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SILAE XXVI

THE ITALO LATIN AMERICAN SOCIETY OF ETHNOMEDICINE

IX Colombian Congress of Chromatography - COCOCRO 2017

SEPTEMBER 25th TO 29th 2017

CONVENTION CENTER AT ESTELAR HOTEL

CARTAGENA DE INDIAS - COLOMBIA

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SILAE XXVI
CARTAGENA DE INDIAS, FROM SEPTEMBER 25th TO 29th, 2017

IX COCOCRO

IX Colombian Congress of Chromatography

Hotel Estelar
Centro de Convenciones
Cartagena´s Room
Cartagena de Indias, September 25th to 29th 2017

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SOCIEDAD COLOMBIANA DE CIENCIAS QUÍMICAS

Abstracts Book
XXVI SOCIEDAD ITALO-LATIN AMERICAN ETHNOMEDICINE CONGRESS – SILAE 2017
IX CONGRESO COLOMBIANO DE CROMATOGRAFÍA – COCOCRO 2017

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Abstracts Book

XXVI SOCIEDAD ITALO-LATIN AMERICAN ETHNOMEDICINE CONGRESS

IX CONGRESO COLOMBIANO DE CROMATOGRAFÍA

IX Colombian Congress of Chromatography

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WELCOME TO SILAE CONGRESS 2017

The Italo Latin American Congress of Ethnomedicine (SILAE) is a scientific event to be held annually and alternately its headquarters between Italy and Latin America. This congress seek to disseminate the scientific research in renowned universities located in Italy, Latin America and the rest of the world; all framed in the systematic study of medicinal and edible plants applied to traditional medicine and phytotherapy, with an anthropological and ethnobotanical approach. Recently, it have been also dispersed worldwide important investigations including areas such as health service, environment, pharmacology, food and nutrition, analytic chemistry and clinic studies. The SILAE congress also seeks to establish collaborative contacts between research centers, academic institutions, governments and specialized organizations from the member countries, for the elaboration, participation and executions of research projects that can be financed both in Europe and in Latin America. On the other hand, the Colombian Congress of Chromatography (COCOCRO), has brought together, by all means since 1996, the Academic, Scientific and Industrial community that have in our country the Cromatography day to day profession. Because of that, the COCOCRO has become the Colombian Society of Chemical Sciences (CSCS) insignia congress. In addition, CSCS' Versatility has allowed Chromatography to be currently, the essential tool for the scientific and industrial development of our country, keeping in mind important sectors of the Medicine such as the Pharmaceutical. Also taking into account COCOCRO's high academic level and capacity of academic meetings, investigators and professionals; it has become an important date for the national community who work around Chromatography, it being the most outstanding issues that are carry out by the Colombian Chemical Community.

In 2017, the Pontificia Universidad Javeriana and the Sociedad Colombiana de Ciencias Químicas joined to another national and international academic institutions will organize the XXVI SILAE congress joined to the Colombian Congress of Chromatography, COCOCRO, that will take place from 25th to 29th of September, at Estelar Cartagena de Indias Hotel and Centro de Convenciones, both located in Cartagena, Colombia. This congress will have worldwide-recognized scientific speakers. As a part of the congress' objectives, it will have the integration of academics, researchers, and students from different universities and institutions of the member countries and the rest of the world, who will introduce their most recent studies from different areas of natural products and its applications. Furthermore, the Congress expects to disseminate significant advances, promote the professional training and the mutual knowledge transfer.

Additionally, the congress will have international and national commercial houses that showed the most important analytic instruments advances and supplies, all applied to the themes reference of the congress. Under the presented perspective, the congress has the pleasure of inviting you to participate in this traditional event of international scope, which will be held for the first time in Colombia.

Dr. Crispin A. Celis
SILAE 2017 President

GENERAL SCHEDULE

MONDAY, SEPTEMBER 25TH			
HOUR	**ROOM**	**ACTIVITY**	**CONFERENCE TITLE**
8:30-12:30	CARTAGENA'S 1 ROOM 8th floor	Pre-Congress courses and Registration	Advances in chromatographic techniques and their coupling to mass spectrometry, Dr. Carlo Bicchi (Italy), Dr. Albert Lébedev (Russia), Dra. Elena E. Stashenko (Colombia)
	CARTAGENAS'S 2 ROOM 8th floor	Pre-Congress courses and Registration	"Supercritical Fluid Chromatography. Primer" Dr. Terry Berger.
12:40-14:00		FREE LUNCH	FREE LUNCH
14:00-14:45	8th floor Lobby	Registration	Organizer committe
14:45-15:30	Main Auditorium	Opening ceremony	Dr. Crispin Celis Zambrano. SILAE-COCOCRO 2017 president. Dr. Uberto Malizia. Italy embassy Dr. German Malagon. SILAE president Dr. Harold Duban Ardila. SCCQ president
15:30-16:15	Main Auditorium	International Lecture	CI 01 Dr. Michael Heinrich: "The Values of Medicinal Plants – Explorations into their Sociocultural and Economic Importance". University College of London.
16:15-17:00	Main Auditorium	International Lecture	CI 02 Dr. Carlo Bicchi: "New trends in analysis of plant volatiles." Università di Torino
19:00-21:00	Hotel Estelar´s restaurant	Opening social event	SILAE and COCOCRO´s registrered assistants

TUESDAY, SEPTEMBER 26TH			
HOUR	**ROOM**	**ACTIVITY**	**CONFERENCE TITLE**
08:00-08:30	Commercial Hall	Posters installation	PPEE 01-46; PPTC 01-33; PPNP 01-20
8:30-9:10	Main Auditorium	International lecture	CI 03 Dr. Alberto Gimenez Turba: "Can Ancestral knowledge become new alternative treatments today?" Universidad Mayor de San Andres
9:10-9:50	Main Auditorium	Technical lecture	CT 01 Dr. Jimmy Yuk: "Unraveling the complexity of traditional medicines using LC/MS coupled with a novel informatics platform." Waters Corporation - Ramguz / Quimicontrol S.A.S.
9:50-10:30	Main Auditorium	International lecture	CI 04 Dr. Albert Lebedev: "GC/HRMS and GCxGC/HRMS in the study of clouds. " Moscow State University
10:30-11:10	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPEE 01-46; PPTC 01-04
11:10-11:30	CARTAGENA'S 1 ROOM	Short communications CC	CC 01 Dra. Elena Stashenko
	CARTAGENA'S 2 ROOM		CC 02 Dr. Omar German Malagon
	STELAR´S 3 ROOM 6th FLOOR		CC 03 Dra. Adriana Basile
11:30-12:45	CARTAGENA'S 1 ROOM	Oral communications PO	Check oral communications schedule
	CARTAGENA'S 2 ROOM		
	STELAR´S 3 ROOM 6th FLOOR		
12:45-14:30	Hotel Estelar´s restaurant	LUNCH	LUNCH
14:30-15:30	CARTAGENA'S 1 ROOM	Oral communications PO	Check oral communications schedule
	CARTAGENA'S 2 ROOM		
	STELAR´S 3 ROOM 6th FLOOR		
15:30-16:15	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPTC 05-33; PPNP 01-20
16:15-16:55	Main Auditorium	International lecture	CI 05 Dr. Terry Berger: "The current state of the Art in supercritical Fluid." SFC Solutions Inc.
16:55-17:35	Main Auditorium	International lecture	CI 06 Dr. Jordi Eras Joli: "Contributions for the renaissance of gas chromatography in the metabolomics analysis" Universitat de Lleida
19:00-21:00	Claustro San Agustin, Universidad de Cartagena (Cra 6 No. 36-100)	Cultural activity	SILAE and COCOCRO´s registrered assistants

WEDNESDAY, SEPTEMBER 27TH			
HOUR	**ROOM**	**ACTIVITY**	**CONFERENCE TITLE**
08:00-08:30	Commercial Hall	Posters installation	PPFF 01-77; PPAF 01-25
8:30-9:10	Main Auditorium	International lecture	CI 07 Dra. Judith Rollinger: "Natural compounds combating the lethal synergism between influenza and pneumococci." University of Vienna/Universität Wien
9:10-9:50	Main Auditorium	Technical lecture	CT 02 Dr. Jeffrey Dahl: "Pesticide Analyses in Cannabis and hops by modified QeuChERS extraction and high speed LC-MS-MS and GC-MS-MS." Shimadzu-Lab instruments / Casa Cientifica
9:50-10:30	Main Auditorium	International lecture	CI 08 Dr. Francisco Macias: "Allelopathy in the search for bioactive compounds." Universidad de Cádiz
10:30-11:10	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPFF 01-50
11:10-11:30	CARTAGENA'S 1 ROOM	Short communications	CC 04 Dr. Luca Campone
	CARTAGENA'S 2 ROOM		CC 05 Dr. Olmedo Luis Morales
	STELAR´S 3 ROOM 6th FLOOR	NUTRIKETO	ROUNDTABLE DISCUSSION
11:30-12:30	CARTAGENA'S 1 ROOM	Oral communications PO	Check oral communications schedule
	CARTAGENA'S 2 ROOM		
	STELAR´S 3 ROOM 6th FLOOR	NUTRIKETO	ROUNDTABLE DISCUSSION
12:30-14:30	Hotel Estelar´s restaurant	LUNCH	LUNCH
14:30-15:30	CARTAGENA'S 1 ROOM	Oral communications PO	Check oral communications schedule
	CARTAGENA'S 2 ROOM		
	STELAR´S 3 ROOM 6th FLOOR		
15:30-16:10	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPFF 51-77; PPAF 01-25
16:10-16:50	Main Auditorium	International lecture	CI 09 Dr. Fabricio Pamplona: "Potential clinical benefits of CBD-enriched extracts over purified CBD in treatment-resistant epilepsy: insights from Brazilian experience and meta-analysis data." Phytolab
16:50-17:30	Main Auditorium	International lecture	CI 10 Dra. Ru Angelie Edrada Ebel: "Using Concatenated Analitical Data for Metabolomic Guided Production and Isolation of Bioactive Natural Product." University of Stratchclyde

THURSDAY, SEPTEMBER 28TH			
HOUR	**ROOM**	**ACTIVITY**	**CONFERENCE TITLE**
08:00-08:30	Commercial Hall	Posters installation	PPQV 01-50; PPQM 01-36
8:30-9:10	Main Auditorium	Technical lecture	CT 03 Giampaolo Rota: "Overcome the challenges in enviromental extraction. A fast, accurate and reliable method to analyse contaminants in enviromental samples." Milestone-Innovatek
9:10-9:50	Main Auditorium	International Lecture	CI 11 Dr. Octavio Luiz Franco: "Development of bioinspired antimicrobials: the new edge of pharmacological design" " Universidade Catolica de Brasilia
9:50-10:30	Main Auditorium	Technical lecture	CT 04 MSc. Victor Mondragon: "Caracterization and analysis of impurities in food and pharmaceutical products." Agilent Technologies-Khymos S.A.
10:30-11:15	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPQV 01-50
11:15-12:45	CARTAGENA'S 1 ROOM	Oral communications PO	Check oral communications schedule
	CARTAGENA'S 2 ROOM		
	STELAR´S 3 ROOM 6th FLOOR		
12:45-14:30	Hotel Estelar´s restaurant	LUNCH	LUNCH
14:30-15:10	Main Auditorium	International Lecture	CI 12 Dr. Alfonso Espada: "Orthogonal LC/MS-based methods for rapid identification of small molecule therapeutics." Elly and Lilly Company
15:10-15:50	Main Auditorium	International Lecture	CI 13 Dra. Silvia Quesada: "Tropical Higland blackberry (*Rubus adenotrichos*) as functional food: evaluation of its biologicals activities. " Universidad de Costa Rica
15:50-16:30	Commercial Hall	Poster session / Coffee Break	Poster evaluation PPQM 01-36
16:30-17:10	Main Auditorium	International Lecture	CI 14 Dr. Luis Cisneros-Zevallos: "The role of oxidative stress in Nutraceutical production and its use. " Texas A&M University
17:10-17:40	Main Auditorium	Closing ceremony	Closing Remarks
17:40-18:10	Main Auditorium	Assembly	General SILAE Assembly
19:00-21:00	Hotel Estelar´s restaurant	Closing dinner	Dinner / Traditional White Night

FRIDAY, SEPTEMBER 29th		
HOUR	**LOCATION**	**ACTIVITY**
7:30-8:30	HOTEL 1st FLOOR	Take the bus
8:30-15:30	Playa Blanca Beach	Tour Lunch Included
15:30-18:00	Bus	Return to the hotel

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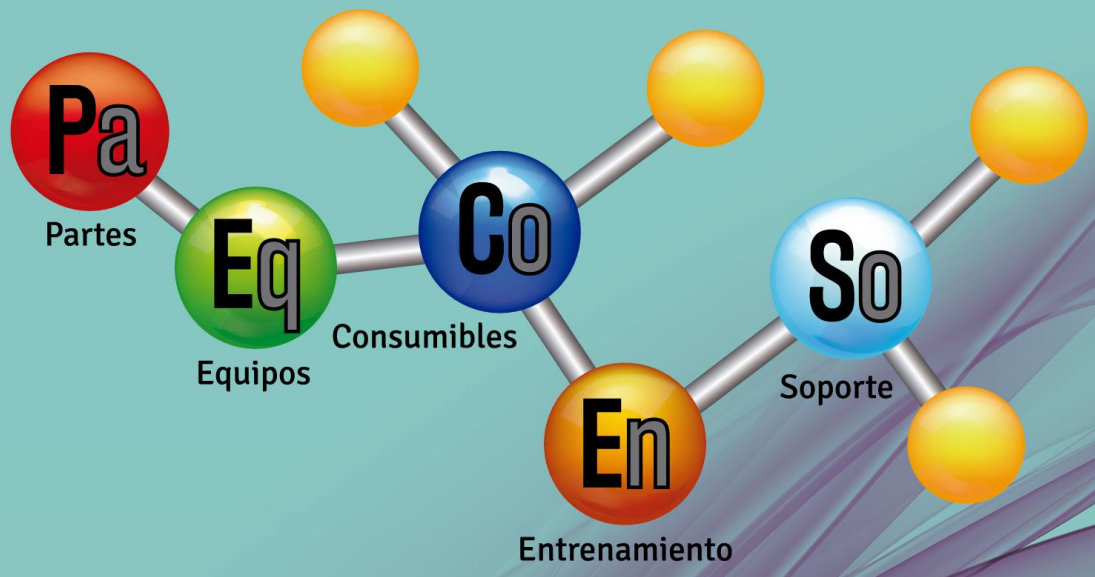

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SILAE XXVI
CARTAGENA DE INDIAS, FROM SEPTEMBER 25th TO 29th, 2017

IX COCOCRO

IX Colombian Congress of Chromatography

CI
INTERNATIONAL LECTURES

The Values of Medicinal Plants – Explorations into their Sociocultural and Economic Importance

Heinrich, M.*

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CI 01

Medicinal (and food) plants are not only a source for new drug leads and high value medical products, but they also highlight a wide range of socio-cultural questions. Using a series of examples from our recent research I will discuss the role of these resources in an ethnopharmacological context. The use of biodiversity be it as a food, a medicine or in any other way also allows a community to highlight their 'uniqueness' and 'special characteristics' as well as the complex interfaces with other cultures. The first example is taken from Ireland, fifteen years after it gained independence from the UK. In 1937 a scheme to collect folklore by agency of senior primary school children was implemented in the National Schools in Ireland. What makes this scheme so fascinating that as early as the late 1930's the political elite in Ireland saw a value in having children recording the 'folk knowledge' in Ireland and to use this also as an educational tool. A large number of remedies as well as many other folk practices were recorded and the data stored in (unpublished) files. While there was no economic value attached to it, relevance clearly lies in helping to define an identity of the young nation and its cultural values. In the last years and in an increasingly interconnected world value chains of medicinal plants have also been highlighted as a core focus of research on medicinal plants. Research into these chains (e.g. Booker, et. al., 2014) highlights problems like exploitation through middlemen, over-harvesting of wild medicinal plants, adulteration and contamination of products at different stages along the chain and a general lack of traceability through the different stages of production. Ethnopharmacology offers both a new framework for research and new strategies for resolving some of the key problems. We need to better understand what core values such products have to the primary producers and through the value chains leading to the final products. Both examples are in different ways of direct relevance to medicinal plant research (ethnopharmacology) in Southern America – they highlight that we need to move away from some of the traditional ideas about what ethnopharmacology is all about, and that we need to critically engage with sociocultural and economic aspects of the field. Value (n.) Look up value at Dictionary.com Latin valere "be strong, be well; be of value, be worth" (see valiant). c. 1300, "price equal to the intrinsic worth of a thing" late 14c., "degree to which something is useful or estimable," from Old French value "worth, price, moral worth; standing, reputation" (13c.), noun use of fem. past participle of valoir "be worth". The meaning "social principle" is attested from 1918, supposedly borrowed from the language of painting. Value judgment (1889) is a loan-translation of German Werturteil. http://www.etymonline.com/index.php?term=value

Keywords: Gas chromatography, Metabolomas

Referencias Booker, A., D. Frommenwiler, D. Johnston, Ch. Umealajekwu, E. Reich, M. Heinrich (2014) Chemical variability along the value chains of turmeric: A comparison of Nuclear Magnetic Resonance (NMR) pectroscopy and High Performance Thin Layer Chromatography (HPTLC). Journal of Ethnopharmacology 152: 292-301.

NEW TRENDS IN ANALYSIS OF PLANT VOLATILES

Bicchi C.[1]

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CI 02

The volatile fraction emitted from a plant is an important biosensor diagnostic of the changes that take place in its metabolism. In chemical terms, the volatile fraction of a plant is a mixture of compounds that can be recovered because of their capability to vaporise both spontaneously and/or through suitable sampling conditions or techniques. The term volatile fraction implies a group of approaches and/or techniques providing samples representative of the volatiles characterizing a plant matrix. The resulting samples may have different and mutually non-comparable compositions, e.g. headspace, essential oils and/or extracts obtained by specific techniques. The overwhelming evolution of analysis over the last three decades as well as the present trend aiming to develop Total Analysis Systems (TAS) have radically changed approaches and strategies also for the investigation of the plant volatile fraction. Gas chromatography combined with mass spectrometry (GC-MS) is the technique of choice for the analysis of volatiles. GC evolution falls in the wider context of the whole analytical procedure in its three main steps (i.e. sample preparation, analysis and data handling) [1-3]. Over this period, ever-powerful techniques have been introduced, including high concentration capacity sample preparation techniques, fast and ultrafast GC, enantioselective GC, GCxGC, tandem and high-resolution mass spectrometry, non-separative methods, etc. However, data handling has been the step that has more dramatically increased in importance; informatics has decisively contributed to the full automation of analysis and instrumentation, and data managing (chemometrics), and gained a role as relevant as those of sample preparation and analysis.

This lecture is an overview of the most recent conventional and non-conventional methods and technologies for routine analysis of the plant volatile fraction not only in terms of instrumentation but also of operative strategies. These topics will be illustrated with real-world examples taken from the author's everyday experience.

Keywords: *Plant volatiles, Dedicated sample preparation techniques, Gas chromatography, Mass spectrometry, Data elaboration*

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1) Rubiolo P., Sgorbini B., Liberto E., Cordero C., Bicchi C., in The Chemistry and Biology of Volatiles – A. Herrmann (Editor) ISBN: 978-0-470-77778-7, Chapter 3, pp 50-93.
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COULD ANCIENT KNOWLEDGE PROVIDE NEW TREATMENTS?

Giménez-Turba, A.[1]

[1]*Universidad Mayor de San Andrés, La Paz, Bolivia.*

CI 03

The Largest Public University in Bolivia The Universidad Mayor the San Andrés (UMSA) and the Swedish International Development Agency (SIDA) are developing quinquennial programs for institutional strengthening at UMSA, based on young talents training within a Swedish scientific sandwich Ph.D. program, that started in 2000. Based on our successful studies on Evanta (*Galipea longiflora*) in the treatment of cutaneous leishmaniasis within the "*UMSA-SIDA Infectious Diseases Project (2004-12)*". The Pharmaceutical Chemistry Area (AQF) at the Institute for Pharmaceutical and Biochemical Research (IIFB) at the Faculty of Pharmaceutical and Biochemical Sciences (FCFyB), is developing now, with Lund University (Prof. Olov Sterner), the program ***"Biomolecules of Medicinal and Industrial Interest"*** (2013-17). Our main goal is building research capacity with scientists, trained at MSc and PhD programs, that are able to search for and study novel lead compounds from the Bolivian biodiversity that could be developed, particularly concerning novel antiparasitic agents. We will initiate, in some cases, and increase, in others, the scientific knowledge on local medicinal plants. Results of our scientific findings, are being returned to the communities, for a better and safer local use of medicinal species useful in the treatment of parasitic infections. There are reviews on discovery of new drugs, that show marked importance for natural products and, today, these are used as models for the synthesis of derivatives and continue to play an important role in the process of discovery and drug development. Local ethnic groups use plant species alone or in semi-elaborated preparation, often, this knowledge transmitted orally from older to younger generations, is lost. Traditional knowledge scientifically evaluated, will aloud to ascertain on the potential of local biodiversity as a source of lead molecules to address general health problems such endemic parasitosis, that constitutes some of the most frequent health alterations in tropical societies. Bolivia, is part of the megadiverse countries. However, according to FAO, Latin American countries conducted deforestation five times more, per rural inhabitant, than Africans and 40 times more than Asians. In this regard, two aspects are of special interest to the study area, first bring scientific knowledge to the conservation of medicinal species and secondly, that despite the great diversity of plants, only a few products based on natural resources region have come to the markets, mainly due to the lack of scientific studies to support their use and effectiveness. WHO Member States urges national governments to respect, preserve and widely communicate traditional medicine knowledge while formulating national policies and regulations to promote appropriate, safe, and effective use; to further develop traditional medicine based on research and innovation. Our current research is based on documentation of the Tacana ethnic group, that thrives on the low lands (Amazon area). Over 100 cultural and medicinal species collected based on Traditional knowledge are part of our studies. Proceedings include harvest, voucher elaboration, taxonomy work by the National Herbarium (HLP), milling, maceration, and *in vitro*, bioguided fractionation against *Leishmania*, *Trypanosoma* and *Giardia* Parasites. The most relevant findings of our research that started questioning if antient knowledge could provide new treatments will be presented and discussed.

GC/HRMS AND GCXGC/HRMS IN THE STUDY OF CLOUDS

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CI 04

Understanding the chemical composition of clouds is crucial, as clouds participate in the formation and transformation of chemical species, production and consumption of oxidants, droplet activation and growth, transport and deposition of pollutants. A large fraction of the organic compounds present in the clouds has not been characterized so far and this presentation addresses that gap. We have focused this study on the SVOCs composition in the clouds. Cloud samples were collected at the Puy de Dôme station (France, 1465 m) in the period from 2013 through 2017. The samples were filtered and kept frozen at -20°C before MS analysis. Sample preparation was carried out according to US EPA 8270 Method. Dichloromethane extracts were analyzed with high resolution time-of-flight mass spectrometer Pegasus® GC-HRT (LECO Corporation, USA) in GC and GC×GC modes. The obtained EI mass spectra were used for the identification by utilizing high mass accuracy data and the various tools provided in the instrument's data processing software (ChromaTOF-HRT). It was very important to take into account all possible sources of contamination during sample preparation. Thus ultrapure water from France and USA, the same water after passing trough the filters used in the experiments, and after contact with glass and metal surface of containers and glassware, as well as 5 samples of dichloromethane were analyzed together with the cloud water samples. Over one hundred compounds were identified in the samples at various levels of reliability. Twelve compounds from the EPA list of semi volatile priority pollutants (EPA 8270 Method) were identified and quantified taking into account their response factors values. Sixty seven compounds were identified at level 2 taking into account library search score, retention indices, accurate masses information, and laws of fragmentation under electron ionization. Forty two compounds were partially identified (elemental composition, some structural units). Accurate mass measurements were very helpful allowing correcting the results of the library search. In many cases correct structural elucidation became possible only due to accurate masses of the ions. Due to high resolution tool more than 10% of the library search results were corrected and the structures of several compounds not present in the library were manually elucidated. The analysis in GC×GC mode has allowed chromatographic separation of closely eluting and coeluting constituents, making analytes identification more reliable. The content of the samples differs from the usual picture expected for cases of water or soil pollution. For example, the levels of concentration of the dibutyl and bis(2-ethylhexyl)phthalates are rather low. Nevertheless only dialkylphthalates and phenols were the representatives of the priority pollutants in the cloud water samples. Another peculiarity involves complete absence of the chlorinated/brominated compounds. We suggest that chlorine is removed from the clouds due to radical atmospheric reactions. More than 90% of the composition is due to oxygen-containing compounds. These results support suggestions of the presence of oxidative condition in the clouds. Ketones, aldehydes, furans, acids, ethers, and esters were also detected. The quantitative levels of SVOC were measured using internal standards (deuterated PAH) method and estimated as being in the range 0.1-10 ng/ml.

THE PRESENT STATE-OF-THE-ART IN SUPERCRITICAL FLUID CHROMATOGRAPHY

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CI 05

Supercritical fluid chromatography (SFC) has been around since the 1960's as a niche technique. This started to change in the 1990's particularly in the pharmaceutical industry where it is now widely used, mostly for analytical and semi-prep scale chiral chromatography. Today, 4 of the largest instrument manufacturers produce analytical scale instruments, often interfaced to MS. Several also produce semi-prep instruments, mostly used in drug discovery. In addition, several other companies produce semi-prep chromatographs. Thus, SFC is in the process of becoming a major technique.

Many of the advances in HPLC column technology over the last 20 years have only recently found their way into SFC. Sub-2µm, a superficially porous particles, with polar stationary phases are now becoming fairly common. Even sub-2µm chiral columns are available that can produce separations in as little as 5 seconds.

Applications are expanding beyond chiral and beyond pharma. Of particular interest to this author is the use of SFC for the analysis, and purification of natural products. The state of the instrumentation, columns and applications will be discussed.

CONTRIBUTIONS FOR THE RENAISSANCE OF GAS CHROMATOGRAPHY IN THE METABOLOMICS ANALYSIS

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CI 06

There is no doubt that the introduction of liquid chromatography has allowed very satisfactory descriptions of the metabolites in biological tissues. It appeared that their combined efficiency with their versatility had relegated to gas chromatography (GC) for certain specific applications and, in general, within the scope of the routine analysis. Gas chromatography faces its great limitation, its dependence on the volatility of the analytes. Derivatization reactions partially solved this limitation, but are often long reactions that are carried out under non-conservative conditions for labile analytes. However, new techniques of sample preparation, derivatization, improvements in injection techniques and the GC equipment have been developed in recent years. These methodological and technical developments combined with the high resolution capacity of the GC and the excellent performance for the identification offered by electronic impact ionization when combined with mass spectrometry allow to approach the analysis of metabolomes with sufficient guarantees in detection capacity. This presentation describes the recent extraction methods such as Dispersive Liquid-Liquid Micro-Extraction (DLLME), the elimination of interferences by QuEChERs beyond their use for pesticide analysis, microwave-assisted derivatizations, microscale silylation reactions and mixed derivatizations in a single step. In relation to the injection stage, the injection-port derivatization and the desorption of *twisters* are discussed. Finally, we detail the performance in the field of metabolomics that allow GC coupled with mass spectrometry with single quadrupole, triple quadrupole, ion traps, time of flight analysers and two-dimensional gas chromatography.

Keywords: *Gas chromatography*, Metabolomas

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NATURAL COMPOUNDS COMBATING THE LETHAL SYNERGISM BETWEEN INFLUENZA AND PNEUMOCOCCI

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CI 07

Influenza, an acute viral infection of the respiratory tract, causes about 3 to 5 million cases of severe illness, and about 250,000 to 500,000 deaths every year worldwide.1 Influenza infections are often associated with secondary complications caused by bacterial pathogens, most commonly Streptococcus pneumoniae[2]. There is a complex interplay of influenza virus and pneumococci, which have developed a lethal synergistic strategy mediated by neuraminidases.2 Intriguingly, these surface proteins are present in both pathogens, and show a high structural homology, particularly in their ligand-binding domain[3].

In the past years, several studies have reported the discovery of influenza neuraminidase inhibitors isolated from natural sources[4]. During an ongoing screening campaign for natural products active on influenza and pneumococcal nauraminidases (Natural Lead Structures Targeting Influenza (FWF P 24587), we identified several herbal agents and thereof derived natural compounds with potent neuraminidase-inhibiting and antiinfluenza activity[5-7].

Here, I will present strategies, which were used for a rationalized discovery of natural lead structures targeting neurmainidase. They encompass (i) chemoinformatics approaches, such as pharmacophore-based virtual screening, molecular dynamic simulations and docking, (ii) information from ethnopharmacological sources, and (iii) the usage of a set of complementary assays (target-based and phenotypic assays). The combination of these approaches will be demonstrated by some recently performed studies, which succeeded in identifying natural compounds with antiviral and anti-pneumococcal activity by disrupting their neuraminidase-driven lethal synergism[8].

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ALLELOPATHY IN THE SEARCH FOR BIOACTIVE COMPOUNDS

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CI 08

Plants have their own communication and defense mechanisms and allelochemicals are, in fact, natural herbicides within others. Allelopathy studies developed new compounds that may lead to obtain growth inhibitors with different target sites tan traditional herbicides. Following the 'economy of resources' principle one defense metabolite is cheaper in terms of resource investment (energy, NADPH, carbon) if it can defend the plants from more than one organism. Here, we illustrate this principle with several examples where allelochemicals, in addition to phytotoxic activities, have sown other interesting biological properties. Thus, epoxycurcuphenols from *Helianthus annuus*, showed potential use as inmunosuppressants.[1] Similarly, a secoguaianolide isolated from *Artemisia gorgonum* showed high activity on phytotoxicity bioassay. Additionally, these compounds were tested on human cell culture apoptosis induction on ovarian cancer cell. Another examples are some compounds of the Benzoxazinoids family,[2] as well as naphtotectone, a natural quinone product isolated from *Tectona grandis*.[3,4]

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POTENTIAL CLINICAL BENEFITS OF CBD-ENRICHED EXTRACTS OVER PURIFIED CBD IN TREATMENT-RESISTANT EPILEPSY: INSIGHTS FROM BRAZILIAN EXPERIENCE AND META-ANALYSIS DATA

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CI 09

Different therapies including cannabinoid compounds have become popular for treatment-resistant epilepsy in the recent years. This was the beginning of a rush of small-scale enterprises to produce "*Cannabis* oils", followed by independent initiatives of patients and patient associations, which decided to produce the "oils" by themselves. In Brazil, there are over 2500 patients importing products and taking medicines of uncertain quality, and there is a lively debate on whether pure CBD or CBD-enriched extracts are the best therapeutic option. This meta-analysis study evaluated all the observational clinical data available in the scientific literature for cannabinoid treatment in treatment-resistant epilepsy in children. The aim is to shine some light on the currently controversial question of whether "Cannabis-based extracts" or "purified/synthetic compounds" would be a preferential therapeutic approach. The meta-analysis study with clinical observational data from 442 patients suggests that treatments using CBD-enriched extracts have higher potency and a better side effects profile (but not higher efficacy) than purified CBD, at least for this group of treatment-resistant epilepsy patients.

USING CONCATENATED ANALITICAL DATA FOR METABOLOMIC GUIDED PRODUCTION AND ISOLATION OF BIOACTIVE NATURAL PRODUCT

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CI 10

High resolution Fourier transform mass spectrometry (HRFTMS) and nuclear magnetic resonance (NMR) spectroscopy were employed as complimentary metabolomic tools to dereplicate chemical profiles of Bioactive Natural Products from their sources.

The innovative strategy involved targeted cultivation, harvest, and isolation of biologically active compounds. Principal Component (PCA), Hierarchical Clustering (HCA), and Orthogonal Partial Least Square-Discriminant (OPLS-DA) analyses were used to evaluate HRFTMS and NMR spectral data of culture extracts. The results of the statistical analysis identified and validated the best culture conditions and extraction procedure which optimized the isolation of novel bioactive metabolites.

Production of secondary metabolites was investigated in several of the bacterial symbionts that were isolated from marine sponges. Novel secondary metabolites were screened using high resolution mass spectrometry and NMR-based metabolomics approaches. Metabolomic profiling using 2D-NMR and HR-ESIFTMS were done at different stages of the growth phase for both solid and liquid culture media. Dereplication studies were accomplished by utilizing the Mzmine software with Antibase and DNP databases. The optimised method in terms of media, incubation time, and maximum production bioactive compounds are taken into account for the scale-up. Metabolomic- and bioassay-guided isolation were carried out to target the compound(s) of interest.

With the metabolomics approach, it was possible to predict and optimize the biosynthetic pathway involved in the production of the target secondary metabolite.

DEVELOPMENT OF BIOINSPIRED ANTIMICROBIALS: THE NEW EDGE OF PHARMACOLOGICAL DESIGN

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CI 11

Peptide rational design was here used to guide the creation of novel compounds that could help on resistant bacteria control. Firstly, two novel short β-lactamase inhibitors with five amino acid residues length were generated. Molecular modeling associated to peptide synthesis improved bactericidal efficacy in addition to amoxicillin, ampicillin and cefotaxime. Docked structures were consistent with calorimetric analyses against bacterial □-lactamases. These two compounds were further tested in mice. Whereas commercial antibiotics alone failed to cure mice infected with *Staphylococcus aureus* and *Escherichia coli* expressing β-lactamases, infection was cleared when treated with antibiotics in combination with peptides, clearly suggesting that peptides were able to neutralize bacterial resistance. Moreover, host-defense peptides derived from mastoparan and clavanin families were redesigned in order to improve antimicrobial activities and decrease mammalian cell toxicity. Both peptides were evaluated in sepsis and wound model infections showing the ability to control the infection caused by Gram-positive and -negative pathogenic bacteria. Moreover in all cases, immune response was also evaluated. In summary, the unusual peptides here described provide leads to overcome β-lactamase-based resistance, a remarkable clinical challenge.

OTHOGONAL LC/MS-BASED METHODS FOR RAPID IDENTIFICATION OF SMALL MOLECULE THERAPEUTICS

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CI 12

The hyphenation of mass spectrometry to liquid separation techniques has become the most demanded analytical approach in the discovery of new drug-like compounds. While straightforward in theory, for successful work within a production environment this approach requires the right combination of orthogonal separation techniques to fully exploit the capabilities of mass spectrometry when dealing with complex matrixes. The first part of this presentation deals with the use of orthogonal separation and detection techniques to overcome the challenges associated with the identification and quantification of bioactive compounds from different sources. Details of new strategies for accurate compound detection by mass spectrometry will be presented.

The second part of this talk is devoted to Hydrogen/deuterium exchange mass spectrometry. HDX-MS is a biophysical tool for the characterization of protein dynamics following ligand binding (where the ligand is a small molecule, a peptide or another protein). HDX-MS has emerged as a rapid and sensitive approach to interrogate protein-protein interactions (PPIs) and transient protein folding states. In this presentation, we report the use of HDX-MS to characterize interactions of small molecules with PPI targets. Our results demonstrate that HDX-MS is able to identify the binding mode for PPI modulators, which is not accessible by conventional structure elucidation techniques. These findings demonstrate that HDX-MS can validate and probe protein-ligand interactions with the concomitant impact on biology and drug discovery.

TROPICAL HIGLAND BLACKBERRY (*Rubus adenotrichos*) AS FUNCTIONAL FOOD: EVALUATION OF ITS BIOLOGICALS ACTIVITIE

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CI 13

Berries have been proposed as fruits that can potentially improve human health due to their high phenolic compound content. The main polyphenols present in the tropical highland blackberries are anthocyanins and ellagitannins. Our group has evaluated antioxidant and anti-inflammatory activities in a polyphenol extract from fresh blackberries. The main polyphenols detected were the anthocyanins: cyanidin-3-glucoside, cyanidin-3-malonyl glucoside and the ellagitannins: lambertianin C and sanguiin H-6. These phenolics compounds protected liposomes and liver homogenates against lipid peroxidation (IC_{50} 7.0 ± 0.5 and 20.3 ± 4.2 mg/mL respectively), also inhibited superoxide production by NADPH oxidase in THP-1 cells and nitrite production in J774 cells stimulated with LPS+IFNγ, because a down regulation of iNOS protein expression. Blackberries are commonly consumed as juice in Latin-American countries. However the juice is easily fermented, hereby, different industrial techniques are being applied to enable the juice to be stored for longer periods. The National Center of Science and Food Technology of the University of Costa Rica developed a microfiltrated blackberry juice, which not only allows longer storage for blackberry juice but also preserves the health-promoting activities of this fruit. This juice showed less polyphenols concentration than the fresh blackberry, however the protection against lipid peroxidation and intracellular oxidation were not significantly different. The same pattern of results was seen after the pasteurization of the microfiltrated juice. Also the effect of this blackberry juice consumption on streptozotocin-induced diabetic rats was assessed. The juice was diluted in water (12.5 and 25 %) and given orally for 40 days to the rats. The higher dose of the beverage significantly decreased glucose (-48.6%), triacylglycerols (-43.5%) and cholesterol (-28.6%) and improved plasma antioxidant capacity. The inhibitory activities found in *Rubus adenotrichos* fresh fruit and in the microfiltrated juice suggest a potential beneficial effect against oxidative stress, inflammatory processes and as a dietary adjuvant to the pharmacological treatment of diabetes, so that it could be considered a functional food.

Keywords: *Rubus adenotrichos*, antioxidant, anti-inflammatory, diabetes, lipid peroxidation, iNOS, microfiltration

THE ROLE OF OXIDATIVE STRESS IN NUTRACEUTICAL PRODUCTION AND ITS USE

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CI 14

When plants are exposed to stresses (e.g., wounding, UV, chemicals, among others) a series of responses are elicited by the abiotic stress including accelerated metabolism and synthesis of secondary metabolites of nutraceutical importance. Here we identify the primary and secondary signals involved in the stress response in different plant species. Overall, once the stress is applied in the plant or plant part a redox imbalance takes place with reactive oxygen species (ROS) playing a major role as secondary signals. In this presentation we will show in detail the different signals involved and their mode of action, the role of calcium ions as well as NADPH oxidase as generator of superoxide radicals and their effects in secondary metabolism as well as quality changes. In addition, by elucidating the signaling mechanism we will revisit the status of the actual technologies being used by different industries dealing with plant and plant products including the fresh industry, cosmetics, functional foods and pharmaceutical. Furthermore, we will propose alternative approaches either by modifying current technologies or proposing novel technologies to enhance the quality of plant and plant products to enhance their nutritional content. Similarly we will discuss how the secondary metabolites produced by oxidative stress in plants have the potential to ameliorate inflammation and several chronic diseases associated to oxidative stress in Human cells and promote health.

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CC 01 ANALYSIS OF PHYTOCANNABINOIDS: FROM PLANT TO FINAL PRODUCTS

Stashenko, E.[1]

CC 02 APPLICATION OF qNMR IN THE CHARACTERIZATION OF HERNANDULCIN IN THE SPECIES *Phyla strigulosa*

Malagon, O.G.[1]

CC 03 FEIJOA SELLOWIANA FRUIT, A SURPRISING AND MULTIFACETED DRUG AND A HOPE FOR CANCER TREATMENT

Basile, A.[1]

CC 04 OPTIMIZATION OF MACROPOROUS RESIN ADSORPTION FOR THE EXTRACTION OF FLAVONOIDS AND LIMONOIDS IN ORANGE JUICE OF OVALE CALABRESE (*Citrus sinensis*) BY DISPERSIVE SOLID-LIQUID EXTRACTION

Campone, L.[1]

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CT
TECHNICAL LECTURES

UNRAVELING THE COMPLEXITY OF TRADITIONAL MEDICINES USING LC/MS COUPLED WITH A NOVEL INFORMATICS PLATFORM

Yuk, Jimmy[1]., Isaac Giorgis[1]., Wrona, Mark[1]., Nikles, Stefanie[2]., Bauer, Rudolf[2]

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CT 01

To fully understand the effectiveness of traditional medicines (TM), it is vital to investigate the chemical components of the raw herbal materials. This is a difficult task due to the complexity of the sample which can contain one or multiple herbs. LC/MS is a widely-used analytical technique as it is highly sensitive to separate and identify the diverse chemical components in the TM. However, due to the large datasets of chemical information, this is a major challenge to screen the chemical components and create results rapidly. Here, we present a novel workflow that enables researchers to quickly identify chemical ingredients from a well-known traditional Chinese medicine, Yu Ping Feng San, in a single LC/MS injection. This presentation will show a thorough analysis of the complex LC/MS data-set and deduce the chemical components using an in-depth data analysis workflow.

Keywords: Metabolomics, Screening, and Mass Spectrometry

OVERCOME THE CHALLENGES IN ENVIROMENTAL EXTRACTION. A FAST, ACCURATE AND RELIABLE METHOD TO ANALYSE CONTAMINANTS IN ENVIROMENTAL SAMPLES

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CT 03

La extracción con disolvente asistido por microondas (MASE) es una técnica de preparación de muestras altamente eficiente que permite extracciones con cantidades reducidas de disolventes mientras trabaja a altas temperaturas y presiones. Esto acelera el proceso de extracción, produciendo resultados equivalentes al método estándar de Soxhlet, pero en una fracción del tiempo y utilizando significativamente menos disolvente.

Los métodos de prueba de la Agencia de Protección Ambiental de los Estados Unidos (USEPA) para Evaluar Residuos Sólidos (SW846) proveen una fuente comprensiva de información sobre muestreo, preparación de muestras, análisis e informes. US EPA 3546 es un procedimiento MASE para extraer compuestos orgánicos insolubles en agua o ligeramente solubles en agua tales como pesticidas organoclorados, compuestos orgánicos semivolátiles, HAP, PCB, herbicidas fenoxiácidos, fenoles, dioxinas y furanos de suelos, arcillas, sedimentos, lodos y residuos sólidos .

Este trabajo demuestra el uso del sistema de extracción de microondas de mesa Ethos X de Milestone con el nuevo rotor fastEX 24 y cómo genera recuperaciones confiables después de la extracción de contaminantes orgánicos de los suelos certificados siguiendo el Método 3546 de la EPA estadounidense. Esto comparado con todas las otras técnicas automatizadas, Extracción de fluido presurizado y extracciones convencionales de Soxhlet. Las muestras se analizaron usando GC-MS.

CARACTERIZATION AND ANALYSIS OF IMPURITIES IN FOOD AND PHARMACEUTICAL PRODUCTS

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CT 04

Manufacturers of pharmaceuticals, drug packaging components, medical devices and packaged food products have come under growing pressure to perform sensitive and accurate analytical studies to detect, identify, and quantify extractable and leachable compounds (E&Ls). E&Ls may be potentially toxic or have otherwise undesirable effects on the efficacy of drugs. Even as regulatory guidance related to the application, performance, and reporting of E&L studies increases and examples and data accumulate, E&L analysis is still an evolving area of investigation.

The US FDA has issued guidance to the industry on container closure systems for packaging human drugs and biologics. Profiling compounds that can be extracted from the packaging materials, or that have leached into a drug substance or product is a complex task due to the wide range of materials used for the construction of primary and secondary containers, diversity of the physico-chemical of the extracted and leached impurities, detection levels in samples ranging from ng to µg and challenges in the detection of these compounds in a wide range of different matrices.

A workflow using different analytical platforms is proposed for the analysis of several matrices to enable confident identification and quantification of potential E&Ls (platicizers, photo-initiators, stabilizers, antioxidants) from extracts derived from a variety of contact closure system components and packaging materials.

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ORAL COMMUNICATIONS

NUTRACEUTIC COMPARISON OF THREE ACCESSIONS OF *Malpigia emarginata* FROM COSTA RICA

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PPAF 01

The growing interest in functional foods has brought in the latest years not only a deep analysis of its composition but also of its function in the organism in order to be used, mainly, in benefit of human health [1]. Such research has included thousands of plants all around the world and one of those is the *Malpighia emarginata* D.C., commonly known as "acerola". The acerola plant can be found in a tropical weather like the one in Costa Rica. This plant produces small and red fruits, with a high vitamin C (ascorbic acid) levels; among other antioxidants compounds [2].

The objective of this research consisted of an evaluation in the content of phenolic and proanthocyanidins compounds, vitamin C, also to measure of the antibiotic and antioxidant activity present in the crude extract of three accession of acerola collected from a farm of Puriscal, San José-Costa Rica.

Three accessions of this fruit, were tested for vitamin C with a chromatographic method obtaining up to 158 mg of this vitamin per gram in a dry weight base (gDW) in a specific accession (INTA-92), phenolic compounds using Folin-Ciocalteu method, showed for the same accession the highest value (150 mg gallic acid eq. per gram of dry weight, GAE/gDW), antioxidant activity using a DPPH method had around 2000 µmol of trolox equivalents (TE)/gDW in the same accession and antibiotic activity by inhibition halo, both bacteria, the gram-positive and gram-negative ones showing an growth inhibition around 78% in comparison with a 30µg chloramphenicol disc of similar characteristics in *E. coli*. Those results allow recommending the introduction of the INTA-92 as a commercial accession do to its high phytonutrients content as a nutraceutic with an excellent benefit.

Keywords: Acerola, Nutraceutic, Antioxidant.

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ANGIOTENSIN I CONVERTING ENZYME (ACE)-INHIBITORY ACTIVITY OF SPERMIDINE DERIVATIVES IN DEHYDRATED LULO (*Solanum quitoense*) FRUIT

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PPAF 02

Lulo (*Solanum quitoense* Lam.) is a tropical bush that usually grows in Andean region between 1600 and 2450m above sea level, with a production in Colombia close to 35.000 ton in 2014. This fruit is widely consumed to prepare juices or jellies because its intense and refreshing aroma [1]; however, during its postharvest handling is highly perishable. For that reason, dehydration is a strategy to increase its shelf-life time. Recently, hot-air drying, freeze-drying and spray-drying techniques were used to obtain lulo powders, which were characterized to study their potential as food ingredient [2]. During this research, it was found that the amount of N1,N4,N8-tris(dihydrocaffeoyl)spermidine and N1,N8-bis(dihydrocaffeoyl)spermidine was increased after the drying, and also that these compounds were responsible for the inhibition of Angiotensin-I-converting enzyme, such showing *in vitro* antihypertensive activity [3]. The IC50 for lulo fruit pulp was 1.08 ± 0.30 ppm, while the values for freeze-dried and spray-dried powders were 83.49 ± 4.10 and 43.17 ± 3.80 ppm, respectively. With the aim to potentiate this bioactivity, spray-dried microencapsulates of lulo mixtures with vegetables that had also shown antihypertensive activity were developed. The mixture of lulo-broccoli (10:1) showed an increase in the ACE-inhibitory activity. These results confirm the potential of lulo fruit for the development of functional foods and/or ingredients that can contribute to the prevention and/or modulation of hypertension. *In vivo* experiments need to be done in order to confirm the bioavailability of spermidine derivatives.

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Keywords: antihypertensive activity, spray-drying, functional food ingredients, Solanaceae.

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CHEMICAL PROFILING OF POLYPHENOLIC COMPOUNDS IN THE FRUIT SKIN OF *Prunus domestica* PLUMS FROM COSTA RICA

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PPAF 03

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Prunus domestica (plum) is a tree from the Rosacea family, native from southern Europe and western Asia, which was introduced to Costa Rica in order to diversify crops production. Studies on extracts from *Prunus domestica* fruits have reported polyphenolic compounds [1,2] and associated bioactive properties such as antioxidant potential and anticancer activity [3,4].

The objective of the present work was to study the polyphenolic contents from a composite of *P. domestica* (satsuma cultivar) fruit skin from Costa Rica's only commercial cultivar, using ultra high-performance liquid chromatography high-resolution multi-stage mass spectrometry (UHPLC-PDA-ESI/HRMS/MSn) analysis. A total of 59 polyphenolic compounds were identified: six hydroxycinnamic acid derivatives, 18 acylated coumaroyl sucroses, 20 glycosylated flavonoids and 15 flavan-3-ols, including monomers [(+)-catechin and (-)-epicatechin)], A-type and B-type procyanidin dimers and trimers as well as B-type procyanidin tetramers.

Keywords: Plum, Polyphenols, Procyanidins, HRMS.

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CHARACTERIZATION AND QUANTIFICATION OF PROCYANIDINS IN AGRAZ (*Vaccimium meridionale* S.) POMACE

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PPAF 04

Agraz (*Vaccinuim meridionale* S.) pomace, a residue from jam production, represents 20% of the fruit weight. Agraz pomace has a high content of phenolic compounds including procyanidins (PAs). Procyanidins are compounds of interest due to their biological properties, including preventative effects against oxidative stress and chronic inflammation, which are the risk factors for chronic diseases. These compounds are commonly present in high concentration in fruit pomace.

In this work, PAs were extracted from agraz pomace. Normal Phase High-performance Liquid chromatography (HPLC) was used to determine PAs composition and content. The pomace contained 21±8.0, 13±3.6, 24±6.2, 15±4.0, 12±3.4, 13±3.2, 8.5±2.1, 8.5±2.5, 18±3.7 y 8.5± 2.1mg/100 fresh weight (FW) from monomers to nonamers, respectively. These data suggest that agraz pomace can be potentially used as a functional food ingredient.

Keywords: Phenolic compounds, HPLC, Oligomers, Functional ingredient.

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IMPROVING REMOVAL OF TOTAL POLYPHENOLS IN DRY FRUITS OF *Vaccinium meridionale* WITH MICROWAVE-ASSISTED EXTRACTION

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PPAF 05

The plant *Vaccinium meridionale* grows in high zones of the department of Boyacá (Colombia) between 2600 and 4000 m.a.s.l. Its fruit contains remarkable quantities of polyphenolic compounds. On the other hand, research studies have verified the suitability of the microwave-assisted extraction technique (MAE) on the removal of total polyphenols (TP) in different plant matrices. In this work, the response surface methodology was applied to study the effect of the independent variables power (P), temperature (T), the liquid-solid ratio (L:Srat.), time (t), and ethanol concentration in aqueous solutions ([EtOH]) on the amount of TP extracted in dry fruits of *V. meridionale* with MAE processes, as well as the determination of the conditions of maximum removal.

A central composite design face-centered with three levels for each variable was used (N = 50): P = 300-900 W; T = 70-110°C; L:Srat. = 30:1-70:1 w/w; t = 5-15 min; [EtOH] = 0-80%. Quantification of TP was performed by applying the colorimetric system of Folin-Ciocalteu reagent using gallic acid as the reference molecule. The analytical method was previously validated by the authors in terms of selectivity, linearity, repeatability, and accuracy. The TP quantities were found in the range of 18.8-40.2 mg GA/g Dw (mg of gallic acid per g of dry fruit), showing an important influence of the experimental conditions on TP removed.

According to the analysis of variance (ANOVA) for response surface quadratic model, a second-order equation with 13 coefficients was established to describe the experimental results ($R2 = 0.9746$). In the same way, the most significant variables in the extraction process were ethanol concentration, temperature, and time. The best removal was obtained in the range [EtOH] = 44-49 %, T = 110°C, and t = 10-15 min. In order to evaluate the suitability of the quadratic equation to describe and optimize the amount of TP extracted, six different extractions were carried out in the range of the maximum removal mentioned above, obtaining high TP recoveries (38.4-41.1 mg GA/g Dw).

On average, there were not significant differences between the experimental results and the values predicted by the quadratic equation. We also found in three of these six assays a major recovery of TP when compared with the quantities obtained in the experimental design. We determined that in terms of quantity, time and consumption of energy, the microwave-assisted extraction is an effective technique for the extraction of total polyphenols in dry fruits of *V. meridionale*.

Keywords: Microwave-assisted extraction, Surface response methodology, Total polyphenols, *Vaccinium meridionale*.

NUTRACEUTICAL EVALUATION OF TWO WILD BERRIES (*Vaccinium consanguineum* AND *Ugni myricoides*) COLLECTED FROM THE VICINITY OF IRAZÚ VOLCANO, COSTA RICA

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PPAF 06

The objective of this research consisted of an assessment in the content of phenolic and proanthocyanidins compounds, also to measure of the antibiotic and antioxidant activity present in the crude extract of two berries collected in the foothills of the Irazú volcano, Cartago-Costa Rica. The parts of the plant used in this research were fruit (ripe and unripe), leaves and stem. The content of total phenolics in the crude extract of *V. consanguineum* using the Folin-Ciocalteu method showed 146 ± 5mg of gallic acid eq/g of dry sample for the leaves, 98 ± 1 for the stem and 24.8 ± 0.5 for both ripe and unripe fruit. On the other hand, the U. *myricoides* results were lower, 84.5 ± 0.4mg of gallic acid eq/g of dry sample for the leaves, 40.8 ± 0.1 for the stem, 91 ± 4 for the unripe fruit and 69 ± 2 for the ripe fruit.

The concentration of PACs using the DMAC method showed the following results; *V. consanguineum* gave 30.5 ± 0.5mg catechin eq. (CE)/g of dry sample for the leaves, 38.1 ± 0.5 for the stem, 5.54 ± 0.07 for the ripe fruit and 12.4 ± 0,5 for the unripe fruit. The *U. myricoides* samples showed 31 ± 3 for the leaves, 24 ± 4 for the stem, 11.6 ± 0.9 for the ripe fruit and 15.4 ± 0.2 for the unripe fruit. The antioxidant activity was determined using the ORAC method. The *V. consanguineum* results were of 69941 ± 5876 µM Trolox eq/g of dry sample for leaves, 62617 ± 1463 for the stems, 23912 ± 739 for the ripe fruit and 32503 ± 3111 for the unripe fruit. For the *U. myricoides* samples, the ORAC results were of 52,241 ± 3106 for the leaves, 23,025 ± 2647 for the stems, 38339 ± 7773 for the ripe fruit and 45053 ± 3728 for the unripe fruit [1,2].

Finally, the antibacterial activities of two types of extracts (crude extract of polyphenols (CEP) and crude extract of proanthocyanidins (CEPACs), 3 mg) of *V. consanguineum* and *U. miricoides* were tested against *S. areus*, *B. subtilis*, *E. coli* and *P. aeruginosa* using the disc diffusion method. The average percentage (%) of growth inhibitions of all the extracts were 92 ± 3, 62 ± 3, 62 ± 4 and 68 ± 3% against *S. areus*, *B. subtilis*, *E. coli* and *P. aeruginosa*, respectively. In general, the percentage of growth bacterial inhibitions was slightly higher with the CEPACs in comparison with the CEP.

Keywords: Nutraceutic, Folin-Ciocalteu, Proanthocyanidins, Trolox, Berry, DMAC, ORAC, Chloramphenicol.

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ANTI-INFLAMMATORY AND ANTIOXIDANT PROTECTIVE ACTIVITIES OF GREEN AND BROWN PROPOLIS: A FOCUS ON THEIR MECHANISMS OF ACTION

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PPAF 07

Propolis is a complex product consisting mainly of vegetable resin and wax produced by bees to isolate and protect the beehive from biotic and abiotic external agents. Moreover, propolis is rich in different types of polyphenols and bioactive components depending on the plant it comes form [1]. Since ancient times, propolis has been considered a healthy product. In fact, it was used in the traditional medicine of Egyptian, Greek and Roman civilization [2]. Today, we find propolis in the formulations of a number of food supplements and medical devices as well as in the composition of some functional foods, due to its biological activities that has been demonstrated both in *in vitro* and *in vivo* conditions [3-5]. There are different types of propolis, which differ in chemical composition, sensorial and biological properties. This variability comes from several factors (i.e. botanical species from which bees collect the resin, geographic origin, and bee species) [6]. To investigate the influence of the different geographical origin on propolis antioxidant [7] and anti-inflammatory [3] well-known activities, and to elucidate the molecular mechanism associated with propolis biological properties, two different types of propolis extracts were studied. In particular, human keratinocytes (HaCat cells) were treated with increasing non cytotoxic concentrations (ranging from 0.78 to 3.125 µg/mL) of a brown propolis extract from Brazil (collected mostly from *Baccharis dracunculifolia* D.C.), and a green propolis extract from Europe (derived principally from *Poplus* species) [8]. The results showed that the expression levels of microRNAs involved in the oxidative stress and inflammation (miR-19a-3p, miR-203a-3p, miR-27a-3p, miR-17-3p) were modulated by both types of propolis, being brown propolis extract more active. These results were confirmed by the modulation of the target mRNAs and proteins (antioxidant enzymes and pro-inflammatory cytokines).

Keywords: Green and brown propolis, Antioxidant and anti-inflammatory activities, microRNAs, mRNAs and proteins.

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CHEMOPREVENTIVE EFFECTS OF HORCHATA, BEVERAGE OF SOUTH ECUADOR

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"Horchata" is an herbal mixture infusion consumed in Southern Ecuador: 66% of its plants are anti-inflammatory medicinal plant and 51% are analgesics [1]. Both activities could be related to chemoprevention [2]. Chemoprevention is the ability to prevent, block, or reverse cancer progression [3]. The aim of this study was to evaluate the cytotoxic potential of horchata (HRCH) as well as its mechanism and antigenotoxic effects. Nine different HRCHs varieties that are popular in Loja were prepared, consumed, and freeze-dried.

Phytochemical and antioxidant activities were evaluated. The cytotoxic activity was evaluated on cerebral astrocytoma (D-384), prostate cancer (PC-3), breast cancer (MCF-7), colon cancer (RKO), lung cancer (A-549), immortalized Chinese hamster ovary cells (CHO-K1) and human peripheral blood lymphocytes via a MTS assay. The pro-apoptotic effects were evaluated with Anexin V/Propidium Iodide and western blot of Bax, Bcl-2, TP53, and TP73. Induction and reduction of ROS were assessed by fluorimetry. Genotoxic and antigenotoxic effects were evaluated with a comet assay and micronuclei on binucleated cells. Phytochemical screening tests on HRCHs samples revealed the presence of saponins, flavonoids (except HRCH 1), terpenoids (except HRCH 1), quinones (except HRCH 7 and HRCH 8) and alkaloids (except HRCH 2, HRCH 3 and HRCH 5). High antioxidant capacity of seven of the nine HRCHs was observed. There was no inhibitory effect on cell growth with normal cell. In D-384 cells, five (HRCH 1, HRCH 2, HRCH 7, HRCH 8 and HRCH 9) of the 9 HRCHs generated cell inhibition greater than 30%. The IC50 range of effective HRCHs was 41 to 122 µg/mL.

We observed an increase in the percentage of cells in early apoptosis and modulation expression of p21, p53 TP73 in all HCRHs. The CHO-K1 cells showed increased ROS, but this was ~50% lower than the values produced a ROS-inducing agent (H2O2). In the comet test also shows an increase in the tail length of the comet assay. Relative to the H2O2 control, the DNA damage was ~ 30% (HRCH 9) and 40% (HRCH 1 and HRCH 7) lower. We observed no increase of micronucleus with respect to basal damage via a DNA damage-inducing agent such as MMC C. The damage decreases even at basal levels with HRCHs. Horchata is a traditional drink in southern Ecuador. It contains various medicinal plants and presents cytotoxic activity toward astrocytoma cells inducing regulated apoptosis in the p53/p73 pathway. However, several HRCHs have great antioxidant and anti-genotoxic capacity with chemoprotective affects.

Keywords: Horchata, Cancer, Antigenotoxicity, Anticlastogenic, Apoptosis.

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MANGO AND GUAVA´S BY-PRODUCTS TO PREPARE FUNCTIONAL INGREDIENTS

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PPAF 09

The processing of tropical fruits generates a large amount of by-products that are rich in dietary fiber and compounds with antioxidant activity, they can be used as ingredients and functional foods [1]. The aim of this work was to evaluate the techno-functional properties of by-products and their use for the preparation of ingredients. Mango (*Mangifera indica* L.) and guava´s (*Psidium guajava* L.) by-products were provided by Agroficial S.A. (Guayaquil, Ecuador).

By-products (peel, pulp and seed only of guava) were dried at 50 °C and the particle size used was 125-212 and 212-250 µm. Water retention capacity (WRC), swelling capacity (SC) and oil retention capacity (ORC) were determined [2,3]. The ratio tested of mango:guava for the agglomerate was 75:25 and 50:50 and for the powder ingredient was 60:40, 70:30, 80:20 and 90:10. The best formulation was chosen using a sensory descriptive test with 9-point scale and semi-trained judges. The attributes evaluated were flavor, color, smell and texture, applying a factorial design 2^2.

The general acceptability of the ingredients was evaluated in the final product (granola and yoghurt) with 30 consumers using a 9-point scale for calculated the acceptability index (%AI). The total dietary fiber "TDF", insoluble dietary fiber "IDF", protein, ash and fat were determined. ANOVA and a Tukey range test (p<0.05) were used to determined significant differences. Mango by-products showed by gram of dry sample, 11.40 to 12.24 g water of WRC, 7.96 to 8.21 mL of SC and 1.24 to 1.38 g oil of ORC.

Guava by-products had 3.18 to 3.88 g water of WRC, 2.44 to 3.26 mL of SC and 0.99 to 2.21 g oil for ORC. The 80:20 ratio was chose for the powdered ingredient, the content of TDF and IDF was 51.6 and 38.31 g/100g, respectively and the AI was 83.3%. In the agglomerated ingredient, the ratio 75:25 (mango:guava) was selected, it had 29.23 g/ 100g FDT and 20.07 g/100g to IDF, the AI was 94.4%. In both ingredients the particle size chosen was 212 to 250 µm. Mango by-products showed high WRC and SC, both by-products showed low ORC. Both ingredients proved to be good resources of TDF and IDF, with a high acceptance by consumers, constituting a versatile, cheap and healthy alternative to being use by the food industry.

Keywords: By-products, Mango, Guava, Functional ingredients.

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RECOVERY OF ANTIOXIDANTS FROM FRUIT BY-PRODUCTS BY SUPERCRITICAL FLUID EXTRACTION

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PPAF 10

Fruits and vegetables are recognized as good source of natural antioxidants, the intake of these foods is related with health and prevention of diseases. The by-products derived from industrialization of fruits and vegetables also have been studied by the high content of antioxidants [1,2]. Supercritical fluid extraction is a technology that has been used in the recovery of bioactive compounds from different vegetal matrixes [3], the aim of this study was the recovery of antioxidants from *Annona cherimola* and *Psidium guajava* by-products. The fruits were obtained in the province of Loja and treated similar as in the industry to obtain the by-products. The dehydrated samples were milled to reduce the particle size until 250 micrometers and then extracted with supercritical carbon dioxide (SC-CO2) during 3 hours, the main operation parameters, pressure and temperature, were varied between 100 to 200 bar and 35-60°C, respectively. The extracts were analysed by quantification of total phenolics content and antioxidant capacity by DPPH and ABTS methods. In the case of *Annona* the highest extraction yield was 1.91% (w/w) at 40°C and 200 bar, the total phenolic concentration was 891mg GAE/100g of extract at 40°C and 100 bar, the antioxidant activities by ABTS and DPPH were 188.5µM TE/g ES at 35°C and 100 bar and 42.47 µM TE/g at 35°C and 200 bar, respectively. While, for *Psidium guajava* the highest extraction yield was 3.45% at 45°C and 150 bar, the total phenolic concentration was 56.6 mg GAE/100 g of extract at 60°C and 100 bar, the antioxidant activities by ABTS and DPPH were 82.11µM TE/g extract at 35°C and 200 bar and 68.7 µM TE/g at 60°C and 200 bar, respectively. At the experimental conditions, pressure and temperature, the solubility of the extracted compounds was not related to the capacity of SC-CO2 extraction. The results of antioxidant capacity would encourage to intensify the studies in the application in food or pharmaceutical industries such as value-added natural extracts.

Keywords: Supercritical fluid extraction, Antioxidants, By-products, *Annona cherimola*, *Psidium guajava.*

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DIRECT LARGE VOLUME INJECTION HPLC DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHs) IN WATER: AN EASY AND FAST ANALYTICAL METHOD

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POTC 01

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The presence of PAHs in aqueous media is an issue of special concern due to the associated health risks for both humans and living beings [1]. This work proposes an easy and fast analytical method for the simultaneous determination of anthracene (AN) and benzo[a]pyrene (BaP), two of the most representative PAHs, at ultra-trace concentrations in water employing high-performance liquid chromatography coupled with a fluorescence detector after direct injection of a large volume. Several factors affecting the separation of the target analytes, such as the injection volume, column temperature, flow rate, strength of the mobile phase in terms of acetonitrile proportion, and the excitation and emission wavelengths, were evaluated for screening purposes using a fractional factorial design of experiments. The statistically significant factors from the screening step at a confidence interval of 95% were optimized from a Box-Behnken multiresponse surface methodology. The optimal operating conditions were 1 mL/min, 90%, 35°C, 100 µL, and 416 nm for the flow rate, acetonitrile content of the mobile phase, column temperature, injection volume and the emission wavelength, respectively. The optimal excitation wavelengths were 254 nm and 267 nm for AN and BaP. Under the optimized conditions, the proposed method was validated and applied to different natural water matrices. Good linearity values and low limits of quantification and detection of 75 and 5.54ng/L for AN, and 30 and 4.26 ng/L for BaP were obtained. Additionally, intraday and interday precisions lower than 2 and 11%, respectively, were found. Accuracy was also verified and relative standard deviations lower than 10% were evidenced. Furthermore, the analysis of AN and BaP in real natural water gave satisfactory recoveries. The developed method showed to be suitable for the identification and quantification of AN and BaP at ultra-trace levels in relatively clean natural water by direct injection in only 5 min of analysis.

Keywords: Polycyclic aromatic hydrocarbons (PAHs), Direct injection, Multiresponse surface methodology.

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DETECTION OF CYANOTOXINS TRANSFORMATION PRODUCTS BY UPLC QTOF MS

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POTC 02

Cyanobacteria have become the focus of extensive research, due to increased blooms and consequent presence of toxic compounds, cyanotoxins, in the aquatic environment [1]. Some cyanotoxins are hepatotoxic, and the most representative are microcystin-LR (MC-LR), cylindrospermopsin (CYN) and nodularin (NOD), which have been detected and studied in different aquatic environments. It has been reported worldwide poisonings, gastro-enteritis mainly, associated to cyanotoxins, and some cases of fatal intoxication has been also reported in humans and animals [2,3].Hepatotoxins are stable in natural aquatic environments, being resistant to various natural elimination processes including chemical oxidation by naturally generated reactive oxygen species and biological transformation by other microorganisms [4, 5]. A high number of studies on the remediation of cyanotoxins using conventional methods have been reported [6-9], as well as several studies using UV radiation as possible tertiary treatment. Other are advanced oxidation processes have been also reported for these compounds [10-12]. Some studies are focused on the identification of transformation products (TPs) of cyanotoxins. To this aim liquid chromatography coupled to time of flight mass spectrometry (LC-QTOF-MS) has been used as an efficient tool for elucidation of cyanotoxins' TPs [13,14]. In this work, a research has been made on identification of the TPs formed in the processes of simulation of sunlight, UV radiation, chlorination and dark conditions or hydrolysis, on three hepatotoxins, MC-LR, CYN and NOD. A total of 22 cyanotoxins TPs were detected and tentatively identified by liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (LC-QTOF MS, as a powerful tool for identification thanks to the accurate-mass full acquisition data provided by this technique [15]. MS data obtained from these tests were processed using MetaboLynx XS application managers (Micromass v 4.1). Possible elemental compositions were calculated using the MassLynx elemental composition calculator with a maximum deviation of 2 mDa from the measured accurate mass [16].

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DETERMINATION OF THYMOL METABOLITES IN BROILER CHICKEN ORGANS THAT CONSUMING FOODS WITH NATURAL ADDITIVES, USING MSPD AND UHPLC-ESI-ORBITRAP-MS

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POTC 03

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The essential oil (EO) of *Lippia origanoides* H.B.K., has pharmacological activity against several microorganisms, this property is associated with the presence of thymol [1]. *In vivo* studies demonstrated that when these compounds are administered orally to broilers, the most representative biotransformation products of thymol are conjugated to sulfate and glucuronide [2]. This work describes the use of the extraction technique matrix solid phase dispersion (MSPD) to determine biotransformation products of thymol in muscle, kidney, liver, lung, plasma and intestine of broilers.

The tissue was lyophilized and subjected to MSPD extraction using octadecylsiloxane (C18) as a dispersing agent and acidified methanol (2% formic acid) as the elution solvent [3]. Analysis and identification of the analytes was carried out in a UHPLC-MS with electrospray interface (UHPLC-ESI(-)-Orbitrap-MS, Dionex Ultimate 3000, Exactive Plus Thermo Scientific, Sunnyvale, CA, USA). Accurate mass of the deprotonated molecular ions [M-H]- were obtained with negative mode ESI. For the identification of the compounds accurate mass *m/z* 325.12928 corresponding to thymol glucuronide and *m/z* 229.05400 corresponding to the thymol sulfate was used. The structure was confirmed from the ion fragment formation *m/z* 149.09719 corresponding to the mass of thymol with 20V collision energy for the sulfate and 30V for the glucuronide.

Based on the analysis, it was found that thymol sulfate was present in all matrices analyzed, the kidney is the organ that presented the most bioacomulation. Thymol glucuronide was not found in liver, muscle, plasma and lung. In the intestine, specifically in the ileum, the largest bioaccumulation of glucuronide was found.

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Keywords: MSPD, Thymol glucuronide, Thymol sulfate, Broiler chicken, UHPLC-ESI(-)-Orbitrap-MS.

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PURIFICATION OF SERRATIOPEPTIDASE PRODUCED BY *Serratia marcescens* ISOLATED FROM SILKWORM *(Bombyx mori*)

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Serratiopeptidase is a metalloprotease produced by a strain of *Serratia marcescens*. This microorganism was originally isolated from the digestive system of silkworm [1]. The production of the protease by this strain is higher compared to reference strains. This enzyme has been used as an anti-inflammatory and fibrinolytic agent [2]. However, it is important to purify the enzyme in order to confirm its biological activity. The present work focused on the purification of serratiopeptidase produced from the C8 isolate of *Serratia marcescens* obtained from a Colombian silkworm hybrid. The bacteria were cultured on a medium composed based in casein. The mixture was incubated at 28 C during 36 hours on a rotary shaker. Then, the mixture was centrifuged at 15.500 x g, at 4 C for 30 minutes. The supernatant was filtered with a cellulose acetate membrane filter (0,45 µm and 0,22µm) and referred as crude protease. The protease activity was measured by the azocasein method and the protein content was determined using the Bradford method.

The crude protease was concentrated using two methods: ultrafiltration with Macrosep (10 kDa) and ammonium sulphate precipitation (55% saturation). The fraction with a molecular weight higher than 10kDa was collected and loaded into a Bio-Scale Macro-Prep DEAE column pre-equilibrated with 25 mM Tris-HCl + 1 mM CaCl2 buffer (pH=8). After washing the column with buffer, proteins were eluted with 1M NaCl containing buffer. The active fractions were collected, applied to an ENrich SEC 70 Column and protein was eluted. The purified enzyme was stored at -20 °C. The molecular weight was determined by SDS-PAGE. The serratiopeptidase was purified by protein concentration (ammonium sulphate precipitation and ultrafiltration), weak anionic and gel filtration chromatography. The specific activity of crude enzyme was of 4,369 ± 323 U/mg protein and 4,507-± 367 U/mg protein after concentration with ammonium sulphate precipitation and ultrafiltration, respectively. The yield was similar in both methods (approximately 98%), however, the purification fold was higher after ultrafiltration (3.17) compared with ammonium sulphate precipitation (2.25). The capture of serratiopeptidase using weak anionic chromatography displayed the highest yield (55%) and purification fold (4.27) in samples concentrated by ultrafiltration. Active fractions were pooled, concentrated and purified by gel filtration chromatography. This step increased the total yield (40%) and purification fold (5.41) in samples submitted to ultrafiltration. The results indicate that protein concentration is a determinant step during the purification process. The molecular weight of serratiopeptidase is 50kDa. Sample ultrafiltration resulted in the highest specific activity (24,384±453 U/mg protein) of the enzyme. The calculated molecular weight is similar to data reported previously. In this work, we did successfully standardized a chromatographic method to isolate and purify serratiopeptidase from *Serrata marcescens*.

Keywords: Purification, Serratiopeptidase, Chromatography, Proteolytic activity.

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POLYCYCLIC AROMATIC HYDROCARBONS PHAS IN COMPLEX BIOLOGICAL MATRICES BY GC /MS

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POTC 05

The systematic research to determine PAHs biological accumulation, requires their sampling and analysis in various biological matrices. However, processing and purification this samples prior to the chromatographic analysis, constitutes a real challenge for the analyst taking into account lipids and proteins interferences and the need to concentrate the analyte for a correct instrumental detection. Most of the methods for analysis of PAHs are based on analyte separation in open columns packed with alumina, florisil and / or silica [3], which involves the use of large volumes of high cost toxic solvents. In order to provide a more efficient alternative for the analysis of PAHs in complex biological matrices, a method was developed and standardized to purify the extract obtained after treating the sample with hexane which includes solid phase extraction (SPE) with commercial cartridges, which optimizes the cost of the analysis by employing less solvent volume, reducing the extraction time, and providing selectivity by having cartridges with a wide range of polarity. In animal origin matrices such as blood serum, seminal fluid, milk, liver, kidney and pancreas, extraction was performed using silica as the stationary phase; while for matrices of greater complexity due to their high fat and protein content such as ovaries, eggs, fish and animal fat tissue, it was necessary to perform the extraction in several successive steps, modifying the polarity of the solid phase. Among the stationary phases used alternately or successively for this type of samples are: fluorisil, silica and alumina.

Prior to the extraction and purification treatment, the convenience of lyophilizing the biological matrices was established, since the decrease of moisture prevents its biochemical degradation without generating losses of the analytes of interest. The lyophilized sample is subjected to two consecutive processes: saponification and liquid-liquid extraction obtaining an extract with the analyte of interest. The extract obtained is purified with solid phase extraction cartridges, concentrated in inert atmosphere and injected into the apparatus. The chromatographic system employs helium as carrier gas, a SHRXI 5MS or equivalent column, autosampler, a temperature ramp between 75°C and 330°C and mass detector. The identification of the 15 PAHs is based on the retention time, and relative abundance of the characteristic masses. PAHs certified standard, external standard, method targets and analytical-substitute recovery controls are used. The extraction technique and the chromatographic process was standardized by statistical verification establishing the linearity, limit of detection, repeatability and reproducibility of the method for each type of analyzed matrix. The efficiency of the extraction process implemented for these matrices was verified by a percentage of analytical-substitute recovery between 70% and 130%.

Keywords: Complex biological matrices, Phase solid extraction, Polycyclic aromatic hydrocarbons, GC/MS.

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QUANTITATIVE ANALYSIS OF COCAINE SAMPLES TO EVALUATE THEIR PURITY AND MAIN ADULTERANTS, USING GAS CHROMATOGRAPHY COUPLED TO A FLAME IONIZATION DETECTOR (GC-FID)

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POTC 06

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According to the latest anti-drug reports from the United States, Colombia is the world's largest producer of cocaine. For this reason is necessary to implement studies that provide information about the purity of the produced and marketed drug and the presence of adulterants in order to evaluate the market dynamics, the chemicals that are included in the production process and additionally have chemical analysis methodologies for its characterization and quantification.

Based on the above, the present study was carried out, where a random sample of 249 forensic samples of cocaine was made in the *Fiscalía Genereal de la Nación de Colombia* chemistry laboratory, and later was made its quantification and analysis of the presence of recognized adulterants.

The study was performed using the instrumental technique of gas chromatography coupled to a flame ionization detector, where the samples were treated with methanol as solvent and Tetracosan (C24H50) as internal standard. Is established like a measurand the concentration of cocaine in each sample, the substances caffeine, levamisole, phenacetin and diltiazem are taken as the main adulterants and these were evaluated in presence and quantity.

The chromatographic method is optimized so that in a time of 15 minutes eluates all substances with excellent resolution and symmetrical peaks. With reference materials of the six interest analytes the calibration curves are constructed with concentration levels approximately from 100 mg/L to 1000 mg/L, for the quantification of each sample and then with the data obtained determine the percentage of cocaine in each one and the most used substances in the country to adulterate and in the combinations being marketed.

Keywords: Cocaine, adulterants, quantification, GC-FID.

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CONTRIBUTION TO THE PHYTOCHEMICAL STUDY OF THE DYES PRESENT IN *Arrabidaea florida* DC. LEAVES

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POTC 07

The species *Arrabidaea florida* DC. (Bignoniaceae), known as Om o Cudi, is widely used as dye by the indigenous communities of the Amazonian trapeze [1]. In Colombia it is distributed in the departments of Chocó, Caldas, Meta, Antioquia and in the Amazon Trapeze. Considering that there are not phytochemical studies on this species, in this work we perform a chemical study of the predominant fixed metabolites in the colorant precipitate obtained by fermentation of the aqueous extract of dry leaves of the species. The components retained in cotton fibers stained with *Arrabidaea florida* were analyzed

The separation and purification by liquid-Liquid fractioning, exclusion and column chromatography, allowed to obtain in fractions of medium and high polarity the flavones: apigenin, luteolin, acacetin, 6-methoxyluteolin and scutellarein, and the 3-deoxyanthocyanidins: 3',4',6,7-tetrahidroxy-5-methoxyflavylium, 4',6,7-tetrahidroxy-5-methoxyflavylium and 6,7-tetrahidroxy 4',5-dimethoxyflavylium, called 3'hidroxyarrabidin, arrabidin and carajurin respectively. Compounds were analyzed and identified using two high performance liquid chromatography systems (HPLC-DAD), with a database of reference compounds of HPLC grade. When it was considered necessary liquid chromatography with a mass detector was employed. HPLC-DAD analysis of the obtained dye extract of cotton fibers stained with *Arrabidaea florida* revealed as main components carajurin, arrabidin and 3'-hidroxyarrabidin and the flavones luteolin, acacetin y apigenin.

These results are consistent with the flavones found in species of the genus *Arrabidaea* [2-5] and have a high coincidence with the compounds determined in *Arrabidaea chica*, a species known for its dyeing and medicinal properties [6, 7], which allows to establish chemotaxonomic affinities and in dyeing properties between these species; In addition, constitute the first report of chemical studies of a plant species that has little scientific information.

Keywords: *Arrabidaea florida* DC, Phytochemistry, Natural dyes, 3-deoxyanthocians.

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PHYTOCHEMICAL STUDY OF THE COLORANTS PRESENT IN THE SPECIES *Berberis meollacensis* L.A. CAMARGO (CHUNU) (BERBERIDACEAE)

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POTC 08

The species *Berberis meollacensis* L.A. Camargo it is one of the colorants sources used by the indigenous community IKA located in the Sierra Nevada of Santa Marta for dying textile fibers, mainly cotton and fique in order to obtain yellow coloring [1].

Taking into account that there are not phytochemical studies about this species and that the stability of its colorants which is traditionally recognized, this work was made a chemical study of the fixed metabolites predominant in the acid, ethereal and chloroform; obtained from the ethanolic root extract of the species. Through of the preliminary phytochemical analysis, it was established the presence of flavonoids, cardiotonic glycosides, terpenes, tannins, and steroids. It is consequent with the previous phytochemical study made to the same kind [2]. The separation and purification by acid-base extraction permitted to get compounds of alkaloid type and of flavonoid type in the different fractions, which were identified through HPLC-DAD, GC-MS and 1H-NMR, using "reference patterns" as method for their identification. Flavonols such as quercetin and alkaloids with protoberberine-like structures such as berberine, jatrorrhizine, berbamine and palmatine and benzylisoquinolines type such as protopine. These alkaloids are common to the phytochemistry of the genus Berberis [3-6] and their presence in *B. meollacensis* is consistent with this chemotaxonomic feature. The analysis by HPLC-DAD of the colorant extracts obtained from cotton fibers stained with an aqueous extract of the species, determined that the main colorants present in the fibers were: berberine and jatrorrhizine. The textile quality tests on dyed material indicated that the coloring compounds of *Berberis meollacensis* give the material photoprotective capacity and fastness to the light, results that contribute to the assessment of native colorants.

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PLASMA MULTIPLATFORM METABOLIC AND LIPID FINGERPRINTING OF BREAST CANCER: A PILOT CONTROL-CASE STUDY IN COLOMBIAN HISPANIC WOMEN

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In the present pilot study, a multiplatform fingerprinting under metabolomic and lipidomic approaches was used to obtain a global picture of metabolic alterations related to breast cancer in Colombian women. The study was performed using plasma samples obtained from 30 breast cancer patients (BCP) and 30 control patients (CP). In order to increase the metabolite coverage, samples were analyzed by the three platforms commonly employed in metabolomics studies (GC-MS, LC-MS and NMR) using protocols previously described. For GC-MS, the samples were deproteinized and derivatized using a two stage process, methoximation and silylation. In LC-MS, both untargeted metabolomics and lipidomics were performed using an HPLC system coupled to Q-TOF. For untargeted metabolomic approach, plasma deproteinization and metabolite extraction were performed by mixing one volume of plasma with three volumes of cold mixture of methanol/ethanol (1:1). For untargeted lipidomic approach, lipids were extracted using the MTBE method, employing a mixture MTBE/methanol/water (10:2:2.5). 1H-NMR profiling was performed using a 400 MHz NMR spectrometer with different pulse sequences that allowed solvent suppression and protein signal suppression.

The samples were mixed with phosphate buffer with deuterated trimethyl silyl propionic acid and deuterated water. Differences between profiles from BCP and CP groups were evaluated using univariate (UVA) and multivariate (MVA) analysis. Statistics showed discrimination between breast cancer and healthy subjects on all analytical platforms. The differentiating metabolites were involved in glycerolipid, glycerophospholipids, amino acid and fatty acid metabolism. This study demonstrates the usefulness of multiplatform approaches in metabolic/lipid fingerprinting studies to broaden the outlook of possible shifts in metabolism.

Our findings propose relevant plasma metabolites that could help in a better understanding of underlying metabolic shifts driven by BC in women of Colombian Hispanic origin. Particularly, the understanding of the up-regulation of long chain fatty acyl carnitines and the down-regulation of cyclic phosphatidic acid (cPA). addition, the mapped metabolic signatures in breast cancer were similar but not identical to those reported for non-Hispanic women, despite racial differences.

Keywords: Metabolic fingerprinting, Breast cancer, Mass spectrometry, NMR.

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CYTOTOXICITY AND LEISHMANICIDAL ACTIVITY OF ESSENTIAL OIL FROM PLANTS PRESENT IN COLOMBIA AND COMMONLY USED IN TRADITIONAL MEDICINE

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POEE 01

Cutaneous leishmaniasis (CL) which is associated with considerable morbidity is still a major health problem in the world especially in developing countries. Over the last 70 years, only a few drugs for CL have emerged and drug resistance has increased; therefore, new drugs are needed.

Plants provide a valuable source of drugs due to the presence of abundant molecules with a variety of pharmacological activities. In the present study we evaluated the cytotoxic and leishmanicidal activity of 18 essential oils extracted from the aromatic plants *Thymus vulgaris*, *Salvia officinalis*, *Rosmarinus officinalis*, *Mentha piperita*, *Schinus molle*, *Origanum vulgare*, *Cinnamomum zeylanicum*, *Cupressus sempervirens*, *Citrus sinensis*, *Pinus pinea*, *Lavandina abrial*, *Hyssopus officinalis*, *Lavandula officinalis*, *Lippia alba*, *Cymbopogon nardus*, *Cimbopogum citratus*, *Eletaria cardamomumm*, *Bulnesia sarmientoi*, *Satureja sp.* and *Aloysia polystachya.* These plants have been associated with antibacterial, anti-inflammatory and antiparasitic activities. The essential oils were solubilized in DMSO not exceeding 0.5%. The cytotoxicity of was evaluated on the human U- 937 macrophages using the MTT colorimetric method. The leishmanicidal activity was evaluated on amastigotes of *L. (V) panamensis* by flow cytometry.

The results are expressed as Lethal Concentration 50 (LC50) for cytotoxicity and Effective Concentration 50 (EC50) for effectiveness evaluated, both values calculated by Probit. None of the essential oils was cytotoxic to the U-937 cells. In turn, the most effective essential oil to *L. panamensis* amastigotes were *Mentha piperita*, *Bulnesia sarmientoi, Cupressus sempervirens* and *Schinus molle* with an EC50 < 20mg/mL, while *Thymus vulgaris* and *Elettaria cardamomun* showed moderate antileishmanial activity with EC50 of 21.0 and 49mg/mL, respectively.

To date, there are no reports of the antileishmanial activity for *M. piperita*, *B. sarmientoi*, *C. sempervirens* annt and anti-ulcerative. *Schinus molle* is used as a healing, analgesic, antiparasitic and anti-inflammatory compound.d *S. molle* essential oils. Considering the antiseptic, analgesic, anti-inflammatory properties of these species, the development of a formulation that combines these properties could be a possible alternative for the management of uncomplicated CL.

Keywords: Essential oil, Antileishmanial activity, Cytotoxicity.

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ANTIMICROBIAL AND ANTIOXIDANT POTENTIAL OF THE ETHANOLIC EXTRACTS FROM *Erythrina edulis* M. FRUITS

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POEE 02

The *Erythrina* genus (Fabaceae - Papilionideae) is an important source of secondary metabolites that have been reported with different biological activities including antimicrobial, anti-inflammatory, antimalarial, analgesic and antipyretic [1-4]. However, many of its species have not been studied, and therefore, the present study aimed to determine the antimicrobial and antioxidant capacity of the ethanolic extracts from the chachafruto seeds, testa and pods (*E. edulis* M.). Once the preliminary phytochemical screening of the extracts [5] were carried out, the antiradical capacity against ABTS and DPPH [6] as well as the antibacterial and antifungal activity (using the optical density method and diffusion agar respectively) were also determined [7,8]. Secondary metabolites such as flavonoids, alkaloids, tannins and terpenes were identified. The extracts showed stabilizing activity against the two radicals at low concentration and inhibited the growth of the evaluated microorganisms. The results suggest that the compounds found in the extracts could be a good antimicrobial and antiradical alternative to be used in the phytopharmacological industry.

Keywords: Chachafruto, Antioxidant, Antimicrobial, Seeds, *Erythrina*.

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PHYTOCHEMICAL STUDY AND ANTIINFLAMATORY ACTIVITY OF BADEA (*Passiflora quadrangularis*) AND GULUPA (*Passiflora edulis* f. *edulis*) LEAVES

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POEE 03

Passiflora quadrangularis and *Passiflora edulis* f. edulis, known as badea and gulupa, respectively, are cultivated at Colombian low lands. Their edible fruits are used for local consumption in juices. Passiflora genus species are well known by their anxiolytic and anti-inflammatory properties. In this sense, the aim of this work was to isolate and identify the major compounds from aqueous extracts of *P. quadrangularis* Linn. and *P. edulis* f. edulis Sims. leave, and to evaluate their anti-inflammatory activity.

The isolation of the main compounds was conducted by high-speed countercurrent chromatography (HSCCC), column chromatography and HPLC-DAD-ELSD. The structure analysis was done by spectroscopic methodologies, including 1D and 2D NMR spectra and ESI-TOF-MS/MS. The aqueous extract of Gulupa (*Passiflora edulis* f. edulis) yielded three previously reported saponins (1, 2, 3) and three minority flavonoids, previously reported from an unidentified variety of *P. edulis*. This is the first research that describe chemical composition of the polar fraction of gulupa leaves. From badea (*P. quadrangularis*) aqueous extract was possible to isolate four novel cycloartane type saponins (4, 5, 9 and 12), two known cycloartane type saponins (10, 11) and two novel saponins were identified in mixture (6, 7).

Finally, other known oleanolic nucleous saponin (8) and the flavonoid 2'-xylosil-vitexin (13) were identified. The last compounds have been also isolated from another *Passiflora* species. Anti-inflammatory activity was evaluated using TPA-induced ear edema model. Saponin 4 and flavonoids fraction of *P. quadrangularis* showed an anti-inflammatory activity similar to these showed by dexamethasone. Myeloperoxidase activity and nitric oxide mediator production in the ear exudates were evaluated, the results showed inhibition of leukocyte degranulation by saponin 1 and lower activity for saponins 2 and 4, related to the myeloperoxidase activity.

Flavonoids fraction for both species showed greater inhibition of leukocyte degranulation than these caused by saponins fractions. Saponins 1 and 2 showed activity in the inhibition of nitric oxide production. Saponins and flavonoids fractions from *P. edulis* f. edulis showed greater inhibition activity in the production of nitric oxide than these caused by *P. quadrangularis* fractions. These results indicate great potential for aqueous polar extract and butanolic fractions of gulupa and badea leaves as anti-inflammatory.

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Keywords: *Passiflora*, Counter-current chromatography, Saponin, Flavonoid, Anti-inflammatory activity.

ANALYSIS OF FLAVONOIDS IN PLANTS OF THE GENUS *Passiflora* BY UPLC-DAD-ELSD

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POEE 04

The plants of the genus *Passiflora* are widely cultivated in the tropics by the value of their fruits, and in Colombia represent a market of great interest whose appreciation has been increasing in recent years [1]. Additionally, plants of this genus are recognized worldwide for their multiple ethnopharmacological uses. With the present work, the development of a method of quantification of vitexin and chrysin by HPLC in aqueous extracts of leaves of cultivable *Passiflora* species was proposed. The first compound corresponds to the chemical marker reported for *P. incarnata* in the European, British and Spanish pharmacopoeias [2-4], and the second was selected because of the many recent studies on its biological activity. This analytical tool will be used for the quality control of both the starting material and finished products that could be developed - for therapeutic, nutraceutical, cosmeceutical or of any other kind - from leaves collected as part of the pruning process of crops, providing an added value to them.

The method developed by ultra-high performance liquid chromatography with diode array detection by external standard proved to be linear, precise, accurate and having adequate detection and quantification limits for the determination of such flavonoids in different *Passiflora* species. In addition, it was established that the recovery of flavonoids from the aqueous extract is greater when XAD-2 resin is used than when using butanol. In this study, banana passionfruit (*P. tripartita* var *tripartita*, *P. tripartita* var *mollisima*, *P. mixta*, *P. cumbalensis*), passion fruits (*P. edulis* var *flavicarpa*, *P. edulis* var *edulis*), granadillas, (*P. ligularis*, *P. quadrangularis*) and sweet passion fruit (*P. alata*) leaves were analyzed.

Of the 9 studied species, only a quantifiable amount of vitexin (6.8 ± 0.06mg g-1 dry extract) was found in *P. mixta*, whereas for *P. tripartita* var *mollisima* (curuba de castilla), the official species in the Vademecum of Colombia, is present but not quantifiable. Regarding the chrysin content, it was observed that it is only present in *P. ligularis* (granadilla).

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Keywords: *Passiflora*, flavonoids, UPLC analysis, validation, chrysin, vitexin.

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ANALYSIS OF VOLATILE COMPONENTS OF NINE SPECIES USED IN TRADITIONAL MEDICINE IN ECUADOR

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POEE 05

This study was designed to examine the physical properties, chemical composition and antifungal, antibacterial and antioxidant *in vitro* activities of the volatile components from some aromatic species such as *Scutellaria volubilis*, *Lepechinia paniculata*, *Baccharis latifolia*, *Baccharis obtusifolia*, *Artemisia sodiroi*, *Siparuna eggersii*, *Tagetes filifolia*, *Clinopodium nubigenum* and *Annona cherimola* which are used widely in traditional medicine in Ecuador. The essential oil was examined by a combination of GC/FID and GC/MS techniques.

The antifungal and antibacterial activities were determined by the broth microdilution method. The antioxidant activity was measured by DPPH and ABTS radical-scavenging activity tests. Thirty seven components were determined in essential oil of *S. volubilis*, the principal constituents are found to be sesquiterpene hydrocarbons: germacrene D (20.4%), ?-caryophyllene (17.5%),?-humulene (14.7%) and ? -bisabolene (5.8%). Thirty four components were identified for essential oil of *L. paniculata*, the principal groups are sesquiterpene hydrocarbons such as aromadendrene (24.6%), viridiflorene (12.4%), ?-selinene (7.4%) and valencene (6.7%). Twenty-nine compounds, representing 90.91% of the oil from *B. latifolia* were identified, the major components were limonene (33.72%); ? -phellandrene (10.32%); sabinene (10.28%); ?-pinene (6,99%); ?-pinene (5.44%). Thirty-one individual compounds were identified and constitute 96.1% of the total composition of the oil from *B. obtusifolia*, the main constituents of the oil were limonene (28.3%), germacrene-D (9.8%), ?-pinene (9.0%), ?-pinene (8.2%), bicyclogermacrene (6.2%) and ?-cadinene (5.7%).

In the essential oil of *A. sodiroi*, the oxygenated monoterpenes were the main group of components, especially sabinyl acetate (65.8 %), while the essential oil of *S. eggersii* was mainly composed by the oxygenated sesquiterpenes among which the epicurzerenone (29.9 %) was the most representative. Conversely, the aromatic hydrocarbons predominated in the oils of *T. filifolia* and *C. nubigenum*, with (*E*)-anethole (72.6 %) and carvacryl acetate (38.1 %) as the main components, respectively. Thirty components were identified for essential oil of *A. cherimola*, the main constituents of the essential oil were Germacrene D (21.8 %), Sabinene (8.9 %), ?-Elemene (7.9 %), Bicyclogermacrene (6.2 %). The essential oil from *B. latifolia* exhibited activity against *Trichophyton rubrum* (ATCC 28188) and *Trichophyton mentagrophytes* (ATCC 28185). *B. obtusifolia* essential oil exhibited a moderate antibacterial effect against *Klebsiella pneumoniae* (ATCC 9997) and *Enterococcus faecalis* (ATCC 29212) and good antifungal activity against *Trichophyton rubrum* (ATCC 28188) and *Trichophyton mentagrophytes* (ATCC 28185). The essential oil from *A. cherimola* showed strong antioxidant activity in both DPPH and ABTS assay.

ANTI-INFLAMMATORY ACTIVITY OF COLOMBIAN TRADITIONAL MEDICINAL PLANTS AND ANALYTICAL STRATEGY FOR BIOACTIVE COMPOUNDS DETERMINATION

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POEE 06

Inflammation is a complex process that is closely related to the development of chronic noncommunicable diseases which are currently the leading cause of death in the world [1,2]. Nowadays, there has been a growing interest on the ingredients and extracts used in traditional medicine systems as potential alternative for the treatment of inflammatory events [3]. A previously ethnopharmacological study carry out in Eastern of Antioquia, revealed some species with high traditional anti-inflammatory use and potential antioxidant profile [4]. To contribute to the preservation of the traditional knowledge and confirm this medicinal use, we investigated the anti-inflammatory activity of the hydroalcoholic extract of the most promising species: *Cuphea calophylla* (Lythraceae), *Tibouchina kingii* (Melastomataceae) and *Pseudoelephantopus spiralis* (Asteraceae), in a cellular model using LPS-activated THP-1 macrophages. Reactive oxygen species (ROS), nitric oxide (NO) and malondialdehyde (MDA) were monitored as inflammatory and oxidative markers. In addition, we evaluated the inhibitory capacity on lipooxygenase (LOX) and cyclooxigenase (COX) activity in a free-cell system. The results showed the potential of the extracts to reduce ROS (26% - 48%) and NO (26% - 48%). The levels of MDA lipid peroxidation marker were reduced between 13%-20%. The hydroacoholic extracts also showed a cytoprotector effect decreasing approximately 40% the quantified levels of dehydrogenase lactate in LPS-activated macrophages. Regarding to inflammatory enzymes, the medicinal plants also attenuated the catalytic activity of LOX (33%-79%) and COX (41%-64%). Complementarily, with the final purpose to identify the bioactive markers into the extracts, we applied modern high-resolution mass spectrometry techniques and multivariate analysis such as principal component analysis and partial least squares discriminant analysis. These findings may confirm the anti-inflammatory potential of these plants, which may represent a valuable source of natural bioactive compounds with benefits for human health.

Keywords: Inflammation, Traditional medicine, Multivariate analysis, High resolution mass spectrometry, Bioactive markers.

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PROTOTYPE OF BIO-REPELLENT LOTION USING ESSENTIAL OIL OF *Bursera graveolens* (PALO SANTO) FROM ECUADOR

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POEE 07

Actualy, several synthetic chemicals have been developed to protect humans from mosquito. The DEET is not only a broad spectrum repellent, but also the most effective and persistent on the skin. There are studies that show its high toxicity, for this reason is important to increase efforts to find repellents of natural origin that are safe and environmentally friendly. In this study was evaluated the essential oil of *Bursera graveolens* specie (Palo santo) like the main component of a naturally bio-repellent lotion. For this, we made studies about pre-formulation and formulation evaluating the interaction between the oil and seven excipients using the experimental design of binary mixtures showing that three components interacts with limonene (majority compound 68% and the one owing the repellent activity).

The analysis of oil and lotion was done in GC-MS. Besides, we have studied the repellent effectiveness four concentrations were tested (0.5% - 1% - 2% - 3%) and the lotion elaborated at 2% is the one that provides protection up to 60% (5 hours, considered repellent category IV) against *Aedes aegypti* mosquitos. Additionally, the stability studies were done during three months under climatic conditions that corresponding to Zona 4 according to International Conference of Harmonization (ICH): 17° C ± 2 (ambient temperature), 30 °C ± 2 and 40 °C ± 2 and a relative humidity of 75 % ± 5 %. The organoleptic, physical and chemical properties were into of normal parameters, like a homogeneous aspect, transparent colour, citric odour, pH 5.9, density 1.0 and viscosity between 10 - 12 cP. Likewise, the microbiological studies showed that there is no growth of microorganisms (*Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa*, Fungi and Yeast). Furthermore, the degradation of limonene was more than 10% when the lotions were stored at climatic conditions previously mentioned. The shelf life prediction of this prototype was 1, 24 months, approximately.

Finally, the obtained formula was subjected to toxicological studies (Acute Dermal Toxicity performed in Wistar rats) demonstrated that the prototype no produces side effects, and lacks pathogenic elements that could put the health in risk. Thus, we believe that the formulation of the bio-repellent constitutes in our country a natural alternative solution opposite to a public health problem such as infection of diseases caused by mosquitos.

Keywords: *Bursera graveolens*, Binary mixture, Repellent lotion, DEET, *Aedes aegypti.*

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INHIBITORY POTENTIAL OF COLOMBIAN MEDICINAL PLANTS AGAINST SIX SEROVARS *Leptospira spp*

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POEE 08

Plants have traditionally been used for disease control but only 15% have been selected for their therapeutic value; being its active principles considered as source of new and novel drugs due to microbial resistance and adverse effects [1]. Colombia for its plant diversity and ecology offers the possibility of studying the medicinal potential of diverse species that may be useful for the control of *Leptospira* spp., a bacterium that causes leptospirosis a zoonosis that affecting the human and more than 160 animal species; their control is an unresolved problem and in the world only three plant species have been studied to evaluate their potential against *Leptospira* spp. [2,3]. Leptospirosis is principally controlled with penicillin G and ampicillin; however, empirical treatment has favored resistance to antimicrobials [4] and the variation in susceptibility of *Leptospira* strains seems to depend of host [5]. Therefore, the objective of this work was to determine the inhibitory potential of Colombian medicinal plants against six serovars of *Leptospira* spp. For this, 13 plants of the traditional Colombian medicine were selected and the extracts were obtained by cold maceration with 96% ethanol. The inhibitory effect of the extracts against six serovars of *Leptospira* spp. by the microdilution technique (MDT) was evaluated, was to determined cell viability by dark field and its effect on DNA cleavage were determined by electrophoresis. Of the promising species *Niphogeton glaucescens* presented a MIC of 4mg/mL against serovar Bratislava and 2mg/mL against serovars Icterohaemorrahagiae and Canicola; *Copaiba officinalis* and *Eucalypto pellita* presented MICs of 4mg/mL and 2mg/mL against these three serovars respectively. Additionally, differences in serovar susceptibility were observed compared to the extracts evaluated.

Therefore, Canicola and Bratislava serovars were inhibited by 46% and 39% of the extracts studied; followed by Icterohaemorrahagiae (23%), Hardjo (15%) and Autumnalis (8%). In contrast, the Pomona serovar was not inhibited by any extract. This study contributes to the knowledge about the medicinal potential of colombian plants for the control of *Leptospira* spp., allowing to evaluate its use for the obtaining of active principles oriented to the generation of bioproducts for the prevention and control of a zoonosis of worldwide interest.

Keywords: Medicinal plants, Antimicrobial potential, Leptospirosis.

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MORPHOHISTOCHEMICAL AND PHYTOCHEMICAL STUDY OF LEAVES AND ROOTS OF *Heliconia latispatha* Benth

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POFF 01

The Heliconias (Zingiberales: Heliconiaceae) are among the most attractive plants of the Neotropical forests, easily recognizable by their inflorescences with large and showy bracts [1]. In Colombian national territory these plants attract attention for the diversity of their colors, most of the species are endemic and are threatened by the destruction of their hábitat [1].

In this study, we present for the first time the morphological description and determination of the primary and secondary metabolites identified in leaves and roots of *Heliconia latispatha* Benth, for which we selected ten vigorous and healthy plants collected in the district of Bajo Grande, Sucre-Sucre, located at 8° 41' 0" North and 74° 51' 0" West in Colombia, South America. From the morphohistochemical view, the root presents the uniestratified epidermis, the vascular system is composed of polyarque xylem strands alternated with the phloem with a clearly defined endodermis. The leaves have paracytic stomata and the central vein consist of aerenchyma and a large number of closed collateral vascular bundles. In the histochemical tests performed for the aerial parts, the presence of carbohydrates, abundant lipids, chalk, cellulose, hemicellulose, lignin, calcium oxalate, phenolic compounds and alkaloids were determined. In the roots were found aleurone granules, lipids, callus, tannins, calcium oxalate and alkaloids. The presence of cardenolides, carbohydrates in leaves, roots and flavonoids, and leucoanthocyanins only in leaves are reported in the ethanol extract of the collected parts of this specie through qualitative phytochemical screening-drop test.

Keywords: Sucre, Heliconiaceae, Morphology, Histochemistry, Primary and Secondary metabolites.

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GASTROPROTECTIVE MECHANISM AND ULCER RESOLUTION EFFECT PROMOTED BY THE METHANOLIC EXTRACT OF *Cyrtocarpa procera*

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POFF 02

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Gastric ulceration is a multifactorial disease characterized by the presence of open sores in the lining of the stomach. *Helicobacter pylori* infection and the chronic consumption of NSAIDs are the two main etiological factors. It is widely accepted that gastric ulcers result from and imbalance between mucosal protective mechanisms (i.e. mucosal integrity, mucus secretion, NO, prostaglandins, and tissue microcirculation) and noxious factors (i.e. gastric acid, pepsin, ROS, *H. pylori* infection, alcohol and NSAIDs ingestion). Current therapies are mainly targeted for *H. pylori* eradication, leaving aside other factors that contribute to the resolution of gastric ulcers. Moreover, actual anti-acid treatments are insufficient to promote a complete ulcer healing and to prevent the relapse of gastric ulcers. It has been suggested that the histological quality with which this repair process occurs, plays a key role in the risk of ulcer recurrence [1]. *Cyrtocarpa procera* Kunth (Anacardiaceae) is a tree endemic to Mexico. Preparations from its bark have been extensively used in folk medicine for treating digestive disorders [2]. Previous research with different polarity extracts of *C. procera* bark, have demonstrated that the methanolic extract (CpMet), obtained by exhaustive maceration, had a remarkable gastroprotective effect (ED50=0.53 mg/kg) in a murine acute ethanol ulcer model and a good *in vitro* anti-*H. pylori* (MIC= 62.5 µg/ml) activity [3]. The present study was conducted to assess: the mechanism by which CpMet exerts gastroprotection, the toxicological safety and the preclinical efficacy in the resolution of ethanol-induced gastric ulcers in mice models during a 20-day repeated-dose oral administration of the extract. The results showed that the gastroprotective activity of CpMet can be mainly attributed to NO and prostaglandins, followed by sulfhydryl groups, and KATP channels. The gastroprotection afforded by the extract does not rely on the increment of the gastric pH. CpMet showed to be effective in the resolution of ethanol-induced gastric ulcers. Compared to the initial ulcer damage generated by ethanol, CpMet (300 mg/kg, twice a day) promoted a 62.65% of gastric ulcer resolution at the 20th day of the treatment; this percentage was practically attained from the 5th day of the regimen. The gastric healing effect of CpMet was confirmed by macroscopic and microscopic evaluation. Macroscopically, the alleviation of gastric mucosal ulcers was evidenced by the presence of flat scars that dovetailed with the histological findings, characterized by the recovery of the gastric epithelial architecture, an increment in mucus production and the absence of inflammatory infiltration at the site of the repaired ulcer. No clinical or biochemical signs of systemic toxicity were observed in the animals orally treated for 20 consecutive days with the extract. These data suggest the safety and efficacy of CpMet in preventing gastric ulceration by acting upon the enhancement of some endogenous gastroprotective mechanisms, and very importantly, by promoting a high quality of ulcer healing.

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Keywords: *Cyrtocarpa procera*, Gastroprotection, Gastric ulcer resolution, Toxicity.

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ANTIOXIDANT ACTIVITY AND POLYPHENOLIC CONSTITUENTS OF *Fumana montana* POMEL

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POFF 03

Cistaceae family consists of eight genera and about 180 species. Five genera (*Cistus*, *Fumana*, *Halimium*, *Helianthemum* and *Tuberaria*) are native to the Mediterranean region. Several phytochemical studies on the Cistaceae family revealed to be essentially rich in essential oils [1] and flavonoid glycosides [2]. *Fumana montana* Pomel is a dwarf shrub growing on rocky ground of Algeria [3]. Extract of this aromatic plant showed larvicidal activity [4]. Thus far, there have been no literature reports on either the constituents or the biological activity of *F*. *montana* extracts, except the larvicidal activity. The phytochemical investigation of the ethyl acetate extract of the whole plant of *F*. *montana* results in the isolation and structural elucidation of four new phenolic compounds consisting of three methylated flavonol glucosides **1–3** and one unusual sulfate flavanone **4**, in addition to fourteen known compounds including seven flavonols, two flavanols, one benzophenone glucoside, one phenolic glucoside and three benzoic acid derivatives.

The structures of the isolated compounds were established on the basis of physical and spectroscopic analysis, including 1D and 2D homo- and heteronuclear NMR experiments (COSY, HSQC, HMBC and NOESY), and by comparison to the respective literature data.

The ethyl acetate and *n*-butanol extracts of *Fumana montana* were also examined *in vitro* for antioxidant activity using different methods including 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging and ferrous ion chelating assays.

Keywords: Cistaceae, *Fumana montana*, Flavonoid glucosides, Antioxidant activity.

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NEW ISOFLAVONOIDS AND BIOLOGICAL ACTIVITIES FROM *Erinacea anthyllis*

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POFF 04

The genus *Erinacea* (family Fabaceae) belonging to the subfamily Papilionoideae and the tribe Genisteae, contains a single species called *Erinacea anthyllis* Link [1]. *E. anthyllis* is a shrub with purplish blue flowers growing in mountains of Algeria, Tunisia and Corsica [2]. This species is used in folk medicine of Algeria to treat rheumatic diseases [3]. In the current study, two new prenylated isoflavonoids, namely Erinasone A and Erinasone B along with 19 known secondary metabolites including 12 isoflavonoids, 3 polyphenols, 1 flavonol, 2 flavanones and 3 phytosterols, were isolated from the whole plant (roots and aerial parts) of *Erinacea anthyllis.* Structures of all isolated compounds **1**-**21** were elucidated by spectroscopic analysis, including 1D and 2D NMR (1H, 13C, COSY, HSQC, TOCSY, HMBC and NOESY), mass spectrometry (ESI-MS), UV-Vis, measurement of optical rotation [α]D and by comparison with the literature data. The total phenolic and flavonoid contents were determined by the Folin-Ciocalteu and AlCl3 methods revealing that EtOAc and *n*-BuOH extracts of *E. anthyllis* contain a great amount of polyphenols. Furthermore, the evaluation of antioxidant activity of the EtOAc and *n*-BuOH extracts, and isolated compounds was carried out by three methods including DPPH, FRAP and PPM. The results of the antioxidant activity show that all extracts and isolated products (±)-erythrinin F, daidzein, genistein and genistein-8-*C*-glucoside**,** act as anti-oxidants. These extracts possessed a moderate antioxidant activity. Their inhibitory concentrations at 50% (IC50) were approximately 0.04 mg/mL (*n*-BuOH) and 0.037mg/mL (EtOAc). In addition, the antibacterial activity of EtOAc and *n*-BuOH extracts was determined by the agar disk diffusion against four strains of microorganisms. The results of the antibacterial activity revealed a sensibility only against Gram positive strain *Staphylococcus aureus* with MIC values at 0.25g/mL. The antibacterial activity of the EtOAc was higher than *n*-BuOH extracts. These findings can be explained by the presence of isoflavonoids which are known for their antibacterial activity. Consequently, *Erinacea anthyllis* is a rich source of polyphenolic compounds particularly isoflavonoids used as chemotaxonomic markers for the subfamily Papilionoideae of the family Fabaceae.

Keywords: Fabaceae, *Erinacea anthyllis*, Isoflavonoids, NMR, Biological activities.

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PHARMACOLOGICAL EFFECTS OF A PRENYLATED FLAVANONE AGAINST AZOLE- RESISTANT *Candida albicans*

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POFF 05

Candida albicans is an opportunistic fungus that produces important infections, particularly in immunocompromised patients. Treatment of candidiasis is generally carried out with azole antifungals and resistance to these drugs has widely developed in the last times. Efflux pumps play a major role in resistance and may represent a new therapeutic target. Thus, by inhibiting such transporters, the concentration of antimicrobials within the microorganisms can be increased and therefore resistance can be reversed. In this paper, we summarize the results obtained with the prenylated flavonoid 2', 4'-dihydroxy-5'-(1''', 1'''-dimethylallyl)-8-prenylpinocembrin (8PP, formerly 6PP), isolated from the roots of *Dalea elegans.* 8PP shows an direct antifungal effect, inhibits rhodamine 6G and reverses fluconazole resistance in azole-resistant *Candida albicans* overexpressing cdr transporters (R*Ca*). The combination of both compounds was significantly more effective than each compound separately. MIC for fluconazole decreased by more than 1000 times in the presence of 100µM 6PP [1,2]. The checkerboard study shows a FICI of 0.61, which together with an isobologram showing a concave shape suggests an additive interaction between them [3]. *C. albicans* viability were decreased by fluconazole, 8PP and their combination. For fluconazole, minimum fungicidal concentration (MFC) and FC50 (the concentration that kills 50% of the fungal cells) were 4-fold reduced in combination with 125µM 8PP. A decrease of 3 log units in viable counts with respect to control was reached. Thus, both fungistatic compounds when combined achieved an almost complete fungicidal effect at lower concentrations respecting of each of them alone them [3]. Cell viability was also measured by reduction of 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2H-tetrazolium bromide (MTT). Fluconazole decreased cell viability in a concentration-dependent manner. Thus, mitochondria may be a therapeutic target for 8PP in R*Ca* [4]. Similar results had been previously reported by some of us in human tumor cells HEp-2 cells and rat hepatocytes. 8PP impairs the hepatic energy metabolism by acting as a mitochondrial inhibitor [5]. In preliminary toxicological assessment, lethal dose 50% (LD50) for 8PP by the i.p. route was 357 and 245 mg/Kg, for female and male adult albino mice, respectively. Fluconazole LD50 was 785 and 650 mg/Kg for female and male animals, respectively. In summary; besides killing *per se*, 8PP helps fluconazole to achieve an almost complete fungicidal effect, which would be crucial to eradicate fungal infections. Part of its effects might be mediated by inhibition of the ABC cdr transporters and mitochondrial functions. These data, added to preliminary in *vivo* studies, would indicate that 8PP deserves further research as a potential therapeutic agent.

Keywords: flavonoids, Fabaceae; rhodamine efflux inhibition, antifungal activity, *Candida albicans*, reversion of fluconazole resistance.

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REMINERALIZING EFFECT ON ENAMEL OF FRACTIONS OBTAINED FROM *Piper marginatum* AND *Ilex guayusa*

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POFF 06

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The disequilibrium of the bacterial flora is the basis of oral diseases. The dental caries is associated with microorganisms of the genus *Streptococcus* and *Lactobacillus*. These microorganisms interact with the diet forming organic acids and generate demineralization the enamel, causing structural damage to the tooth and pain for sensitivity [1]. The aim of this study was to observe if the fractions of *Piper marginatum* and *Ilex guayusa* have the remineralizing effect on demineralized enamel. Ultrasonic-assisted extraction was used to obtain the total extract in ethanol (Total ext.). Then solid-liquid fractionation was performed using hexane (Fr. Hex), ethyl acetate (Fr. EtOAc), dichloromethane (Fr. DCM), butanol (Fr. BuOH), acetone (Fr. Me2CO), ethanol (Fr. EtOH), methanol (Fr. MeOH) and water (Fr. H2O). Human premolar teeth cuts were used, which were demineralized with demineralizing gel (Etchant Gel, 3M). Sodium fluoride, Recaldent ™ and Clinpro were used as positive controls. Water and artificial saliva (SalivaryR) as negative controls. The cuts were left in contact with the solutions of the treatments (Total extract and fractions) between 0 and 96 hours, then analyzed using Raman spectroscopy. The results shown that some fractions (Fr. DCM and Fr. BuOH) of *Piper marginatum* and *Ilex guayusa* could have a remineralizing effect on tooth enamel. In conclusion, the remineralization of the adamantine tissue was observed in this study.

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Keywords: Remineralización, *Piper marginatum*, *Ilex guayusa*, Enamel, Raman spectroscopy.

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EVALUATION OF THE ANTIOXIDANT POTENTIAL OF FIVE ESSENTIAL OILS FROM THE KUTUKÚ BIOLOGICAL STATION

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POFF 07

The Kutukú mountain range is located in the southern Amazon region of Ecuador, is an intermediate mountainous system between the eastern Andes mountain range and the Amazon plain. Universidad Politécnica Salesiana possesses a biological station extending 400 Ha and located in the Sevilla Don Bosco town, in the Province of Morona Santiago. In this place, it is possible to find a great variety of aromatic plants.

The present work researched the antioxidant potential of essential oils from the leaves of five species located at the Kutukú biological station: *Ocotea quixos* (ishpink); *Psidium guajava* (guayava); *Eugenia stipitata* (arazá); *Piper auritum* (sacha anis); *Piper imperiale* (ampar). The free radical scavenging capacity was evaluated by the DPPH and ABTS spectrophotometric methods and protocols, obtaining the best results in *P. auritum* IC50 DPPH 4.9µL/mL and IC50 ABTS 2.9µL/mL and *O. quixos* IC50 DPPH 11.2µL/mL and IC50 ABTS 7.9 µL/mL. The antioxidant assay of beta carotene bleaching test showed higher activity for *P. auritu*m IC50 0.0031µL/mL, *P. guajava* IC50 0.021 µL/mL and IC50 *O. quixos* 0.048µL/mL. HP-TLC-DPPH bioautographic evaluations performed showed safrol activity in *P. auritum*; Trans Caryophyllene E, Humulene ? Cupene and ? Caryophyllene oxide in *O. quixos* and *?* cadinene in *E. stipitata* [1]. The two remaining oils showed no antioxidant activity. Of the 5 evaluated oils, the best results were obtained in the oil of the plant known as sacha anis, that showed an safrol abundance of 25.7%, a compound that is already known to have this activity [2].

Keywords: *Piper auritum*, DPPH, ABTS, ?-carotene bleaching, Antioxidant bioautography.

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DRUG DISCOVERY OF NOVEL ANTICANCER COMPOUNDS FROM PUERTO RICAN MEDICINAL PLANTS

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POFF 08

Cancer is the second leading cause of death in USA, preceded by cardiovascular disease according to World Health Organization (WHO) reports. Recent studies revealed that approximately 60% of cancer patients use vitamins or herbs as chemotherapeutics. However, in most of the plant species there is little information about the chemical constituents responsible for its anticancer activity. Specifically, the Caribbean plants have been less studied than those from Africa, India and Europe.

Therefore, our rationale comes from the literature and from our own study that Puerto Rican and Caribbean plants provide an important source of new leads for in depth investigation as new cancer therapeutics. The objective is to investigate the pharmacologic effects of chemical constituents from *Simarouba*, *Croton*, *Moringa* and *Guaiacum* Puerto Rican species. The specific aims of this project are to assess the therapeutic potential of extracts from plant species in different cancer cell lines derived from solid tumors including ovarian (A2780, SKOV3), breast (MCF-7, MDA-MB-231), and prostate (PC-3, LNCAP), to isolate and characterize the secondary metabolites of the plant extracts responsible for the biological activity against cell lines, and to study the major reasons of cell proliferation inhibition induced by plant cell extracts.

The plants were collected and extracted with solvents of different polarities. From the three Puerto Rican plants species studied, at least one extract of each plant showed high growth inhibitory potency with GI50 <0.1mg/mL against A2780CP20 and MDA-MB-231 cancer cell lines. Based on this preliminary results, we are performing a bioactivity-guide fractionation of extracts using different chromatographic techniques to obtain the compounds with the most potent anticancer activity. We expected that novel compounds will be discovered and analyzed as potential cancer therapeutics.

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Keywords: Puerto Rican plants, drug discovery, anticancer activity, pharmacognosy.

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INTRINSEC APOPTOSIS INDUCED BY MICROTUBULE DISRUPTING AGENTS IN PC3 PROSTATE CANCER CELL LINE

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POFF 09

Resistance of PC3 cell line is associated with negative response to androgens, glucocorticoids, or epidermal or fibroblast gowth factors. Microtubule disrupting agents (MTAs) are frequently used in androgen independent prostate cancer chemotherapy [1]. These compounds lead to cell death by induction of proteins involved in mitochondrial pathway of apoptosis, with cytochrome c release and caspases activation [2]. An *in silico* analysis of the protein interaction network associated to paclitaxel and vincristine interactome was done. The network had more than 100 nodes and 2500 connections, and revealed that BimEL, p53, Bax, Casp-3 and Bcl-2 proteins are essential topological nodes. *In vitro* experimental interactome validation was performed on PC3 prostate cancer cells treated with IC50 of the compounds. Paclitaxel and vincristine compounds induced apoptosis with a significant increase of BimEL and Bax proteins, nevertheless, the concentration of p53, Bcl-2, and Casp-3 proteins was dependent of type of treatment. Interestingly, activation of pro-Caspase-3 was not significant and more than 40ug of protein was necessary to detect the active form in cells treated with paclitaxel and p53 protein treated with vincristine. The complex formation between BimEL and Bax increased at 48 hour of treatment with both compounds, and a favorable decrease between Bax and Bcl-2 complex was observed. Interaction of p53 and Bcl-2 was not significant after treatments. We conclude that apoptosis induced in prostate cancer cells involve intrinsic pathway but the mechanism and interactions between topological nodes, depending of the chemical compound as literature suggest [3]. The study suggests that the effectiveness of MTAs treatments in resistant types of cancer cells could be established after monitoring complexes occurrence and expression levels of pro-apoptotic proteins.

Keywords: Apoptosis, Chemotherapy, Prostate Cancer, Interactome.

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ANTIOXIDANT AND ANTIFUNGAL ACTIVITY OF *Solanum dolichosepalum* EXTRACTS AND FRACTIONS: CORRELATION STUDY

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POFF 10

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Solanum dolichosepalum belongs to the family Solanaceae, its leaves and fruits have been used as a healing, to eliminate lice and in the treatment of renal diseases. This species has been reported as an inhibitor of *Candida albicans* and *Trichophyton rubrum*. The objective of this research was to evaluate the antioxidant and antifungal activities of extracts and fractions through a correlation study between the variables analyzed, as well as to identify some phenolic compounds and alkaloids present in each matrix. The extracts were obtained in soxhlet equipment with five different solvents (acetone, methanol, ethanol, chloroform and dichloromethane) and subsequent concentration under reduced pressure.

Then, the antioxidant activity was determined by the methodologies of ABTS and DPPH with Trolox as standard antioxidant, and the total phenols compounds were quantified using the Folin-Ciocalteu method with gallic acid as reference. Antifungal activity against *C. albicans* and *F. oxysporum* was performed by the PDA agar diffusion method with fluconazole (0.06mg/mL) as positive control. Acetone extract was fractionated by vacuum column chromatography, eluting with hexane, dichloromethane and finally with acetone. Antioxidant and antifungal activity was analyzed to the fractions, in the same way as with the crude extracts. Acetone extract had the highest content of total polyphenols and total antioxidant capacity, followed by methanol, ethanol, chloroform and dichloromethane extracts.

The IC50 values for ABTS are lower than those of DPPH, given their effectiveness with lipophilic and hydrophilic antioxidants. All extracts used had inhibitory activity against *C. albicans* and *F. oxysporum*. It was found that *F. oxysporum* was more sensitive to acetone and ethanolic extracts, whereas *C. albicans* was more sensitive to methanol and acetone. *F. oxysporum* was the most sensitive microorganism with minimum inhibitory concentration (MIC) values of 26.5 ±8.9 and 24.6 ±11.5mg/mL for the acetone extract, which was the most active. The primary fractionation to extract the acetone removed low polarity compounds (carotenoids and lipophilic vitamins), concentrating the total phenolic compounds and increasing the antioxidant activity with DPPH and ABTS in the acetone fraction, compared to the crude extracts. The obtained fractions inhibited the analyzed microorganisms, being drastic differences between them. The most active fraction was acetone and *F. oxysporum* was more sensitive than *C. albicans*. It was determined that the content of total polyphenols has a direct proportionality with the inhibition of the ABTS and DPPH radicals, and inhibition of the analyzed microorganisms.

In contrast, the IC50 of the two radicals and the MIC of the two fungi have inverse proportionality with the total polyphenol content. By comparison of retention times and UV-Vis spectra the following compounds were identified in the extracts and fractions of *S. dolichosepalum*. Phenolic acids: p-hydroxyobeozoic, vanillic, ferulic, trans-cinnamic, Caffeic, p-coumaric, and rosmarinic acid; xanthines caffeine and theobromine; and the flavonoids quercetin and luteolin.

Keywords: *Solanum dolichosepalum*, *Fusarium oxysporum*, *Candida albicans*, Antifungal activity, Antioxidant activity, Correlations.

SYNTHESIS OF ACYLATES FROM RICE STARCH CATALYZED BY THE *Candida antarctica* LIPASE B (CALB)

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POQV 01

The application of the green chemistry principles in the processes of biotransformation and synthesis of materials from plant by-products is of the main biotechnology challenges. Such process has some economic and environmental advantages since it allows the production of products with an added value. In this sense, those biotechnologically modified starches have better structural and functional characteristics compared to their native precursors, allowing their use in the pharmaceutical and cosmetic industries [1].

Starches were extracted from some rice varieties including the F60, F50 and other 473 varieties (grown in the department of Tolima) by using an alkaline method. This material was enzymatically acetylated by using lipase B as biocatalyst (from *Candida antartica*), linoleic and stearic acids as acyl donors, and dimethylsulfoxide (DMSO) as organic solvent. A starch-fatty acid equimolar ratio and a constant stirring of 100 rpm and a temperature of 60ºC were maintained. The reaction systems were evaluated with intervals of 3 and 6 hours. Subsequently, the physicochemical and structural characteristics of the starch acylates were determined through IR spectroscopy, X-ray diffraction and optical microscopy. The functional properties were determined through the Water Absorption Index (WAI), swelling power (SH) and water solubility index (WSI) [2].

Reaction yields above 70% were achieved for all synthesized materials. An increase in the absorbance in the acute band was observed at 1644.6 cm-1; probably due to the vibration and extension of the carbonyl group (C=O) caused by the acylation agents that were used. This confirms the presence of acetylated products in the samples [1-2]. Native starch showed strong diffraction peaks at 15.12°, 17.08°, 18.09° and 23.01°, indicating a crystalline-type C structure. The displacement or loss of these crystalline patterns makes noticeable the effect of the modification on the crystalline structure as observed in the synthesized materials. Likewise, the microscopic analysis confirms the change in the shape and size of the granules of the starches after the reaction. Functional properties such as WSI and SW show a tendency to increase in those modified materials with reference to the native starches [2]. After 3 hours of reaction, there was not any significant difference in the starches compared to the those that reacted during 6 hours. in this sense, it is clear that the maximum point of modification is achieved by keeping all the conditions during 3 hours of acetylation.

Starch acylates that were biocatalytically synthesized from rice residues (used during the production chain) showed variation in their crystallinity, morphology and functional properties once they were acetylated. Expanding their potential application in industries such as pharmaceuticals as encapsulation materials, bioplastics and cosmetics.

Keywords: Lipases, Starch, Biocatalysis, Modification.

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INFLUENCE OF DIFFERENT EXTRACTION TECHNIQUES ON ANTIOXIDANT ACTIVITY AND PHYTOCHEMICAL PROFILE OF *Ocimum basilicum* L. EXTRACTS

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POQV 02

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Researches unraveled the role of plants, as *Ocimum basilicum* L. (basil), utilized as important sources of effective antioxidants. In our work, we analyzed the effects of different extraction techniques on antioxidant activity and phenolic profile of *O. basilicum* extracts. The aerial parts of *O. basilicum* were extracted by different methods: maceration with methanol:water 80:20 (MAC), hydroenzymatic extraction using cellulase, xylanase, pectinase, and their mix, buffer based digestion, and accelerated solvent extraction using water (ASE H20) and ethanol (ASE EtOH). Successively, the obtained extracts were tested by 4 *in vitro* assays for screen the antioxidant potential. In particular TPC [1], DPPH [2], FRAP and BCB [1] have been used. Relative Antioxidant Capacity Index was also calculated to compare data obtained from different methods [1]. Metabolites identification and quantification was also performed by RP-HPLC-DAD. According to obtained assays results, ASE EtOH and ASE H2O were the samples with highest RACI values. The samples extracted by enzymes, instead, showed the lowest values. After that, quali-quantitative analysis of the extracts was made by RP-HPLC. The data confirmed that the highest content of compounds was found in MAC (22447.47 ± 563.70 mg standard/Kg of extract), followed by ASE H2O. The other extraction techniques, does not affect the quantity of metabolites and neither the yield when results were compared with ASE technique. Our results indicated that ASE H2O show the highest activity; and MAC showed the highest content of secondary metabolites compared to other extracts.

Keywords: Basil, Antioxidants, Phenolics, HPLC-DAD, Extraction techniques.

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NEW METHOD BY DIFFERENTIAL SCANNING CALORIMETRY (DSC) FOR CHARACTERIZATION OF ORGANIC EXTRA VIRGIN OLIVE OILS (eVOOS) FROM DIFFERENT INTERCONTINENTAL GEOGRAPHICAL AREAS

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The thermal properties of many organic extra Virgin Olive Oils (eVOOs) coming from different Intercontinental areas of the world were investigated by Differential Scanning Calorimetry (DSC). Different studies have shown that DSC provides significant information about the authenticity of an oil, its cultivars, its changes and its geographical origin [1]. DSC applications include the measurement of the melting point of vegetable oils [2], the determination of thermally oxidized olive oil, the determination of quality of frying oil [3], the detection of adulterated extravirgin olive oil [4] and of seasonal changes. In this paper, we report the results obtained by using an improved methodology concerning DSC in combination with an unsupervised multivariate statistical analysis such as the Principal Component Analysis (PCA). This technique, through a series of heating and cooling cycles, provides a specific curve, i.e., a thermogram, which represents the fingerprint of each eVOO sample. In fact, variations due to the different cultivars, geographical origin or chemical composition can be highlighted because they produce changes in the corresponding thermogram. In particular, we apply the PCA to the melting thermogram characterizing the fusion temperatures of fatty acids and triacylglycerols (TAGs) after proper cycles of crystallization.

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DETECTION OF FLAVONOID GLYCOSIDES IN *Swinglea glutinosa* LEAVES, USING LC/Q-TOF-MS TECHNIQUE

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POQV 04

Swinglea glutinosa Merr. Rutaceae family, is a plant of Asian origin, introduced in Central and South America where it is used as a live fence and ornamental plant. This plant has been attributed several biological properties such as allelopathic effects, insecticides, antifungal, as well as antimalarials and anti-inflammatories, among others. Phytochemical analyzes of different organs of *S. glutinosa* have reported mainly flavonoids, coumarins and alkaloids, but alkaloid only in roots and bark. [1-4]. In this work, were isolated several phenolic acids, cinnamic, caffeic and ferulic acid. A flavonoid glycoside was also isolated, which was identified as Apigenin 7-O-neohesperidoside (Rhoifolin), Identification was made using 1D and 2D NMR techniques, this compound has been previously reported in other citrus plants [5-6]. A deeper understanding of composition of *S. glutinosa* leaves was performed using LC/Q-TOF-MS technique. For this, *Swinglea glutinosa* leaves were collected in the southwest region of Antioquia, Colombia. The leaves were dried and blinder with ethanol. The solvent was removed under reduced pressure. The ethanolic extract was filtered on Sephadex LH-20, removing chlorophylls and fats. The remaining fraction was concentrated and analyzed in an ACQUITY UPLC equipment coupled to a high-resolution mass spectrometry equipment Xevo G2 QTof (Waters). Using different voltages in cone. Possible elemental compositions were calculated using the MassLynx elemental composition calculator with a maximum deviation of 5 mDa from the measured accurate mass. Using LC-QTOF MS as a powerful tool for identification thanks to the accurate-mass full acquisition data provided by this, four more glycosides flavonoids were detected. Which was possible by comparing the exact molecular weight and its fragmentation pattern. In conclusion, 3 phenolic acids, 1 glycosidic flavonoid, were isolated. And in addition, 4 more glycosidic flavonoids were detected using an HRMS technique. Indicating that leaves of *Swinglea glutinosa* have a high concentration of phenol type compounds. And the possibility that the reported biological activities of this plant come from the presence of these compounds.

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NEW STRATEGIES FOR THE DEVELOPING BIO-BASED MATERIALS WITH BIOLOGICAL PROPERTIES

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POQV 05

The presentation addresses the development of new bio-based materials with selected physicochemical, and biological properties [1]. The materials are based on a bio-degradable biopolymer (poly-lactic acid) and the addition of polyphenols (oligo-, and polyflavonoids) from woody plant barks. Isolated products, and polymer blends show antibacterial properties, and high UV-filtering behavior. The dissertation is focus on the polymer blends formulation (torque rheometer), as well as the physical-, chemical-, and mechanical characterization of the resulting materials. In addition, the antibacterial assays (liquid and solid media) [2], the thermal resistance (thermo-gravimetry analysis) [3], and the UV-adsorption [4] spectra are presented.

Keywords: Polyphenol, Polymer, Antibacterial, Tannin.

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OPTIMIZATION AND STABILITY EVALUATION OF *Passiflora quadrangularis* LEAVES EXTRACT WITH SEDATIVE ACTIVITY

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POQV 06

Passiflora species have been used in folk medicine as tranquilizer [1]. Pharmacological studies performed specifically for *Passiflora quadrangularis* leaves extracts have corroborated sedative activity proposing the flavonoids present in these species as the responsible compounds of that effect [2,3]. The aim of this work was to contribute to the *P. quadrangularis* leaves extract standardization with sedative activity considering: the optimization of the extraction of total flavonoids (TF), the evaluation of the effect of locality and collection period on the content of TF, evaluation of the stability of TF on extract under stress conditions and the determination of the shelf life of the optimized extract from *P. quadrangularis* leaves. Sedative activity was verified by the ethyl ether-induced hypnosis test in Swiss ICR mice. Percolation was used as extraction method and it was assessed as variables drug-solvent ratio, extraction solvent (EtOH:H2O) and time. Response surface methodology (RSM) was employed to determine the optimal conditions of extraction. Stability studies under stress conditions were performed adapting to "Guidance on Conduct of Stress Tests to Determine Inherent Stability of Drugs" [4]. Shelf life was calculated according to "Guidelines of Stability Testing of Active Pharmaceutical Ingredients and Finished Pharmaceutical Products". Concentration of TF was monitored during 6 months under controlled storage conditions: intermediate stability (T=30°C±2; RH=75%±5) and accelerated stability (T=40°C±2; RH=75%± 5) [5]. According to the results it was able to determine that drug-solvent ratio of 1:15, extraction solvent EtOH:H2O (1:1) and time of 48 hours allow to obtain the highest concentration of TF. The locality and collection period influences the content of TF, finding the highest TF concentration in the vegetal material cultivated in Neiva (Colombia). Regards to stability under stress conditions, it was found that the optimized extract is practically stable under hydrolysis and oxidation, labile by acidic hydrolysis and basic hydrolysis and photostable. In addition, it was identified two degradation products and the shelf life for the extract was estimated as 2 months. Finally, it was demonstrated that the optimized extract improve the sedative effect exhibited by the aqueous extract in the ethyl ether-induced hypnosis test.

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Keywords: *P. quadrangularis*, C-glycosidic flavonoids, Standardization, Stability, Apparent shelf-life and sedative activity.

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LIPOSOMES FOR THE CO-DELIVERY OF NATURALLY OCCURRING POLYPHENOLS (QUERCETIN AND RESVERATROL): CHARACTERIZATION AND *IN VITRO/IN VIVO* EVALUATION

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POQM 01

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Polyphenolic compounds, such as quercetin and resveratrol, have gained great interest in the pharmaceutical research area due to their beneficial properties, namely antioxidant, antiradical, antiinflammatory, anticarcinogenic, antibacterial, and antiviral effects [1,2]. This wide spectrum of therapeutic activities, coupled with their safety profile and natural origin (they are commonly found in fruits and vegetables), make quercetin and resveratrol very attractive candidates for the development of novel pharmaceutical products [3]. However, the use of these two polyphenols is limited by their poor water solubility and instability, which lead to subtherapeutic levels and require higher doses to be administered, thus hampering their beneficial properties and potential health benefits [4,5]. In this framework, nanoparticulate delivery systems have been proven to be effective in protecting, controlling the release, and enhancing the action of different bioactive compounds. The current study was carried out to determine whether the combination of the two polyphenols delivered by liposomes would increase their bioactivity in coping with oxidative stress and inflammation implicated in pre-cancerous/cancerous skin conditions. The formulation is also expected to have superior efficacy as compared to the free agents, owing to the advantages offered by the nanovector, specifically tailored for skin delivery. Quercetin and resveratrol co-incorporated in biocompatible liposomes were characterized in terms of physico-chemical and antioxidant properties. Their morphology and lamellar assembly were also probed. The *in vitro* cytotoxicity/cytocompatibility and uptake of the two polyphenols were tested in human fibroblasts, as well as their activity against free radicals (ROS). Further, the efficacy and safety of the co-formulated polyphenols were assessed *in vivo* by testing their activity against chemically-induced oedema and leukocyte infiltration. Therefore, the proposed approach based on polyphenol vesicular formulations may be of value in the treatment of pre-cancerous/cancerous skin conditions associated with inflammation and oxidative stress.

Keywords: Quercetin, Resveratrol, Liposome, Antioxidant, Fibroblast, Skin lesion.

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STUDIES IN VITRO AND IN VIVO OF ANTILEISHMANIAL ACTIVITY AND DIFFERENTIAL CYTOTOXICITY OF *Cannabis spp.*

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POQM 02

Current research looks at the scientific findings on the potential of *Cannabis* to treat skin lesions, discovering the role played by the endocannabinoid system in maintaining healthy skin and wound healing, and validating the potential of *Cannabis* in the topical treatment of cutaneous lesions. Due to its anti-inflammatory and healing properties, the study aimed to confirm the *in vitro* and *in vivo* antileishmanial effect of *Cannabis* spp.

Three ethanol extracts from *Cannabis* Nicole Kush strain (75% *C. indica* and 25% *C. sativa*) were prepared by percolation. The cytotoxicity was evaluated on different cell lines and primary culture cells using the 3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium Bromide (MTT) colorimetric method while the antileishmanial activity was evaluated on *L. braziliensis* amastigotes by flow cytometry. The results were expressed as median Lethal Concentration (LC50) for cytotoxicity and the median Effective Concentration (EC50) for effectiveness [1]. The content of cannabinoids was determined by chromatography. A cream and a lotion formulations were prepared and tested in hamsters experimentally infected with *L. braziliensis* [2]. The most active extract *in vitro* (EC50 24 mg/mL) was the extract with the higher percentage of THC (18%). The remained two extracts had moderate activity (EC50 28.2 and 32.8 mg/mL, respectively). No differential cytotoxicity was observed.

The cream formulation of the most active extract showed cure 80% of hasmters after treatment. This is the first report of antileishmanial activity in *Cannabis* spp. Since this plant has been associated with anti-inflammatory effects, is possible to think that *Cannabis* extract could be a good alternative for the management of uncomplicated cutaneous leishmaniasis.

Keywords: *Cannabis*, Antileishmanial activity, Cytotoxicity.

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STUDY OF MARINE DITERPENES OF ALGAE OF THE GENUS *Dictyota* OF THE COLOMBIAN CARIBBEAN

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POQM 03

The Algae of the genus *Dictyota* have been consider as a rich source of diterpenes [1,2]. Those metabolites have great biological value and function as chemotaxonomic markers [3]. We performed the analysis of diterpenes from our collection of brown algae using 1D and 2D-NMR experiments. From this collection, we choose *Dictyota pinnatifida* for a chemical study, being the first time worldwide that this species is analyzed (ICN 596747). This study allowed the identification of six diterpenes, five of them novel: (1*R**,5*S**,6*S**,7*R**,11*R**) 6-epipachydictyol A, (1*R**,5*S**,6*S**,7*R**,10*R**,11*R**) 6-epidictyol C, (2*S**,3*R**,10*S**) 18-acetoxy-dilophol, (1*R**,3*S**,4*R**,5*S**,7*S**,9*S**,10*R**, 11*R**) 3,4-epoxy-9,hydroxy-6-deoxy-dictyol C, which we called dictyol L, (1*S**,4*S**,5*S**,6*R**,7*S**,9*S**,10*S**,11*R**,14*R**) 1,10-3,5-diepoxy-6,9,14-trihydroxy-15-methoxy-pachydictyol A, which we called dictyol M; and dictyoxepin, a diterpene previously reported. In addition, we find a new photosynthetic pigment free of magnesium that we called Pheophytin *j*. In the metabolome of *Dictyota pinnatifida*, the following compounds were observed: germacrene D [5], pentadecene [6], pentadecane [7], heptadecene [6], ineleganene [8] and dictytriene A [9], through GC-MS and NMR.

Data from GC-MS of 6-epipachydictyol A, 6-epidictyol C, 18-acetoxy-dilophol and dictyoxepin were included in our database of marine-derived diterpenes for future dereplication [4]. The chemotaxonomic analysis of diterpenes isolated from *Dictyota pinnatifida* coincides with the reported molecular approaches [10], since species close to *Dictyota pinnatifida* such as *Dictyota caribaea* and *Dictyota mertensii* are characterized by the production of diterpenes with prenylated germacrene nuclei. Related to biological activity, Dictyol M and dictyoxepin showed to be no active against *Escherichia coli* and *Pseudomonas aeruginosa* as antimicrobials. In the case of *Pseudomonas aeruginosa*, it was observed that the two compounds, promote the production of pyoverdine. Dictyol M showed a strong inhibition of biofilm production in *Pseudomonas aeruginosa*, seven times better than the positive control. Dictyoxepin was able to inhibit the biofilm formation in *Escherichia coli*. The results suggest that, this diterpenes are potential control agents for bacterial biofilm.

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Keywords: Brown algae, marine diterpenes, prenylated germacrene, xeniane, chemotaxonomy, biofilm inhibition, *Dictyota pinnatifida*.

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PLANTS OF SOUTHERN ECUADOR WITH CYTOTOXIC AND ANTHELMINTIC ACTIVITY

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POQM 04

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Cancer and parasitic infections are significant global health problems. Cancer is a leading cause of death worldwide, and more than 1.5 billion people are infected with soil-transmitted helminths (STHs) [1]. The main infantile intestinal parasites are Strongyloides, Ascaris, and Taenia [2]. Natural products have served us well in combating cancer, helminth and other parasitic infections, and other diseases [3]. The search for plants that are potentially useful against diseases has recently increased because of the growing resistance of some diseases to available synthetic agents. Furthermore, plants represent a reliable resource for the production and supply of effective drugs with less side effects and low toxicity [4]. In Ecuador there are approximately 20,000 different plant species, 20 % of which are endemic. In this country, as in many other developing countries, up to 80% of the population relies on medicinal plants for primary medical care [5]. Because of the importance of finding new treatments for diseases with a global impact, such as cancer and STH infections, 12 species of native plants were selected for which, to date, there have been no reports in the literature of their cytotoxic and/or anti-parasitic effect. The species were selected based on ethnomedical knowledge and reports in the literature. The plants were collected in Loja and Zamora Chinchipe and identified. Extracts from each species were obtained using solvents: hexane (Hex), ethyl acetate (EtOAc) and methanol (MeOH). The fractionation of the extracts was performed by open column chromatography. NMR and MS were used to characterize and identify the secondary metabolites. All extracts were evaluated in an MTS in vitro cell proliferation assay to evaluate anticancer activity and a larval motility assay to assess anthelmintic activity. For the evaluation of antitumor activity, 4 human cancer cell lines were used: PC-3 (prostate), RKO (colon cancer), D-384 (astrocytoma), and MCF-7 (breast cancer). For the anthelmintic evaluation, L3 larvae of *Strongyloides venezuelensis* were used for 24 and 48 h. Thirty-seven compounds were isolated and identified as alkanes, fatty acids, flavones, sterols, or terpenes. Of these, 2 were identified for the first time in the species studied. The extracts with the most cytotoxic activity were EtOAc from *Echinopsis pachanoi* (in all 4 cancer cell lines evaluated) and Hex from *Pentacalia vaccinioides* (in 3 of the 4 cell lines). The MeOH extracts from *Echinopsis pachanoi* and *Peperomia inaequalifolia* demonstrated antiparasitic activity at doses greater than 500µg/ml.

Twelve plant species were selected from southern Ecuador, and their antitumor and anthelmintic activities were evaluated. The results obtained so far identify some promising species for possible use in treating cancer and helminth infections. We are evaluating isolated secondary metabolites to validate the ethnomedicinal use of plant species.

Keywords: Cytotoxicity, Anthelmintic activity, Ecuador, *Strongyloides venezuelensis.*

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CYANOBACTERIAL COMPOUNDS AS LARVICIDES AGAINST THE MOSQUITO *Aedes aegypti*

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POQM 05

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The mosquito *Aedes aegypti* is an important vector of viral diseases such as dengue, chikungunya, zika and yellow fever [1–4]. Currently, there is a global concern about the prevention of these diseases due to several epidemic outbreaks worldwide, including Colombia. Larvae control [5] is regarded as an important control strategy to curb mosquito populations. This study reports the potential of Caribbean marine cyanobacteria as sources of larvicidal compounds against *Ae. aegypti*. Organic extracts of 16 cyanobacterial mats were evaluated in 3 different bioassays, lethality against *Ae. Aegypti* larvae; lethality against *Artemia salina* as an ecotoxicity indicator and inhibition of acetylcholinesterase in order to ascertain a possible mode of action. We selected three cyanobacterial samples for further chemical studies. The first sample, identified as *Lyngbya* sp. (IBUN-02213) yielded fatty acids, FAMES (14:0 y 16:0), malyngolide seco-acid and malyngolide. The malyngolide seco-acid, a novel natural product, showed strong larvicidal activity against *Ae. aegypti* without ecotoxicity, and also showed acetylcholinesterase (AChE) inhibition, suggesting a possible action mode. The second cyanobacterial sample, a green turf mat (IBUN-02224), yielded two new cyclic depsipeptides, dolastatin D analogs and fatty acids. Both peptides showed interesting larvicidal activity, no ecotoxicity and no AChE inhibition. The third sample, identified as *Moorea producens* (IBUN-03496) yielded fatty acids, FAMES (14:0, 16:0, 16:1, 18:0 and 18:1), sterols such as cholesterol, clionasterol and campesterol and lipopeptides including neodysidenin and the novel compound 10-dechloroneodysidenin. Some of the identified fatty acids and FAMES were evaluated as larvicides against *Ae. aegypti*. Oleic acid (18:1) was the most active (91% lethality, 50 µg/mL). Myristic acid and neodysidenin showed moderate larvicidal activity with low ecotoxicity and no AChE inhibition. Neodysidenin however, also exhibited growth disruption and the larvae remained in instar II after 6 days of development. Our results show that the chemical diversity from marine benthic cyanobacteria from the Colombian Caribbean is promising in controlling important disease vectors such as *Ae. aegypti*.

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Keywords: Cyanobacreria, *Lyngbya*, *Moorea producens*, *Aedes aegypti*, Peptides, AChEI, *Artemia salina*.

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NEW STATISTICAL STRATEGY FOR THE ANALYSIS OF CYTOTOXIC ACTIVITY OF 42 OCTOCORAL EXTRACTS FROM COLOMBIAN CARIBBEAN

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POQM 06

The rising rate of cancer mortality around the world makes necessary to be continuously searching for medicines that can fight this disease. One of the potential sources of compounds with cytotoxic activity is the marine invertebrates such as Octocorals, that belong to the Anthozoa class, Cnidaria phylum, and produce metabolites with novel structures that confer them potent biological activities such as cytotoxic activity. In Colombia, the study of these metabolites has been focused on different biological activities such as anti-inflammatory, antifouling and inhibition of quorum sensing, leaving the cytotoxic potential of the Colombian octocorals almost unexplored. Therefore, in this project we established the cytotoxic potential of 42 octocoral extracts from the Colombian Caribbean, by means of cytotoxic activity assay against a panel of cancer cell lines (prostate, lung, breast and cervix), which are highly relevant in the country due to its high mortality rate. The cytotoxic activity of extracts, fractions and compounds was tested against SiHa (ATCC® HTB-35?), MDA-MB-231 (ATCC® HTB26?), A549 (ATCC® CRM-CCL-185?), and PC3 (ATCC® CRL1435) cell lines by means of MTT assay2 during 48 h, using five different concentrations against the cells by triplicate (10, 25, 50, 100 and 200 µg/mL), using a negative control (without any extract) for each cell line. The absorbance results measured at 570 nm were analyzed through two different approaches: first one, the IC50 values were calculated by a non-linear regression 4PL3 for the extracts for each cell line. The second one, a Kruskal Wallis test of analysis of variance was performed to compare the absorbance obtained by the control for each cell line with the absorbance obtained by 200 µg/mL concentration for each extract against each cell line; then an area under the curve analysis was performed to find the most active extract and allowed to group the extracts with the same type of activity. Finally, the above together with an AMMI analyzes showed an active group of extracts that statistical behaves in the same way, being the 40% of the extracts evaluated in this work active against at least one cell line. In addition, it showed a group of extracts that has no statistical activity against the cell lines (60% of the extracts evaluated). In conclusion, the comparison of the two approaches, allowed to establish that the area under the curve method is a good way to analyze the cytotoxic activity of octocoral extracts.

Keywords: Cytotoxic activity, octocorals, statistical approaches.

DOLABELLANE DITERPENE SEMISYNTHESIS WITH ANTI-ZIKA AND ANTI-CHIKUNGUNYA ACTIVITY

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POQM 07

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Viral diseases are a permanent threat to the human health due its capacity to generate resistant strains together with fast and lethal outbreaks [1]. Compounds with antiviral activity represent the main alternative of treatment, especially in diseases where the objective of a vaccine has not been achieved [2]. Therefore, the search for antivirals with improved properties is still an important part that contributes to strengthen the antiviral therapy.

Marine organisms are an outstanding source of bioactive and structurally diverse compounds. Between marine sources, brown algae and soft corals represent the most prolific source of dolabellanes, a family of diterpenes who has exhibited a remarkable spectrum of biological activities [3]. Dolabellanes have shown a remarkable *in vitro* antiviral activity against HSV and HIV and it has been reported that dolabellanetriol, isolated from *D. pfaffii,* inhibits HIV-1 replication acting as a non-nucleoside reverse transcriptase inhibitor [4]. Furthermore, oxygenated dolabellanes obtained by semisynthesis from compounds isolated from soft corals showed an impressive antiviral activity compared with their natural precursors [5]. In this work, we constructed a chemical library of dolabellanes by simple and straightforward semisynthetic modifications in order to obtain derivatives with improved antiviral activity.

A total of 21 dolabellane analogues were obtained from the natural isolated dolabellatrienone (**1**) and (1*R*, 7*R*, 8*R*, 11*S*)-13-keto-7,8-epoxy-dolabella-3,12(18)diene (**2**) through semisynthesis. We employed allylic oxidation reactions (**3-6**), reductions (**7-13**), acid catalysed ring opening epoxides (**14-18**) and acetylations (**19-21**). In some cases, acid catalysed dehydration of some hydroxylated derivatives to obtain dienes (**22-23**) was observed. All compounds were identified through nuclear magnetic resonance (NMR) mono and bidimensional combined with electronic impact mass spectrometry and X-ray diffraction. The antiviral activity of derivatives and their natural precursors was evaluated against Zika and Chikungunya virus, using a 20 µM concentration. In general, most of the semisynthetic derivatives improved their antiviral activity inhibiting the virus replication and seven of them showed more than 95% of inhibition. The results encourage us to continue exploring the antiviral activity of dolabellanes and their more oxygenated derivatives.

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Keywords: Antivirals, Dolabellane diterpenes, Semisynthesis, Zika, Chikungunya.

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ISOLATION, BIOACTIVITY AND METABOLOMIC ANALYSIS OF A DIVERSE ACTINOBACTERIA COLLECTION FROM ARAUCA RIVER SEDIMENTS (COLOMBIA)

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POQM 08

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Antimicrobial resistance and cancer research are looking forward to the development of innovative approaches for detecting new antimicrobial and cytotoxic agents, taking as a primary tool the use of bioprospective studies. The primary goal of bioprospecting studies in microorganisms is to generate useful information about the potential of a microbial collection in different samples as a source for natural product discovery. From microorganism group, *Actinobacteria* have proven to be a prolific source of this compounds [1-2]. However, since the late 1980's the rate of discovery of new natural products has declined thus requiring the development of new strategies to isolate different species.

Herein, we describe a combinatorial strategy for detecting low-abundance actinobacteria from an understudied environmental sample like Arauca tropical river sediment in Colombia Orinoquía, using different physico-chemical pretreatments and dereplication analysis through MALDI-TOF MS and UPLC_HRMS approach. Five physico-chemical pretreatments were chosen such as the use of solvents, thermal energy, non-ionizing energies, sonication and pH changes. A total of 790 actinobacteria-like isolates were fermented and their antimicrobial activity was assessed against methicillin-resistant *Staphylococcus aureus* (MRSA), Vancomycin-resistant *Enterococcus faecium* (VRE), extended-spectrum β-lactamase *Klebsiella pnumoniae*, clinical isolates of *Cladosporium cladosporioides* and *Epicoccum nigrum*.

Seventy-eight isolates, belonging to the Streptomytaceae family according to 16s rRNA analysis were found to have antimicrobial activity and were categorized as low abundance actinobacteria by MALDI-TOF MS after dendrogram analysis. Cytotoxic bioactivy assay through MTT analysis was performed with 100 ppm ethyl acetate extracts from these strains, founding 16 isolates with at least one positive hit against PC3, MDA, A549, SiHa, HeLa and HTB26 cell lines. Metabolomic analysis of these sixteen bioactive isolates by UPLC-HRMS and AntiBase 2014 database was made founding one possible novel ion in one isolate. Scale-up to 3L broth culture of the strain having the possible new metabolite was made and further purification of the suggested novel metabolite is still in process using Teledyne Isco CombiFlash instrument.

The results suggest that the combination of physico-chemical pretreatments and dereplication of microbial collections through MALDI-TOF MS and UPLC-HRMS, in understudied tropical Colombian river samples, facilitates the detection of low abundance actinobacteria isolates with antimicrobial and cytotoxic activity that can be taken as a new source of novel metabolites.

Keywords: Actinobacteria; Dereplication; Bioprospecting; MALDI-TOF MS; UPLC-HRMS.

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ACETYLCHOLINESTERASE INHIBITORS FROM CHILEAN PLANTS

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POQM 09

Inhibition of acetylcholinesterase (AChE), the key enzyme in the breakdown of acetylcholine, is considered as a promising strategy for the treatment of neurological disorders and development of insecticides. Natural cholinesterase inhibitors have been found in many biological sources. Compound with agarofuran (epoxyeudesmane) skeleton were isolated from seeds and aerial parts of *Maytenus disticha*, *M. boaria* and *Euonymus japonicus* belonging to Celastraceae family. On the other hand, pentacyclic triterpenes with ceanothane skeleton were isolated from aerial parts of *Trevoa quinquenervia*, *Colletia spinossisima* and *Trevoa trinervis* belonging to Rhamnaceae family. From isolated compounds it was evaluated inhibitory activities for the rate of hydrolysis of acetylthiocoline and butirylthiocoline in comparison to reference compound galanthamine. These natural compounds, which possessed mixed-type or noncompetitive mechanisms of inhibitory activity against AChE, may be considered as a models for the design and development of a new naturally occurring drug for management strategies for neurodegeneratives disease or pest control.

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Keywords: Celastraceae, Rhamnaceae, Agarofurans, Ceanothanes, Acetylcholinesterase.

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Jatropha dioica ITS CITOTOXIC, CHEMOPROTECTIVE AND ANTITUMORAL EFFECTS

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POQM 10

Jatropha dioica (Moc. Et Sessé), known in Spanish Dragon's blood, is a small shrub of 1 to 3 feet, with tiny pink or white flowers in clusters. The sap turns red blood when exposed to the air. Root infusions have been used to treat alopecia, oral and cutaneous lesions. The objective of the macro project was to determine its toxic and chemoprotective capacity using the micronucleus test, the kite test and the antitumor test. Decoction was prepared by boiling 1g of dried root and ground in 250 ml of commercial bottled water for 15 minutes. Decoction of the root, as well as, its aqueous (5mg/ml) and methanolic extracts (5mg/mL) showed antioxidant capacity with the DPPH test and also avoided the oxidation of linoleic acid. For the bioassays, the groups of five male mice, strain ICR, with an average weight of 25 g, were treated as follows: negative control with purified water and 3.5, 10.71 and 21.42ml/kg of decoction by oral route, cyclophosphamide (CPP) (10 mg/kg), daunorubicin (DAU) (10 mg/kg) and methyl methanesulphonate (MMS) (40mg/kg) IP. Route. For the sub-chronic micronucleus test, decoction showed a slight cytotoxic effect and the genotoxic effect was not evident. For the antigenotoxic assay, the results showed a decrease in EPCMN induction with DAU, CPP and MMS, effects after 4 weeks of treatment with the highest dose of root infusion. For the comet assay, after an acute administration of decoction and mutagenes, the animals were sacrificed at 3, 9, 15 and 21 hours. Liver, kidney and bone marrow were dissected to prepare cell suspensions. The slides were analysed using Metasystem Image Analyser and COMET 2.0 software, with Carl Zeiss Axioimager Fluorescence Microscope with 20X / 0.065. The chemoprotective effect was observed against the two alkylating agents at 3 h in the liver, kidney and bone marrow, but the protective capacity was observed only for CPP at 9 and 15 h. For the DAU, chemoprevention in the three organs was observed until 21 h. The difference between the effects on the two alkylating agents could be related to the antioxidant capacity of the compounds present in the decoction, which could inhibit CPP bioactivation while apparently only blocking the initial alkylation caused by MMS on DNA, and for DAU its antioxidant capacity. The antitumor ability assessed in the Balb C strain against murine L5178Y lymphoma was observed with the higher doses of decoction that inhibit tumor growth and increase the life span over the control of vincristine.

Keywords: *Jatropha dioica*, Chemo protection, Antitumoral effect.

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TRYPTAMINE ISOLATED FROM *Warszewiczia schwackei* (Rubiaceae)

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PONP 01

Rubiaceae family possess about 609 genres and 13,673 species, with a cosmopolitan distribution. Most of them were analyzed by phytochemical and biological studies showing that these family have a huge variety of chemical important secondary metabolites such as triterpenes, anthraquinones, iridoids and indole alkaloids mainly. Some of them can be used as taxonomic markers for discovery of new therapeutic compounds [1]. In this work the species *Warszewiczia schwackei* was chosen to realize a phytochemical study due to not showed previous studies.

Leaves and branches were collected in Reserva A. Ducke/INPA, Manaus-AM. The methanolic extracts of the leaves (10.0g) was fractionated by liquid-liquid partition. The ethyl acetate phase was fractionated by open chromatographic column on Sephadex LH-20 and the subfractions 3 and 4 were mixed and fractionated on column using Alumina, which allowed the isolation of a fraction with yellow amorphous solid, that showed to be an alkaloid by TLC analysis. It was analyzed by 1H and 13C NMR, including COSY, HMBC and HSQC experiments, dissolved in DMSO-d6. The 1H NMR spectrum showed the signals corresponding to the hydrogens of the aromatic ring of the indole system, characterized by the presence of four hydrogens with chemical shifts at H 7.09 (1H, dd, J= 8.5 and 7.5Hz), 7.00 (1H, dd, J= 8.5 and 6.6Hz), 7.56 (1H, d, J= 7.6Hz) and 7.38 (1H, d, J= 7.5Hz), was also observed a singlet in ?H 10.98 integrating for one hydrogen. The correlation between these hydrogens with the carbons at C 120.98, 118.29, 118.09 and 111.40, was confirmed by gHSQC spectrum. The signal at H 10.98 do not showed correlation with carbon at the same spectrum, indicating whether it was a heteroatom-bound hydrogen. Nevertheless, it was observed the correlation of this hydrogen with the signals in C 136.17, 122.98, 110.46 and 126.84 in the HMBC correlation map spectra confirming the presence of the indole group. It is also observed the presence of two methylene carbons at C 24.92 and 40.13, both of them coupling with the hydrogens at H 2.97 (4H, m), which were confirmed by HMBC correlations. The ESI-MS spectrum (both positive and negative mode) suggested 160 m/z as a molecular weight concerning to the molecular formula C10H12N2. All these data indicates the alkaloid tryptamine as the main compound of the fraction. The NMR data were compared to literature and confirmed [2].

This substance is produced by several species of the genus *Acacia*. It is important to highlight, that tryptamine is an important precursor in the indole alkaloids biosynthesis, as showed by studies realized with species of Condamineeae tribe belonging to Rubiaceae family indicating that 24.54% of compounds isolated are alkaloids and 81.18% of this alkaloids are indolic [3]. This is the first report of this compound in the genre *Warszewiczia*.

Keywords: Alkaloid, Phytochemical, Amazon.

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IDENTIFICATION OF ANTIBACTERIAL COMPOUNDS FROM THE EXTRACTS OF *Phaseolus vulgaris*, USING BIOAUTOGRAPHY TECHNIQUE

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PONP 02

Phaseolus vulgaris is part of the Colombian agricultural economy, due to have high nutritional value and great possibilities of cultivable species; it generates agricultural, nutritional and economic advantages, among others. However, there are factors affecting production, such as phytopathogens (*Xanthomonas axonopodis* (XCP123)), and (*Rhizoctonia solani* (RH17)), which cause losses between 20% and 50% of total production [1,2].

Control methods are based on the addition of commercial fungicides and the removal or burning of the infected crop. An alternative to counteract the negative effects caused by these phytopathogens and to mitigate the environmental impact is the search and selection of resistant materials [3], which can be used as inputs in plant breeding processes. The present work aimed to establish the relationship between the production of defense molecules and the tolerance/ susceptibility response to phytopathogens (XCP123) and (RH17) in four bean varieties three of these cultivars and one from the CIAT germplasm bank.

The chemical response was determined under greenhouse conditions. Methanolic and protein extract of leaf were quantified relative to the accumulation of low molecular weight compounds of protein and phenolic type. By means of microdilution in wells and thin layer chromatography (TLC) coupled to the technique of direct immersion bioautography with development by MTT to determine the antimicrobial activity. The four varieties exhibited two bands with Rf (0.65 and 0.91) that inhibited bacterial growth against XCP123, the red cargamanto variety had the greatest effect, however, it did not show inhibition upon fungus (RH17) growth. The concentration of total phenols was 9.07 E g Gallic acid /g sample.

The Nima Calima variety had fungistatic effect against the strain (RH17), and its antibacterial effect was significant, however, the higher concentration of total phenols was found (18,35 E.?g gallic acid / g sample). The protein extract obtained from the four varieties did not show to be related to the antimicrobial response. The ability of defensive response to the phytopathogen RH17 was directly related to a higher production of total phenolic compounds, in contrast, the defensive mechanism against the phytopathogen XCP123 does not correlate with an increase in the phenolic concentration, the protein concentration is not related to the defensive capacity of this beans varieties plant.

Keywords: *Phaseolus vulgaris, Rhizoctonia solani, Xanthomonas axonopodis,* Defensive response, Bioautography.

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BIOLOGICAL ACTIVITY OF VOLATILE ORGANIC COMPOUNDS RELEASED BY MARINE ORIGIN BACTERIA CULTURES

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PONP 03

The biological activity of volatile compounds has always been associated with the smell of our environment. For example, the odor that is perceived after a rainy afternoon, is due to geosmin and 2-methylisoborneol compounds, which are released by actinobacteria present in the soil [1]. In addition to the odor, others biological activities mediated by Microbial Volatile Organic Compounds (MVOCs) has been identified. Although these MVOCs have long been considered as degradation products of biosynthetic pathways, they are now recognized for their regulatory role in various ecological relationships [2,3]. There are examples of MVOCs involved in microorganism growth regulation, bacterial pathogenicity, and inhibition of Quorum Sensing (IQS) [4]; and also in the promotion or inhibition of plant growth [5,6] and the control of phytopathogenic fungi [7].

On the other hand, the study of marine microorganisms as source of biological active compounds has been increasing, and great developments are expected in this field in the near future. However, the study of MVOCs has barley studied. In this sense, our group has evaluated the MVOCs produced by some bacteria isolated from marine environments as antifungal against phytopathogenic fungi (*Fusarium* spp and *Colletotrichum* spp), and as quorum sensing inhibitors (using *Chromobacterium violaceum* biosensor). The extraction conditions, the effect of culture media and seeding time were evaluated in the production of MVOCs. For some of the identified compounds antimicrobial *in vitro* tests have been conducted.

The results showed that the exposition of phytopathogens to MVOCs produced by marine bacteria can reduce fungi growth and inhibit spores production in phytopathogenic fungi, and are able to inhibit quorum sensing. The identification of bioactive MVOCs allowed to propose this bacteria as agents for the biological control of pathogens in plants.

Keywords: microbial volatile organic compounds (MVOCs), l, inhibition of quorum sensing, antifungal, antibacterial, SPME-GCMS.

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EVALUATION OF ANTI-ALZHEIMER ACTIVITIES AND COMPARATIVE ANALYSIS OF ALKALOIDS COMPOSITION FROM TWO *Lycopodium* SPECIES GROWN IN COLOMBIA

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PONP 04

Alzheimer's disease (AD) is a complex condition involving many genetic and environmental factors. Among these, increased levels of acetylcholine, oxidative stress and inflammation within the brain have been implicated in the pathogenesis and progression of AD. Therefore, anti-inflammatory and antioxidant agents as well as inhibitors of the Acetylcholinesterase (AChE) enzyme might be beneficial for the treatment of AD. *Lycopodium* alkaloids produced by Chinese folk herb *Huperzia serrata* (Lycopodiaceae) such as Huperzine A, have been shown to be promising agents for the treatment of Alzheimer's disease due to their potent AChE activity. The members of this family are widely distributed in Colombia, but there is only one research study on their chemical composition and biological activities. Thus, two Lycopodiaceae species endemic of Colombia (*L. Thyoides* and *L. Jussiae*), were collected in paramo areas, their alkaloids content extracted with ethanol and their *in vitro* AChE inhibition and antioxidant activities determined. Weak antioxidant activities, evaluated through two different assays (DPPH and ABTS radicals), were observed for the ethanolic extracts of *L. thyoides* and *L. jussiae*: EC50 (DPPH)= 23,02 mg/mL and EC50 (ABTS)= 4,52 mg/mL for the; EC50 (DPPH)= 12,04 mg/mL and EC50 (ABTS)= 3,17 mg/mL respectively. The AChE activities of the whole ethanolic extracts were found to be significantly reduced *in vitro* (*L. thyoides* IC50= 7,64mg/mL; *L. jussiae* IC50= 12,04mg/mL). The whole extracts were subsequently fractionated and analyzed by HPLC-MS/MS in order to identify the compounds responsible for the biological activity. Several alkaloids were assigned to the two different species of Lycopodiaceae. Thus, it appears that *L. thyoides* and *L. jussiae* alkaloid extracts show weak antioxidant activities and good inhibition of the acetylcholinesterase *in vitro*, suggesting that the *Lycopodium* species from Colombia may constitute a promising source of compounds with pharmaceutical interest for Alzheimer's disease.

Keywords: Alzheimer disease, antiAch activity, antioxidant activity, HPL-MS/MS, alkaloids.

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METABOLIC PROFILING OF THE OCTOCORAL *Erythropodium caribaeorum* FROM THE COLOMBIAN CARIBBEAN SEA

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PONP 05

The octocoral *Erythropodium caribaeorum* produces erythrolides, chlorinated briarane diterpenoids, with an ecological role as feeding deterrent compounds [1]. Briarane diterpenoids also have shown different biological activities as cytotoxic, antimitotic etc [2]. In Colombia, this octocoral can be found at different locations in the Caribbean Sea including Santa Marta, Islas del Rosario, and Providencia [3]. The organic extracts obtained from samples collected at these places were analysed by HPLC-HRMS. The LC-MS data were processed by MZmine software, and the principal component analysis (PCA) and hierarchical analysis cluster (HCA) showed that the diterpenes profile changes according to the place in which the sample growth.

Diterpenes from samples of each location were isolated to describe each one of the three chemotypes. The one from Santa Marta (2 samples) was a highly diverse chemotype, with two new erythrolides W and X along with eight known erythrolides identified by direct derreplication as 16-acetylerythrolide H, erythrolide D, erythrolide E, erythrolide F, erythrolide I, erythrolide J, erythrolide U and erythrolide V. Samples from Islas del Rosario (14 samples) showed a low diversity chemotype constituted by high amounts of erythrolide A and B. These samples also showed by principal component analysis (PCA) and hierarchical cluster analysis (HCA) of their NOESY-1D NMR spectra great similarity among them. Finally, the chemotype from Providencia showed low chemical diversity with only two main compounds identified as erythrolide V and R.

These results indicate the potential that Colombian specimens of *E. caribaeorum* have in the production of compounds with potential biological activity. This information will be helpful for future approaches of aquaculture of *E. caribaeorum* for the production of these compounds [4].

The Ministerio de Ambiente y Desarrollo Sostenible granted permission to collect samples and perform this research (Contrato de acceso a recurso genético No 109). Financial support from Colciencias and Universidad Nacional de Colombia is acknowledged.

Keywords: *Erythropodium caribaeorum*, Erythrolide, Briarane, Diterpene.

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MARINE MICROORGANISMS FROM THE COLOMBIAN CARIBBEAN SEA AS A SOURCE OF BIOACTIVE COMPOUNDS

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PONP 06

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Marine microorganisms are one of the most prolific sources of compounds with biological activity, besides sponges and cnidarians [1]. In our country, plants and marine invertebrates have been the main focus in natural products research during the last decades. Also, they represent one of the most promising answers for the problem of supply compounds and extracts for the industry. This presentation shows the results of our studies of marine microorganisms recovered from the Colombian Caribbean Sea as a novel source of bioactive compounds. Our first approaches search for compounds form marine benthic cyanobacteria and Firmicutes.

Several new peptides as the almiramides B-G and cereusitin, and poliketides as the calibolide A, among other compounds have been isolated from extracts obtained from envrionmental samples of cyanobacteria and from the culture of Firmicutes belonging to the genera *Bacillus*, *Oceanobacillus* and *Jeothgalicoccus*. These compounds showed activities as cytotoxic, antiparasitic, antimicrobial and quorum quenching activities. In addition, we explored their application in the control of phytophatogens and insects. In our most recent approach, we include techniques of derreplication such as direct derreplication, metabolic barcoding and mass networking, as well as techniques of metabolic profiling (HCA, PCA, OPLS) to select the most interesting strains of microorganisms as a source of interesting and bioactive compounds. Also, these approaches allow following metabolite production of compounds during their culture process.

With this, we have identified amides and peptides such as tetrapeptides, diketopiperazines and antimycines with potential uses as agrochemicals for the control of phytopathogenic strains of bacteria and fungi. In addition, from 15 strains of marine recovered fungi, a strain of *Purpureocillium lilacinum* PNM-67 showed to produce four new peptides named lilacinines A-D, related with the structure of leucinostatins. Mass networking studies on the extract showed an unexplored chemical diversity allowing propose the structure of new lilacinines and leucinostatines. These results encourage us to continue the search of bioactive compounds and interesting structures from marine microorganisms collected at the Colombian Caribbean Sea.

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Keywords: Marine microorganisms, Bioactive compounds, Metabolomics, Derreplication.

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INTERLOCATION AND ONTOGENIC-RELATED VARIABILITY OF METABOLIC PROFILES OF *Lupinus bogotensis*

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PONP 07

Lupinus plants are legumes members that form root nodules to fix atmostpheric nitrogen and produce more nitrogen-containing secondary metabolites than other plants. Despite this behavior, a lack of information regarding variability of *Lupinus* plants on highlands is still missing as well as metabolic-mediated variability. Thus, the aim of the present study was to observe the interlocation and ontogenic-related variability of metabolic profiles of wild, highlands-growing *Lupinus bogotensis.*

On this context, the metabolite profiles of unfractionated ethanol-soluble crude extracts from leaves, stems, flowers, pods and seeds of accessions from different locations and stages were determined using HPLC-DAD-ESI-MS and NMR techniques. LC and NMR profiles were compared by Principal Component Analysis (PCA) and were correlated to their location, plant part and stage by means of Orthogonal Partial Least Square-Discriminant Analysis (OPLS-DA). The set of extracts exhibited a chemical profiles involving several common compounds (flavonoid and quinolizidine-type) between samples but other constituents were found to be restricted to some accessions, part and stage.

This fact indicated a marked chemical variability throughout *L. bogotensis* samples that could be correlated to its capacity to be invasive. Thus, unsupervised and supervised multivariate statistical analysis showed significant differences between extracts according to location (e.g., natural and modified environments), plant parts and stages, involving particular metabolites serving as metabomarkers. This fact was supported by Monte-Carlo cross-validation (MCCV) using area under ROC curves. This study therefore constitutes as the first evidence of metabolomics-based variability of *L. bogotensis.* The present work is a product derived by the Project IMP-CIAS-2293 financed by Vicerrectoría de Investigaciones at UMNG.

CHEMICAL STUDY AND MASS NETWORKING DEREPLICATION OF THE FUNGI *Purpureocillium lilacinum*

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PONP 08

Agriculture represents an important part of the Colombian economy. One of the most common problems related with agricultural practices is the rising of resistant strains of phytopathogens as a consequence of the intensive use of agrochemicals [1]. Currently, environmental friendly methods to control plagues and diseases are widely encouraged, and microorganisms represent a remarkable alternative among these methods [2]. In the last decades, marine natural products research has focused its attention on microorganisms and especially on marine-derived fungi [3] and their applications in agriculture are increasing with time [4].

Therefore, this work was designed with the aim to contribute with the study of fungi isolated from samples collected at the Colombian Caribbean by evaluating their capability to produce antimicrobial compounds against the rice pathogens. The ethyl acetate extract of a strain of *Purpureocillium lilacinum* PNM-67 grown in PDB media was studied by traditional methods. This allowed the identification of four peptides that share the N-terminal residues of leucinostatin A, whose structures were not found in databases (Antimarin and Scifinder), and were named as lilacinins A-D. Compounds 1 (lilacinin A) and 3 (lilacinin C) exhibited mild activity against *Burkhorderia gladioli* at a concentration 442 µM for compound 1 and 300 µM for compound 3.

In the dereplication by the mass networking strategy, MS/MS data were used to construct networks through the data-driven platform offered by the GNPS (Global Natural Products Social Molecular Networking) [4]. The obtained results allowed us to identify five already known leucinostatins and to propose the structure of 22 new peptides, among them, 10 new leucinostatins and 12 lilacinins. The Ministerio de Ambiente y Desarrollo Sostenible granted permission to collect samples and perform this research (Contrato de acceso a recurso genético No 121). Financial support from Colciencias and Universidad Nacional de Colombia is acknowledged.

Keywords: Dereplication, Molecular networks, Phytopathogen, *Purpureocillium lilacinum*.

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IN VITRO AND *IN SILICO* EVALUATION OF BENZYLISOQUINOLINE-TYPE ALKALOIDS AS ANTIFUNGALS

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PONP 09

Novel compounds with fungitoxic potential can be found on plant or bacteria metabolites, since several phytopathogenic fungi represent a threat for various crops around the world, not only by the damage they can cause but also by their progressive resistance to traditional fungicides. On this context, it is necessary to find compounds to fight them efficiently. Some candidates for the above-mentioned purpose are plants from *Zanthoxylum* genus (Rutaceae), which produce some metabolites with fungitoxic potential such as alkaloids, amides and coumarins. Among the *Zanthoxylum* genus-occurring metabolites are benzylisoquinoline alkaloids, which have reported a large number of applications including antimicrobial agents, making these compounds promissory agents for antifungal control.

Thus, in the present work, the antifungal activity of an alkaloidal extract from *Zanthoxylum schreberi* was assessed *in vitro* against phytopathogenic fungus *Fusarium oxysporum*, and the binding mode of some *Zanthoxylum*-derived benzylisoquinoline metabolites into a fungal enzyme was *in silico* explored. Alkaloidal extracts were then obtained from bark and leaves of *Z. schreberi*, and were separately tested against *F. oxysporum* by means of a micro-scale amended-medium method at 0.1-5.0 ?g/?L. After 48 h, a growth inhibition was observed above 81% for leaves extract and 100% for bark extract.

Extracts were analyzed by HPLC-ESI-MS in order to achieve a peak annotation by mass spectra data. The binding mode of identified benzylisoquinoline alkaloids within the active site of Lanosterol 14?-demethylase (LDM) as target enzyme was evaluated through molecular docking using Autodock/Vina. Results were examined through Vina scores and ligand-residues interactions. Good Vina scores were obtained for docked structures at different levels. Most stable conformers of LDM and alkaloid 1 were found to exhibit comparable docking energies to that of control. Benzylisoquinoline-related compounds might be considered as good candidates for structural optimization leading natural product-based design of anti-phytopathogens.

The present work is a product derived by the Project INV-CIAS-2293 financed by Vicerrectoría de Investigaciones at UMNG - Validity 2013.

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POSTERS

COSMETIC PHYTOTHERAPY

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PPEE 01

Herbs and spices have been used in maintaining and enhancing human beauty because herbs have many beneficial properties, such as sunscreen, antiaging, moisturizing, antioxidant, anticellulite, and antimicrobial effects. The merging of pharmaceutics and cosmetics is known as cosmeceuticals, which consists of products with medicinal properties that shows beneficial topical actions and provides protection against degenerative skin conditions (1). We describe the use of some natural products in cosmetic preparations with a brief description of the major use, plant parts used and the benefits of such products; the plants, commonly used in domestic medicine and home remedies, by those of different cultures, are traditionally used for the remedy of hair and scalp diseases where the main focus, currently, is on their “cosmeceutical” purposes. The use of herbal products in skin care; such as dryness, eczema, acne, and as free-radical scavenging, antiinflammatory, antiaging and skin protection effects are also discussed; as well the use in hair care as hair growth stimulants, hair colorants, and scalp complaints such as dandruff. A novel concept in this field is the treatment of photoaging and preventing its progression by repairing and optimizing the stratum corneum barrier, while reversing and inhibiting chronic cutaneous inflammation, has now been proven (2). Research has shown that a disrupted stratum corneum permeability barrier coupled with chronic inflammation induce signs of extrinsic aging (photoaging) (3). The herbal-based product cosmeceutical regimen are used to reverse these two anomalies. As compared with synthetic cosmetic products, herbal products are mild, biodegradable, and have low toxicity profile. To enhance these properties, research is being done in the development of newer approaches, which could improve both the aesthetic appeal and performance of a cosmetic product. Many plants used in traditional medicine represent rich sources of natural bioactive substances with health-promoting effects and no side effects. Nowadays, over 65% of the world population relies on traditional medicine for health care (4). Therefore, nutracosmetics are an emerging class of health and beauty aid products that combine the benefits of nutracosmetical ingredients with the elegance, skin feel, and delivery systems of cosmetics (4). Since the term "cosmeceutical" was coined over 2 decades ago, the number of products in this category that claim to combat dermal aging has grown dramatically (5). There are many effective treatment options including surgical measures and nonsurgical modalities, such as fillers, neuromodulators, lasers, and light technology, but these are costly and have the potential for greater side effects. Therefore, a minimally invasive treatment, such as a topical cosmeceutical, is often the desired first line of skin treatment. This review discusses the efficacy of herbal-based products for cosmetic purposes or even therapeutic effects.

Keywords: Phytotherapy, Cosmetic medicine, Cosmoceuticals

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ETHNOPHARMACEUTICAL FIELDWORK IN THE PERUVIAN AMAZON AND PHYTOCHEMICAL ANALYSIS OF TRADITIONAL RECIPES. NEW INSIGHTS FROM LOCAL HERBAL MEDICINAL KNOWLEDGE

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PPEE 02

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Ethnopharmaceutical research investigates the modes of preparation through which plants are transformed into medicines, and may offer a valuable arena to investigate the culturally recognized procedures and standards necessary for the wanted formulation of the end medicinal product in a given context.

In the present work, ethnopharmaceutical fieldwork was performed in the region of San Martin, Peru, by the means of semi-structured interviews with experts in the field of traditional Amazonian herbal medicine preparation. Phytochemical data based on HPLC-UV/DAD metabolite fingerprinting analyses were also acquired on selected herbal medicinal products. In accord with literature data on other traditional pharmacopoeias [1, 2], our results show how specific manufacturing steps do affect the chemistry of the finished product, indicating the relevance of the study of traditional processing methods for a more comprehensive understanding of the chemistry of herbal medicines at large.

Anthropological contributions, however, contend that a purely chemical outlook in ethnopharmaceutics does not capture the broader beliefs and practices linked to the efficacy of herbal medicines [3]. In the present study we pursue an interdisciplinary approach to ethnopharmaceutics and, by recording informants' discourses on the production process, we shed light on the underlying concepts of quality, safety, and efficacy in traditional herbal medicine, making us rethink the model of the “Active Ingredient” in other pharmacopoeias.

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ESSENTIAL OIL COMPOSITION OF *Hedyosmum racemosum* FROM ECUADOR

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PPEE 03

The genus *Hedyosmum* (Chloranthaceae) comprises approximately 45 species distributed throughout the tropical and subtropical regions of America. Sixteen of them have been reported in Ecuador. *Hedyosmum racemosum* (Ruiz & Pav.) G. Don, is known by the indigenous population as, “guayusa”, “guayusa de monte”, and “jicamilla”. This genus is considered of high importance under the ecosystem. The species is widely used under the folk medicine to treat inflammations together with Bixa orellana. It is also used with Cordia to treat snakebites. The essential oil from leaves of *Hedyosmum racemosum* (Ruiz & Pav.) G. Don collected in Ecuador was obtained by hydrostillation and analyzed by GC and GC-MS. Monoterpenes (44.38 %) constitute the majority of 32 compounds identified, with estragole (14.18%) as the main constituent. Sesquiterpenes accounted for 24.64 % of the oil. Gurjenene (12.47 %), alpha phellandrene (11.80 %), terpinolene (8.40 %), alpha pinene (8.11%), o-cymene (5.59 %), and gamma amorphene (5.25 %) accounting for compounds with high concentration in the oil. In a research were the phytochemical and bioactivity of this species was undertaken, the oil was characterized. Comparing our results with some species of the same genus [1-3] the composition of the essential oil of *H. racemosum* was significantly different of other species in qualitative and quantitative differences. In two of the species reported in the literature, *H. mexicanum* and *H. bomplandianum* sabinene was the most abundant compound, but estragole, the major component in *H. racemosum*, is present in very low percentages in the survey of species previously described in the publications. Estragole, the main compound present in the oil, have been associated with high antimicrobial activity [4].

Keywords: *Hedyosmum racemosum*, Essential oil, Estragole, Composition

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PPEE 04

PHYSICOCHEMICAL PROPERTIES AND TOXICITY OF PULP OIL OF MAXIMILIANA MARIPA (AUBL) DRUDE

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The inajá (*Maximiliana maripa* (Aubl.) Drude) is a Palm in the Arecaceae family and is found in Colombia, Venezuela, Trinidad (Caribbean), Guyana, Ecuador, Peru, Bolivia and Brazil. Both the almond and the pulp of the fruit represent the raw material that can be consumed as food in its natural state, also serving for the production of wines, juices and ice creams. It is also important for the cosmetics and health products industry. It presents physicochemical characteristics that allow its use as an energy food, as well as raw material of an oil character. This work presents the chemical, physicalchemical and toxicity study of the *M. maripa* pulp oil of natural occurrence in the state of Roraima. Its objective was to determine the physical-chemical properties by 1H-NMR, to identify the main functional groups present, through the infrared spectrophotometer, and to evaluate the nauplii toxicity of *Artemia salina*. The pulp extracted a colouring light yellow oil with 44.20 percent yield, obtained by Soxhlet extraction with hexane. Physicochemical properties were calculated using the values of the integrals of the 1H-NMR spectrum, where direct measurement were calculated iodine, acid value, saponification value, oleofínic/aliphatic hydrogens ratio, average number of establishment by triglyceride, estimated percentage of unsaturated fatty acids derivatives totals and degree of unsaturation, demonstrating that the pulp oil inajá physicochemical features that enable your enjoyment on both human as animal feed. Infrared spectroscopy, showed Absorptions bands characteristics of triglycerides, as a strong and intense band, for the C=O group, at 1.732 cm-1, the carboxylic acids. In the test against *Artemia salina*, an LD50 of 0.96 µg.mL-1 was determined, being considered toxic. The results obtained provide new information for literature and suggest future studies of chemical and biological exploration of this species with the purpose of developing bioproducts.

Keywords: *Maximiliana maripa*; 1H-NMR; Infrared; Toxicity

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COMPARISON OF FOUR ANTIMICROBIAL METHODS WITH EXTRACTS OF PLANTS USED IN TRADITIONAL MEDICINE FOR THE TREATMENT OF UROGENITAL DISEASES FRONT TO *Escherichia coli* and *Pseudomonas aeruginosa*

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PPEE 05

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Infectious diseases have been a challenge for humanity and despite advances in science there are many conditions that do not yet have control mainly due to the resistance of the pathogens from different commercial antibiotics (1,2). Urinary tract diseases caused by bacteria are among the three leading causes of infection after the respiratory and gastrointestinal (3), reporting at least 150 million people affected annually (4). Within the treatment alternatives, to reduce the resistance of bacteria associated with urogenital infections (UI) it is the use of medicinal plants (5); however, differences have been reported in evaluating the antimicrobial potential depending on the method used; this probably due to limitations in the reproducibility and reliability of the techniques due to lack of standardization (6). For this reason, the objective of this study was to compare four antimicrobial methods with six plant extracts used in the Colombian traditional medicine for urogenital infection control. The vegetal species (ortigón, grama, vira vira, cola de caballo, caracola and parietaria) were obtained from a local of sale of medicinal plants of the place Restrepo (Bogota), and these were subjected to maceration with ethanol at room temperature. Subsequently, by methods of disk diffusion, dilution in tube, microdilution and HT-SPOTi, assessed the antimicrobial activity against *E. coli* (ATCC 25922) y *P. aeruginosa* (ATCC 9027) of the ethanol extracts at a concentration of 30 mg/mL in DMSO and used as controls dimethyl sulfoxide to 10% and gentamicin (10 mg/mL). This work allowed to know that the results of the antimicrobial potential were consistent in the four methods performed and that four of the extracts present inhibitory effect against the evaluated strains. The evaluation of the antimicrobial potential allowed to identify the advantages and disadvantages of each one of the methods used and learn about the antimicrobial potential of plants used in traditional medicine for the treatment of urinary tract infections. This type of research promotes studies aimed at the isolation of active principles that can be used in the development of drugs for the treatment of UI.

Keywords: Antimicrobial methods, medicinal plants, Escherichia coli, *Pseudomonas aeruginosa*.

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CHEMICAL COMPOSITION OF ESSENTIAL OIL FROM *Tagetes filifolia* LAG. (SACHA ANIS)

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PPEE 06

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The plant sacha anise (*Tajetes filifolia* Lag.) belongs to the Asteraceae family; it is herbaceous and grows wild in the region inhabited by the Saraguros. The Saraguro community uses it as medicine to relieve stomach pain, for colds and for the cough; in food to prepare infusions and as aromatic additive of horchata (a drink prepared with a mixtures of plants). This species that grows in considerable quantity has a seasonal production and is collected from April to July.

In order to use the sacha anis produced in the Saraguro region in a sustainable manner, a cooperation agreement was signed between the UTPL and the Council of healers of Saraguro Hampiyachakkuna for the purpose of extracting, characterizing chemically and using the essential oil in a Traditional alcoholic beverage called aniseed.

In the first stage the chemical composition of the essential oil has been studied, as well as its physical chemical properties. The Saraguro community has collected the material (sacha anis) necessary for the research. The oil was obtained from the fresh plant material, three extractions were carried out through the method of steam distillation in the laboratories of the UTPL using a clavenger equipment. The oil presented a light yellow color; its yield was 0.25%, the average density of 0.983 g / cm 3, and the refractive index was 1.5524; identifying forty components, in which the majority were: Anethole <(E) -> (77.221%) and Methyl chavicol (20.43%). The second stage aims to evaluate the use of the oil to make the alcoholic beverage and establish the parameters for its elaboration in a craft process that can be developed by members of the Council of healers of Saraguro as an agroindustrial enterprise that generates resources to the community. Likewise, the use of a stainless steel artisan distiller that can be used in the community will be evaluated.

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OBTAINING A NATURAL COADJUVANT FOR THE TREATMENT OF DIABETES MELLITUS, FROM KALANCHOE PINNATA

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PPEE 07

Diabetes mellitus, is considered an epidemic disease by the World Health Organization (WHO) and is thought to be the seventh cause of death in 2030. In 2014, Costa Rica reported 8 743 diabetes new cases (incidence rate: 183.17 cases per 100 000 Hab.) and 720 deaths (mortality rate: 15.08 cases per 100 000 Hab.)[5].Some methods to control this disease are: hypoglycemic drugs, insulin, diet and exercise. Even though, some people prefer home remedies or medicinal plants. *Kalanchoe pinnata* (Crassulaceae) is use in folk medicine, because it is capable to reduce glucose blood levels when people consume fresh leaves or infusions. Its leaves have been reported to contain: alkaloids, bufadienolides, flavonoids, triterpenoids, steroids, phenols, tannins, macroelements, microelements and vitamins. Leaf extract experiments showed antidiabetic activity tested on *in vivo* model, but did not showed the responsible metabolite [1,3]

This project aims to study, for the first time in the country, phytochemical characteristics of *K. pinnata*, in order to identify secondary metabolites related to diabetes control and scientifically support of the antidiabetic capacity of the plant, through an *in vivo* animal model, in order to obtain a natural coadjuvant extract for diabetic patient's treatment. *Methodology*: The plant material was collected from land and greenhouses. It was botanically identified by the National Herbarium. *Justicia spicigera* ("insuline") was included. Three disinfection methods and four M&S culture medium have been tested on *in vitro* introduction of *K. pinnata*. The zinc concentration was also quantified both vegetative material and commercial natural products. The second part of the research, includes DNA characterization from three species of *Kalanchoe spp*. using mat-K region, phytochemical identification of extracts metabolites (kaempferol and kaempferitrin mainly because their hypoglycemic activity) and α–amilase inhibition test. Extracts will be obtained from fresh material, oven-dried and lyophilized, using water and ethanol:water and different extraction techniques (decoction, maceration and infusion). The better extracts will be tested on *in vivo* animal's models. [2,4]. *Results and conclusions*: *K. pinnata, K. blossfeldiana y K. daigremontiana* were identified. Introduction and *in vitro* multiplication of *K. pinnata* showed better results in M??&S culture medium without growth regulators. *K. blossfeldiana* presented the largest amount of Zinc (97mg/Kg) it might contribute to glycemic control. Significant results have been obtained, but better conclusions are expected upon completing the research.

Keywords: *Kalanchoe sp, Diabetes mellitus, Justicia spicigera*, Zinc, *in vitro*

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ANTIFUNGAL ACTIVITY *in vitro* of *Oxandra venezuelana* R.E. FR. (ANNONACEAE) EXTRACTS AGAINST *Candida spp*. IN MONTERIA, COLOMBIA

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PPEE 08

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The incidence of fungal infections caused by *Candida spp*., has increased significantly in recent years, coupled with the increase of antifungal resistant strains due to the increase in immunocompromised population has generated a serious public health problem worldwide, becoming increasingly complex treatment for these infections, generating high rates of morbidity and mortality in this population [1]. All this, emphasizes the interest in the search for new antifungal agents from natural sources. Plants are an invaluable source of biologically active molecules; from them, a great diversity of secondary metabolites has been isolated, which have been shown important biological activity among which stand out antitumor, cytotoxic, anti-inflammatory and antimicrobial [2].

The present study aimed to evaluate the in vitro antifungal activity of *Oxandra venezuelana* extracts against clinical isolates of *Candida spp*., using microdilution and agar diffusion using wells methods. The antifungal activity of the extracts: leaf oil benzine, leaf acetone, bark and wood of *Oxandra venezuelana* were evaluated against 12 clinical isolates of *Candida spp*., and the strain ATCC 10231 of *Candida albicans*. The results obtained show an inhibitory effect of all the extracts in the highest concentrations evaluated, being the leaf acetone extract that showed a greater inhibitory effect by Microdilution method, however, the tests performed with the agar diffusion method did not show evident inhibition halos, which confirms the sensitivity of the microdilution method.

The activity of the extracts is possibly attributed to the presence of alkaloids, flavonoids, terpenoids, saponins, tannins and coumarins found in the phytochemical gait performed on this species and which have been reported in other studies of antimicrobial activity [3,4]. These results show a possible antifungal potential of the *Oxandra venezuelana* extracts at the highest concentrations studied, once again revalidating the potentiality shown by isolated compounds of various species of the Annonaceae family.

Keywords: Fungal infections; secondary metabolites; Microdilution; Diffusion in agar and inhibition of growth.

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EXTRACTION AND CHARACTERIZATION OF CLINOPODIUM BROWNIE (SW) KUNTZEN ESSENTIAL OIL

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PPEE 09

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This research is part of a collaborative project between the Healing Council of Saraguro Hampiyachakkuna. (Consejo de Sanadores de Saraguro Hampiyachakkuna), UTPL and the Ministry of Health of Ecuador, whose objective is to study the natural therapeutic resources used by the Saraguro people and determine which natural resources can be taken advantage in sustainable agroindustrial ventures.

The essential oil was obtained from the medicinal species *Clinopodium brownie* (Lamiaceae), commonly known as poleo chico or poleo pequeño who is used in traditional medicine Saraguro community for treating colds and intestinal problems [1].

The plant was collected by the Saraguros themselves in the sector of Tuncarta-Saraguro. Its leaves and stems were steam distilled in a clevenger device to obtain the essential oil. The recognition of their compounds was performed in a gas chromatograph with a DB-5MS column coupled to mass spectrometry and flame ionization detector. The essential oil had a light-yellow color and an efficiency of 0.068%, the major compounds that have been recognized were the following monoterpenes Anethole (E) (13.99%), Methyl Chavicol (5,07%), Bicyclogermacrene (0,37%) Isopulegone (0.35%) and Menthone (0.29%). The antimicrobial activity was evaluated against micrococcus luteus (ATCC 10240), Escherichia coli (O157: H7) (ATCC 43888), and Candida albicans (ATCC 10231) with a minimum inhibitory concentration of 4000, 8000 and 2000 µl / ml respectively. The essential oil had a refractive index of 1.4819 at 20.1 ° C and a polarimetry of 0.566.

Keywords: *Clinopodium brownie* (Sw) Kuntzen, Essential Oil, CG-MS, Ecuador

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COMPOSITION OF *Baccharis oblongifolia* ESSENTIAL OIL

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PPEE 010

The plant *Baccharis oblongifolia* (Asteraceae) in the Saraguro community (southern Ecuador) is used for the treatment of stomach and liver diseases, as well as to reduce inflammatory processes and to cure ulcers and skin wounds. (Gonzales, 2015).

The essential oil was obtained by means of steam distillation, the oil had a yellowish color, its density was 0.8657 g / cm3, the refractive index was 1.4844 and a specific rotation of 5.333. For the identification of the compound was used a gas chromatograph, model 6890N Network ºC System coupled with a mass spectrometer 5973 Inert and a flame ionization detector (GC-FID) of DB-5MS capillary column (30m, 0.25mm, 0.25 Mm), the sample injected into the equipment was a mixture of 10ul of oil and 990ul of dichloromethane. It was possible to identify 94 compounds, having in greater abundance: Thujene (4.566%); Pinene(3.110%); Sabinene (4,397%); Pinene<β-> (6.47%); Myrcene (2,740%), Terpinene (3,006%); Limonene (39.084%); Anothole <(E) β-> (5.41%); Candinene (5,650%); Cadinene (2.036%); Phenyl ethyl octanoate (2.369%).

Keywords: Ecuador, Essential oil, Baccharis Oblongifolia, (GC-FID), DB-5MS,

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ANTIHYPERTENSIVE AND ANTIOXIDANT POTENTIAL OF ETHANOLIC EXTRACTS FROM *Passiflora vitifolia* Kunth and *Passiflora edulis* Sims f. edulis seeds

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PPEE 11

The present study evaluated the antihypertensive and antioxidant capacity of the ethanolic extracts obtained from the seeds of *P. vitifolia* Kunth and *P. edulis* Sims f. edulis. The presence of secondary metabolites was evidenced by using qualitative tests and thin layer chromatography (CCD) (Murillo and Méndez, 2012). The antioxidant capacity of the extracts was measured by the stabilization of the ABTS and DPPH radicals, according to the methodology proposed by Sánchez, Murillo and Méndez, (2010). The antihypertensive potential was determined by using Wistar rats that where induced to hypertension through the administration of a L-NAME inhibitor (30mg/Kg, i.p.) (nitric oxide synthase inhibitor). In order to establish the vasodilator effect and its possible mechanism of action, a vasodilation protocol model based on aortic rings was used as proposed by Bareño (2015). High presence of terpenes, anthraquinones, flavonoids, tannins, phenols and anthocyanins was found. The antiradical evaluation showed that the radicals were stabilized by the extracts at low concentrations. In terms of the *in vivo* antihypertensive potential, the extracts exhibited a preventive effect on hypertension during the six weeks of treatment ($p \leq 0.05$); similar to that of the standard (enalapril) and control (normotensive rat). The evaluation of the possible mechanisms of action through an isolated organ in *ex vivo* (treated rats), pre-contracted (with phenylephrine) and relaxed (with acetylcholine and sodium nitroprusside) aortic rings did not show a relaxing effect greater than the one from the untreated rings of rats without induced hypertension. Otherwise, those isolated aortic rings from untreated rats that were precontracted with phenylephrine, KCl and phenylephrine, showed a relaxing effect when in contact with the extracts. Such effects are not reversed in the presence of propanolol, atropine, methylene blue and indomethacin, but are partially reversed in the presence of L-NAME, besides, they inhibit the angiotensin II-induced contraction. The results suggest that the extracts from the seeds of *P. vitifolia* and *P. edulis* f. *e*dulis, contain secondary metabolites with antihypertensive and antioxidant potential that could be of interest in the phytopharmaceutical industry for the production of possible antihypertensive products.

Keywords: *Passiflora vitifolia*, *Passiflora edulis* var. edulis, antioxidant, antihypertensive, L-NAME, angiotensin-II.

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CYTOTOXIC PROPERTIES OF THE ENDEMIC VASCULAR FLORA OF THE CLIFFS FROM VALPARAISO REGION

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PPEE 12

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The cancer is one of Chronic Non-Transferable diseases (CNTD) of higher occurrence with result of death in the world. With respect to the incidence of the principal kinds of malignant neoplasms ills that affect world's populations are lung, liver, stomach, colon and breast. The conventional therapies given a palliative solution for the diseases but it bring with a number of unwanted side effects. In additions the low selective of the drugs often complicates the treatment of cancer by limiting the therapeutic doses of these, and the poor quality of life of patients during and after treatment. These reasons confirm the need to find new methods for the treatment of this disease, thus avoiding more deaths and / or side effects and preventing economic losses, since the value of these new methods is lower than conventional treatments, Being the alternative the secondary agents synthesized by the plants. We decided to evaluate the cytotoxic effect and cell viability of the vascular plants endemic to the cliffs of the Valparaíso region1 on neoplastic cell lines.In this scenario, sixteen sequential extracts from fourth plants endemic to the cliffs of the Valparaíso region as *Blepharocalyx cruckshanksii, Adesmia microphyla, Franoca apendiculata, and Modiola caroliniana* were evaluated *in vitro* for their antiproliferative activity against Ht-29; PC-3; MCF-7, and a healthy epithelial cell lines. Plants were extracted using n-hexane, chloroform, ethyl acetate, and ethanol. The antiproliferative activity was measured by SRB assay2 and daunorubicin was used as the positive control. Ethyl acetate extract of *Adesmia microphyla* was the most active extracts against Ht-29, PC-3 and MCF-7 cells with IC50 of 10.96, 25.32 and 30.78 µg/mL, respectively and was less toxic against epithelial cell line. However, daunorubicin is at least one hundred times more active as an anticancer compound against three cancer cell lines with IC50 of 0.38 ug/mL than ethyl acetate extract of *Adesmia microphyla*. Other extracts showed lower activity against cancer cell lines. TLC was used to identify active fractions. Based on the results obtained we have demonstrated the potential of the native flora of the cliffs of Valparaíso as a source of future neoplastic agents such as terpenes, phytosterols and flavonoids. The information obtained in this study gives us the opportunity to obtain new uses and applications of these plants for the treatment of cancer and other pathologies.

Keywords: *Blepharocalyx cruckshanksii, Adesmia microphyla*, cancer cells, antiproliferative activity

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ETHNOBOTANICS OF 30 SPECIES OF NATIVE MEDICINAL PLANTS IN THE MUNICIPALITIES OF SANTUARIO, CELIA, AND QUINCHÍA (RISARALDA) AND CALARCÁ (QUINDÍO)

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A quantitative ethnobotanical study was carried out on the use and knowledge of 30 species of medicinal plants in the municipality of Quinchía, Celia, and Santuario (Risaralda) and Calarcá (Quindío), with the purpose of knowing the level of importance that these medicinal species have for treatment and prevention of diseases in rural communities, also to identify the current use of these resources. Structured surveys were applied to 40 families with agricultural activity in each zone, following the methodology of Informant Consensus. The data were analyzed using the Value of Use Indices (VUI) and The Significant Level of Use Tramil (SUT). The species with the highest VUIs were: sauco (*Sambucus* sp) 1.1 – 2.5, acedera (*Oxalis corniculata*) 1.0 – 2.4, cidrón (*Aloysia triphylla*) 1.2 – 2.1, paico (*Chenopodium ambrosoides*) and pronto alivio (*Lippia alba*) 1.0 – 1.9, matarratón (*Gliricidia sepium*) 1.0 – 1.3; at the same time, the species that reported the greatest cultural acceptance (SUT) were: sauco (*Sambucus* sp) and matarratón (*Gliricidia sepium*) with 100%, paico (*Chenopodium ambrosoides*) with 99%, pronto alivio (*Lippia alba*) and acedera (*Oxalis corniculata*) with 98% and cidrón (*Aloysia triphylla*) with 97%. The analysis of the descriptive information showed that the 30 species evaluated contributed with their therapeutic properties to the attention of 66 average health conditions, the municipality of Quinchia was the one where a greater number of uses are reported for the species under study, - 100 health conditions - . Fever, the flu, infections and inflammations are the most attended diseases, pronto alivio (*Lippia alba*), anamú (*Petiveria alliacea*) and bencenuco (*Asclepias curassavica*) are considered the species used for the treatment of the greatest number of diseases. It is confirmed that the knowledge about medicinal plants is more representative in women (61.37%), and in informants with ages ranging from 51 to 70 years (48.89%), 100% of the respondents acquired the knowledge by oral transmission, through the family. Communities highlight other uses for plants under study such as bioside one, ornamental one, spiritual one and nutritional one.

Keywords: Native species, quantitative ethnobotany, Value of Use Indices (VUI), Significant Level of Use Tramil (SUT).

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TRAINING OF NEW GENERATIONS OF TRADITIONAL HEALERS (YACHAK) IN SARAGURO COMMUNITY.

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PPEE 14

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During the colonial period, the indigenous Saraguro (Southern Ecuador) maintained their traditions, knowledge, and practices to restore and preserve the health of their members. Unfortunately, many of their practices and medicinal resources have not been documented. Under a technical and scientific cooperation agreement among the UTPL, the Department of Salud Intercultural (MSP), and the Saraguro Healers Council (Consejo de Sanadores de Saraguro), was possible the organization of an academic course to form the new generations of traditional healers Saraguros, In this project the Saraguro Healers Council selected the 3 healers (yachak) most recognized for their knowledge and use of natural therapeutic resources. (**1**) a midwife, partera or *wachak*, (**2**) a herbalist, yerbatero or *yurak* (**3**) an orthopedist, sobador or *kakuy*.

The Department of Salud Intercultural (MSP) selected the Saraguros instructors in topics as **(i)** Cosmovision of the Saraguros people and **(ii)** Use of Andean foods. The UTPL accredited the course academically, organized the logistic, train in the elaboration of herbal products academically and delivered the certificates. In the first edition, all the participants (40) in 210 hours of course (154 classroom hours and 56 hours distance learning) have been able to visit the places where medicinal and sacred plants are collected, know their common names, uses, the form of preparation, administration and doses.

They also learned, the traditional diagnoses most used for the diagnosis of diseases and the use of sacred species for the treatment of supernatural diseases. This project is in line with the priorities and strategic research lines of the National Secretary for Science and Technology (SENESCYT) of Ecuador, especially with the concept of "*buen vivir*" (good living) that includes the efforts for preserving the indigenous ancestral culture by using the methods of modern science, while respecting the environment, nature, life, traditions and sovereignty of the indigenous communities.

Keywords: Ecuador, Saraguro, Traditional healers, yachak, Cosmovision, Ecuador.

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ANTIFUNGAL ACTIVITY OF THE SPECIES OF THE GENUS *Piper* AGAINST PHYTOPATHOGENIC FUNGI ISOLATED FROM COCOA FRUIT (*Theobroma cacao* L.)

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PPEE 15

Cocoa is one of the agricultural products with the greatest economic projection in the country. Low yields of cocoa production are attributed to many factors, including diseases caused by phytopathogenic fungi. To control this kind of fungi, there are usually employed expensive chemical products, with low selectivity and effectiveness, making necessary to find new antifungal substances. Plants offer a potential source of these substances due to the diversity of metabolites that they produce. The objective of this research is to determine the antifungal potential of various species of genus *Piper* against phytopathogenic fungi that affect the cocoa fruits.

The methodology included the isolation and preliminary characterization of fungi present in diseased cocoa fruits, the obtaining of ethanolic extracts of *Piper* species collected in the Cundiboyacense region, preliminary phytochemical analysis, and evaluation of antifungal activity by the direct bioautography method. Two fungi belonging to the genus *Fusarium* and one belonging to the genus *Colletotrichum* were isolated. 46 ethanolic extracts were obtained from 14 species of genus *Piper*. The preliminary phytochemical analysis together with the bioautographic tests allowed to determine that the main metabolites with antifungal activity against the evaluated fungi corresponded to triterpenes and/or steroids and phenols. The most promising extracts against the evaluated fungi correspond to those obtained from leaves and inflorescences of *P. marequitense*, and the extracts obtained from inflorescences of *P. asperiusculum* and *P. peltatum.*

Keywords: Preliminary phytochemical analysis, Phytosanitary agents, *Colletotrichum*, *Fusarium*, *Piper*, Theobroma *cacao* L.

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BIOACTIVE POTENTIAL IN AGRO-INDUSTRIAL RESIDUES OF CHOLUPA *Passiflora maliformis* AND GULUPA *Passiflora edulis* var *edulis* OF

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PPEE 16

Passiflora species are important native phytogenetics resources with sedative, antispasmodic, antibacterial, antioxidant, antiproliferative (1) and insecticide properties (2). Previous studies of fruits show the presence of phenolic compounds and flavonoids (3). Currently, major part of this metabolites are wasted by fresh fruit trade, where agro-industrial residues are frecuently discarded. The present research evaluated biological funcionality of bio-active compounds isolated from juice and fruit subproducts (Peel and seeds) of *Passiflora maliformis* (Cholupa) and *Passiflora edulis var. edulis* (Gulupa).

Fruits of both species coming from municipality of Rivera, Huila (*P. maliformis*) and municipality of Anzoátegui, Tolima (*P. edulis var edulis*), were processed, obtaining juice, pulverized peel, fatty oil and seed "cake". With peel and "cake", phytochemical screening, total phenols quantification and antioxidant potential by DPPH were performed. For the seeds was also performed a bromatological analysis. For the oil, following indexes, percentages and contents were determinated: Yield, density, brix degrees, saponification, esterification, acidity, free fatty acids, iodine, peroxidation, total phenols content, and antioxidant potential by DPPH. In peels of *P. edulis* were detected phenols, flavonoids and terpenoids; the first two absent in P. maliformis. In the "cake" of both species was found a high content of phenols, flavonoids, tanins and terpenoids. Phenols were above of 90 mg galic acid equivalents / g of sample; contrary for peles, where values don´t exceed 22 mg galic acid equivalents / g of sample (*P. edulis*).

The capacity for stabilize DPPH in both species show a better performance in the "cake", however, peel also show this potential but in minor degree, being major the antioxidant potential in P. edulis (Peel and "cake"). Oil show values in phenols of 9.55 mg galic acid equivalents / g of sample for P edulis and 1.17 mg galic acid equivalents / g of sample for *P. maliformis*, respectively.

A similar case occurred with antioxidant potential, where is evident a better behaviour in *P. edulis* with values that duplicate the registered values for P. maliformis. Oil physicochemical properties, according with parameters described previously, were similar in both species of *Passiflora*. Present study show the high potential of juice and agro-industrial residues of studied species, opening the posibility of recover compounds of high interest and value in the industry.

Keywords: Native, phytochemical, antioxidant, seeds, peel.

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MANAGEMENT PLAN AND EXPLOITATION OF ASAÍ (*Euterpe precatoria* Mart)

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PPEE 17

The formulation of the management plan for the use of the Euterpe precatoria Mart. Palm in the department of Amazonas is carried out with the aim of making a sustainable use of its fruits for commercial purposes by the rural community based in the Amazon, Corregimiento of La Pedrera (Amazonas), as an economic alternative within the activities developed by the community in its territory.

From the statistical forest inventory, the species with the highest ecological value in these flood forests was Asaí, with a high density and frequency, followed by Canangucha palm (Mauritia flexuosa) and Oxandra polyantha anonácea. From the census conducted for the estimation of Asaí individuals, the average individual per hectare greater than 10 cm of DBH was found to be 120, of which 78% are actively reproductive with an average of 2 clusters each. It is estimated that the area identified for its use (250 ha) can produce 70.5 tonnes of fresh fruit per year. Of this total, under the norm established for the use of non-timber products, in which 25% of the population and 40% of the production per palm are left untapped for their regeneration and conservation, it is estimated that the maximum volume To take advantage of is 26 tonnes per year.

The negative impacts that can be generated by the use, are minimal, and the form of mitigation are based mainly on the implementation by the villagers of good management practices. The proper implementation of the Asaí management and exploitation plan will allow the value chain to be consolidated around a non-timber forest product and it is hoped to achieve environmental and socio-economic sustainability of the species over time.

Keywords: Sustainable management, Non-timber forest products, Sustainable economic alternative

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PHYTOCHEMISTRY AND ETHNOPHARMACOLOGICAL RESEARCH ON ISLA GRANDE, CARTAGENA

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PPEE 18

An identification and knowledge of native plant species of Isla Grande, Cartagena has been done. We worked in association with traditional local healers about knowledge medicinal plants on the Island and we now know for what the plants are used for there. The informative data was based on semi-structured interviews, group discussions, questionnaire and field visits. The goal of this project is to diffuse the knowledge about medicinal plants of the island to the Colombian population and to tourists visiting the region. But, we can only diffuse how to use these plants only if the use is scientifically verified. We use in our research the Vegetal Caribbean Pharmacopeia [1,2] where the use of medicinal plants reported is scientifically tested. We compared the use done by the traditional local healers with the use referenced in Vegetal Caribbean Pharmacopeia.

Currently, we found 12 species of medicinal plants of Isla Grande which are used on the Island in the same way as described in the Pharmacopeia. In that place the plants are used as first aid to treat diverse ailments such as weakness, flu, asthma, gastric or urinary disorders. These ethnobotanical researches take place within a project of the "Grupo de Investigación en Química de Medicamentos" (Research Group in Drugs Chemistry) of the University of Cartagena. This Project, financed by COLCIENCIAS and University of Cartagena (CODE: FP44842-484-2016), is named Design and implementation of an ecotourist trail for a sustainable use of the mangrove and tropical dry forest ecosystems of Isla Grande (Cartagena, Colombia). In this Project, a pound with native plants of the island will be created. A part of the pound will be dedicated to a garden of medicinal plants and a place to sell them. It is in the place that we will be able to diffuse the medicinal knowledge of the traditional local healers of the Island.

We would like to thank the community council of Isla Grande, Hernando Goméz and the traditional local healers for their efforts and help which allowed us to realize the project that we had.

Keywords: Ethnobotanical, Identification, Knowledge, Diffusion

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EFFECT OF *Cryptocarya alba* HYDROETHANOLIC EXTRACT ON CELL VIABILITY IN TUMOR CELL LINES.

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PPEE 19

Prostate and Colorectal cancer are the first and third most common cancer in America, according to the World Health Organization (WHO). In Chile, 1300 to 1600 men die annually due to prostate cancer, and colorectal cancer has increased 0.8 points in the last decade (MINSAL-Chile). It has been evidenced a correlation between antioxidant activity of natural products and their anticancer effects [1, 2]. *Cryptocarya alba* (Peumo) is a Chilean tree whose principal use is decorative. Peumo can be found from fourth to tenth region in Chile. In ethnomedicine, this tree is used to treat hepatic illness and rheumatism since its bark is rich in tannins and has high antioxidant activity [3,4]. Herein we determine the effect of extracts of *C. alba* on viability of tumor and non-tumor cells. The hydroethanolic extract was prepared in ethanol 85% with dried and mashed Peumo leaves at 3% w/v. and 72 hours later, the extract was rotary evaporated and resuspended in DMSO in a 100 mg/mL final concentration. Measurement of total phenolic concentration was made through Folin Ciocalteu assay. The results show that the content of phenols in Peumo leaves was 199,7 mg of acid galic equivalent/mg of extract. To measure cell viability, we used two cell lines; HT29 (colorectal adenocarcinoma) and LnCap (prostate carcinoma), and cell line derived of non-tumoral mammalian stromal cells as control (RMF-EG). Cell lines were incubated with Peumo extract at 0, 5, 50 and 500 µg/mL and 48 hours later cell viability was determined by MTS assay. Peumo extract only at 500 µg/mL decreased cell viability about 60.5 % in HT29 and 70.7% in LnCap while in RMF-EG 27%. These results suggest that Peumo hydroethanolic extract has antitumoral properties without significant effects on normal cells, probably by its high phenolic concentrations.

Keywords: *Cryptocarya alba*, Cancer, Cell Viability.

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DETERMINATION OF SACHA ANÍS PROPERTIES

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PPEE 20

The plant "sacha anis" (*Tagetes filifolia Lag*.) belongs to the Asteraceae family, this annual species is native to Central and South America, can reach up to forty centimeters in height. With respect to its resistance in adverse conditions it has been proven that the minimum temperature range it can withstand ranges from -7 °C (20 °F) to -1 °C (30 °F).

The medicinal properties of anise are used mainly when there is stomach pain. The firming of the leaves or stem is used for nerves, weakness and cough. The cooking of the leaves is usually used to give baths in general. Although it is also advisable to ingest it or in rub, in order to lower the fever and remove chills. It is recommended to use in colic, for children, flatulence and to eliminate the coldness, headache, spasm, heartbeat and bad air.

Samples of plant material are collected at the chosen time, may be during or after flowering. A complete sample of leaves, flowers, stems and roots is obtained, allowed to air dry and leaves, stems and flowers are separated, taking them to a drying chamber until having a constant weight. If necessary, the plants are crushed with a mill, although grinding can be carried by hand.

A series of physicochemical tests were carried out, which allowed us to know the composition of the plant as its humidity, determination of ash, nutrients and metals present in “sacha anis”.

In the tests of humidity it was possible to determine that the drying is optimal because the plant started with a humidity of 78.26% and at the end of drying we obtained 10.13%.

The ashes give a mineral content of the plant. Its determination is important because mineral matter may be responsible for some pharmacological action. 5g of sample was taken and calcined at 400 °C for 3 hours and dissolved in hydrochloric acid (1:9), from this solution was taken 1ml and dissolved in 100ml of HCl (1:9) to reduce the ash concentration.

Finally, the analytical determination of metals was performed, which was satisfactory, by atomic absorption spectroscopy. The sample was examined for the presence of sodium (Na), potassium (K), calcium (Ca), iron (Fe), zinc (Zn), magnesium (Mg) and phosphorus (P). Of which potassium predominates with 5,723 g / L in the sample analyzed.

Keywords: Aches, humidity, atomic absorption spectroscopy, mineral

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BIOCONTROL ACTIVITY OF Annona reticulata ETHANOL EXTRACT AGAINST *Corythucha gossyppi* INSECT PEST

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PPEE 21

Corythucha gossypii is a serious pest affecting over 24 hosts including ornamental, wild, and commercially important plants [1, 2]. No botanical pesticides have been reported for its control. For lace bug control insecticides are commonly used, such as neonicotonoids and methyl carbamates with long residual effect [3]. In the present study *A. Reticultata* ethanol extract was evaluated as a biological insect-pest control against *Corythucha gossypii*. Extract was obtained by passive maceration of ground and dried material at room temperature. Ethanol was then used for extraction as a solvent at a 1:4 sample-solvent ratio with constant agitation for a week [4]. Brine shrimp lethality bioassay based on McLaughlin was employed with some modifications [5]. An in vitro model was implemented with *Corythucha gossypii*. Brine shrimp lethality assay evidenced active compounds presented a median lethal concentration of 0,0672, 0,049 and 0,0716 µg/mL. In addition, for insecticide assay a mortality percentage of 13.33% at 10 µg/mL after 24 h was observed. Chemical characterization studies revealed the main active metabolites contributing to extract activity were acetogenins and isoquinoline alkaloids.

Keywords: Acetogenins, Biocontrol, *Corythucha gossypii, Annona reticulata.*

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CITOTOXIC EVALUATION OF THE EXTRACT OF *Justicia spicigera* ON THE CELL LINE OF BREAST CANCER MDA-MB-231

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Cancer is the cause of millions of deaths globally, it originates when cells in some part of the body start to grow in an uncontrolled way. There are different types of cancer, among them the breast cancer that is the accelerated, disordered and uncontrolled proliferation of the cells of the tissues of the mammary gland, cells with mutated genes, which act normally suppressing or stimulating the continuity of the cellular cycle. At present, new therapeutic options are being sought against this disease, although many of them have a high cost and are aggressive, as is the case of chemotherapy. An alternative that could help the treatment of breast cancer is the use of natural compounds. Plants are a source of medicinal drugs that could be harnessed for clinical use in order to counteract many diseases. Since ancient times man has used plants for the treatment of cancer. *Justicia spicigera* (muitle), a native plant in Mexico and attributed various medicinal properties, including antitumor properties, is a good element in the search for alternative treatments that have more or equal antitumor activity to the anti-cancer agents currently employed, and Possibly with the generation of minor side effects. For this reason, in this work is presented as an anticancer alternative to the plant *Justice spicigera*, which according to the literature has important antitumor pharmacological activity. Comparison of percent viability of the MTT assay in MDA-MB-231 cells interacted for 24 hours with extract of Justicia spicigera and paclitaxel

According to our first results, an increase in concentration of the positive control paclitaxel exerts a greater damage in the cells MDA-MB-231, since to compare the percentages of viability of this against the extract of *Justicia spicigera*, it is possible to be observed that *Justice Spicigera* causes greater damage at the same concentrations

Keywords: Breast cancer, *Justicia spicigera*

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CYTOTOXICITY OF METHANOL EXTRACTS OF MEXICAN MEDICINAL PLANTS TOWARDS HUMAN COLON CANCER CELL LINE

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One of the diseases that represent a big challenge for medicine is cancer, which is the third cause of death in Mexico and the second worldwide. Nowadays, the treatments used for this disease, like chemotherapy with synthetic drugs, radiotherapy and surgeries, are not an effective solution at all, can be expensive, inefficient, toxic and induce side effects in the patient, like immunosuppression, hepatic and renal damage, heart and pulmonary problems, as well as psychological and emotional problems, among others. Recent researches aim in discover of new metabolites to treat cancer. The use of natural products, particularly from plants, are an alternative healing modality that has been proposed for the prevention and treatment of cancer. Plants contains secondary metabolites that are pharmacologically important. These natural compounds obtained from plants has been used in many countries as traditional medicine. The aim of this work was to evaluate the toxicity and cytotoxicity activity of the methanolic extract of Croton lechleri, Castela texana, Borrichia frutescens, Salvia divinorum and Humulus lupulus. The preferred method to test the natural compounds toxicity is the assay with Artemia salina, that has been standardized globally. In this study, the methanolic extract of C. lechleri, C. texana, B. frutescens, S. divinorum and H. lupulus were performed by the assay with A. salina. Our results showed that only H. lupulus has a DL50 of 365.83 µg/ml. Cytotoxic assays were performed on HTB-38 human cancer cell line (colorectal) using the MTT method. The five methanolic extracts were tested by this method, having a survival rate of 37%, 35%, 18%, 17% and 15% respectively. Our results provided new evidence for anticancer activities of these plants which could be useful for developing new anticancer therapies.

THE WAYUU PHARMACOPOEIA AND ITS IMPORTANCE IN THE PREVENTION, RELIEF AND CURE OF THE PAIN

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The Wayuu Pharmacopoeia, has been used traditionally by the Wayuu in the prevention and cure of their diseases. The Piaches (Ouutsü and Ouutshi) have an important role in this process, since they have the ability to transit between the physical and the spiritual world through their "altered state of consciousness," invoking allied spirits who reveal the Patient's disease, plants that cure the disease, sites where they are found, preparation and application of the plant (Perrin, 1982; Rosado, 2009; Rosado & Ramírez, 2017). The aim of this research was to identify the plants used by the Wayuu in the prevention and cure of pain in order to motivate the scientists of the area to carry out phytochemical studies that serve as a basis for validating their effects on the mitigation of pain in the future. Structured surveys were carried out on Piaches (Ouutsü and Ouutsi) and Yerbateras Wayuu settled in the municipalities of Riohacha, Maicao, Uribia and Manaure, obtaining information on the medicinal plants used in the cure and prevention of diseases. The information collected was tabulated, selecting those plants that use against pain, emphasizing the name of the plant, parts used, preparation and application. We then proceeded to determine the kind of pain, family, species and gender associated with this symptomatology. In the Wayuu Pharmacopoeia, 150 medicinal plants are used related to 175 diseases. Of these, 65 species (43%) use them to counteract 17 kinds of pain. The pains with the highest number of associated species were: Stomach pain (30), head (17), body (11), toothache (10) and belly pain (9). There are 35 families that cover 57 gender, with the highest number of species: Euphorbiaceae (6), Caesalpiniaceae (5) and Malvaceae, Cactaceae and Verbemeceae with 3 species. The gender that reached the highest percentage were: *Lippia alba* (15.4%), *Croton malambo* (9.2%), *Castile erecta* (7.7%) and *Prosopis juliflora* (7.7%). There is a great biodiversity of medicinal species reported in Wayuu pharmacopoeias and used in the prevention, relief and cure of pain that should be the reason for future research in the phytochemical and pharmacological field, many of them are the pharmacochemical and pharmacochemical studies to define Su Biological activity, others have not been studied; Therefore, this research contributes to reduce the gap as it relates to the symptomatology of pain.

Keywords: Wayuu, pharmacopoeia, medicinal plants, pain.

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EFFECT ARISTOTELIA CHILENSIS EXTRACT ON FEMALE REPRODUCTIVE TRACT TUMOR CELLS

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Chilean maqui (*Aristotelia chilensis*) is an evergreen tree whose habitat ranges from Coquimbo to Chiloe. Many handicrafts and musical instruments are made of its wood, and the fruits are edible. Moreover, *A. chilensis* has more total phenolic compounds and antioxidant capacity than other common berries **(1)**. It has been shown that some phenolic compounds have anti-breast cancer properties and prevent breast carcinogenesis **(2)**. Herein, we investigate the effect of Chilean maqui extracts in cell lines derived from cervical carcinoma and endometrial adenocarcinoma. Cervical cancer is the third most common cancer in women in the world and the fourth in mortality, and endometrial cancer is one of the most frequent gynecological cancers in postmenopausal women **(3)**. Maqui hydroethanolic extract was prepared with ethanol 85% from dehydrated fruits collected of the Bío Bío region in Chile. Then, the extract was rotary evaporated and resuspended in DMSO. HeLa (cervical cancer) and Ishikawa (endometrial cancer) cell lines were treated with 0, 5, 50 and 500 µg/mL of Chilean maqui extract for 48 hours and then cell viability was measured by MTS assay. Treatment with 5 µg/mL of extract did not show any effect in both cell lines, compared with cells without treatment; however, when cells were treated with 50 µg/mL, a decrease of cell viability at 25% was observed in Ishikawa cells. Furthermore, both cell lines treated with 500 µg/mL of maqui extract showed a decrease of cell viability at 45%. These results suggest that *A. chilensis* extract have antitumor effect in female reproductive tract cancer enhancing its applications in biomedicine.

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Keywords: *Aristotelia chilensis*, Cancer, Cell Viability, Female reproductive tract

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ANALYSIS OF THE ESSENTIAL OIL OF *Myrteola phylicoides* (BENTH.)

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This research is part of an interagency project between El Consejo de Sanadores de Saraguro “Hampiyachakkuna” (Saraguro Healers Council) and the Technical University of Loja (Universidad Técnica Particular de Loja), whose purpose is to study and validate the ancestral therapeutic resources used by the people Saraguro in the Southern Region of Ecuador.

The essential oil was obtained from the aerial part of the medicinal plant *Myrteola phylicoides* (Benth.) (Myrtaceae), known as white Romero the hill and is used by the Saraguro community to treat bad air. The sample was collected in the sector Patunada, San Lucas (2050 m) by members of the community Saraguro own and then transported to the UTPL for extraction of essential oil. The species in the databases consulted does not present previous phytochemical or pharmacological type [1].

To obtain the essential oil is carried out three different extractions of the material in the fresh state, through steam distillation using a Calverger equipment. The average yield of essential oil was obtained (0,148%). The mean values of the refractive index, density and polarimetry were (1.3830), (0.8844g/ml) and (-5.318), respectively. The identification of the components of the oil was carried out using a gas chromatograph model 6890N Network º6C System coupled with a mass spectrometer 5973 Inert and a flame ionization detector (GC-FID), the analysis will use a capillary column DB-5MS (30m, 0.25mm, 0.25µm). The sample is injected into a relationship: 10µl of oil and 990µl of dichloromethane, being able to identify 49 compounds being the majority; the α-pinene (26.94%), caryophyllene-E (21.93%) and the α-humulene (9.56%). The essential oil of Myrteola phylicoides is characterized by its content in monoterpenes and sesquiterpenes hydrogenated oils. The investigation will continue with the full oil identification and evaluation of its antibacterial activity. After the study is completed the results are socialized to the Saraguro community with the aim of establishing promising natural resources that can be used in a sustainable way in agro-industrial enterprises and/or be preserved or used in programs of rural tourism (eco-tourism) [2].

Keyword: *Myrteola phylicoides*, Essential oil, CG-MS, Ecuador

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PARTICIPATIVE ETHNOBOTANY: CONSERVATION AND LOCAL DEVELOPMENT AMONG RESIDENTS OF QUILOMBO DO CAMBURY, BRAZIL

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Studies on ethnobotany that use a participatory approach propose active involvement of local people in its various stages, in order to promote, among other things, local culture strengthening and their empowerment on decision-making about the use of resources available at their environment, aiming local development (Etkin and Ticktin, 2005). To develop an ethnobotanical survey at “Quilombo do Cambury” in Serra do Mar State Park - Picinguaba, Ubatuba, Brazil - with participation of its residents called "local partners"; and to produce potential conservation diagnosis of raised plant species. This project is being developed in two phases. In phase 1, courses have been offered to "local partners" about plants collection and ethnobotanical data. The partners, together with technical team, utilized ethnobotany methods and techniques to select and interview experts about various categories of plant use: construction, medicine, food, fuel, among others. Data of each plant are were noted on specially chips designed for this project, respective plant were collected and deposited in herbaria: Municipal-SP Herbarium (PMSP), and on herbaria: Forestry Institute (SPSF). In phase 2, potential conservation diagnosis of plants (the ones collected in Phase 1) will be performed by calculating the Conservation Priority Index (CPI), associated with ecological and phenological data, as well as bibliographic data of each plant conservation status. Local collaborators were trained on anthropology methods for interviews and botany, aiming at collecting the plants indicated during the interviews. During 45 days of fieldwork, seven specialists have been interviewed by the three “local partners” and have indicated 147 plants for 177 uses. For medication it was cited 62 plants; 50 for food/ spices; 33 for handicraft; 21 for construction; among others. Some plants are used for more than one indication, as it is the case of some palms which they eat the fruit and the apical meristem, use the bract for handicraft and the wood and leaves for construction. Moreover, such data are being used for the production of booklet and an audiovisual documentar (available on youtube: “Herança Quilombola”), as well as on themed trails construction, contributing to tourism activity. The development of this study will contribute to advancement of ethnobotany research, promoting participation of local inhabitants in the registration of their own knowledge; above all, it will bring progress to ethnobotanic methods that aim conservation and local development, since these have been one of the focus of current studies in this knowledge area.

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Keywords: Ethnobotany, conservation, local development, traditional knowledge.

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ETHNOBOTANICAL STUDY OF MEDICINAL PLANTS IN ISLA GRANDE, CARTAGENA-COLOMBIA

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PPEE 29

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Isla Grande is one of the 28 islands belonging to the Islas del Rosario archipelago, with different tropical dry forest ecosystems and mangrove forest. Its Afro-descendant population makes use of these natural resources as a fundamental element of their traditional medical system due to the lack of primary health care. According to data from the World Health Organization, more than 80% of the world population uses ethnobotany as a fundamental tool for the use of plants as a therapeutic alternative [1, 2]. The objective of this study is to know the traditional use of the medicinal plants of Isla Grande. An identification of the main plants used by the region's experts was carried out through guides illustrated with the vegetation present in the island, accompanied with interviews the traditional use of these species was investigated, validated by the Caribbean vegetable pharmacopoeia of TRAMIL [3]. A total of 128 species were identified, 35 plants were reported with medicinal use, within 21 families where *BIGNONIACEAE, EUPHORBIACEAE, AMARANTHACEAE* and *FABACEAE* are the most representative in this study, only 12 species reported the same use of the pharmacopoeia, for example, the Paico (*Chenopodium ambrosioides*) reported as antiparasitic and the Papaya (*Carica papaya*) reported in problems of skin grains and White brush (*Sida rhombifolia*) with healing effects. This work contributed to the validation of information on the use of traditional medicine and, in turn, valuation of natural resources and biodiversity in the Caribbean islands of Colombia.

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Keywords : Isla Grande, Medicinal plants, Traditional medical

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TRYPANOCIDAL EFFECT OF PLANT EXTRACTS AGAINST *Trypanosoma cruzi* AND INDUCTION OF CYTOKINE PRODUCTION IN CD8+ T CELLS

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PPEE 30

Chagas disease (ChD), caused by the protozoan parasite *Trypanosoma cruzi*, is an important cause of mortality and morbidity, and a health problem in the worldwide [1, 2]. Actually, there are two nitroheterocyclic compounds for treatment of ChD (nifurtimox and benznidazole), they not approved by the FDA. Indeed, both compounds are toxic and its efficacy is still a matter of debate [3]. Looking for alternative treatment for ChD, trypanocidal and cytotoxic effect of fifteen ethanolic plant extracts were evaluate against epimastigotes and trypomastigotes forms of *T. cruzi*, their immunomodulatory effects in the interferon gamma (IFN-γ) and tumor necrosis factor alpha (TNF-a) production on CD8+ T cells from healthy donors (HDs). The extracts of plant were processed and dissolved in 1% dimethylsulfoxide until use. To evaluate the trypanocidal and cytotoxic activity of total ethanolic extracts on epimastigotes and trypomastigotes of *T. cruzi* or peripheral blood mononuclear cells (PBMCs) obtained from HDs were treated with a range of decreasing concentrations of plant extracts. Assays were tested in triplicate, in three independent experiments and the half maximal inhibitory concentration (IC50) for parasites, as well as the half-maximal cytotoxic concentration (CC50) for PBMCs were calculated using a non-linear regression curve fit with a sigmoidal dose-response curve with variable slope model. In addition, it was calculated the selective index (SI) by determining the ratio of the IC50 values to the CC50 values, as previously described [4]. To assess the ability of extract to induce the IFN-g and TNF-a production in CD8+ T cells from HDs, PBMCs were stained with antibodies to identified cytokine production in CD8+ T cells, in presence of ethanolic extracts or 1% DMSO [5]. All plant extracts demonstrated an inhibitory effect on the parasite growth, but *A. vacciniaefolia*, *A. muricata*, and *C. fimbriata* extracts were the most effective against epimastigotes forms, with a IC50 less than 100 mg/mL. Then, when the effect of ethanolic extracts in PBMCs from HDs were determined, it was observed that *A. vacciniaefolia*, *C. fimbriata*, and *S. sessiliflora* ethanolic extracts had a CC50 higher than 250 mg/mL. Given these results, it was evaluated the degree of selectivity of these extracts, shown a SI higher than 3 value to *A. vacciniaefolia*, *C. fimbriata*, and *S. sessiliflora* ethanolic extracts. Additionally, it was observed a high inhibitory capacity for *C. fimbriata* extract against trypomastigotes with a low IC50 (42.9 mg/mL) compared with *A. vacciniaefolia* and *S. sessiliflora* extracts. Subsequently, it was evaluated the frequency of CD8+ T cells producing IFN-g or TNF-a in presence of ethanolic extracts, and was found a high frequency of CD8+ T cells producing IFN-g and TNF-a with *S. sessiliflora* extract stimulation, but the *C. fimbriata* extract stimulation leads to the TNF-a production on CD8+ T cells, but not in the IFN-g production compared with cells cultured with DMSO. After *A. vacciniaefolia* extract stimulation, similar to the found in DMSO cultured cells, a low frequency of CD8+ T cells that producing both cytokines were found. These results suggest that the ethanolic extracts of *C. fimbriata*, and *S. sessiliflora* had a trypanocidal effect against *T. cruzi* and an induction of cytokine production in CD8+ T cells from HDs.

Keywords: Trypanocidal effect, *Trypanosoma cruzi*, Cytokine, Plant extracts

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CARNOSOL FROM *Lepechinia mutica* (BENTH.) EPLING: A PROMISING COMPOUND AGAINST *Pyricularia oryzae*

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Lepechinia mutica (Benth.) Epling (Lamiaceae), local name '*casa casa*'; is an endemic plant of Ecuador, the plants of the genus *Lepechinia* are used in folk medicine for the treatment of uterine tumors, stomach ailments, diabetes mellitus control and diarrhea; in particular, the leaves of *L. mutica* are used to treat headache and nervous affections1. In this study the leaves of *L. mutica* were collected in Quilanga, Loja-Ecuador, in September 2012. The plant was extracted with ethyl acetate, followed by methanol and methanol-water. Chromatographic fractionation of the EtOAc extract afforded a phenolic diterpene known as carnosol (**a**) and described for the first time in this species. The structure of (**a**) was established by X-ray analysis. The crystallographic data were the same as those reported in literature2: orthorhombic crystal. P2121; a = 15.762 (1), b = 13.757 (1), c = 7.7747(7) Å, *Z* = 4, *V* = 1688.2 Å3, and *R* = 0.031. The structure of (**a**) was also supported by the comparison of 1H-NMR, 13C-NMR, and ESI-MS data with those of literature3. The 13C-NMR spectrum indicated the presence of four methyl groups, four methylenes, two methines, one oxymethine, six aromatic carbons, two quaternary carbons and one ester carbon. The aromatic ring must be penta-substituted and one substituent was an isopropyl group, according to 1H-NMR.

Antifungal activity for (**a**) was measured as minimum inhibitory concentration (MIC) and minimum fungicidal concentration (MFC). Carnosol showed potent antifungal activity against *Pyricularia oryzae*. This fungus is responsible for the *'blast disease'*, the most important disease in rice cultures worldwide. The MIC and MFC values determined for carnosol against *P. oryzae* are very close to those of the reference pesticide flutriafol.

Keywords: Carnosol, *Lepechinia mutica*, Antifungal activity, Ecuador, *Pyricularia oryzae*.

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CHEMICAL STUDY OF THE ETHANOLIC EXTRACT OF WOOD OF *Oxandra longipetala* R. E.FR. (ANNONACEAE) AND EVALUATION OF ITS ANTIOXIDANT ACTIVITY

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Plants due to their chemical diversity possess a high bioactivity that has allowed the development of many drugs and in fact, the majority of drugs used clinically for the treatment of infectious agents are derived from natural products. There is great interest in the study of many vegetable families that present a high pharmacological potential1. Within which it is possible to emphasize to the family Annonaceae. The phytochemical study of *Oxandra longipetala* R.E. FR. wood allowed the isolation of the compound of name 2-Isopropyl-3,6-dimethoxy-5-methylphenol (Isoespintanol) corresponding to 15% by weight to the petroleum benzene sub-extract. The structure was established using 1H NMR, 13C NMR in 1D and 2D, As well as gas chromatography coupled to mass spectrometry and by comparison with bibliographic data2-3.

On the other hand, in the evaluation of the antioxidant activity the subextracts of dichloromethane and chloroform presented promising results with IC50 values 1.64 and 1.22 mg/L against the cationic radical ABTS+? And for the DPPH radical method? we found IC50 of 9.42 and 8.45 mg/L respectively.

Keywords: Annonaceae, Oxandra longipetala, Antioxidant.

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ANTINOCICEPTIVE ACTIVITY OF *Croton guatemalensis* Lotsy

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Croton guatemalensis Lotsy, popularly known as “copalchi” in Chiapas, Mexico, is used for the treatment of fever, abdominal pain and malaria. In Guatemala, it is valued as a remedy for chills and for treating rheumatism. The aim of this study was to evaluate whether aqueous extracts from the bark of *Croton guatemalensis* Lotsy possesses indeed antinociceptive properties.

The putative antinociceptive activity of extracts from *Croton guatemalensis* bark was assessed in this work in two different animal models of nociception, the acetic acid-induced writhing test and the hot plate model. To elucidate the mechanism of action from *Croton guatemalensis*, animals were pre-treated with naloxone (opioid receptor antagonist, 5 mg/kg, i.p.), atropine (muscarinic receptor antagonist, 2 mg/kg, i.p.), or glibenclamide (an ATP-sensitive K+ channel inhibitor, 2 mg/kg, i.p.).

The results of this study showed that intraperitoneal administration of this extract at the dose of 200 and 400 mg/kg, 30 min prior pain induction produced a significant dose-dependent antinociceptive effect in the acetic acid-induced writhing test but not in the hot-plate model. This effect was not reversed by naloxone, atropine or glibenclamide, suggesting that the endogenous system of opioid, muscarinic or ATP-sensitive K+, does not underlie the antinociceptive effects of the *Croton guatemalensis* Lotsy extract in the acetic acid-induced writhing test.

Our results indicate for the first time that aqueous extracts from *Croton guatemalensis* bark contain pharmacologically active constituents endowed with antinociceptive activity. It is suggested that cyclooxygenase inhibition might be at least partially involved in the antinociceptive effects of this extract. The above results justify its popular therapeutic use in treating clinical conditions associated with pain in humans.

Keywords: *Croton guatemalensis*; Antinociception; Acetic acid-induced writhing test; Hot plate test

PHYTOTHERAPY AND PATHOGENIC MECHANISMS

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The disease comes from general pathogenic mechanisms and specific alterations of tissues, organs or systems. Among the general pathogenic mechanisms are inflammation, oxidative stress, decreased vasodilatory action, alterations in cell differentiation, endothelial and epithelial damage, pathological cell migration, degenerated cell and tissue repair, capillary fragility and carcinogenesis. All organic tissues are intimately connected to inflammation, which is the innate defense system of the body for removing harmful stimuli and participates in the tissue healing response. Besides, sustained inflammation and other pathogenic factors and the corresponding regenerative healing response can induce the development of fibrosis, and eventually cancer. Oxidative stress is associated with the activation of inflammatory pathways, while chronic inflammation is found associated with some human cancers. Inflammation and cancer may be connected by the sequence of inflammation-fibrosis-cancer. In a second level of complexity are the general processes of organic or systemic damage such as immune deficiencies, kidney function, metabolic, hepatic, biliary excretion, digestive, elimination function, hemostasis, among others. Medicinal herbs display abilities in protecting the mammalian organisms compared to conventional drug therapies, as many herbal medicines have been shown as effective anti-inflammatory, anti-oxidative agents and many other anti-pathogenic actions. We review the relationship between substances present in medicinal herbs with its anti-pathogenic properties either inespecific or specific ones. Our purpose is to provide new insight into how medicinal plants works and its mechanisms in therapeutic strategies for diseases.

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ANTIFUNGAL COMPOUNDS FROM *Endlicheria oreocola* (Lauraceae)

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Anthracnose is a plant disease that causes great losses of crop production. In the case of tree tomato (*Solanum betaceum*) crops, the fungus that causes this disease is *Colletotrichum tamarilloi* (Damm et al., 2012). In this work a screening of antifungal activity against *Colletotrichm tamarilloi* of Laureceae species is carried out, as result we obtain that the ethanolic extract of the bark of *Endlicheria oreocola* showed one of the best inhibitory activities of this fungus growth.

The genus *Endlicheria* is a neotropical genus that has 60 species so far reported, most of which are found in the northern part of South America, and some others in different parts of Latin America, it is important to note that the highest concentration of Endlicheria species is located in the Amazon rainforest (Chanderbali, 2004).

Endlicheria oreocola bark extract was fractionated by vacuum liquid chromatography (CLV) from it obteined 11 total fractions. The phytochemical bioguided study of these fractions led to the isolation and characterization of the following compounds: Palmitic acid, Caryophyllene oxide, 1,5-epoxysalavial-4(14)-ene, 4(15)-eudesmene-1,6-diol, o-methylmoscatoline, and a mixture of sterols: campesterol, stigmasterol and ?-sitosterol.

The antifungal activity test against the fungus *Colletotrichum tamarilloi* was carried out by the microdilution method (Rashmi and Rajkumar, 2011). For *Endlicheria oreocola*, the sterol mixture and the stigmasterol pattern showed a MIC and IC50 equal to or close to that of Benomyl. Once the MIC was obtained, the minimum fungicide concentration (MFC) has been determinate (Meletiadis et al., 2007). From this test it showed that most compounds have a MIC equal a the MFC, except for the mixture of sterols and the Sesquiterpenoids.

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Keywords: Lauraceae, Endlicheria, Sesquiterpenoids, Palmitic acid, Sterols, Oxoaporphine alkaloid.

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POTENTIAL INHIBITORY OF COLOMBIAN PLANTS FOR THE CONTROL OF *Pseudomona aeruginosa*

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Infectious diseases cause 25% of global deaths, with 44% of cases in America continent, of which 40% correspond to new pathogens and 31% to antimicrobial resistant strains (1). The Pan American Health Organization has suggested establishing control and surveillance strategies to prevent the spread of microorganisms such as *P. aeruginosa*, a bacteria that survives in unfavorable conditions, grows in different environments and is resistant to most antiseptics and antibiotics. It is considered an important and frequent opportunistic pathogen, typically nosocomial, causing several infections in immunocompromised patients or with homeostatic problems (2). Between health care-associated infections, 8-10% are related to *P. aeruginosa*; being 13% multiresistant strains (3,4). This pathogen produces a mortality of 30-40%, mainly in the first 24 to 48 hours of its spread, especially in relation to lung disease and inadequate antimicrobial treatment (5). The work with natural products based on traditional knowledge is an effective method for the identification of medicinal plants and bioactive principles, which can be used as alternatives to conventional antibiotics (6). Colombia is a megadiverse country where few studies that evaluating the medicinal potential of its species have made, allows to propose multidisciplinary research aimed at finding molecules that can be used as alternatives for the treatment of *P. aeruginosa* infections. Therefore, the objective of this work was to determine the potential of plant species of the Colombian flora against *P. aeruginosa*. For this, were selected 113 ethanolic extracts from ethnopharmacological and phytochemical studies that were screened by HT-SPOTi and disk diffusion against P. aeruginosa ATCC 9027. The results obtained suggest that 35 species present promising activity to inhibit the growth of this bacteria, including 12 species commercialized in Colombian traditional medicine and 23 species of Colombian flora belonging to *Piper* (13) and *Zanthoxylum* (6) genus. The extracts of these species constitute a starting point for initiate biodirigid chemical studies, with the objective of isolating and identifying the active constituents against P. aeruginosa, which can subsequently be used for the development of new, more effective, selective and safer drugs, contributing to the current challenges facing medicinal chemistry.

Keywords: Medicinal plants, Antibacterial, *Pseudomona aeruginosa*, Ethnomedicine

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ETHNOBOTANICAL STUDIES IN TRADITIONAL COMMUNITIES IN NITERÓI MUNICIPALITY, RJ, BRAZIL

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Ethnobotany is the study of the relationship between humans and plants and the way those plants are used as resources. This science, through its interdisciplinarity, facilitates de dialogue between specialists and traditional people in hope of generating new forms of knowledge an new philosophical, ethical, epistemological and institutional demands, as well as provide useful information for the elaboration of pharmacological, phytochemical and agronomic studies about plants resources [1]. Biodiversity should not be understood just from biological concept, it might be considered as the result of local community practices which domesticates species and increases the local diversity. The tropical ecosystems face problems such as degradation, occupational patterns and how natural resources are explored [2]. Brazil presents one of the richest flora in the world, as well as estimated 4,5 million people belonging to different traditional groups, inserted in various biome. Amongst the Brazilian biodiversity, we find the Atlantic Forest, representing a great floristic richness of species. Advances in the anthropic urban-industrial actions has made it a critical issue for conservation in Brazil [3]. It`s estimated that only 7,5% remain of the original area occupied by the Atlantic Forest. Inserted in one of those areas we find the county of Niterói that makes home to seven traditional communities: Comunidade do Morro das Andorinhas; Sapê/Fazendinha; Comunidade do Engenho do Mato; Comunidade da Praia do Sossego; Pescadores Artesanais de Itaipú; Sitiantes da Serra da Tiririca; Comunidade Duna Grande.The native people from Nitetói, have been proving a large folk knowledge that must be investigate more deeply, especially about medicinal and food plants. Partial data shows among 68 % of 357 collected species was from food category and 32 % was from medicine uses. Little is known about the occupational process, history and ways of living on these communities. It is known though that they are under constant pressure because they are placed near conservational units and real estate speculation. The Laboratório de Botânica Econômica e Etnobotânica of Universidade Federal Fluminense seeks to investigate the history behind these communities and their knowledge by collecting data about local species and their traditional use. The studies being developed will contribute for the register of traditional knowledge, for recognizing these individuals as traditional populations as well as helping those individuals to maintain their traditionally occupied sites. These communities detain great understanding about the vegetation in which they are inserted showing promising results, especially when concerning medicinal and alimentation purposes, where we can find the most representative species.

Keywords: Traditional knowledge, traditional communities, Atlantic forest, applied botany

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ANTIBACTERIAL ACTIVITY OF ETHANOLIC EXTRACT OF *Artocarpus altilis* LEAVES

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Colombia is extremely rich in biodiversity and shows a great variety of plants to which are empirically attributed medicinal properties. The Breadfruit (*Artocarpus altilis* (Parkinson) Fosberg 1941), is a tree widely spread on America and produces many specialized compounds (secondary metabolites) of pharmaceutical interest[1]. In order to develop drugs at the future for fighting against human pathogens based on bioprospecting, the antibacterial activity of ethanolic extracts obtained from breadfruit leaves were tested on Gram negative bacteria strains (*Escherichia coli* ATCC 25922, *Klebsiella pneumoniae* ATCC 70503 and *Pseudomonas aeruginosa* ATCC 27853) and Gram-positive strains (methicillin resistant *Staphylococcus aureus* ATCC 43300) by using microdilution methodology[2]. Then, the leaves were harvested, dried, grounded and mixture with ethanol in a ratio of 1:3; afterwards several colorimetric, chromatographic techniques and foam action tests were performed to determine the groups of secondary metabolites and the phytochemical components by using TLC and GC-MS. The results show the presence of compounds such as: 9, 12, 15-octadecatrienoic acid, linoleic acid Methyl ester, Phytol and hexadecanoic acid. Furthermore, the ethanolic extract from *A. altilis* shows a differential inhibitory effect among Gram-negative bacteria and Gram-positive bacteria, exhibiting the highest percentages of inhibition to *E. coli* and *P. aeruginosa* with 65,43 and 57,02, respectively; and the lowest percentages of inhibition to *K. pneumoniae* and *S. aureus* with 15.25 and 35.06, respectively. The final analysis corroborates differences statiscally significant to all treatments in comparison with controls. In addition, the susceptibility of the bacteria strains to *A. altilis* ethanolic extracts were observed, demonstrating the potential of the secondary metabolites produced by this tree for the treatment of infections caused by these bacteria at the future[3].

Keywords: *Artocarpus altilis*, Antibacterial activity, Secondary metabolite, Phytol.

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THE ANTIDIABETIC PRINCIPLE FROM ECUADORIAN PLANT *Clinopodium taxifolium* (Lamiaceae)

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Clinopodium taxifolium (Kunth) Govaerts is a small tree widely distributed in the southern of Ecuador, It is known with the names of "cerro del inca", "culantrillo de cerro", "romero" "cerro del campo" (De la Torre et al., 2008). The species is used traditionally in the folk medicine to treat internal inflammations, stomach pain, malaria and cough. The diabetes is a serious health problem in Ecuador, representing one of the more important causes for diseases in our population. In our continuing search for plants with antidiabetic properties (Torres et al, 2016), the aim of this study was to identify the bioactive metabolites of *Clinopodium taxifolium* on the α-glucosidase inhibitory activity, which is an important assay to find hypoglycemic compounds. The dry leaves of the plant were macerated with solvents of increasing polarity, n-hexane, ethyl acetate and methanol. Each one of these extracts were submitted to column chromatography according to the best conditions found by TLC. From the hexane extract was isolated the carvacrol, a monoterpene with recognized antimicrobial activity, the squalene was also isolated from the same extract. The fractionation of the ethyl acetate extract afforded the triterpenes uvaol, erytrodiol, and ursolic acid, and from the methanol extract the flavonoid salvigenin. Hypoglycemic activity-guided separation of the extracts using the enzymatic assay with the α-glucosidasa was realized. The excellent results obtained with ursolic acid, were consistent with the values of the ethyl acetate extract from which was isolated this compound. Ursolic acid (3-beta-hydroxy-urs-12-en-28-oic acid), is a natural pentacyclic triterpenoid carboxylic acid and is well known for its biological effects, such as antioxidant, anti-inflammatory, anticancer, as well as the ability to induce apoptosis (Meng et al., 2012). Previous reports in the literature indicate the antidiabetic activity of this ubiquitous triterpene (He et al., 2015)

Keywords: *Clinopodium taxifolium*, Diabetes, Ursolic acid, Ecuador

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PHYTOCHEMICAL PROSPECTING AND EVALUATION OF BIOLOGICAL ACTIVITY OF LEAF EXTRACTS OF *Hyptis dilatata* BENTH

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The species *Hyptis dilatata* Benth belongs to the family Lamiaceae, composed of herbs and shrubs consisting of approximately 400 species. It has as popular synonym: mint of the field is used in folk medicine for the treatment of diarrhea, infections and skin ulcers, coughs, expectorant, cold and other inflammatory processes. The purpose of this study was to determine the phytochemical profile, as well as the biological activity front of fungi and Gram-positive and negative bacteria, the leaf extract of *H. dilatata*, in different conditions of air humidity (dry and rainy period). The fresh leaf extract was extracted using solvents hexane and ethanol, with filtration and the filtrate, periodical gathering in Soxhlet apparatus. From the extracts, the route of detection of the chemical constituents was carefully carried out. Were identified in the etanolic and hexanic extracts of the leaves in the rainy season (catechins and coumarins) and dry (flavones, flavanols, flavanones, flavanonols and xanthones). Condensed tannins, phenols and saponins were found in all extracts from the dry and rainy season. In the evaluation of the biological activity on yeast *Candida albicans*, the hexanic extracts of the dry and rainy periods presented IC50 22.5 µg/mL and IC50 136.5 µg/mL and the ethanolic extracts of the dry and rainy periods presented IC50 14.1 µg/mL and IC50 72.6 µg/mL, respectively. About the bacteria *Staphylococcus aureus*, etanólicos extracts of dry and wet periods presented IC50 161.4 µg/mL and IC50 58.5 µg/mL. Hexanic extract of the rainy and dry periods presented in *Salmonella typhimurium* IC50 43.4 µg/mL, *Bacillus cereus* IC50 101.1 µg/mL and *Citrobacter freundii* IC50 130.4 µg/mL. Thus, *H. dilatat*a is a candidate species for bioguided studies because it shows good activity regarding the inhibition of bacteria, aiming quantitative investigations, as well as isolation and structural elucidation, of the active substances.

Keywords: *Hyptis dilatata*; Phytochemistry; Bacteria.

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PHYTOCHEMICAL ANALYISIS AND MICROPROPAGATION OF A NATIVE BLUEBERRY (*Vaccinium consanguineun*) FROM COSTA RICA

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Wild species of cranberry in Costa Rica produce fruits comparable in color and size to imported fruits (Jiménez-Bonilla and Abdelnour-Esquivel 2013). In the absence of information on fruit nutritional and antioxidant qualities, Jimenez-Bonilla and Abdelnour-Esquivel (2013), through the ORAC chemical analysis , determined their antioxidant capacity that ranged from 545.12 to 676.19µM Trolox Equivalent to g / dry sample), indices greater than those reported for commercial blueberries (94 and 92 µM of Trolox equivalent / g fresh sample) (INKANATURAL 2008), and values ??reported for plum (73), blackberry (53), raspberry 48), apple (43) and orange (18). A preliminary phytochemical analysis of leaves and fruits was carried out by means of the formation of precipitates and colorimetric reactions to determine the presence or absence of useful secondary metabolites in the prevention of multiple diseases Associated to the oxidative processes, showing presence of flavonoids, leucoantocianidinas, triterpenes, steroids, and saponins only in the leaves. The antioxidant activity of the crude extract of fruits and leaves was determined by the DPPH test, obtaining an EC50 of 293.90 and 7.10 ug / mL, respectively. From the crude fruit extract a simple syrup was prepared for human consumption. These results show the usefulness of the chemical and agronomic characteristics of this wild species for the establishment of crops because they are species well adapted to the highlands of our country that allow a rational use of our natural resources as a source of regional and national development . An alternative is micropropagation, a technique that allows massive clonal multiplication and rescue of improved and wild varieties with desirable characteristics (George 2008). It has been possible to establish in vitro field material with the use of immersions in enzymatic soap (5 ml.l-1), sodium hypochlorite (3% ia), for the sprouting and multiplication of the established material a thermal shock was applied at 5ºC For 15 days, using the WPM medium with 120 gl-1 sucrose and 0.1 mgl-1 Z. Subsequently, the materials were transferred to liquid WPM medium supplemented with 30 gl-1 sucrose and 0.1 mgl-1 of Z with filter paper bridge, which reduced the oxidation of the explants and improved the nutritional conditions of the culture being reflected In higher growth and better appearance of the outbreaks.

Keywords: Flavonoides, arándano, antioxidante, *Vaccinium consanguineum*

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EVALUATION OF THE ANTIMICROBIAL POTENTIAL OF EXTRACTS OF PLANTS AGAINST *Staphylococcus aureus*, ORIENTED TOWARDS THE SEARCH FOR ALTERNATIVES FOR BACTERIAL CONJUNCTIVITIS

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Infectious diseases are a global problem that affects public health, its persistence is increasingly common because of the resistance that present microorganisms to commercial antibiotics (1). Within the most common ocular infectious diseases, is bacterial conjunctivitis reaching is present in 65% of consultations in countries such as the United States (2). Conjunctivitis is inflammation or infection of the conjunctiva that can have different etiologic as bacteria, viruses, fungi and parasites agents. Among the most common bacteria associated with this infection is *Staphylococcus epidermidis* (48.46%) and *Staphylococcus aureus* (35.38%), being this genre which has presented a greater resistance to antibiotics such as oxacillin and Methicillin, traditionally used for the control of infection (3). Therefore, this study evaluated the antimicrobial potential of four plant extracts (Belladonna, Calendula, basil, annatto and annatto fruit) (*Atropa belladona, Calendula officinalis, Ocimum basilicum, Bixa Orellana*) against *S. aureus.* For which we selected the four plants most used in traditional medicine for the treatment of conjunctivitis and without previous studies of antimicrobial activity. Subsequently, the respective ethanol by cold maceration extracts (4) were obtained and the antimicrobial potential against *S. aureus* (ATCC 6538) was evaluated by the disc diffusion and dilution in tube technique, as well as evaluate commercial antibiotics susceptibility. In this way (5), found that oxytetracycline and ciprofloxacin are antibiotics that present greater zone of inhibition with an average of 2.9 cm and 2,7 cm respectively and was determined that extracts of Marigold and Basil showed inhibitory effect against the evaluated strain introducing halos of inhibition of 1.97 cm and 1.52 cm, respectively. Additionally by the dilution in tube technique of determined that extracts had a value of minimum inhibitory concentration (MIC) of 7.5 mg/mL for both extracts and that commercial antibiotics had an MIC of 2 mg/mL value. This work constitutes the basis of future research aimed at the development of Bioproducts for ocular use that can be considered as an alternative in the treatment of eye infections caused by *S. aureus.*

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PAPAYA CARICA LEAVES AND GINGIVITIS REDUCTION BY PLATE

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Leaves of carica papaya are very effective in plaque reduction, bacterial. The applied experimental scientific research was carried out in Educational Institution Pitágoras of Puente Piedra Lima - Peru, 2016. Considering the clinical effectiveness of papaya leaves rinsing in the treatment of plaque - associated gingivitis in children aged 6 to 8 years of the Educational Institution Pitágoras de Zapallal - Puente Piedra, it is concluded that the rinsing Elaborated from the papaya leaf after used by the child, manages to heal the gingivitis present. Take into account the results, to use hygiene papaya leaf rinse Oral cavity of the children, being able to completely improve its gingival process and therefore its quality of life, for a sustainable development in the places of low economic level.

Regarding bleeding, the total number of participants (88) did not present this sign in the first and second controls. Regarding the color of the gingiva in the first control, the total number of participants (88) was red, and in the second pink control. Regarding the consistency of the gingiva in the first control, the total number of participants (88) presented soft consistency and in the second control firm consistency. It was appreciated that in the first control the group presented diminished signs, and in the second control they were healthy. The general CONCLUSION was reached: considering the clinical effectiveness of papaya leaves rinsing in the treatment of plaque - associated gingivitis in children aged 6 to 8 years of the Educational Institution Pitágoras de Zapallal - Puente Piedra, it is concluded that the rinsing Elaborated from the papaya leaf after used by the child, manages to heal the gingivitis present.

Keywords: *Carica papaya* leaves, gingivitis by plate

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CHEMICAL CONSTITUENTS OF MEDICINAL PLANTS USED IN THE COMMUNITY SARAGURO, ECUADOR

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PPEE 44

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Plants are fundamental part of the health system in ethnic groups living in Ecuador. Especially in Saraguro community [1]. Nevertheless many of these plants do not have chemical studies and are used without consider the possibilities of toxic compounds. In a research project, financially supported by the Ecuador government (SENESCYT), a group of plants used by the Saraguro population with different medicinal uses, were validated. All the plants included in this study were submitted to toxicological evaluation in animals' models to identify signs of possible toxicity of these species. None of the included plants, *Oreocallis grandiflora* (Proteaceae), *Bejaria resinosa* (Ericaceae), *Maclania rupestris* (Ericaceae), *Otholobium mexicanum* (Fabaceae), *Rubus urticiflius (*Rosaceae*)*, and *Geranium diffusum* (Geraniaceae), showed toxicity at the evaluated doses. Each one of these species was phytochemically investigated to isolate and identify the major metabolites, which could be responsible for the medicinal activity claimed for the inhabitants of the Saraguro community. From *O. grandiflora* were isolated Beta-sitosterol, catequine, galocatequine, and one glucose disaccharide. From *B. resinosa*, triterpenes such as ursolic acid, alpha, and beta amyrin, taraxerol and the flavonoid quercitrin were identified [2]. *O. mexicanum* gave bakuchiol and 3-hydroxy bakuchiol as the major compounds [3], from *R. urtucifolius* eryodictiol and eryodictiol-5-O-glucosa and *M. rupestris* and *G. diffusum* yield maltose and hydrolysable tannins as the more important metabolites.

Several of these chemical constituents are considered as the bioactive compounds present in these species. A series of these known metabolites are recognized to have activity in the ailments or diseases claimed by the population. In this presentation will be shown the results of this interesting project.

Keywords*:* Ecuador, Saraguro comminity; medicinal plants; toxicity; metabolites.

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PHARMACOGNOSTIC AND PHYTOCHEMICAL EVALUATION OF OIL OBTAINED FROM THE SEEDS OF *Passiflora quadrangularis* L. (BADEA) CULTIVATED IN ECUADOR

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PPEE 45

Several species of the genus *Passiflora* are distributed all over South America, and many of these species are used in popular medicine, mainly as sedatives and tranquilizers [1]. The Badea, *Passiflora quadrangularis L.* also called "purple passionflower" is a climbing species of the family *Passifloraceae.* The name *quadrangularis* is for its stem with four sides of quadrangular type. This planta is originally from Ecuador, province of El Oro [2,3]. The use of fruit pulp has been limited mainly to its consumption like juices, baby foods, nectars and jellies [3]. The decoction of the leaves is used as a vermifuge and to treat skin afflictions like poultices. Tea leaves for high blood pressure and diabetes [2]. The pharmacognostic parameters obtained comply with the international criteria: residual moisture 5.8%, total ash 2.5%, insoluble ash 0.26%, and phytochemical screening was positive for: alkaloid, steroids and reducing sugars. The seeds oil extraction of Badea, was make using the soxhlet method with hexane like solvent. Its yield was 39.2% and the physicochemical analyzes showed a density of 0.96952 g/mL, acidity index 11.8%, saponification index 112.2, unsaponificable compounds 1.0006%, and refractive index 1.4591. The lipid profile by GC-MS analysis showed a high content of unsaturated fatty acids being linoleic acid with 77.07% and oleic acid 9.69%, the most abundant. These values are reported for the first time for the species and are similar to those reported for *P. pinnatistipula* [4] and *P. edulis* [5].

Keywords: *Passiflora quadrangularis*, pharmacognosy, seeds oil

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ANTIFUNGAL ACTIVITY OF EXTRACTS AND FRACTIONS OF PLANTS OF TRADITIONAL USE IN THE SIERRA NEVADA OF SANTA MARTA - COLOMBIA

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PPEE 46

Mycoses have had a significant increase in recent years and constitute a therapeutic challenge, due not only to the development of resistance but also to the emergence of new species that are not susceptible to the available treatments[1]. One important mycosis, mainly in tropical regions is sporotrichosis, which usually only compromises the skin and subcutaneous cellular tissue, while can cause disseminated infections[2]. The treatment of choice in developing countries is potassium iodide and secondly itraconazole. However, the adverse effects of the first, and the cost and resistance in some species to the second, limit their uses[1,3]. Natural products derived from plants are important sources of agents with different biological activities and potential uses. The indigenous ethnia of the Sierra Nevada de Santa Marta (SNSM) traditionally use plants for curative purposes[4]. Considering the need of new antifungal agents with potential for topical use, the aim of this work was to evaluate the antifungal activity of global extracts and fractions derived from different plants with ethnomedical antecedents. Global extracts (ethanolic or methanolic) and fractions derived from their fractional insolubilization or liquid/liquid extraction were obtained from *Piper peltatum*(4 samples); *Baccharis inamoena*(3), *Neurolaena lobata*(1), *Clibadium arboreum*(2) and *Castanedia santamertensis*(2) specimens collected in the SNSM (Colombia). The alcoholic extracts were treated with MeOH/CH2Cl2(1:20) to separate an insoluble fraction (that contain polar waxes), the another soluble. The latter was treated with MeOH/CH2Cl2(20:1) to separate the insoluble fraction (that contain non-polar waxes), from the another soluble fraction. Subsequently was evaluated the *in vitro* activity of the 12 samples against different yeasts(11) and filamentous fungi(13). In addition, 21 isolates of *Sporothrix schenckii* complex were evaluated with a fraction of *Clibadium arboreum* extract. The determination of the antifungal effect was carried out following the protocol of the European Committee for the evaluation of antifungal susceptibility (AFST-EUCAST)[5]. The extracts and fractions were evaluated at a concentration of 500 µg/mL and with a final inoculum of each microorganism of 0.5-2.5x10^5 CFU/mL. In cases where total inhibition of fungal growth was observed, the minimum inhibitory concentration (MIC) was determined. Test controls include *Candida krusei* ATCC 6258, *C. parapsilosis* ATCC 22019, *Aspergillus fumigatus* ATCC 204305 and *A. flavus* ATCC 204304 strains evaluated with itraconazole and amphotericin B. The activity of the samples varied among the strains. With yeasts(5), five samples were active (MIC ≤31.25-500 µg/mL). Only activity with two genera of filamentous fungi was observed: *Trichophyton interdigitale* (CMI value) and *S. schenckii* (31,25-500 µg/mL). One fraction of the *C. arboreum* extract showed a broad-spectrum activity. Of importance is the activity of this fraction against clinical isolates of *S. schenckii, sensu stricto* (MIC range ≤31.25-500 µg/mL) and *S. globosa* (≤31.25-250 µg/mL), because the structure of the wall of this genus has characteristics that may give indications on the possible target. In addition, the mycosis they cause is cutaneous/subcutaneous, so the application of a topical formulation prepared with this fraction could be feasible for clinical use. **Acknowledgments:** Financing from JCyL and MINECO, Spain (projects SA221U13 and AGL-2016-79813-C2-2-R, respectively), COLCIENCIAS and the FPIT of the Banco de la República, Colombia (projects No 111745921459 and 3756, respectively).

Keywords: Antifungal activity, plant extract, ethnomedical, mycoses

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COMPARISON BETWEEN CHROMATOGRAPHIC TECHNIQUES GC-µECD AND HPLC-DAD FOR THE QUANTIFICATION OF CEFEPIME IN URINE

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PPTC 01

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Today, many compounds of anthropic origin enter the environment because there are no regulations on its disposal, an example of this are β-lactam antibiotics (BATB). In this work, cefepime (CEP) was studied as a representative compound of BATB, which belongs to the family of fourth generation cephalosporins. Due to its broad spectrum of action against Gram-positive and Gram-negative bacteria, CEP is highly consumed at the hospitalary level. The antibiotic once administered and metabolized, is excreted through the urine in greater proportion (85%) without alterations and to a lesser extent in metabolized form. The excessive incorporation of CEP into the environment is a problem at the international level, since it generates an antimicrobial resistance cycle.

The objective of this work was to compare two chromatographic techniques, GC-µECD and HPLC-DAD, for the validation and quantification of CEP in urine matrix. In a first step, solid phase extraction was performed using cartridges with C18 resin, to extract the analyte from the matrix. The conditioning was performed with 10 mL of methanol and 10 mL of water, and then 50 mL of urine fortified with CEP (0.4 µg/mL) was charged. The resin was washed with 20 mL of water and the analyte eluted with 10 mL of methanol. Finally, it was brought to dryness under a nitrogen flow at 45°C and the sample was reconstituted in 2 mL of methanol. The urine samples were analyzed by GC-µECD, and confirmed by Direct Sample Analysis-Time of Flight-Mass Spectrometer (DSA-TOF-MS). In another part of the study, the analysis of CEP in aqueous matrix was carried out by HPLC-DAD. In all the techniques used, the operating conditions were optimized.

Due to the physicochemical characteristics of CEP, the results obtained by GC-µECD indicate that an adequate resolution of the analyte is not achieved, despite having tested different chromatographic conditions. Therefore, a derivatization step was required, for which an acylation was performed with MSTFA (N-Methyl-N-(trimethylsilyl) trifluoroacetamide), this compound provides a functional group reactive to the molecule, which has been shown to give good results in other BATB. In relation to the confirmation by DSA-TOF-MS analysis, the m/z of 86 was observed, which corresponds to N-methylpyrrolidine, the main metabolite of CEP. The results obtained by this technique, both in water and in urine, present a good linear correlation of the data with R2 of 0.999 and 0.995, respectively, in a linear concentration range of 7 to 57 µg/mL. In relation to the quantification of the analyte by HPLC-DAD, the results present a good linear correlation, with R2 of 0.999, in a concentration range of 0.5 to 201 µg/mL, with limits of detection and quantification of 0.13 and 0.48 µg/mL, respectively.

Through this study, it can be concluded that the techniques of lower complexity for the quantification of CEP in water and urine matrix are HPLC-DAD, and its confirmation through DSA-TOF-MS. The GC-µECD technique would allow to determine lower concentrations, but with the incorporation of an analyte derivatization step.

Keywords: Cefepime,Urine,HPLC-DAD,GC-µECD

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A VIRTUAL CHROMATOGRAPHY BASED ON SUPERVISED LEARNING FRAMEWORK

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PPTC 02

High-performance liquid chromatography (HPLC) is a technique in analytical chemistry widely used in different industrial sectors to obtain reliable information about the composition of a mixture. This technique separates, identifies and quantifies each component in a mixture based on different flow rates for the different components caused by the interaction of each one with an absorbent material in a pressurized column. Nevertheless, when the components are separated, the sample can no longer be analyzed by itself. Further, HPLC is a costly technique and requires knowing a standard solution to accomplish the separation what can be hard when the sample is complex [1].

Nowadays, the analytic measure techniques are looking for a sensible, precise and selective ways to do it in shorter operational times than classic methods. Important progress has been made with respect to the instrumentation used, such as coupled measurement systems, modified sensors, among others. On the other hand, the progress in computer sciences provide tools to achieve these objectives. Our proposal is a virtual chromatography based on machine learning techniques. This can be divided into two stages. The first stage consists of a set of selected electrochemical sensors regarding its molecular affinity to characterize the mixture behavior by voltammogram signals. The second stage involves three sub-stages: 1) voltammogram analysis by Fourier transform, voltammogram energy and derivate of signals, 2) a relevant analysis stage run out by KPCA methodology and 3) a supervised learning based stage to generate a function capable of estimating the components of a mixture using SVM classification [2]. As result, we obtained a system capable of estimating the components of a mixture in our database of products from the voltammogram signals collected by the electrochemical sensor set. To test our proposal, we used a set of 12 products with 12 principal components or attributes. We obtained promising results both good approximation to HPLC values about 3% k-fold cross-validation error rate and a significant decrease in time (about 10 minutes) with respect to HPLC methods (about 4 days depending on the machine). As a conclusion, this proposal provides an alternative way to classic chromatography techniques with comparable results opening the door to new methodologies in this field of chemistry[3].

Keywords: HPLC, Chromatography, KPCA, SMVs.

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CHROMATOGRAPHIC ANALYSIS OF THE ESSENTIAL OIL OF *Rosa centifolia* L. (Rosaceae) PETALS GROWN IN COLOMBIA

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PPTC 03

Rosa centifolia L. (Rosaceae) ecological cultivars produce good quality, highly appreciated worldwide essential oil, with notable biological properties. High quality rose essential oils are applied in pharmaceutic, cosmetologist and food industry. Promotion and development of certified organic orchards is one of the most important strategies in preservation and environmental conservation and to protect health and welfare of consumers. *R. centifolia* native from Asia known as "*May rose*" is very well recognized by its delicious fragance. Its essential oil is astringent, antiseptic, digestive and anti-inflammatory [1]. Previous work in this species, by Góra *et al*. [2], in polish cultivars and by Shabbir *et al.* with samples from Faisalabad (Pakistan) [3], reported yields for petals of 0.05 % and 0.23% with determination of 31 and 13 identified constituents, respectively [4].

In this work, essential oil was extracted by hydro-distillation from 4 Kg of fresh petals recently cut, and purified water by the Ecosmarte® method, with a yield of 0,17%. Ethereal extract by HRGC-MS was analyzed in HP-5 capillary column in 30 m fused silica, columns with the same temperature program (AR-8). According the chromatographic profiles more than sixty signals were detected and by application of chromatographic and spectrometric criteria was possible to detect the 95% of the constituents in relative amounts. For this genotype, the major compounds are 2-phenylethyl alcohol (27%), β-caryophillene, terpenols as geranyol, nerol, linalool 1,8-cyneol, rose oxide, citronellol and the linear hydrocarbons nonadecane (C-19, 8.2%) and heneicosene (C-21, 3%); terpenols are very important components for fragrance quality. Presence of methyl-eugenol (1.8%) is a decisive factor for the biological properties recognized for the *R. centifolia* essential oil [5]. This is the first report about the chemical composition of the *R. centifolia* petals organically cultivated in Colombia.

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AN IMPROVED ANALYTICAL METHOD FOR THE QUANTIFICATION OF ACRYLAMIDE IN FOOD USING A GAS CHROMATOGRAPHY - TANDEM MASS SPECTROMETRY (GC-MS/MS)

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PPTC 04

Acrylamide (2-propenamide, C3H5NO) is a neurotoxic compound considered as a probable human carcinogen substance which is formed during the processing and/or cooking some food by roasting or frying. A safe limit of 500 ng/mL acrylamide in drinking water have been set by The World Health Organization (WHO). However, higher levels over 500 ng/g are detected in some processed foods. Usually, acrylamide is present in a variety of cooked food and formed from carbohydrate-rich foods. Acrylamide is formed by the Maillard reactions between the non-essential amino acid, asparagine and glucose. Also acrylamide can be produced by acrylic acid and acrolein resulting from sugar and glycerol. The mechanism of formation of acrylamide that involved an amino acids and the reduction of a sugar has not well understood, yet. Determination of trace amount of acrylamide on processed food and foodstuff is not easy task because it is a complex matrix. Therefore, development of analytical method for quantitation of trace levels of acrylamide in food which have been baked or fried with accuracy, speed, and repeatability is urgently requested. Most of methods reported for the determination of acrylamide on food are based on derivatization step before the GC injection. Derivatization consists of substitution of acrylamide double bond with bromine atoms by potassium bromide or potassium bromate to produce 2,3-dibromopropionamide (2,3-C3H5Br2NO). Acrylamide is a polar substance soluble in water having a logP value of -0.65. Reported methods to determine acrylamide often require derivatization to improve the sensibility. In this case, acrylamide was injected without derivatization before injection on GC-MS/MS. Acrylamide method was developed to determination on potato chips. The potato chips were finely divided and 1 g was weighed into a vial. Sample was spiked with 10, 25, 50, 100, 250, 500, and 1000 ng/g of acrylamide standard in 2% formic acid / water. The sample was then filtered through a filter membrane. Evaporate methanolic extract and reconstitute with 1 mL of 1 µg/mL of internal standard in methanol to the SPE cartridge. The analysis of acrylamide was performed on a Gas Chromatography - Tandem Mass Spectrometry (GC-MS/MS) in the electron impact positive ionization mode (EI+) and multiple reaction monitoring (MRM) as acquisition mode. MRM was performed by monitoring transitions of 72 ¦ 55 m/z for acrylamide and 75¦ 58 m/z for 13C3-acrylamide. Determination was carried with a GC capillary column of 30 m × 0.25 mm × 0.25 µm with a stationary phase based on polyethylene-glycol. The method had a limit of detection of 5 ppb and the calibration curve was made for acrylamide on the matrix over the range of 10 -1000 ng/g. The coefficient of determination (R2) for the linearity of the method was 0.999. Accuracy of the method for 13C3-acrylamide used as spike isotope label internal standard was 90%.

HILIC-ESI-MS/MS METHOD FOR NITROGEN PRIMARY METABOLITES ANALYSIS

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PPTC 05

Nucleotides are some of the most important nitrogen primary metabolites. *De novo* synthesis of pyrimidines is one of the most relevant metabolic pathway that produce nucleotides. It starts with amino acids and other small molecules going through orotate (ORA) and dehydroorotate (DHO) and finalizing with uridine monophosphate (UMP) [1-3]. Regarding biochemistry of plants, there are some hypotheses showing that levels of nucleotides and its intermediaries vary when plants are affected by different biotic and abiotic process, such as infections, hydric stress among others. Based on the foregoing, the research goal is to develop an analytical method to analyze and quantify metabolites involved on *De novo* synthesis of pyrimidines in plant-pathogen interaction systems. To achieve this goal, we improved the methodology by using Hydrophilic Interaction Liquid Chromatography coupled to tandem Mass Spectrometry (HILIC-ESI-MS/MS). We used ZIC-HILIC column (3.5 µm, 2.1*150 mm) with gradient concentration of ammonium acetate and acetonitrile for the separation and detection of 13 intermediaries of pyrimidine pathway. A series of designed experiments were run to select a suitable condition of column temperature (25, 40 and 55°C) and concentration of additive (5, 10 and 15 mM) that produced higher sensibility for most compounds. The area of chromatographic peak was evaluated as a parameter to establish the most appropriate method for primary metabolite analysis. We gave special attention to ORA, DHO and UMP specific metabolites on this metabolic pathway. All variables and interactions were significant for ORA, DHO and UMP. According to the results, the chromatographic analysis of ORA and DHO reached higher areas for high temperature and low additive concentration, while UMP reached higher areas for low temperature and low additive concentration. In conclusion, the conditions HILIC-MS/MS tested allowed the separation and detection of nitrogen primary metabolites such as nucleotides, nucleosides, and organic acids and bases belonging to the pyrimidine pathways. Additionally, this method is useful to be applied in complex matrixes.

Keywords: HILIC, HPLC-MS/MS, Primary Metabolites, Nucleotides.

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ANALYSIS OF SYNTHETIC PEPTIDES BY HPLC: COMPARATIVE STUDY USING ELUTION GRADIENT, IN REVERSED PHASE AND HILIC MODES

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PPTC 06

Peptides are molecules of great interest in the field of health sciences by presenting biological activity, specifically as antimicrobial, antigens, biocatalysts, probes for biosensors, among others. Peptide chemical synthesis is a powerful tool; it allows obtaining molecules with non-natural modifications, which enhance the biological activities. In this context, analysis by RP-HPLC is fundamental for characterization of both crude and purified products [1-3]. In this context, different gradient analysis protocols were tested using a peptide derived from Protein L1-HPV (C-Ahx-SPINNTKPHEA) as model. Three columns were evaluated, two in reverse phase (RP) mode: Kromasil EternityXT 5-C18 (packed column) and Chromolith® HighResolution RP-18e (monolithic column) and one in HILIC mode: 60-5-HILIC-D (packed column). RP columns showed better profiles than the HILIC column, providing a higher resolution at the adjacent peaks in relation with the major peak. Additionally, the monolithic column, by having a one-piece stationary phase, provided the best chromatographic analysis for peptides.

Keywords: HPLC, Column, Monolithic, Resolution.

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GC-MS BASED METABOLOMICS ANALYSIS OF *Avena sativa* ROOT EXUDATES UNDER CADMIUM STRESS: PHYTOSIDEROPHORES ELUCIDATION

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PPTC 07

In this work, a gas chromatography mass spectrometry (GC-MS) based metabolomics analysis of Avena Sativa root exudates under cadmium (Cd) stress was proposed in order to elucidate some phytosiderophores that make possible the Cd mobility from plant growth medium to roots and leaves.

Oat seeds were manually scarified and then sterilized according to the next steps: NaClO, ethanol, NaClO, ethanol followed by washing and soaked in sterile distilled water and then placed into wet cotton in a petri dish. The seeds were kept in the dark at room temperature for 3 days. Sprouted seeds were transplanted into a Magenta growth box (width 77 mm x length 77 mm x height 97 mm) containing Agar and Murashige and Skoog medium. For heavy metal stress experiments, Cd concentration was fixed to 10 mg/L using 3CdSO4.8H2O solution during agar preparation. The oat plants grow in a made in house growth chamber with a 16/8h light/night regime. After two weeks, roots and leaves were sampled and used for measuring the amount of Cd and root exudates extraction. Ten biological replicates were grown for each treatment. Cd in roots and leaves samples was measured using microwave assisted digestion and atomic absorption spectrometer.

For exudates extraction, about 50 mg of roots were immersed in liquid nitrogen and then 2 mL methanol:water solution (80:20 v/v, 0.1 % in formic acid) were added and mechanically stirred. The solution was transferred to a new vial and blown until dried by using a gentle nitrogen flow. Ribitol and docosanol were used as internal standards and added after the mechanical agitation. Dried sample was reconstituted in n-hexane and derivatized by 40 µL methoxiamine (20 mg/mL in pyridine, 2h, 37 °C) and 70 µL N-methyl-N-trimethylsilytrifluoroacetamide w/1% trimethylchlorosilane (30 min, 37 °C). Derivatized samples were transferred to an amber 2 mL vial and used in GC-MS analysis. Into the GC (Agilent 7890A) 1 µL of the sample was inyected using a Rxi-5ms column (30 m x 250 µm, 0.25 µm film) for chromatographyc separation at a constant helium flow rate of 1mL/min. For detection an Agilent 5975C MSD was used and spectra recorded in full scan mode from m/z 50-600 with temperatures of source and quadrupole of 230 and 150 recpectively.

GC-MS data were statistically analyzed using Principal Component Analysis (PCA) and Partial Least Square Discriminant Analysis (PLS-DA). PCA was used in order to verify quality control samples (QCs) behaviour as a measure of instrumental variability and PLS-DA to construct the discriminant model using the variable importance in the projection (VIP) as a method of variable selection in order to explain differences in root exudates between control and Cd treated samples.

Root exudates were identified using the Golm Metabolome Database (GMD) and the results would facilitate the elucidation of the phytosiderophores mechanism that make possible the heavy metal absorption.

Keywords: Metabolomics, Phytosiderophores, Cd stress.

CHEMICAL COMPOSITION AND BIOLOGICAL POTENTIAL OF AN ECUATORIAN PROPOLIS SAMPLE

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PPTC 09

In this work one sample of ecuatorian propolis from Arenillas was studied. The chemical study allowed the identification of sugars, fatty acids, flavonoids and triterpenes in the propolis sample by gas chromatography coupled to mass spectrometry. The content of reducing substances was determined to be 51.76 mg EAG/g extract, using the Folin-Ciocalteu assay. The antimicrobial activity of the sample against Group A β-hemolytic Streptococcus, anti-inflammatory activity from the mouse TPA-induced atrial inflammation model and the inhibitory activity against L. amazonensis and cytotoxicity against peritoneal macrophages of BALB / c mice were also determinated. The ethanolic extract of propolis showed all the activities tested, which were supported by the suggested chemical composition.

Keywords: propolis, biological activity, antileishmania, antimicrobials.

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DEVELOPMENT AND VALIDATION OF SCREENING METHOD FOR THE ANALYSIS OF PESTICIDES RESIDUES IN FRUITS AND VEGETABLES BY GC-MS

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PPTC 10

Agriculture is one the most important sectors of Colombian economy, it´s geographic and climatic diversity allows the production of a grate variety of fruits and vegetables. Which ones have recently gained and important place in the international market, then it´s key the develop of analytical methodologies for pesticide residue analysis that produce reliable results in a short time to guarantee the quality of this products. Recently screening methods have proven to be a great alternative for the identification of pesticides residues, they offer the possibility of a fast identification of compounds pounds present in a sample without the requirement of quantitation. Most of the screening methods require the use of high cost instrumentation such as LC(GC)-HRMS and little research have been published for low budget laboratories. Then this study aims to develop a very efficient and reliable qualitative screening method for the analysis of pesticide residues in fruits and vegetables of high water content. The methodology was based on the European QuEChERS extraction method with and additional clean up step by Gel Permeation Chromatography (GPC). The analysis was carried out by gas chromatography coupled to mass spectrometry with a single quadrupole mass analyser in the selected ion monitoring mode (SIM). The method validation was based on SANTE/EU 2015 document and the European Commission Decision EU 657/2002 requirements. The parameters included in the validation were the selectivity, screening detection limit and the to me suitable applicability. The method proved to be suitable for the qualitative analysis of 31 pesticides currently used in Colombia at their respective maximum residue limits. The results of the screening methodology for the analysis of several contaminated samples were consistent with the results obtained by a routine quantitative methodology and the GPC clean up step help to reduce the amount of matrix compounds in the final extract improving the method selectivity and equipment performance.

Keywords: Pesticide, Screening, Qualitative, Validation

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DETECTION OF CHLORPYRIFOS IN MILK BY GAS CHROMATOGRAPHY AND THE USE OF AN AMPEROMETRIC ACETYLCHOLINESTERASE-BASED BIOSENSOR

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PPTC 11

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Chlorpyrifos is a commercial and organophosphorus insecticide, in Colombia its usage embraces different crops pasturelands and urban sites [1]. Chlorpyrifos works as an inhibitor of the enzyme acetylcholinesterase that produces accumulation of the neurotransmitter acetylcholine in the synapsis mediated by this molecule, both insects and mammals, affecting directly the central nervous system [2]. In the milky herds the misuse of the chlorpyrifos can produce milk with pesticides residues since it can enter to the animals through the mouth, the lungs or the skin, then it passes fastly from the intestine to the bloodstream, which distributes it to the rest of the body. Colombia is a country milk producer whose quantity in the 2015 was approximately three thousand eighty-six millions of liters [3]. Due this reason it is important the chlorpyrifos be monitored inside the milk to guarantee an innocuous product to the consumer. According to the World Health Organization the limit of concentration allowed of chlorpyrifos in the cow's milk is 0.02mg/L [4]. This works explores the usage of an enzymatic amperometric biosensor as a tool able to determine the presence of chlorpyrifos in the crow cow's milk, in comparison to the technique of gas chromatography. The enzyme Acetylcholinesterase was used as the biological element, that was inmobilized over electrods of different material as "screen printed" through the "cross linking" method. Kinetic constants of the free enzyme and the immobilized enzyme was determined. A prototype was developed that allows measurements of voltammetry on printed sensor, with characteristics of low cost, portability and easy operation. It was used for the quantification of the biochemical signal produced in the enzymatic reaction given on the electrode previously immobilized and used in the tests of inhibition and optimization of the biosensor. The validation of the technique for the detection of chlorpyrifos by gas chromatography resulted in the fact that this analytical technique meets the criteria of linearity, precision, accuracy and specificity for the quantification of trace values from 10 µg / L to 100 µg / L and that the method has a matrix effect. On the other hand, the technique of detection of chlorpyrifos in milk by the biosensor resulted in linearity in a concentration range of chlorpyrifos of 10 µg / L up to 30 µg / L, but this technique was not reproducible at these levels so low concentration, in addition, it was obtained that the technique is accurate, but does not meet the acceptance criteria for accuracy and specificity and a matrix effect is evidenced. It is concluded that the biosensor can serve as a qualitative technique for the pesticide detection in milk but not quantitative, for that reason the biosensors can be tools capable of detecting the presence of chlorpyrifos in milks in real time, it allows to reject in the same dairy herd milks that have presence of chlorpyrifos and for the quantification can be used a more robust technique like gas chromatography.

Keywords: Gas Chromatography, Chlorpyrifos, Validation, Biosensor.

CHEMICAL COMPOSITION OF ESSENTIAL OIL OF LEAVES OF *Senecio madagascariensis* (Asteraceae)

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PPTC 12

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Senecio madagascariensis is a plant species belonging to the family Asteraceae commonly known as yellow flower or guerrilla weeds. It is classified as toxic due to the chemical composition of its secondary metabolites and of high ecological impact since it displaces native species and upholstery the native grasslands ruining its productive use.

As for its chemical composition, the reported studies are scarce except for one performed by Gardner and co-workers [1] where different alkaloids were identified: seneciovernin, senecionine, integerrimine, senkirkine, mucronatinine and usaramine; As regards the composition of its volatile metabolites, there are no reports, which is why in the present work from fresh leaves of the species harvested in the municipality of Subachoque - Cundinamarca (04 ° 56 'N 55 ° 11"W) The essential oil was obtained by the technique of steam distillation; Its determination was made by Gas Chromatography coupled to mass spectrometry, comparison of retention index, mass spectra and data reported in the literature. The essential oil was obtained in 0.052% yield; In which 29 compounds were identified which constitute about 89.7% of the total composition, among which are 8 monoterpenes, 10 sesquiterpenes, 3 oxygenated sesquiterpenes, 1 ester, 1 aldehyde, 1 ketone, 1 carboxylic acid and 4 alcohols among which is the majority compound, which in this case corresponds to 1-nonanol (45.65%).

The monoterpenes found represent 27.37%, highlighting the presence of a- and b-pinene; The identified sesquiterpenes correspond to 12.47% of the total chemical composition of the oil where the caryophyllene and germacrene D are found as the components in the highest concentration of this group of compounds. In addition, three oxygenated sesquiterpenes were identified: espatulenol, epiglobulol and caryophyllene oxide, which represent only 0.87%. Other carbonyl compounds such as acids, esters, aldehydes and ketones represent 1.18% and some alcohols corresponding to 47.67%.

The present study is a contribution to the phytochemical investigations of the Asteraceae family in Colombia and in particular of the genus *Senecio*, since this is the first report at the national level regarding the constitution of volatile metabolites of a genus that has few chemical studies .

Keywords: *Senecio madagascariensis*, Essential Oil, Nonanol.

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ANALYSIS OF VOLATILE COMPOUNDS OF MUSHROOMS BY HEADSPACE - SOLID PHASE MICROEXTRACTION - GAS CHROMATOGRAPHY/MASS SPECTROMETRY HS-SPME-GC/MS

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PPTC 13

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The study of macromycetes on a global scale, and particularly in Colombia, is still incipient, the mushrooms inventories are limited and the monitoring of these organisms and their characteristics have been little explored; the studies reported in the literature are mainly focused on the content of macro-nutrients but has been studied very little regarding its content of volatile compounds and the relationship of these volatile metabolites with biological activity of mushrooms. The aim of this work is to generate the profile of the volatile composition of mushrooms *(Agaricus bisporus, Pleurotus ostreatus, Ganoderma lucidum, Grifola frondosa, and Lentinula edodes)*, The methodology used included the extraction, separation and identification phases, extraction of the volatile metabolites was carried out by solid phase microextraction in the headspace (HS-SPME), using samples of the mushrooms in the fresh state, and dehydrated in powder form, The separation and identification were conducted by gas chromatography coupled to mass spectrometry (GC/MS), the analyzes were performed in the chromatography laboratory of the University of Caldas. Once evaluated the appropriate combination of variables for the extraction process, were able to determine that the best results were obtained with an exposure time of 20 minutes at a temperature of 40 °C, and 10 grams of sample in saline solution, it was established that the fiber (PDMS/DVB 65 µm) Extracted more efficiently the volatile analytes that fiber (CAR/PDMS 75 µm), in terms of the separation process was worked under the chromatographic conditions: injection temperature 230 °C, 67.4 KPa of pressure, 36.0 cm s-1 linear speed, and splitless injection mode, and a 30 m long, 0.25 SHRVGC column was used mmID, 1.4 µm df and a 30 m length column DB1 DG, 0.25 mmID 0.25 um df, the masses spectrometry identification threw majority volatile compounds characterized for having chains of eight carbons and the presence of alcohols, aldehydes and ketones, the predominant compounds with the most significant areas were 3 – octanol; 1 – octen, 3 – ol; 1 - octen, 3 – one; 1 – octanol; 1 – octanal; 3 – octanone; 3 – octenal; 2 – ethyl, 1 – hexanol. These results are important considering the scarce information that exists of the volatile composition of the study mushrooms and the interest to know these characteristics that can allow to establish the moment for the harvest, as well as improve the methods of conservation and packing to increase the useful life of mushrooms in general.

Keywords: Gas Chromatography, Solid Phase Microextraction, Nutraceutical Mushroom, Volatile Compounds in Mushrooms.

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FUNCTIONALIZATION OF POLY(GMA-CO-EDMA) WITH p-AMINOBENZOIC AND 6-MALEIMIDEHEXANOIC ACIDS

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PPTC 14

The polymeric stationary phases derived from methacrylate are currently modified in order to improve the selectivity, separation, extraction, purification and quantification of components in complex mixtures [1-3]. Among compounds used for its modification *β*-cyclodextrins, aminoalcohols, sulfates and proteins can be found [4]. These modified surfaces have been used in (i) ion exchange chromatography, (ii) capillary electrochromatography, (iii) enantioseparation of chiral compounds, (iv) hydrophilic interaction chromatography, (v) bio-affinity chromatography [5-7].

Here in, the synthesis of *poly*(GMA-*co*-EDMA) monolithic supports and the chemical modification of its surface, using organic acids, were explored. First, copolymer functionalization with *p*-aminobenzoic acid was performed in order to determine if a carboxylic group, catalysed with an ammonium salt, reacts with the epoxide group generating an ester bonding. Second, optimized reaction conditions were used for the copolymer surface modification using 6-maleimidohexanoic acid. Maleimide group presents a high potential, since it can react by Michael addition in a very sensitive and specific way with the thiol group, which is present in the cysteine residue [8]. A support (containing maleimide motif), could be chemically modified with a peptide wearing a cysteine residue and this could be used for affinity enrichment (e.g. antigen-antibody interaction).

The starting copolymer and the functionalized copolymers were characterized by ATR, Raman and scanning electron microscopy. Additionally, the quantification of organic acids not chemically anchored to the copolymer was performed by UV-Vis or RP-HPLC, finding that 99% of the acid reacted with the copolymer. These results confirm that the carboxylic acids can be used to modify the methacrylate derived polymeric surfaces and extend the field of application of these stationary phases.

Keywords: Polymeric stationary phases, Methacrylates, Maleimide, functionalization, Copolymer

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DETECTION OF OTA IN ROASTED AND SOLUBLE COFFEE BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY WITH FLUORESCENCE DETECTOR AND IMMUNITY COLUMN

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PPTC 15

Ochratoxin A (OTA) is a mycotoxin produced by secondary metabolism of Aspergillus and Penicillium fungi. The principal group of food that contaminates are cereals and derivatives like wine, coffee, spices, cheese and processed foods [1]. The Colombian Coffee is one of the main agricultural products; by its quality level, is exported to other countries in 90% of its production, leaving in the country a coffee of lower quality and missing volumes to supply the demand, which can be contaminated. For this reason, it was decided to develop a biosensor for the detection of Ochratoxin A in coffee of domestic consumption. The method used to verify its performance, was the high performance liquid chromatography (HPLC) with flow detector and solid phase extraction (SPE) [2]. In the chromatographic conditions, was used temperature: 40°C, mobile phase: isocratic mixture of acetonitrile-water-acetic acid (50+50+1), flow: 0,6mL /min, fluorescence detector of variable wavelengths with excitation: 330nm and emission: 460nm and retention time: 7.5min+/-1min. In this procedure, a simple linear regression with C=50ng/mL, initial and final verification was performed, to analyse the possible variations in the method. The value of C is determined by the permissible limit of the analyte in the food product which is 5ng/mL relative to the permissible concentration of the secondary metabolite in the roasted and ground coffee, with points at concentrations 0.5-1-5-10-20-30-40-45-50ng/mL; R2=0.9998 was obtained. During verification, it was proposed to perform all the activities of the MICOTOX LTDA protocol repetitively for six different days and in duplicate. The recovery percentage. 1000g of coffee were taken; 20g per day for the procedure were required; 5g of coffee doped with 1mL of standard solution of OTA 5ng/mL dissolved in methanol and 5g without doping. As the days passed, it was possible to show a different behavior in the treatments, with a coefficient of variation in n=12 of 11% in samples of non-doped coffee, compared to doped samples with n=12 of 15%. This value is at the maximum allowed, according to the Horwitz Trumpet diagram, and for trace level measurements is tolerable up to 45% [2]. According to the results, it´s evident that the used method is reliable to perform the verification of the biosensor operation for Ochratoxin A in coffee of internal consumption.

Keywords: Achratoxin A, Micotoxins, Coffee, Immunoassay .

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CHEMICAL COMPOSITION, GC-O AEDA AND ENANTIOMERIC ANALYSIS OF THE ESSENTIAL OIL DISTILLED FROM LEAVES OF *Lepechinia mutica* BENTH. (LAMIACEAE)

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PPTC 16

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Lepechinia mutica (Benth.) Epling is an endemic plant of Ecuador, present only in the province of Loja, where it grows between 2200 and 3400 m [1]. The volatile fraction composition of leaves from this species was first described in literature in 2003 [2]. In the present study, our group performed a new analysis of the same essential oil, based on updated literature and with enantiomeric and sensorial evaluation. These results are currently in press (June 2017). GC-MS and GC-FID analyses resulted in the characterization and quantification of 79 components, corresponding to 97.30% of the total sample. Sesquiterpene hydrocarbons (38.50%) and monoterpene hydrocarbons (30.59%) were found to be the most abundant volatiles. A non-polar capillary column, DB-5ms, 30 m x 0.25 mm, thickness 0.25 µm film, was used. Samples were dissolved in dichloromethane. An autosampler (series 7673) was used. Helium was the carrier gas at a flow rate of 1.0 mL/min in constant flow mode; the detector and injector temperatures were set at 250 ºC. The injector operated in split mode (split ratio 20:1). The oven temperature was set at 60 ºC for 5 min, then increased to 110 ºC, with a gradient rate of 5 ºC/min, followed by an increase to 148 ºC with a gradient of 2 ºC/min. A third gradient rate of 20 ºC/min increased the temperature to 250 ºC, which was hold for 2.4 min. For a better characterization of the oil aroma, a GC-O AEDA analysis was performed. Moreover, enantioselective GC analysis of *L. mutica* essential oil revealed the presence of twelve couples of enantiomers and two enantiomerically pure chiral monoterpenoids. Furthermore, the essential oil exhibited moderate in vitro activity against five fungal strains, being especially effective against *M. canis*. The Minimum Inhibitory Concentration (MIC) of the essential oil was determined by broth-microdilution method using 96 well flat-shaped microtitre plates, according to Gadd and the Clinical and Laboratory Standards Institute procedures, with minor modifications. The MIC is defined as the lowest drug concentration completely inhibiting observable fungal growth compared to the control. To determine the Minimum Fungicidal Concentration (MFC) by broth-microdilution method, the initial inoculum was sub-cultured from microwell plates containing the extract where no fungal growth was observed (100% inhibition) in fresh culture medium, free of the essential oil, and Petri plates were examined for 10 days at 24 h interval. The MFC is defined as the sample lowest concentration causing total reduction of the initial inoculum on culture medium. All bioassays were performed in triplicate.

Keywords: *Lepechinia mutica*, GC-O, AEDA, Essential oil, GC-MS, Ecuador

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HEADSPACE SPME GC-MS/EI IDENTIFICATION OF TERPENE PROFILES FROM DIFFERENT STRAINS OF *Cannabis sativa* GROWN IN BOGOTÁ - COLOMBIA

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PPTC 17

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In direction of the development of a regulatory framework to the use of *Cannabis* and its derivatives in medical and scientific fields, this year Colombia approved the Decree 613 of Law 1767 - 2016 [1]. The main psychotropic cannabinoid, delta-9-tetrahydrocannabinol has been during years well studied, nevertheless there is not a good knowledge of the terpene profiles present in the plant. These compounds in union with cannabinoids not only have been associated with pharmacological properties but also with applications in the cosmetic field to develop perfumes and/or essences [2]. Besides, it could be highlighted that the studies of varieties of cannabis often have been about creepy and these are the result of crosses among others varieties. For this reason, the interest of this study will be focused on the pure varieties of culture in Colombia.

The aim of the present study was development a methodology in order to identify the volatile substances of three different strains of *Cannabis sativa* by HSS-SPME (Headspace static solid phase microextraction) and gas chromatography electron impact ionization mass spectrometry (GC-MS/EI). This is an advantageous method among the methods that have been used to extract volatile substances with subsequent identification, because of the no-use of solvents, it is not need extra steps during the characterization and identification of compounds, the reduction of steps during the treatment of the sample and the low cost that results from the use of this method [3].

Three varieties of *Cannabis sativa* cultivated in Bogotá (female Red point, female Mango and female Corinth) were analyzed. HSS-SPME fiber of PDMS was worked with a sample of 200 mg. The analysis of volatile terpenes was carried out using a GC-MS/EI with a TR1 capillary column. The oven temperature started at 40 °C for 1 min, increases to 280 °C at 5 °C/min and kept for 3 min, The conditions that resulted in maximum extraction were: 60 °C and 10 minutes. Under these operating conditions the main volatile compounds obtained from the three varieties are monoterpenes (α-pinene, β-pinene, β-thujene, β-myrcene, linalool, β-ocimene) and sesquiterpenes (*trans*-α-bergamotene, iso caryophyllene, humulene, farnesene, β-bisabolene, aromadendrene).

The main volatile constituents are: β-myrcene (8,77%), terpinolene (10,28%), α-bergamotene (7,80%) humulene (13,06%), caryophyllene (38,03%) by Red point, β-pinene (15,07%), terpinene (7,17%), linalool (16,45%), α-bergamotene (11,48%), caryophyllene (30,13%) by Corinth, and α-pinene (5,54%), β-myrcene (6,17%), β-ocimene (9,01%), humulene (13,08%) caryophyllene (53,37%) by Mango. The main chemotype between the three strains is Caryophyllene. To the best our knowledge there are not methodologies in Colombia in order to identify volatile substances in these three strains of *Cannabis*. The combination of HSS-SPME and GC-MS/EI showed satisfactory results for both identification and creation of the volatile profiles of each one of the varieties.

Keywords: *Cannabis sativa*, Terpene-profiles, Volatile, HS-SPME-GC-MS/EI

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DEVELOPMENT OF A METHOD OF ANALYSIS FOR PESTICIDES RESIDUES IN DRINKING WATER BY LIQUID-LIQUID EXTRACTION (LLE) AND CHROMATOGRAPHY GAS COUPLED TO MASS SPECTROMETRY AND ELECTRON CAPTURE DETECTOR

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PPTC 18

According to ISO17034, the characterization of reference materials can be carried out using four different approaches: (i) use of a primary method, (ii) use a single method, for value transfer between closely matched materials (iii) use of one or more methods, performed by a network of competent laboratories, (iv) use of two or more independent methods in one or several laboratories [1]. In this context, we development two measurement methods for determining pesticides residues of different physicochemical characteristics presents on drinking water. This work presents the development results of an easy, rapid and low-cost sample preparation approach for the determination of pesticide residues in water by gas chromatography coupled to mass spectrometry and electron capture detector.

The methodology considers a liquid-liquid extraction and drying step. For this study, were evaluated four extraction solvents or solvent mixtures (hexane, heptane, ethyl acetate-hexane, diclorometh ane), mechanical and ultrasonic shaking, ultrasound times and multiple injection modes in the gas chromatograph. The quantification of individual compounds was based on matrix-matched calibration curve with residuals less to 10 %. For all methods, the recovery studies were performed over drinking water spiked at two concentration levels, 10 µg kg−1 and 100 µg kg−1.

Hexane and heptane showed the better recoveries for the most of pesticides, however for difenoconazole, dimethoate, ?-cyhalothrin presented recoveries less to 70%. On the contrary, the ethyl acetate-hexane mixture showed the higher recoveries and the lowest coefficients of variation for these same pesticides. The comparison between ultrasound and mechanical shaking indicated that no significant differences were found ($p < 0.05$) for the most of pesticides.

The repeatability results indicated that for most of the compounds showed coefficients of variation below 10% and recoveries up to 70 %. Furthermore, it was found that the method is accurate for determination of pesticide residues from different chemical groups such as azoles, organophosphorus, organochlorines, among others.

Keywords: Pesticides, Drinking water, Reference materials, Liquid-liquid extraction.

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CHARACTERIZATION OF ODOUR-ACTIVE COMPOUNDS IN RON VIEJO DE CALDAS BY GAS CHROMATOGRAPHY-OLFACTOMETRY-MASS (GC-O-MS), COMPARISON BETWEEN DYNAMIC HEAD SPACE-SOLID PHASE EXTRACTION (DHS-SPE) AND HEADSPACE- SOLID PHASE MICROEXTRACTION (HS-SPME)

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PPTC 19

In this work, several samples of Ron Viejo de Caldas of different aging ages are been analysed by GC-O-MS. Two extraction techniques were compared. A carboxen/PDMS/DVB fibber was used for SPME in headspace mode. The DHS-SPE was assayed also, employing LiChrolut EN resins (polystyrene/divynilbencene) of 400 mg packed in 3 mL polypropylene cartridges and N2 as purge gas. The extraction conditions were optimized. The chromatographic conditions were: splitless injection mode for SPME extraction, at 250 °C, the column used was a DB624, the MS device were used in EI mode at 70 eV, 230 °C, ion source at 150 °C and transfer line at 150 °C. The chromatograph is equipped with an olfactory detector port ODP by Gerstel, with recognize voice system using the Dragon software.

The DHS-SPE with 80 mL of sample diluted 50% (17%v/v of ethanol aprox.), 1h and 30 minutes of extraction time and 500 mL/min of nitrogen flow allowed the extraction of about 28 odorants from the rum samples and 21 odorants were perceived by olfactometry. The SPME with 5 mL of sample diluted 50%, 1 hour of extraction with stirring and 6 M NaCl allowed the extraction of about 60 compounds and about 50 compounds were perceived in the olfactometry port. The modified frequency (%MF) values were estimated with the support of a trained sensorial panel. Most of the odorants have been identified by their mass spectrum, Kovats Index and aromatic descriptor. The preliminary results showed that esters such as: isoamyl and butyl acetate, ethyl hexanoate, butanoate, pentanoate, octanoate, decanoate and benzoate were scored with the highest MF values (>50%) in all rum samples, these may provide sweet and fruity notes to the rum. Also, other important and non-identified odorants with RI (DB-624 column): 990, 1165, 1196 and 1401 have citric, floral, herbal and caramel notes. Guayacol with a medicinal aroma was an important odorant in rum samples of 3 and 5 years of aging. The acetals: 1,1-diethoxyetane and 1,1-diethoxy-2-methyl-propane and anethole, with fruity and aniseed notes, were highlighted in the sample of 8 years. Alcohols such as: isoamylic and heptanol were well perceived in the sample of 3 years, but less in 5 and 8 years samples, statistical differences by Chi-squared test were observed between samples.

Keywords: Rum, Olfactometry, Odour, HS-SPME, DHS-SPE, GC-MS-O

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PROBABILISTIC MODEL FOR THE ASSESSMENT OF SELECTIVITY IN MS-MS SPECTROMETRY TECHNICS: APPLICATION FOR THE SELECTION OF IDENTIFICATION IONS

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PPTC 20

The selectivity is an important metrological parameter to establish the extent in which a measurement method, will be use to quantify an analyte in a given matrix, without the interference of other compounds with similar behavior [1]. Several studies had propose mathematical models to establish qualitative or quantitative descriptors for the selectivity in multicomponent analysis involving information about detectors, channels, etc. [2], nevertheless the use of these models is often impractical at the analytical laboratory. In chromatographic methods with mass spectrometry detection such as LC-MS/MS, the join selectivity from the chromatographic and detector systems, provide measurement methods highly selective, reason why LC-MS/MS in one of the chosen technics for the identification and quantification in measurements to support normative or legislative decisions [3].

In so much as, the selectivity is a mandatory validation parameter in qualitative and quantitative methods, many guides (e.g for analysis of chemical contaminants) give general guidance for setting up the method selectivity, providing some guidance criteria for the choice of product ions for identification. Berendsen, et.al. [4], put forward a statistical model to describe the selectivity of an LC-MS/MS method, with the aim of estimate the probability of unequivocally identify a given analyte. This model use chromatography and mass spectrometry information about the product and precursor ions. In this work, we present a practical probabilistic model for the selectivity, build with experimental data from the interest matrix and analytes and considering the conditional probability of the product ions for the compounds of the measurand. Additionally we present an application for the proposed model for the choice of the product ions for identification, in a method for the quantification pesticides residues in purple passion fruit “gulupa”, showing the usefulness of the model for made the best choice of the identification ions, based on a quantitative descriptor for the selectivity.

Keywords: Selectivity, Probabilistic model, Mass spectrometry, Identification ions.

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CHEMICAL PROFILING TO SEIZED ECSTASY PILLS BY SOLID-PHASE MICROEXTRACTION (SPME) AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC/MS)

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PPTC 21

Ecstasy is a common drug in night clubs since early 2000´s. The main substance in ecstasy pills, which cause hallucinogenic and empathogenic effects, is the 3,4-methylendioxymethamphetamine (MDMA), although it is commonly adulterated with caffeine and paramethoxymethylamphetamine (PMMA). The aim of this work was to profile ecstasy -MDMA containing- samples by extracting from them precursors, intermediates and byproducts, compare them to previous reports and establish possible synthetic routes based on them.

The samples were prepared by using SPME from ecstasy–MDMA containing-pills, which were seized in Bogotá´s streets, and then analysed by GC/MS. During the SPME extraction, the following parameters were optimized: sample amount, fiber exposition's temperature and time. Each impurity found was correlated to reported synthetic routes. The GC/MS method was used following the UNODC recommendations for synthetic drugs. The analysis was performed using GC-MS IT on an Agilent 7890A-240MS instrument (Santa Clara, CA, USA). A PDMS/DVB 65 µm Supelco fiber was exposed in the chromatograph's injection port (Bellefonte, PA, USA).

During the analysis of the samples, different types of substances such as safrole, piperonal, 3,4-Methylenedioxyphenyl-2-propanone (MDP2P), N-formyl-MDMA, piperonyl chloride, 3,4-Methylenedioxyphenyl-2-propanol, among others, were found, which according to previous reports could be precursors, intermediates or by-products of the Leuckart reaction or reductive amination based on different reagents. Identification of the compounds was done by comparing the mass spectrum against the NIST2.0 Forensic Library, with an acceptation criteria score of minimum 85%.

Analysed samples do not show any prevailing synthetic route; some of the samples show a mixture of compounds of interest, meaning that each pill is actually a blend of different MDMA batches and each comes from different synthetic routes. SPME technique allows preparation of the samples for synthetic drugs profiling. Trace-level compounds as reagents, intermediates and by-products are extracted using this method.

DETECTION AND QUANTIFICATION OF MEROPENEM IN PLASMA BY HPLC-DAD AND ITS CONFIRMATION BY DSA-TOF-MS.

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PPTC 22

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In 1928 was discovered the penicillin which is the mother drug of current antibiotics, among which are the antibiotics beta lactam, whose consumption has been increasing in recent years due to its broad spectrum bactericidal action. Meropenem (MP) is prominent within this group of drugs because it is administered as an empirical treatment prior to the identification of the microorganism causing the disease. The prolonged and incorrect use of MP are among the problems of this compound since the established dose is calculated based on pharmacokinetic parameters of healthy patients. Usually the dosage does not adjust with the intrahospitalary reality, which can generate inconveniences ranging from damages to the patient to antimicrobial resistance.

Due to the above, it is important to develop and validate new methodologies to determine MP in blood plasma, to confirm the dose at the intrahospitalary level.

In a first step, a methodology for the extraction of MP from the plasma matrix was optimized, then the quantification was carried out by HPLC-DAD, for which the plasma was fortified with MP. Two methods were tested for the preparation of the sample; the first one was a simple and low cost method that consisted of the precipitation of proteins with acetonitrile (ACN) and then the separation of the supernatant by centrifugation. The second methodology was the solid phase extraction (SPE), using a C18 resin where the working conditions were optimized [1]. The following chromatographic conditions were used: analytical column C18, mobile phase: methanol/sodium phosphate buffer with flow of 1.2 ml/min and an optimized gradient program. Confirmation of the analyte was carried out by the DSA-TOF-MS technique, using as solvent water and NaOH. To evaluate the positive ionization of the MP, the conditions were positive polarity, crown 3.0µA, APCI 300°C, voltage 2900 V and injection volume 10 µL.

From the results obtained, it is observed that in both water and plasma it is possible to quantify the MP by HPLC-DAD with correlations of 0.998 and 0.997, respectively. The limits of detection and quantification of the technique were 0.001 mg/L and 0.5 mg/L, respectively. The recovery percentages obtained for the ACN extraction methodology were 60% for the concentration of 2 mg/L and above 90% for the concentrations between 4 and 10 mg/L. The SPE methodology allowed to reduce the matrix effect observed in the chromatograms. In relation to the results obtained by DSA-TOF-MS, no significant differences were found between the areas obtained from samples diluted in water and NaOH, obtaining a correlation in water of 0.966, for a linear range of concentration between 10-90 mg/L. The presence of the analyte was confirmed by the *m/z* of 358 corresponding to the degradation product of MP.

This study concludes that it is possible to quantify MP in the plasma matrix by HPLC-DAD and DSA-TOF-MS, which would allow the evaluation of the dosage in real samples.

Keywords: Meropenem, Plasma, Extraction, Chromatography.

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DETERMINATION OF CAROTENES AND ANTHOCYANINS IN *Passiflora edulis* Sims BY UHPLC: A REVIEW

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Anthocyanins and carotenoids are natural pigments present in fruits and vegetables which have generated great interest due to their intense range of colors, safety, and good benefits for health. These compounds are extracted mainly from the fruits peels and have a great potential in order to replace synthetic dyes. Passion fruit or "gulupa" (*Passiflora edulis* Sims) stands out as an exotic and good acceptance fruit because of its organoleptic and nutritional properties. During the year 2014, the department of Antioquia, Colombia presented the highest percentage share in the production of this fruit (29%). In the period from 2010 to 2016, the exports of this fruit grew 150%, making the country as the leading exporter of this fruit in European markets. In order to increase the yield and decrease the pollution in extraction and quantification of natural bioactive compounds, new methods have been developed. The aim of this work was to identify methodologies of extraction and quantification using liquid chromatography for the determination of anthocyanins and carotenoids in plant matrices. This review took the publications of the last 10 years, highlighting the use of efficient and modern techniques like the Ultra High-Performance Liquid Chromatography (UHPLC) to quantify and Supercritical fluids (FSC) to extract the bioactive compounds in the preparations stage of the samples. Therefore, the low solvent consumption and lower generation of the waste make the FSC method advantageous compared to conventional methods, following the principles of green chemistry, and could be used as a procedure to extract bioactive compounds in fruits and vegetables. Simultaneously, the UHPLC technique confers an increase in the sensitivity and efficiency in the separation, reflected in a better resolution and making possible the analysis of a greater number of samples per time, which decrease times of analysis and stabilization of the column, generating fewer wastes and lower mobile phase consumption. The combination of FSC and UHPLC allows enhancing the determination of bioactive agents in various plant matrices.

Keywords: Anthocyanins, Carotenoids, Gulupa, Bioactive Compounds, Green Chemistry, FSC, UHPLC.

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DETERMINATION OF AFLATOXINS IN CEREALS BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC) WITH POST-COLUMN PHOTOCHEMICAL DERIVATIZATION

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PPTC 24

Aflatoxins are secondary toxic metabolites produced by some *Aspergillus* species that contaminate field crops, under favourable conditions of temperature and humidity. The most important aflatoxins are B1 (AFB1), B2 (AFB2), G1 (AFG1) and G2 (AFG2), and contaminate maize, wheat, rice, peanuts, pistachios, cottonseed, copra and spices. Such contamination causes serious economic problems and affects human health, especially in tropical areas. AFB1 is the most prevalent and toxic of aflatoxins and has been classified by the International Agency for Research on Cancer as a first-class carcinogen for humans, mainly affecting the liver.

Taking into account the toxicity of aflatoxins and the established acceptable maximum limit, their analytical identification and quantification at such low levels should be performed using reliable methods. Most current methods include chromatographic methods such as Thin Layer Chromatography (TLC), High Performance Liquid Chromatography (HPLC) and Liquid Chromatography of Tandem Mass Spectrometry (LC-MS/MS). HPLC with fluorescence detector (FD) is the most used chromatographic technique for the quantitative analysis of aflatoxins, because these molecules are naturally fluorescent.

However, the fluorescence of AFB1 and AFG1 is attenuated by the eluents of the reverse phase and, for this reason, it is necessary to improve their response by a derivatization. Such a reaction can be done before or after the sample passes the column. Post-column derivatization is based on the reaction of the 8,9-double bond of aflatoxins with halogens. Said reaction can be achieved by addition of iodine or bromine, or by photochemical derivatization which is based on the formation of hemiacetals of AFB1 and AFG1 by ultraviolet radiation.

The present work aims to validate an HPLC-FD method with post-column photochemical derivatization to determine aflatoxin levels in arepas, rice and bread samples from the department of Caldas.

The method was validated by verifying its selectivity, linearity (R2> 0.9993), LOD (> 0.01 ng/ml) and LQ (> 0.03 ng/ml), precision (mean RSD% 8.7%) and average recovery (99.5%). To date, 185 samples of arepas, rice and bread have been analyzed, finding that 25.4% have aflatoxin contamination (rice=29, arepas=15, and bread=3). Of the positive samples, 22.4% contain AFB1, and almost half exceed the limits established in international regulations (2 µg kg-1).

Keywords: High-performance liquid chromatography, Aflatoxins, Post-column derivatization, Cereals

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OBTAINING A METHOD OF EXTRACTION OF ABSCISIC ACID IN MAIZE SEEDS (*Zea mays* L.)

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PPTC 25

Maize (*Zea mays* L.) is one of the cereals grown by man since ancient times, actually is recognized as one of the most productive plantations with an average global yield of more than 4000 kilograms per hectare [1]. The development of these seeds is intimately related to the presence of a series of hormones, being that the most influential are gibberellic acid (GA3) and abscisic acid (ABA) [2], which are responsible for favoring the germination process and dormancy respectively, provided that adequate environmental signals exist that favor the synthesis of these molecules [3,4].

In order to compare and determine an appropriate method for obtaining abscisic acid in maize (Z*ea mays* L.) seeds, two extraction techniques were used: Solid-liquid extraction or leaching, and dynamic extraction solvent assisted by sonication (DSASE) considered a miniaturized technique, which is attributed to short processing times and a decrease in solvent consumption [5]. Samples were extracted in 6 time ranges ranging from zero to 48 hours of seed development. For leaching extraction, a final volume of 15 mL was obtained by depletion, and for DSASE 10 mL at a flow rate of 0.4 mL / min. The extracts were quantified and data were analyzed by STATGRAPHICS centurion software latest demo mode. The results showed statistically significant effects of each process on the concentration of abscisic acid in maize (*Zea Mays* L.) seeds. In this way, it was determined that the best method of extraction of this phytohormone is leaching with a concentration of 0.122028 mg/kg, a value significantly higher than obtained dynamic extraction solvent assisted by sonication (DSASE) with a concentration of 0.0410778 mg/Kg. The concentration of ABA was also analyzed in different time ranges and it was determined that there were no statistically significant differences with a 95% confidence level.

Keywords: Abscisic acid, leaching extraction, dynamic extraction solvent assisted by sonication (DSASE).

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HPLC-UV/DAD PROFILES, PHENOLIC CONTENT, AND FREE RADICAL SCAVENGING CAPACITY OF COMMERCIAL AMAZONIAN HERBAL MEDICINAL PRODUCTS

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The Peruvian Amazon is known worldwide for its rich biodiversity of medicinal plants and as an important historical centre of traditional medicine. Despite this region is largely considered a great source of potential bio-active natural products, the majority of even locally well-known and commercially available herbal medicines from the Peruvian Amazon, are still poorly characterized especially in terms of phytochemical bio-markers identification. As an important category of phytochemicals, phenolic compounds are dietary constituents widely existing in plants and have been considered to have high antioxidant activity and free radical scavenging capacity. Phenolic compounds have attracted more and more attention as potential agents for preventing and treating many oxidative stress-related diseases. Over the last 20 years, polyphenols have been studied for their potential involvement in many areas including cancer, cardiovascular problems, inflammation and microbial diseases [1, 2].

In the present work, five (5) commercial Amazonian Herbal Medicinal Products, Hydro-ethanol extracts (Tinctures) of *Abuta grandifolia, Mansoa alliacea, Phyllanthus niruri, Maytenus macrocarpa, Dracontium loretense* obtained from the Natural Product Laboratory of Takiwasi Center, have been studied and compared for their native extracts ratio, as well as for the phenolic content and radical scavenging capacity through Folin-Ciocalteu and DPPH spectrophotometric methods, respectively; HPLC-UV/DAD fingerprinting profiles of the crude herbal extracts were also acquired. The overall set of data allowed the acquisition of qualitative and quantitative results, useful for the quality control analysis to support batch to batch reproducibility and extracts standardization. Moreover, by comparison of different batches of Mansoa alliacea Tinctures, three (3) flavonoids derivatives were also selected as potential markers for the stability assays.

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CHEMICAL PROFILE AND ANTI-LEISHMANIAL ACTIVITY OF THREE ECUADORIAN PROPOLIS SAMPLES FROM QUITO, GUAYAQUIL AND COTACACHI REGIONS

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PPTC 27

Three propolis samples were collected from diferent regions of Ecuador (Quito, Guayaquil and Cotacachi) and their methanolic extracts were prepared. Preliminary information supplied by TLC and NMR data, allowed us to define two main types of propolis: Cotacachi propoli sample (CPS), rich in flavonoids and Quito and Guayaquil samples (QPS and GPS) containing triterpenic alcohols and acetyl triterpenes as the main constituents. Two diferent approaches based on RP-HPLC preparative procedure and NMR structural determination (CPS) and GC–MS analysis (QPS and GPS) were successfully used for the chemical characterization of their major compounds. All three propolis extracts were able to inhibit *Leishmania amazonensis* growth but propolis sample rich in flavonoids was the most active (IC50=17.1 ± 1.7 μg/mL). In the literature this is the first study on propolis from Ecuador.

Keywords: Ecuadorian Propolis, *Leishmania amazonensis*, GC-MS; Flavonoids

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DETERMINATION OF WHEY IN RAW MILK, FROM THE QUANTIFICATION OF CASEIN GLYCOMACROPEPTIDE BY HPLC

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The adulteration of raw milk with milk whey is one of the main problems in the milk industry, because it can generate an alteration in the quality of the food and its nutritional value [1]. The European Standard 213/2001 [2] and Royal Decree 2021/1993 [3] show this type of adulteration by the identification of glycomacropeptide, casein [4] by the high performance liquid chromatography (HPLC) technique. In our country there is the decree 616 of 2006 which prohibits the addition of milk whey in any part of the milk production process [5]. However, there is no standardized and validated quantitative technique for the adulteration of milk with milk whey.

This work focuses on identifying the presence of milk whey by the quantification of casein (glycomacropeptide) by HPLC for the quality control of raw milk, in order to verify its possible adulteration. A calibration curve was elaborated using samples of raw milk to which milk whey was added in different amounts, varying the percentage of adulteration (0, 2.5%, 5%, 7.5%, 10%, 12.5%, 15%, 20%, (m / m) to raw milk. After three hours of incubation with the milk whey, trichloroacetic acid (24%) was added to precipitate the proteins, then one hour later it was centrifuged at 3000 rpm, the supernatant was filtered using a 0.22 μm pore diameter membrane, injected a 20μL volume into the HPLC equipment using a particle size exclusion (SEC) column, with a flow of 0.9mL / min using a mobile phase of phosphate Buffer [3,4]. Next, 24 samples collected from different farms were analyzed.

These samples were subjected to the mentioned pre-treatment to evaluate the percentage of milk whey adulteration by means of HPLC. In the chromatograms obtained a signal with a retention time of 10 minutes, which shows proportional increases between the chromatographic area of the signal as the percentage of adulteration with milk whey increases, a calibration curve was obtained showed linearity with a value of R2 " 0.994 ". From the curve and with the chromatograms obtained from the farm samples, were found adulterations up to 9.3%. The chromatographic signal of interest was collected and the technique validated using stick c-GMP in order to confirm the presence of GMP. For the first time, a methodology with a calibration curve is used to identify the percentage of adulteration with milk whey using analytical and quantitative methods; in addition, using HPLC and GMP in order to have a better quality control in milk.

Keywords: Glycomacropeptide, Caseín, Raw milk and Milk whey.

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DEVELOPMENT AND VALIDATION OF A THIN-LAYER CHROMATOGRAPHY/DENSITOMETRY METHOD TO QUANTIFY BETULINIC ACID IN NATURAL EXTRACTS

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Betulinic acid is a pentacyclic triterpene widely distributed in different species such as *Morus alba* L. [1], *Dillenia indica* L. [2], *Licania tomentosa* (Benth) Fritsch [3], *Davilla rugosa* Poir [4] and *Eugenia florida* DC [5]. A wide range of biological activities is reported for betulinic acid including antiviral, antibacterial and anti-inflammatory properties, as well as a potential to inhibit the growth of human cancer cells [6]. A large number of analytical techniques have been developed for betulinic acid analyses in plants. Gas chromatography is described as the best option for assay and purity testing of betulinic acid while the thin-layer chromatography (TLC) is commonly used for its qualitative analysis. While some studies use inappropriate validation procedures for TLC methods, others imply compare their results to traditional techniques without the appropriate statistical treatment to meet international acceptance standards. These limited the use of planar chromatography as an analytical technique method for the assay of botanicals samples. Determination of betulinic acid in differents extracts of plants to quality control through a fast, cheap and efficient technique was the challenge of this work. Betulinic acid was identified using a thin layer chromatography/densitometry method. The analysis were obtained on plates Si60 F254 with hexane:ethyl acetate:acetic acid (7:3:0.3). The quantitation was performed at 190 nm. The system gave compact spots for betulinic acid (Rf 0.5) and exhibited linearity (R2= 0.999). The method was validated and applied successfully to distinguish betulinic acid from the interfering materials and quantify this measure and in a complex matrix such as the extracts of natural samples. This can be an alternative to GC technique. The developed methodology overcame all the failures, misconceptions and misleading pointed in the literature providing a methodology with results comparable to GC results. We believe that this methodology provide a correct and proper validation of TLC methodology for assay of natural samples. The validation protocol developed can be applied to other natural products during its TLC methodology development.

Keywords: TLC/densitometry, Validation, Betulinic acid, Quality control

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ASPECTS TO CONSIDER FOR ANALYSIS OF CANNABINOIDS IN HUMAN HAIR BY GC-MS

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PPTC 31

Nowadays, Colombia doesn't have an analytical method able to detect chronical consumption of marijuana. Laboratories responsible of cannabinoids detection in biological matrixes use fast screening tests in urine by immunoassay approaches, with a detection window of maximum seven days, and is not possible to quantify or identify the cannabinoids Δ9-tetrahydrocannabinol (THC) or one of its main metabolites 9-carboxy-11-nor-Δ9-tetrahydrocannabinol (THC-COOH), reason why it's required an analytical method which could quantify and identify cannabinoids with a wide detection window (greater than 30 days). Then, development of a method of analysis of cannabinoids in hair by gas chromatography coupled to mass spectrometer was proposed. The authors reviewed PubMed and Science Direct databases using the MeSH terms: hair analysis, hair testing, cannabis, decontamination, extraction and chromatography, during twelve months. The review aims to provide an overview of main characteristics of human hair as biological matrix, relationship between melanin content and metabolites retention, and requirements of decontamination and extraction procedures [1]. In addition, a comparison of three extraction protocols was carried out: washing with (a) deionized water, (b) dichlorometane and (c) methanol, segmentation, digestion with sodium hidroxide 1N, and extraction with (a) isooctane and (b,c) n-hexane:ethyl acetate 9:1. Extraction procedure (b) seems to be the best protocol.

Testing drugs in human hair is an approach which has been of special interest in last years, hair is a biological matrix with multiple advantages over urine and blood, being the broad time detection window of hair its main strength, allowing retrospective analysis of chronical or single-dose exposure to drugs [2]. Hair is a non-invasive, stable, easy to obtain, transport and storage matrix [3]; composed by proteins, lipids, melanins and water. Substances are incorporated to hair from blood, sweat, sebum and from external contamination, incorporation process depends on substance's physical and chemical properties (hydrophobicity, acidity and molecular weight), melanin hair content and composition [4] (per the color), hair growing rate (which depends on age, sex, race, nutrition and hair stage) and hair healthy. Hair testing requires a decontamination protocol to guarantee analytes are in hair structure due to active exposure and not as contaminants, as is common to occur with passive exposure to cannabinoids in marijuana smoke [5–7].

Keywords: Hair Analysis, Extraction, Decontamination, Cannabinoids, Marijuana.

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DEVELOPMENT AND VALIDATION OF A METHODOLOGY FOR THE DETERMINATION OF ORGANOCHLORINE PESTICIDES AND PCBS IN RAW MILK BY GC- µECD

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PPTC 32

Polychlorinated biphenyls (PCBs) and organochlorine pesticides have been widely used around the world in industry and agriculture, respectively. Their use has been restricted or banned in many countries even in Latin America. These compounds are characterized by their persistence, slow biodegradation, stability and their accumulation in fatty tissues.

The main route of human exposure of these compounds is dietary intake, particularly food rich in fat such as meat, fish, poultry and milk, because these contaminants are lipophilic and tend to accumulate in fatty tissues.

The persistence and extensive use of these pollutants has led to a wide distribution in the environment, causing a constant concern for the levels to which a population is subjected. Colombia has signed the Stockholm Convention on Persistent Organic Pollutants, so it is mandatory to develop analytical methodologies that can determine the presence of these compounds in accordance with international regulations.

The present work describes the development and validation of a fast and easy methodology for determination of PCBs and organochlorine pesticides in raw milk with a modified European QuEChERS approach. The compounds were extracted with acetonitrile saturated with n-hexane. The extracts were cleaned up by dispersive solid phase extraction with PSA and the final determination was carried out by gas chromatography with a pulsed splitless injection mode and detection by µ-Electron capture detector.

The method is specific and selective, precise and accurate.The calibration curve shows a linearity in the concentration range from 0.0015 mg/kg to 0.16 mg/kg with a quantification limit of 0.0015 mg/kg for all compounds. Recoveries of majority of organochlorine compounds from spiked samples range from 81% to 101% and RSD values lower than 10%. The validation was performed with the objective of analyzing real samples as an indicator of environmental contamination.

Keywords: Polychlorinated Biphenyls (PCBs), Organochlorine Pesticides, GC- µECD, POPs.

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OPTIMIZATION OF A METHOD FOR DETERMINATION OF PESTICIDE RESIDUES USING LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY

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The analytical instrumentation for pesticide residue analysis has presented a great development in the last decades; however, in spite of this progress, it is always necessary to improve and optimize measurement methods to meet the requirements for higher accuracy, higher sensitivity and selectivity and better sensibility. For the production of reference materials, these requirements are much more demanding, since the measurement methods are intended for applications such as certification, stability monitoring, among. For this reasons, the aim of this work was to optimize a multiresidue pesticide methodology for homogeneity testing and stability assessment on candidate to reference materials.

In this context, a simple, selective and fast multi-residue method was optimized to determine 50 pesticides residues in fruits by high performance liquid chromatography coupled to tandem mass spectrometry. The selected pesticides include organophosphorus, organonitrogen, carbamates and neonicotinoids. An extraction procedure based on QuEChERS methodology (quick, easy, cheap, effective, rugged and safe), consisting of a liquid extraction of the fruit samples with acetonitrile and finally a sample clean up step. The pesticides were detected by electrospray ionization in positive ion mode with multiple reaction monitoring.

For this study, the mass spectrometric conditions were optimized in order to increase selectivity and sensitivity by two ways (manual and automatic), finding that pesticides such as carbofuran, heptenophos and pyrazophos presented better responses with the manual optimization methodology. In a second stage, chromatographic conditions were studied in order to achieve narrow peaks, good separation and symmetrical peaks. These experiments indicated that the best results were obtained by using methanol- ammonium formiate with formic acid (0.1%).

Finally, we evaluated different internal standards and the compositions of the sample injection solvent varied in the ratios of water and methanol ranging from 100% (methanol) to 5%. The results indicated that the use of two internal standards guarantees reliable quantification and the methanol mixed with water in a ratio of 1:1 was the better composition of the sample injection solvent.

Keywords: Optimization, Multiresidue pesticide methodology, Candidate to reference materials.

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MOLECULAR IDENTIFICATION OF FUNGAL IMMUNOMODULATORY PROTEINS (FIPs) FROM *Ganoderma australe.*

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Macromycetes belonging to the genus Ganoderma produces compounds called Fungal Immunomodulatory Proteins (FIPs) that exhibits biological activity with potential to be used in medicine. Recent studies have shown that FIPs could be used as adjuvants to the treatment of cancer, inflammatory and autoimmune diseases; due to their ability to stimulate the immune system [1,2]. Given their pharmacological potential, several studies focuses on identifying, isolating and characterization of new FIPs produced by macromycetes diversity. In addition, genetic engineering techniques are used to express those molecules in different systems due to not only their higher yield and biological stability, but also the possibility of scaling through industrial production [3]. Therefore, the objective of this study was the identification of the open reading frame (ORF) of the FIP of *Ganoderma australe* by using molecular biology techniques.

G. australe mycelium was supplied by the Universidad del Valle (Colombia), initially was used Sabouraud Dextrose Agar and then, it was inoculated in liquid medium at 100 rpm, 27°C for 10 days. Afterwards, genomic DNA was extracted by using the protocol described by Moncalvo *et al.* (1995) [4] with modifications. Finally, in order to amplify the ORF of FIP specific primers was used, forward 5′-ATGTCCGACACTGCCTTGATCTTCAGG-3′ and reverse 5´CTAGTTCCACTGGGCGATGATGAAGTC-3′. A 336 bp PCR product was then cloned into p-GEM T-Easy vector (Promega, Madison, WI), sequenced by Sanger 's Technology at Macrogen - Korea, in order to confirm molecular identity.

Fungal Immunomodulatory Proteins constitute a family of small proteins, isolated from different species of macromycetes that show high structural and functional similarities with immunoglobulins. Therefore, they are candidates for drugs developing for treating diseases (e.g. cancer) [2]. In this study we identified a 336 bp DNA fragment related to ORF of Fungal Immunomodulatory Protein of *Ganoderma australe* with 97% homology of the *G. lucidum* isolated FIP LZ-8 protein, these results agree with the reports that determine the ORF is made up of 330-350 bp and with high homology in its primary structure. In conclusion, the identification of the ORF of the Fungal Immunomodulatory Protein constitutes an advance for the evaluation of the biological activity in peripheral blood mononuclear cells. This, at the same time, will allow comparing the results with other previously reported in species of the genus *Ganoderma* and other basidiomycetes and ascomycetes.

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ANTIFUNGAL ACTIVITY AGAINST *Colletotrichum musae* BY THE ETHANOLIC EXTRACT OF *Sapindus saponaria* L.

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Sapindus saponaria L. popularly know as ?saboneteira, sabão-de-mico, sabonetinho or saboeiro? is a Brazilian tree belong to Sapindaceae family. The extract from different parts of this plant has been described for interesting biological activities: Molluscicidal, antifungal, larvicidal and antiinflamatory. Considering the agroindustry development approaches, ethanolic and hexanic extracts of fruits of *S. saponaria* was studied in the treatment of three species of Colletotrichum (Colletotrichum musae 226/12I, Colletotrichum gloeosporioides 09/05I and Colletotrichum boninense 21/10I), common pathogens of legumes, grains, vegetables and fruits. The ethanolic extract showed significant in vitro antimicrobial activity against C. musae by disk diffusion method. Bioassay-guided fractionation of this extract using liquid-liquid extraction and semi-preparative thin layer chromatography resulted in the identification of a fraction rich in a pentacyclic triterpenoid saponin: 3-O-(Beta-D-xylopyranosyl)-(1?3)-alpha-L-rhamnopyranosyl-(1?2)-alpha-L-arabinopyranosyl-hederagenin. Chemical characterization was done using mass spectrometry (MS), 1H and 13C NMR. The most active fraction and the standard thiabendazole were tested in the same concentration (62.5 µg/disk) and the results revealed MIC values of 9.09 ± 0.01 mm and 9.69 ± 0.59 mm, respectively. The present results are the first to show that ethanolic extract and semi-purified fractions from *S. saponaria* can act as antifungal agents against C. musae, an important phytopathogen of banana crops that cause post-harvest losses in a country like Brazil that produces seven million tons of bananas a year and ranks third in world in this crop production.

MARINE BACTERIA AS SOURCE OF QUORUM QUENCHER COMPOUNDS

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PPNP 03

Marine bacteria are considered as a promising source for the discovery of novel biologically active compounds that can be used to overcome the supply problem displayed by marine natural products. In this study, marine microorganisms were isolated form sediment, invertebrates and algae samples. We were recovered 203 isolates including 162 bacteria and 41 fungi [1]. All the isolates were assayed against *Chromobacterium violaceum* ATCC 31532 *in vivo* seeking for quorum quenching activity, 17 bacteria showed the activity. Then, the aqueous and organic extracts of bioactive strains were tested; 13 organic extracts and 2 aqueous phases showed activity, while two strains extracts did not showed activity.

The active strain belongs to Actinobacteria and Firmicutes Phyla. The *Streptomyces* sp (IBUN 090-02089) yielded an active organic extract, the bioguided chromatographic isolation allowed to identify a bioactive peptide by NMR study. The production of this compound is very dependent on culture conditions. From the organic phase of *Micromonospora* sp (IBUN 090-02100) a lipid fraction was identified as responsible for the bioactivity. The study of aqueous phase of *Paenibacillus* sp. (IBUN 090-02110) allowed the isolation and characterization of an antimicrobial lipopeptide, similar to those produced by *Paenibacillus ehimensis* [2].

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PHYTOCHEMICAL ANALYSIS FROM *Rhizophora mangle* BARKS: FIA-ESI-IT-MS/MS AND MALDI-TOF APPROACH

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PPNP 04

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Rhizophora mangle L. (Rhizophoraceae) is a mangrove species, popularly used to the treatment and prevention of several diseases, such as gastrointestinal, inflammation and pain [1]. The main goal of this work was to recognize the chemical composition of the acetonic extract of the barks of *R. mangle* (AERM) using mass spectrometry analyses. The first series of experiments involved [Liquid Chromatography] or Flow Injection Analysis coupled to an Electrospray Ion Trap Tandem Mass Spectrometer {[LC]-FIA-ESI-IT-MS/MS}. The chromatographic separation led to 11 separated catechins. FIA-IT-MS/MS experiments allowed to identify catechin polymers of up three units (DP 3). However, the characterization of the bulk of the condensed tannins of *R. mangle* was limited, since using only these experiments we could not detect compounds with higher molecular weight. To solve this problem, a second series of experiments involving MALDI-TOF experiments was performed to establish the degree of polymerization of the proanthocyanidins as well as of their glucosylated forms. The spectra obtained by MALDI-TOF of the AERM presented two homologous series: one based on polymers of *m/z* 288 Da increments (up to 12 DP) and another series based on polymers of *m/z* [288+162] Da increments (up to 11 DP). In addition to these series of flavan-3-ol compounds, each DP presented additional subsets of masses with variation of -16 Da and +16 Da. These subsets could be explained bythe presence of heteropolymers of flavan-3-ol units containing an additional hydroxyl group (+16 Da), characterizing a third homologous series of gallocatechins (m/z 905 ~ 3497 Da) and a fouth series (-16 Da) based on an homologous series of afzelechins (m/z 873 ~ 3465 Da). A similar pattern with homologous series of gallocatechins and afazelechins could also be observed through the presence of a fifth and a sixth monohexoside series: glucogallocatechins (m/z 779 ~ 3371) and glucoafzelechins (m/z 747 ~ 3339). These results could reveal the full chemical composition of the bark of this tree, and helped us to understand the mechanisms of action inherent to the biological activities described by the traditional knowledge, which had little scientific support.

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4,9-DIHYDROXY-1,2,11,12-TETRAHYDROPERYLENE-3,10-QUINONE ISOLATED FROM *Graphium jumulu* ENDOPHYTIC FUNGUS FROM *Duroia macrophylla*

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PPNP 05

Endophytic fungi are an important source of bioactive molecules. This work had as a main aim to find out the biotechnological potential of the endophytic fungus *Graphium jumulu*, which was isolated from the specied *Duroia macrophylla* (Rubiaceae). The fungus was cultured in potato liquid medium supplemented with 0.2% of yeast extract, distributed in 12 erlenmeyer of 500 mL, each one was filled with 300 mL of medium. They were cultured in an orbital incubator at 120 rpm, at 30 oC for 20 days. Mycelium metabolites were extracted with ethyl acetate using ultrasound for 20 min, procedure repeated three-times. The ethyl acetate extract was assayed against 12 bacterial strains by diffusion agar method and was active against *Pseudomonas aeruginosa*, *Edwardsiella tarda*, *Providencia rettgeri*, *Salmonella enteritidis*, *Escherichia coli* and *Serratia marcescens*. So, it was fractionated by open chromatographic column on Silica gel. The fractions 23-33 were mixed and analyzed by Nuclear Magnetic Resonance (1H-NMR, COSY, HMBC and HSQC experiments, dissolved in CDCl3). The 1H-NMR spectrum showed the signals corresponding to the hydrogens of the aromatic ring, characterized by the presence of two signals with chemical shifts at δH 7.30 (2H, *d*, *J* = 9,3 Hz) and 8.70 (2H, *d*, *J* = 9,3 Hz). In the aliphatic region it was also observed two signals in δH 3.00 (4H, *t*, *J* = 7,0 Hz) and 3.45 (4H, *t*, *J* = 7,0 Hz). One hydroxyl group was present in δH 13.19 (2H, *s*). The ESI-MS spectrum indicates 319 *m/z* as the ion *quasi*-molecular (M+1), which was compatible to the molecular formula C20H14O4. The correlation between the observed hydrogens and the carbons were possible to determine by the HSQC and HMBC spectra and the HxH coupling by the COSY spectrum. The analysis allowed the identification of the perylene quinone: 4,9-dihydroxy-1,2,11,12-tetrahydroperylene-3,10-quinone. This is the first report of this compound isolated from the endophytic fungus *Graphium jumulu*, which was isolated from the amazon species *Duroia macrophylla*.

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Keywords: Endophytic fungus, *Graphium jumulu*, Perylene quinone.

IMPLEMENTATION OF THE HPLC-BASED ACTIVITY PROFILING APPROACH TO THE ISOLATION OF ANTIPROTOZOAL COMPOUNDS

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PPNP 06

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Natural products (NPs) play a dominant role in drug discovery for the treatment of human diseases. Particularly, several well-established antimalarial drugs such as quinine and artemisinin have their origins in nature and ethnopharmacological knowledge [1].

Tracking bioactivity in extracts obtained from natural sources, which are complex matrices, remains a highly challenging task. However, high performance liquid chromatography (HPLC) is one of the most powerful tools in chemistry to separate and identify compounds when it is coupled with other analytical tools such as ultraviolet detection and mass spectrometry. When fractions obtained from HPLC separations are tested in a bioassay and both results are combined and matched, an HPLC-based activity profiling is obtained. The HPLC-based activity profiling allow us not only to dereplicate known active compounds, but also to carry out a target preparative isolation of the active principles present in the active fraction, saving resources and time in comparison with the classical methods of isolation [2].

Malaria blights the lives of hundreds of millions of people worldwide. Most of the drugs available to treat this diseas have serious drawbacks. Hence, new drugs are urgently needed. As a result, the HPLC-based activity profiling helps us to speed up and optimize the process of isolation of new drugs from natural sources [3].

The aim of this work was to adjust the HPLC-based activity profiling in the available setting at the Department of Pharmacy of the National University of Colombia, as a new approach to identify and isolate compounds from extracts by applying it to an active plant. The chloroformic extract of *Miconia theaezans* was tested in an *in vitro* assay of inhibition of the development of *Plasmodium falciparum* FCR-3 strain. It showed promising activity with an IC50 of 2,0 µg/mL.

An HPLC-based activity profiling was obtained for the chloroformic extract of *M. theazans*. The HPLC separation was performed, one minute fractions were collected, 45 in total and the resulting chromatogram was matched with the IC50 of each one of the fractions. As a result, we were able to identify the 28-minute fraction, as the most active one (90,2% of *P. falciparum in vitro* inhibition). Currently, we are working in purifying this fraction by HPLC to obtain the isolated compound responsible for the antiplasmodial activity.

Keywords: *Miconia theaezans*, *Plasmodium falciparum*, HPLC-based activity profiling.

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EFFECT OF DIFFERENT EXTRACTION TECHNOLOGIES ON QUANTITY AND QUALITY OF SECOIRIDOIDS IN EXTRA VIRGIN OLIVE OILS. FOCUS ON CALABRIA REGION (SOUTHERN ITALY) MONOCULTIVAR EVOO FROM CAROLEA, OTTOBRATICA AND GROSSA DI GERACE

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PPNP 07

Olive oil is a rich source of fatty acid (mainly Monounsaturated fatty acids) and poliphenolic compounds which are largely attributed both health promotion functions and organoleptic properties. One of the most important health claim authorized from European Union (regulation EUn.432/2012) is: "*Olive oil polyphenols contribute to the protection of blood lipids from oxidative stress*" if EVOOs contains at least 5 mg of hydroxytyrosol and its derivatives (e.g. oleuropein complex and tyrosol) per 20 g of olive oil. Thus, it is very important that extraction technologies maximize the olives content of these substances by favoring the maximum extractive yield in the derived oils.

The aim of the present work was to compare the efficiency of polyphenols extraction by three different oil extraction systems: traditional three-way decanter (3W) with the addition of water, modern two-way decanter system (2W) without the addition of water, and the innovative multi-functional decanter (DMF), from olives of three different cultivar: Carolea, Ottobratica and Grossa di Gerace. Polyphenols content of the three monovarietal olive oil, obtained by the three differents extraction technology, were extracted by the International Olive Council (IOC) recommended method [1] and analyzed by high resolution mass spectrometry (HRMS) and high resolution tandem mass spectrometry (HRMS/MS), in positive and negative electrospray ionization (ESI) modes, coupled to fused-core reverse phase chromatography as previous developed by the research team.

The results showed that the DMF extraction was the more efficient technology in biophenols extraction followed by the 2W and, finally, the 3W method. This could be attributed to the absence of added water in the DMF and 2W processes that minimizes the loss of the hydrophilic component such as polyphenols. The 3W system involves longer contact between oil and added water, and, therefore, allows the transfer of greater amounts of phenols from oil to water.

The results obtained are in good agreement with those of Antonini et al. (2016) [2], which describes a higher content of secoidridoids and lignans in oils extracted by the two-way decanter respect the three-way decanter. In addition, the present study showed that with DMF technology can be obtained oils with the highest content, even if compared with the two-way decanter.

Keywords: extra virgin olive oils, polyphenols, DMF extraction

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MAIN CONSTITUENTS AND ANTIDIABETIC PROPERTIES OF Otholobium mexicanum

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PPNP 08

Two phenols, bakuchiol (**1**) and 3-hydroxybakuchiol (**2**), and two isoflavone glycosides, daidzin (**3**) and genistin (**4**) were isolated from *Otholobium mexicanum* J. W. Grimes (Fabaceae). Moreover, the ability of the raw extract and isolated metabolites to inhibit the enzymes α-amylase and α-glucosidase was evaluated *in vitro*. In the α-amylase assay, the methanolic extract exhibited a moderate inhibitory activity with an IC50 of 470 µg/mL, while inhibition percentages of bakuchiol (**1**), 3-hydroxybakuchiol (**2**), and daidzin (**3**) were less than 25% at the maximum dose tested (1 µM). Genistin (**4**) exhibited a poor activity with an IC50 of 805 µM. In the α-glucosidase assay, the methanolic extract exhibited a strong inhibitory activity with an IC50 value of 32 µg/mL, while 3-hydroxybakuchiol (**2**) exhibited a moderate inhibitory activity with an IC50 of 345 µM. Daidzin (**3**) and genistin (**4**) exhibited lower inhibitory activity with IC50 values of 564 µM and 913 µM, respectively. Bakuchiol (**1**) exhibited a poor inhibitory activity with an inhibition percentage less than 10% at the maximum dose tested (1 mM).

Keywords: *Otholobium mexicanum*, α-amylase, α-glucosidase, Bakuchiol, 3-OH-bakuchiol, Diabetes

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PPNP 09

FUNGI ASSOCIATED TO AGROINDUSTRIAL RESIDUES AS POTENTIAL SOURCE OF NEW ANTIBIOTICS

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One of the best-known aspects of fungi that having a direct impact on the quality of life of humans, is the ability to produce molecules with antimicrobial activity [1]; since they are considered as natural laboratories where a large number of chemical compounds are biosynthesized, especially products from the secondary metabolism. From this kingdom, macroscopic fungi are commonly associated to the production of enzymatic complexes that facilitate the recycling processes of organic matter; this makes that most of studies on this group of fungi focus on their potential use for bioconversion, by-products production or bioremediation processes [2]. In order to explore the antibiotic properties of these secondary metabolites on *Escherichia coli* (ATCC 25922), *Klebsiella pneumoniae* (ATCC 70503), *Enterococcus faecalis* (ATCC 27853), *Staphylococcus aureus* (Wild type) and Methicillin-resistant *Staphylococcus aureus* (mr) (ATCC 43300); macroscopic fungi were isolated from residues of cocoa cultures and identified by using molecular techniques. Afterwards, liquid extracts were produced and assayed by microdilution methodology. From twenty-six (26) fungi tested, the results show that five (5) had stronger antibacterial activity on *S. aureus* wt than others, with percentages of inhibition ranging from 19% to 75%, eight (8) showed inhibition on *S. aureus* (mr) ranging from 2% to 20%, two (2) showed activity on *E. faecalis* ranging from 1% to 27%, two (2) had lowest activity on *K. pneumoniae* ranging from 2% and 3.5% whereas for *E. coli* only one (1) fungus showed antibacterial activity with 21%. An interesting finding in this study is the fact that the highest percentages of inhibition were obtained against *Staphylococcus aureus*. These results can be attributed to the ability of the fungi to produce molecules with selective inhibitory effect on this bacterium as demonstrated by Sujatha and collaborators (2005) [3]. In recent years, the bacterial resistance to drugs have increased significantly worldwide, so the search and the discovery of new antimicrobial compounds from diverse sources as culture residues represent a biotechnological alternative and an economically interesting field to improve sectors such as medicine, agroindustry and cosmetics.

Keywords: Fungi, Residues, Antibiotic, Bacteria.

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PRELIMINARY CHARACTERIZATION OF CHEMICAL COMPOUNDS FROM SKIN OF *Colostethus imbricolus* USING HPLC-ESI-TOF

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PPNP 10

Dendrobatidae family is known for the great diversity of lipophilic alkaloids present in the skin of different colorful species. Nevertheless, there is a gap of knowledge about alkaloid profiles of less colorful species. Recent publications have demonstrated that toxicity is not exclusive of colorful frogs, even in comparisons of single species with polimorphic coloration. *Colostethus imbricolus*, a presumable non-poisonous frog of dark skin coloration has demonstrated to produce paralysis effects on mice after intraperitoneal injection of skin's extracts of this frog [1]. To analyze chemical composition of skin from *C. Imbricolus*, 4 individuals were collected in Cantón de San Pablo, Chocó, Colombia and euthanized by pithing. Full skin extraction with acidified MeOH /H2O (80:20) assisted by ultrasound bath for 20 min was used. For HPLC-ESI-TOF analysis Luna CN column was employed (Phenomenex, 100 mm x 2.0 mm x 3.0 um) and mobile phases selected were A: ACN 95%, FA 10 mM, AF 10 mM. B: H2O, FA 10 mM, FA 10 mM. The only alkaloid previously reported on *Colostethus* was tetrodotoxin (TTX), so we tested the hypothesis of TTX presence using standard TTX (BocScience ®) for comparison. Chromatographic analysis obtained show that TTX was not found in skin's extracts of *C. imbricolus*, which denies our previous hypothesis. Instead, we found other hydrophilic compounds with similar retention time to TTX and still unknown structure.

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EFFECTS OF ORGANOCHLORINE PESTICIDES EXPOSURE THROUGH METABOLIC PATHWAY ANALYSIS BASED ON METABOLOMICS STUDY IN LIVER CELL LINE AND HUMAN BLOOD PLASMA

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PPNP 11

The motivation of this research is to understand the effects of organochlorine pesticide in human exposure. The interest is driven because is not a simple laboratory test to detect and measure organochlorine intoxication. Moreover, there is not a biomarker that could be easily measured in rural areas.In this vein, we set up a metabolomics study in two different systems: in vitro and in vivo samples in order to identify potential biomarkers and the metabolic pathway analysis. For the in vitro experiment, we exposed a HepG2 Cell line to a different organochlorine pesticide (separately and the mixture of the pesticides), the endogenous metabolites were analyzed by GC/MS-TOF and the results of the potential biomarkers were already published [1]. For the in vivo assay we analyse a hundred blood plasma samples from agricultural workers of Quindío department that have been exposed to organochlorine pesticides and thirty samples from no exposed people by GC/MS. We used methoxyamine hydrochloride and MSTFA for plasma derivatization and follow an untargeted metabolomics procedure for data processing using MZmine software. After the data processing we obtained 504 signals. Then, the data was normalized and scaled using log transformation and Pareto scale. Subsequently, a PCA was performed to visualize the data and we found a clear separation between the two groups (exposed and control) using two Principal Components. Afterwards, a PLS-DA was run in order to identify the representative signals for the exposed plasma samples compared to the control. Once the signals were selected the identification was performed using the Human Metabolome Database and PubChem database and we found that 2-oxoglutarate, L-lysine, L-glutamine and Malondialdehyde were the metabolites with the highest fold change. These results were similar to the results obtained in the cell line model. Finally, the metabolic pathway analysis was performed using Metaboanalyst 3.0 using both the metabolites found in plasma and then the metabolites found in the cell line model. The results showed that alanine, aspartate and glutamate metabolism was altered in both blood plasma and in the HepG2 cell line model. This metabolism could be associated with a deficiency in ion transportation through the cellular membrane. The characteristics of this deficiency includes psychomotor retardation, muscular hypotonia, hyperreflexia, lethargy, electroencephalogram abnormalities and refractory seizures, which are symptoms commonly observed in agricultural workers.

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MINERAL PROFILE AND TRACEABILITY OF SICILIAN *Opuntia Ficus Indica* L. Miller (WHITE CULTIVAR)

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PPNP 12

Opuntia ficus indica, originated from the central Mexico, thanks to its ability to adapt to different environmental conditions (Gurrieri et al. 2000), is actually cultivated in different areas of Africa and South Europe. Particularly, Sicily (Italy) is the first producer in Europe of prickly pear fruits for the great importance in agriculture, food and cosmetic industry due to its nutritional value and biological effects (Piga, 2004).
The Sicilian variety *Opuntia ficus indica* L. Miller exists in red, yellow and white cultivars. In this study were analyzed prickly pear fruits of white cultivar, named "muscaredda", from San Cono, protected by the Product Origin Denomination (POD) (EU Regulation n.510/2006), Roccapalumba, guaranteed by a protection brand, and Pantelleria (Trapani). All samples were submitted to analysis of multi-elements profile by ICP-MS and to PCA analysis, in order to individuate how mineral elements may represent a valid marker of geographic origin.
The results obtained showed that Cr, Se, As, Cd and Pb levels were under the LOQ values in all samples. Among samples of the different areas considered, San Cono (Catania) and Pantelleria (Trapani) showed the highest values of Zn, Cu, Ni, Mg, Ca while (Roccapalumba (Palermo) the lowest for all element analyzed. The PCA analysis, in fact, has allowed to verify that the trace elements content is influenced by geographical origin of prickly pear fruits. In fact, it was observed that 2 principal components accounted for 73.67 % of the total variance in the data and, more detailed, PC1 explains 39.00% and PC2 34.67%, respectively.
This study demonstrated that PCA is an integrated tool for the traceability of *Opuntia ficus indica* L. Miller and, at the same time, an useful method of authentication of a protection brand for this typical local fruits.

Keywords: *Opuntia ficus indica* L. Miller, Traceability, ICP-MS, PCA analysis.

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PHYTOCHEMICAL STUDY OF *Muntingia calabura* (MUNTINGIACEAE) AND EVALUATION OF ANTIOXIDANT CAPACITY

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PPNP 13

Muntingia calabura is a plant species belonging to the family Muntingiaceae, which is distributed from Mexico through Central America and the Antilles to Colombia, Venezuela, Peru, Brazil and northern Argentina; Has traditionally been used as an antiseptic and in the treatment of stomach discomfort. Several studies in Southeast Asia have reported the presence of bioactive compounds such as flavonoids, phenolic compounds and steroids and their direct relationship with antimicrobial, anti-inflammatory and antioxidant effects (Jih-Jung Chen et al., 2005).

The main objective of this work was to contribute to the phytochemical study of the leaves of this species and to evaluate its antioxidant capacity. For this purpose, the extracts of hexane and ethanol were obtained from vegetable material collected in the municipality of Honda (Tolima) and identified in the Colombian National Herbarium under COL number 586231, which were obtained through separations by Column chromatography (CC), thin layer (CCD) and preparative thin layer (CCDP), allowed to obtain a mixture composed of an oxygenated sesquiterpene and a lignan (a-eudesmol and sesamina) in addition to the isolation of an aliphatic hydrocarbon (hexatriacontano), a coumarin glycosylated (scopolin) all first determined for the species and finally a flavonoid identified as 3,5,7,3 ', 4' pentahydroxyflavone (quercetin); The structural elucidation of the isolated compounds was carried out using GC-MS and NMR techniques (1H, 13C, COSY, J-MOD, HSQC experiments) and through the comparison with data reported in the literature.

The determination of the antioxidant capacity was performed by the DPPH method to the extracts and fractions obtained, where it was possible to establish that they had a significant uptake of the DPPH radical (greater than 40%) taking as reference the uptake of gallic acid.

Keywords: *Muntingia calabura*, metabolomic, antioxidant capacity.

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COMPARATIVE EVALUATION OF FATTY ACID METHYL ESTERS PRECEDENTS OF STRAINS *Mycobacterium tuberculosis* BY GC-MS

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PPNP 14

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Mycobacterium tuberculosis (Mtb) is the principal causal agent of Tuberculosis (TB). In 2016 the World Health Organization (WHO) reported that about 10.5 million of incident cases and 1.4 million deaths are produced by Mtb around the world. Rifampicin (Rif) and Isoniazid represent the first-line antibiotics used in TB treatment. However, 5% of new cases of symptomatic TB are resistant to the treatment with Rif and Isoniazid. Some characteristics of resistance to antibiotics and host defence mechanisms of Mtb are associated to its complex cell wall consisting mainly of lipids.

Therefore, this work aims to evaluate possible lipids that might serve as biomarkers to differentiate between strains resistant and sensitive to treatment with Rif. In order to do so, three strains of Mtb were growth (one control strain, one susceptible and another resistant to Rif) using Mycobacteria Growth Indicator Tube (MGIT) culture media. Subsequent extraction of the lipids from Mtb was performed with chloroform:methanol (2:1), dried with nitrogen gas and resolubilized in hexane. On the obtained lipid extracts, different esterification processes were evaluated varying concentration, reaction time and temperature. The derivatization reagents studied were tetrabutylammonium hydroxide solution ~ 40% in water/hexane, trimethyl sulfonium hydroxide ~ 0,25M in methanol/methyl *tert*-butyl ether and acetyl chloride/dry methanol. The results show that only the last two methods generated the expected Fatty Acid Methyl Esters (FAMEs), with the latter producing the complete conversion to FAMEs. The FAMEs correspond to methyl tetradecanoate (C14), methyl hexadecanoate (C16) and methyl stearate (C18).

The differences between the chromatographic profiles of FAME in the three strains were evaluated using methyl nonanoate as internal standard. Using an ANOVA, we identified that the factor of the strain is significant to explain the variation in the relative area of the different lipids. In addition, the Tukey test assigns this variation to the fact that the susceptible strain has a smaller relative area of each one of the three FAMEs compared to the other two strains at 95% confidence, allowing for the identification of susceptible strains to be developed by means of GC-MS in relation to the relative area of the methyl esters from the lipids present in Mtb.

Keywords: *Mycobacterium tuberculosis*, Tuberculosis, Derivatization, FAME, GC-MS.

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SYNTHESIS OF A NEW STEROIDAL DIMER DERIVED FROM ESTRONE

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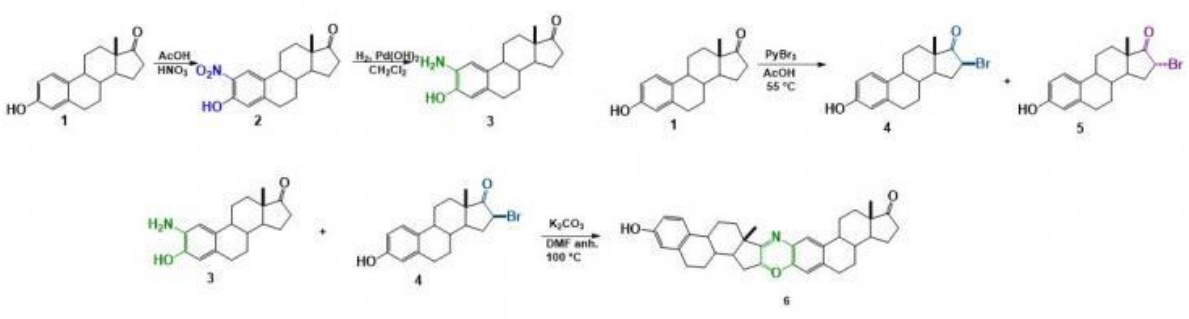
PPNP 15

Steroids are a class of important compounds which exhibit different biological activities in living organisms. The chemical modification of the rings of steroids is a way of altering the functionality of the groups, the size of the rings and numerous structure-activity relationships have been established by such synthetic alterations [1]. Steroid dimers are an important family of pharmacologically active compounds that are predominantly biosynthesized by various marine organisms or synthesized in laboratories [2]. A dimeric steroidal structure possesses unique characteristics that make this kind of compounds interesting targets of study in different specialties. There is remarkable the use of steroidal dimers as citotoxic or antimalarial agents [3].

Herein we describe the synthesis of a new steroidal dimer derived from estrone (**1**) attached through a morpholine scaffold between rings A and D. In the first place it was performed a nitration reaction of the A ring of estrone (**1**) followed by a reduction of the nitro group affording the fragment **3** with a yield of 40%. Moreover the a-halogenation of the D ring of estrone (**1**) gave the diasteroisomeric mixture **4** and **5** with yields of 42% and 6%, the rest corresponds to the raw material. Treatmen of **3** and **4** with K2CO3 in anhydrous DMF at 100 °C drove to the desired compound **6**.



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OPTIMIZATION OF THE PHENOLIC COMPOUNDS PRODUCTION BY *Thevetia peruviana* CELL SUSPENSION CULTURE

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PPNP 16

Thevetia peruviana (Pers.) K. Schum is an ornamental native shrub from Central America. It is widely distributed in tropical regions of America, Asia and Africa. Phenolic compounds with antimicrobial, antioxidant and anti-HIV activity have been identified in fruits and leaves of *T. peruviana* [1, 2]. However, metabolites production in field is highly variable and depending of biotic and abiotic factors. The objective of this research was to optimize the production of total phenolic compounds (PC) and flavonoids (FC) *in vitro* plant cell suspension cultures of *T. peruviana* at shaken flask scale. Culture was established from friable callus obtained from fruit pulp by a protocol previously established [3]. The effect of elicitors, Salicylic Acid (SA) and Methyl-Jasmonate (MeJA), on metabolite production was studied. A factorial experimental design was used to optimize elicitor concentration, elicitation and harvest time. Intracellular concentrations of PC and FC were determined by Folin-Ciocalteu and AlCl3 methods, respectively. In addition, metabolites profile was investigated by thin layer chromatography (TLC) and liquid chromatography (HPLC-DAD). Significant statistical difference was found between PC and FC concentration in fruits, elicited cultures and non-elicited cultures (p-value = 0.000). Optimized conditions were: Elicitation at 4-day of culture and harvest time of 96h. Highest PC and FC concentration were obtained with 300µM of SA, 5.48 ± 0.77 mg of gallic acid equivalent per gram of dry biomass (mgGAE/gDB) and 8.34 ± 0.66 mg quercetin equivalent per gram of dry biomass (QE/ gDB); with 3µM MeJA, 5.13 ± 0.20 mgGAE/gDB and 7.5 ± 0.07 mgQE/gDB; and cultures without elicitor, 4.27 ± 0.57 mgGAE/gDB and 6.32 ± 0.32 mgQE/gDB respectively. TLC showed differential expressions of phenolic and flavonoids compounds during cell growth. Metabolites Quercetin and Kaempferol were identified in elicited cultures by HPLC-DAD. This work presented *in vitro* plant cell suspension cultures of *T. peruviana* as a promising and efficient system for secondary metabolites production.

Keywords: *Thevetia peruviana*, Plant cell culture, Phenolic compounds, Flavonoids, elicitation.

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CHEMICAL AND CYTOTOXIC CHARACTERIZATION OF A GLYCOPROTEIN PRESENT IN THE AQUEOUS EXTRACT OF LEAVES OF *Petiveria alliacea*

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PPNP 17

Petiveria alliacea is a widely distributed worldwide plant known for its ethnobotanical reports going from the treatment of symptoms such as headaches, stomachaches, rheumatoid, inflammation; to diseases like cancer, among others [1], from aqueous infusions and decoctions of both its roots and its aerial parts (stems, leaves, and inflorescences). In the last decades diverse researchers have contributed significantly to the knowledge of the secondary metabolites of this shrub present in several organic extracts, among which are benzaldehyde, benzylthiol, dibenzyl disulfide and dibenzyl trisulfide [3]; nevertheless, the main effects described in diseases and symptoms occur with aqueous extractions of the different parts of the plant; being this type of extracts little studied, finding only two reports of glycosylated proteins present in the roots of this plant [4] which were obtained with water as a solvent. This work was focused on the process of obtaining a glycoprotein present in the aqueous extract derived from leaves of *P. alliacea* by extraction with water and the help of an ultrasonic bath, later to initiate the purification, which was developed through separation of chromatographic methods. The process started with the extraction of the aqueous extract and then fractioned starting with a Sephadex G-100 gel column producing a "crude extract" which was injected into a preparative chromatograph with a Q-sepharose ion exchange column generating 5 chromatographic signals. Each of these signals were collected separately and injected into a Sephacryl S-200 molecular weight exclusion column. The signals obtained in this last column were injected into a Shimadzu Prominence HPLC with DAD detector at 280 nm using a Shodex KW-804.5 molecular weight exclusion column showing the purification of a highly-glycosylated protein with an estimated molecular weight of 5.8 kDa By SDS-PAGE electrophoresis and confirmed by MALDI-ToF mass spectrometry. Cytotoxicity tests on 3T3 fibroblast cells and MCF-7 human cancer cells showed cell viability values ??close to 90%; however, the importance of this research lies in the report of a glycoprotein not reported for this species.

Keywords: Glycoprotein, *Petiveria alliacea*, HPLC chromatography, MALDI-ToF mass spectrometry, Electrophoresis.

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DNA FINGERPRINTING AS POTENTIAL TOOL FOR WHEAT BAKERY PRODUCTS TRACEABILITY

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PPNP 18

Wheat products are of great importance in human diet, consumed yearly in many phases (bread, pasta, pastries, ecc.). Traceability, a major requirement of EU food legislation, is a central issue to protect consumers and producers against fraudulent substitution of quality products in food chain, but the tools available are not always appropriate. It is particularly strict for crop varieties above all for ancient accessions of durum wheat, most of which cultivated in South of Italy and main ingredient of artisanal products such as pasta and bread characterized for their good taste and fine qualities. Wheat traceability is a central issue for the value chain identification, for the qualitative standards maintenance and for authentication. DNA-based markers proved very effective for food authentication.

Durum wheat (*Triticum turgidum* L. subsp. *durum*) is the only tetraploid (AABB, 2n=4x=28) species of wheat of commercial importance that is widely cultivated today. In the cereal industry wheat assignment may play a key role in order to certificate bakery products linked to specific and ancient wheat ecotype. Indeed, traceability of durum wheat cultivated in South Italy and authentication of their cereal-based typical products can contribute to improve profitability and sustainability of durum wheat productions with significant impact on the rural economy of particular geographic areas and on biodiversity conservation. With the goal of developing a durum wheat genetic traceability system for bakery products, the aim of this study was to identify specific microsatellite markers able to discriminate among the most important South Italy durum wheat accessions. A total of 15 microsatellite markers (EST-SSR) were analyzed on 45 flour and pasta samples. Specific microsatellite markers useful for traceability of bakery products and genetic characterization of ancient durum wheat accessions were identified.

The levels of genetic diversity and the performed analysis showed that all of the EST microsatellites tested were polymorphic with a different numbers of variants per locus.

Electropherograms analysis showed, for the first time the coincidence between the result of DNA fingerprint of pasta sample, obtained with Senatore Cappelli flour (Colacchio Foods srl), barcoded with the EST-SSR comp39 marker (191 bp) with Senatore Cappelli flour, due to the same repeat (CT)15 of the mark locus.

This study highlights as microsatellite markers could be applied for authentication of durum wheat in a genetic traceability system to detect adulteration in bakery products.

Furthermore, data confirms the EST-SSR usefulness to build a database to monitor genetic diversity and for traceability of processed food.

Acknowledgment: This work was financially supported by project PON03 PE_00090_1 "*Innovazione di prodotto e di processo nella filiera dei prodotti da forno e dolciari*" and by Research Infrastrcture Saf@med - ***Food Safety platform*** (PONa3_00016). We would also like to show our gratitude to the partner of project Colacchio Foods srl.

Keywords: DNA fingerprint, Traceability, Bakery products, Durum wheat

BIOPROSPECTING: CHALLENGES AND OPPORTUNITIES FOR BIODIVERSITY STUDIES USING COMPUTATIONAL BIOLOGY APPROACHES

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PPNP 19

The exploration and sustainable use of biodiversity is a challenge for scientists in Colombia and represents, in turn, a striking opportunity for the development of different industrial sectors that are increasingly interested in research and development processes. Particularly, the bioprospecting of plants of traditional use in Colombia is focused on the identification of active ingredients with potential use in the cosmetics and nutraceutical industry [1]. For this purpose, an alliance has been established that includes the scientific sector, represented by the Center for Bioinformatics and Computational Biology BIOS and the Alexander von Humboldt Institute, and the industrial sector, represented by four companies in the cosmetic and nutraceutical sector, to generate technological and scientific capabilities in bioprospecting. To achieve this, we intend to establish a model of in vitro and *in silico* analysis of the metabolism of plants of traditional use, which allows the identification of the potential of production of metabolites of interest and facilitates their transfer to the industry. The implementation of *in silico* tools of bioinformatics and systems biology, together with in vitro methods, traditionally used in bioprospecting, constitute an innovative complement to optimize the process of identification of genes and metabolites of industrial interest in plants that have been traditionally used by indigenous and peasant populations. The methodology of analysis for bioprospecting contemplates the genomic and metabolic characterization of the plant [2], complemented with the physicochemical characterization (HPLC - MS-MS and GC - MS profiles) and measurement of the efficacy and safety of the extracts obtained from specific tissues [3], [4]. These characterizations will be integrated within a model that will guide the development of prototypes of cosmetic and nutraceutical products for the participating companies. We expect to obtain a catalog of genes of the studied plant species, their metabolic profiles and metabolic networks that allow us the evaluation of the production of metabolites of interest. In addition, the results will enable companies to make a significant technological leap in their natural products generation processes, based on the sustainable use of biodiversity. This pilot project will allow us to consolidate innovative methodologies in bioprospecting, to promote collaborative work between the scientific sector and industry, to advance the molecular and metabolic knowledge of plants of traditional use and to generate technological and scientific capabilities to obtain value-added products.

Keywords: Bioprospecting, Genomics, Metabolomics, Metabolic networks, Cosmetics industry

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MORPHO-ANATOMICAL, PHYTOCHEMICAL AND CHROMATOGRAPHIC CHARACTERIZATION OF *Gomphrena perennis* var. *perennis* L.

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PPFF 01

Gomphrena perennis var. *perennis* L. "flower of paper" or "always alive of the field" (Amaranthaceae) is a perennial species distributed in South America, mainly Paraguay, Brazil, Argentina and Uruguay [5]. It was used in traditional medicine as a stomach purifying, emollient, and diuretic [3]. Its presence has increased in the last decade because it behaves as a weed tolerant to the herbicide Glyphosate (Round-Up®), widely used in the production system of direct seeding. The objective of this work was to describe morpho-anatomically the vegetative organs: root, stem and leaf of *G. perennis* as well as characterize phytochemistry and chromatographically the extracts of its aerial part. The vegetal material was herborized, botanically identified and analyzed in La Plata, Argentina. Epidermal studies were performed using the diaphanization technique [1], the observations and microphotographs of the evaluated organs were carried out with optical microscope Nikon Photolab II and the study of waxes and foliar ornamentations by scanning electron microscope (SEM) Jeol JSM-35CF. The aerial part was extracted with 70 ° Ethanol by maceration in cold and with solvents of increasing polarity (Dichloromethane, Ethyl acetate, methanol). These extracts are analyzed by characterization reactions [2] and thin layer chromatography (TLC) in mobile phases suitable for each of the main phytochemical groups [4]. The methanolic and hydroalcoholic extract was investigated using HPLC-UV. Morpho-anatomical studies revealed anomalous secondary growth of the herbaceous stems of *G. perennis* with abundant trichomes, a tuberous root system and a structure called xylopodium with the ability to regrow when generating aerial branches of adventitious origin. Its leaves are simple, with Kranz structure of atriplicoide type, which indicates that *G. perennis* has C4 metabolism and it is covered by abundant multicellular trichomes, which have deposits of epi-cuticular waxes called teicodes. Phytochemical tests established the presence of polyphenols, alkaloids, steroids and saponins. The TLC investigation allowed describing the chromatographic profiles of the extracts relative to markers of the main phytochemical groups. The HPLC chromatographic profiles of the methanol and hydroalcoholic extracts were also obtained. All of the above contributes to the botanical and phytochemical knowledge of the Argentinean flora and specifically of *G. perennis.*

Keywords: *Gomphrena perennis var. perennis*, Morpho-anatomical characterization, HPLC profile, TLC profile, Phytochemical characterization

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CHEMOPROTECTIVE EFFECT OF MEXICAN PLANTS

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PPFF 02

The usage of natural products as chemopreventive agents has risen substantially in recent years, since the broad diversity of secondary metabolites (SM) that plants produce is an important source of bioactive compounds. In this context, the Mexican biodiversity plays an important role due to the sheer number of plant species it harbors.

Our group investigates the properties of whole extracts and derived compounds of Mexican plants such as *Buddleja cordata*, *Lippia graveolens*, *Hyptis mociniana* and *Dyssodia tagetiflora*. We have evaluated the antioxidant, cytoprotective and photoprotective effects of the obtained extracts and of a number of characterized SM at the tisular, cellular and molecular levels in bacterial and cellular cultures, as well as mouse models.

The *Buddleja cordata* methanolic extract contains verbascoside. Both the methanolic extract and verbascoside alone had a photoprotective effect on HaCaT cultured cells and on the skin of SKH-1 mice exposed to ultraviolet radiation (RUV), so we considered them candidates for chemoprevention of chronic and acute RUV damage. The global protein expression pattern of SKH-1 mouse skin was disrupted by RUV, and partially rescued when either whole extract or verbascoside alone were applied prior to RUV exposure. Finally, we probed the p53 gene for mutations using HRM-PCR and found that the number of mutations was significatively reduced by either treatment.

The *Lippia graveolens* methanolic extract, was rich in galangine. In a bacterial model, cell death was considerably reduced due to the photoprotective effect of the whole extract. In SKH-1 mice, this extract delayed the onset of skin lesions substantially and prevented the development of malignant cells within them, as demonstrated through histological analysis.

The *Hyptis mociniana* methanolic extract protected bacterial cells from RUV damage for up to 75min, and showed good antioxidant activity. Its photoprotective effect in the SKH-1 mouse model is currently under evaluation.

Quercetine, methoxliated quercetine, hiperoside and avicularine were present in the *Dyssodia tagetiflora* methanolic extract. The whole extract and each of the isolated compounds showed good antioxidant activities. We assayed this extract in *V. faba* roots and found no genotoxicity and a cytoprotective effect.

Currently, our research group aims to evaluate the DNA damage response under the effect of the protection exerted by Mexican plant extracts and the SM present in them, as part of our constant search for new chemopreventive agents.

Keywords: Chemoprevention, Secondary metabolites, Antioxidant activity, Photoprotection, Cytoprotection.

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CHEMICAL CONSTITUENTS OF *Muehlenbeckia tamnifolia* (KUNTH.) MEISN. (POLYGONACEAE) AND ITS *IN VITRO* Alpha-AMILASE AND Alpha-GLUCOSIDASE INHIBITORY ACTIVITIES

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PPFF 03

Muehlenbeckia tamnifolia (Kunth.) Meisn., known as *Anku yuyu lutu yuyu*, is used by indigenous communities in Ecuador to treat kidney diseases, in baths to relieve bone pain, as mouthwash for toothache and, in combination with other plants, to treat bumps and inflammation. It is also applied as a disinfectant and to treat purulent skin wounds. Previous chemical studies on the roots of *M. tamnifolia* showed the presence of anthraquinones such as chrysophanic acid and emodin. The aim of this work was to evaluate the inhibitory activities of different extracts and isolated compounds of *M. tamnifolia* on α-amylase and α-glucosidase.

The phytochemical investigation of *M. tamnifolia*, collected in Loja, Ecuador, led to the isolation of nine known compounds identified as: lupeol acetate, cis-*p*-coumaric acid, lupeol, β-sitosterol, trans-*p*-coumaric acid, linoleic acid, (+)-catechin, afzelin and quercitrin. The structures of the isolated compounds were determined based on analysis of NMR and MS data, as well as comparison with the literature. The hypoglycemic activity of crude extracts and isolated compounds was assessed by the ability to inhibit α-amylase and α-glucosidase enzymes. The hexane extract showed weak inhibitory activity on α-amylase, with an IC50 value of 625μg·mL−1, while the other extracts and isolated compounds were inactive at the maximum dose tested. The results on α-glucosidase showed more favorable effects; the hexanic and methanolic extracts exhibited a strong inhibitory activity with IC50 values of 48.22 μg·mL−1 and 19.22μg·mL−1, respectively. Four of the nine isolated compounds exhibited strong inhibitory activity with IC50 values below 8 μM, much higher than acarbose (377μM). Linoleic acid was the most potent compound (IC50 = 0.42μM) followed by afzelin, (+)-catechin and quercitrin.

Keywords: *Muehlenbeckia tamnifolia*; α-Glucosidase Inhibition; α-Amilase inhibition; Linoleic acid

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CHEMICAL AND ENANTIOMERIC COMPOSITION OF THE ESSENTIAL OIL DISTILLED FROM FLOWERS OF THE ECUADORIAN SPECIES *Lepechinia mutica* (BENTH.) EPLING (LAMIACEAE)

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PPFF 04

Lepechinia mutica (Benth.) Epling is an endemic plant of Ecuador, present only in the province of Loja, where it grows between 2200 and 3400 m1. The volatile fraction composition of leaves from this species was first described in literature in 20032. However, in a recent study, our group performed a new analysis of the same essential oil, based on updated literature and with enantiomeric and sensorial evaluation. These results are currently in press (June 2017).

In this communication we are presenting, for the first time, the chemical and enantiomeric composition analysis of the volatile fraction, distilled from flowers of the same species. Its yield is similar to the one of leaves (about 0.40% w/w) but the chemical composition is quantitatively quite different.

The qualitative analysis was performed by GC-MS, in an Agilent Technologies 6890N GC, coupled with a single quadrupole mass spectrometer detector model 5973. The GC was configured with a 30 m DB-5ms column, with internal diameter of 0.25mm and stationary phase thickness of 0.25µm. The injector was operated in split mode (30:1), with He as carrier gas (flow: 1ml/min). The injections (1µl) were carried out at the concentration of 1µl/ml in cyclohexane, with the oven operating in thermal gradient, according to the following program: 60° for 5', from 60° to 180° at 3°/min, from 180° to 250° at 15°/min, 250° for 5'. The MS was set in SCAN mode, with a mass detection range of 45-350 amu. The identification of constituents was obtained by comparing each EIMS spectrum (70 eV) and linear retention index (C8-C22 n-alkane series) with literature3. Quantitative analysis was performed by GC-FID, quantitating each metabolite with a compound of the same chemical family as external standard. Quantitative analysis was then converted to percentage, referred to total injected amount.

Keywords: *Lepechinia mutica*, Essential oil, GC-MS, Ecuador

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CONTRIBUTIONS TO THE PHARMACOGNOSTIC STUDY OF *Eugenia florida* DC. (MYRTACEAE)

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PPFF 05

The vegetable raw material is one of the most important factors in the processing of herbal products and their identification and purity are indispensable to the safety and efficacy of these products. *Eugenia florida*, known as black cherry, belongs to one of the most representative genera of the Myrtaceae family. The objective of this work was to evaluate samples of *E. florida* aiming to establish important parameters for its diagnosis and for the control of the quality of vegetal products. For the anatomical and histochemical characterization, adult leaves of the 4th and 5th nodes were used and paradermic cuts were made on the adaxial and abaxial surfaces, transversal in the regions of the central rib, intercostal and border, in the median portion of the leaf, besides the median and distal from the petiole, at the free hand with steel blade.

The sections were clarified, neutralized and stained with safranin and astra blue. The diagnostic anatomical structures were compared with data from the specific literature, revealing that the best parameter for diagnosis of the species is the reniform cell that covers the subepidermal secretory structure. Histochemical tests revealed the presence of phenolic substances, alkaloids, and lipids. Physical integrity evaluation tests, as recommended in the 2nd edition of the Brazilian Pharmacopoeia, were carried out with two lots of previously dried and crushed leaves of *E. florida* collected at Oswaldo Cruz Foundation campus. The determination of desiccation loss was 5.9% ± 0.1% and 8.8% ± 0.1%, respectively. The values found for total ash contents were 6.9% ± 0.005 and 5.8% ± 0.005 and for acid insoluble ash were 0.62% ± 0.002 and 0.65% ± 0.002.

The evaluation of the metabolic production of *E. florida* was made through thin-layer chromatography using mobile phase and specific developers for the main classes of secondary metabolites. The results suggest the presence of tannins and other polyphenols, flavonoids, anthraquinones, triterpenoids, steroids, coumarins, saponins. These results are relevant for the control of the quality of vegetal products based on *Eugenia florida*

Keywords: Myrtaceae, Quality control, Anatomy, *Eugenia*

HYPOGLYCEMIC ACTIVITY OF EXTRACTS FROM WILD AND in vitro PLANTS OF Tecoma stans

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Ethnopharmacological relevance: *Tecoma stans* is a plant traditionally used as an alternative treatment for diabetes in Mexico, whose effect has been proven by several studies, this plant accumulate compounds as tecomine, tecostanine, chlorogenic acid, luteolin, verbascoside, apigenine among others. However the current studies are not conclusive from which are the compounds responsible for this activity. In the same way, the objective of this work was to obtain fractions with hypoglycemic activity. Materials and methods: the wild plant material of *T. stans* was collected at the University of Papaloapan Campus Tuxtepec in Oaxaca, Mexico. A hydroalcoholic extract (HAE) was performed, followed by a bipartition, obtaining the aqueous phase fraction (APF) and the organic phase fraction (OPF). Subsequently the OPF (2.5g) was subjected to a phytochemical study and chemical fractionation. The extracts and fractions F12, F14 and F16 were subjected to hypoglycemic evaluation due to it compounds groups profile present, using diabetic CD-1 mice, induced by intraperitoneal administration of streptozotocin (STZ) (40mg/kg) and Nicotinamide (68mg/kg). The *in vitro* seedlings of *Tecoma stans* in a culture medium of Murashige & Skoog (MS), were collected at 2 months of age, subsequently the *in vitro* hydroalcoholic extract (HAE *in vitro*) was performed, which was subjected to a bipartition obtaining an aqueous phase fraction (APF *in vitro*) and organic phase fraction *in vitro* (OPF *in vitro*), OPF *in vitro* was subjected to chemical fractionation and hypoglycemic evaluation using diabetic CD-1 strain mice. Conclusions: The HAE wild and HAE *in vitro* plant extracts showed hypoglycemic activity (37.09% and 15%, respectively at doses of 270 mg/kg. The OPF wild and its fraction 16 both presented hypoglycemic activity with 62.23% and 52.57% of decrease of glucose in blood, respectively at doses of 50mg/kg. This hypoglycemic activity could be attributed to bioactive compound as chlorogenic acid.

Keywords: *Tecoma stans*, Diabetes, Hypoglycemic activity, Phytochemical.

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IN VIVO EFFECTS ON INTESTINAL TRANSIT AND BEHAVIOR OF THE ARGENTINIAN PLANT *Fuchsia magellanica*

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Fuchsia magellanica Lam. (Onagraceae) grows in the cold forest of Patagonic Andes mountains, in Argentina and Chile. It is known as "chilco" and leaves and flowers have been traditionally used by mapuche community to alleviate uterine and intestinal spasms. It was also domesticated in the temperate Pampa region of Buenos Aires [1]. Its pharmacological activities never have been studied, but in previous communications we showed that tinctures of leaves and tinctures of flowers from both regions had antispasmodic effect in *ex vivo* experiments on intestinal smooth muscle [2] and isolated rat uterine tissue [3]. The mechanism of action evaluated through concentration-response curves was the non-competitive inhibition of both, cholinergic contraction and Ca2+ influx [2,3]. In the phytochemical profile there were detected flavonoids such as quercetine, hiperoside, isoquercitrin, canferol and vitexin. The aim of this work was to evaluate the *in vivo* effect of tincture of *Fuchsia magellanica* leaves from Patagonia (Fm-P) and from Buenos Aires (Fm-BA) on the intestinal transit and behavior tests such as open-field and elevated plus-maze.

Leaves of plants from Patagonia were collected in the summer of 2014, and leaves of plants from Buenos Aires were collected in the winter of 2013, in both cases leaves were dried at air. Tinctures (T) were prepared by maceration in ethanol 70° and dilluted in saline solution the day of the experiment. Tests were performed in Swiss mice (20-30g weight). The intestinal transit was evaluated by i.p. injection of T 30 min before the oral administration of the osmotic laxative PEG3350, followed after 30 min by 10%carbon-1% CMC in saline. After other 30 min the % of small intestinal length covered by carbon was measured. A negative control with ethanol-saline and a positive control with 5mg/kg atropine were done. The open-field test was performed to measure the number of crossed lines (CL) and rearings (Re) of mice in 5 min versus time. In the plus-maze the time remained and the entrance number in open and closed arms were measured. In both tests 0.5 mg/kg diazepam was used as positive control.

The T-Fm-P (73.5mg/kg) reduced the intestinal transit to 28.64 ± 6.83% while atropine reduced it to 15.26 ±6.01% (all $p<0.05$ vs vehicle), but the T-Fm-BA (62.5mg/kg) changed it to 48.74 ±6.82% (NS vs vehicle of 55.12 ±6.39%) (n = 8). In the open-field test both T reduced CL and Re during the first 30-60 min. However, in the plus-maze neither of T significantly changed the ratio of open/closed arms entrances or time.

The tinctures of *Fuchsia magellanica* showed in vivo inhibition of intestinal transit, in agreement with the *ex vivo* results, as well as a slight sedative effect but were not anxiolitic.

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CHARACTERIZATION AND ANTICONVULSANT EFFECTS OF A *Cannabis sativa* EXTRACT

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Epilepsy is a chronic neurological disorder that affects people of all ages around the world, compromising their quality of life. About 50 million people have epilepsy, making it one of the most common neurological disorders. Approximately 80% of these patients live in poor and middle-income countries [1]. Of the total number of patients, 70% have a good answer to treatment, while the remaining 30% is resistant to currently available pharmacological therapy [2]. In Colombia, according to a neuroepidemiological study published in 2003, there are approximately 400,000 people with active epilepsy [3]. Currently, there is a need to find new, safe and effective alternatives for the treatment of epilepsy, especially against those forms resistant to conventional pharmacological therapy. For that reason the aim of this work is, estimate the profile of cannabinoids of a chloroform extract from *Cannabis sativa* variety cultivated in Colombia and evaluate the anticonvulsive effect in a murine model.

This study was done with material cultivated and collected in the Faculty of Agricultural Sciences of the Universidad Nacional de Colombia, Bogotá. A voucher specimen was deposited in the Herbario Nacional de Colombia. With the remaining material, a chloroform extract was obtained by percolation [4]. Qualitative (thin layer chromatography and colorimetric tests) and quantitative tests (GC-MS/EI and GC-FID) were performed for cannabinoid detection and characterization [5]. The chloroform dried extract, dissolved in an oily vehicle, was administered to ICR mice, supplied by the Department of Pharmacy's Bioterio. The anticonvulsive potential of the extract was evaluated in a series of tests at three different doses (75, 150 and 300 mg/Kg; p.o) [6]. Preliminary results showed the protective effects of the *Cannabis* extract, in a dose dependant manner, against maximal electroshock induced seizure model. Our results contribute to support the therapeutic potential of this species as an anticonvulsant. Further studies are needed to confirm this activity.

Keywords: Epilepsy, Cannabinoids, Anticonvulsivant, Murine model, Electroshock

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EFFECTS OF FEMALE SEX HORMONES ON THE HEALING OF GASTRIC ULCER IN RATS TREATED WITH *Eugenia punicifolia*

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Eugenia punicifolia is an Amazonian medicinal plant popularly used in the treatment of inflammation, wounds and infections. This study evaluated the healing effect of the hydroalcoholic extract from the leaves of *E. punicifolia* (HEEP) in Wistar rats. The gastric ulcers were induced by nonsteroidal anti-inflammatory drugs (NSAIDs) [1] or ethanol 80% [2]. At NSAIDs model, the rats (male and intact females) received 15 mg/kg of indomethacin for 3 consecutive days. On the 4th day, animals received the respective treatments: vehicle (saline - 0.9%, 10mL/kg), lansoprazole (LZ; 30mg/kg) and HEEP (125mg/kg). After 2 days of treatments, the animals were killed and the stomach removed for analysis of lesion area and biochemical parameters [myeloperoxidase (MPO), pro and anti-inflammatory cytokines].

For the experiment with ethanol, the rats (male, intact and ovariectomized females) received 80% ethanol (p.o) at dose of 8mL/kg for 2 consecutive days. On the 3th day, animals received their respective treatments: vehicle, carbenoxolone (CARB; 100mg/kg) and HEEP. After the 1st, 2nd, 4th and 6th day of treatment, the animals were killed and the stomach removed for analysis of lesion area and biochemical parameters [MPO, superoxide dismutase, malondialdehyde, catalase and reduced glutathione (GSH)]. The results are expressed as mean ± S.E.M. and statistical significance was determined by ANOVA followed by Dunnett's test ($p<0.05$). Animal Research Ethical Committee, n. 675. On NSAIDs model, the treatment with LZ and HEEP was able to heal the gastric ulcer only in male rats after 2 days of treatments (90.43% and 66.07%, respectively) when compared to the control group (vehicle).

These results indicate that HEEP administered for 2 days presents healing effects in male rats against the NSAIDs induced lesions decreasing de IL-5 levels (pro-inflammatory cytokine, 30.76%). In the model of ethanol 80%, the treatment with CARB and HEEP was able to heal the gastric ulcer in male and intact females rats after 4 consecutive days (82.52% and 63.23% [male]; 69.47% and 78.10% [intact female], respectively) and in ovariectomized females rats after 6 consecutive days (65.24% and 67.35%, respectively) of treatments when compared with control group (vehicle). Our results indicate that HEEP administered for 4 days presents healing effects against the ethanol-induced lesions decreasing MPO activity (a marker of inflammation, 40.21%, male) and increasing GSH levels (antioxidant, 1,12x, intact female). HEEP reduces MPO activity (21.03%) after 6 days of treatment in ovariectomized females. HEEP was able to inhibit gastric lesions, protecting the mucosa of highly damaging agent such as NSAIDs and ethanol and we can observe that there is interference of the female sex hormones in the healing of the ethanol-induced lesion, since the intact rats showed healing before the ovariectomized rats and corroborating, thereby, with an indication of this popular plant for wounds and infections.

Keywords: *Eugenia punicifolia*; Ethanol, Nonsteroidal anti-inflammatory drug, Antioxidant, Anti-inflammatory; Sex hormones

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PROTECTIVE EFFECT OF COLOMBIAN *Scutellaria spp*. AGAINST C2-CERAMIDE-INDUCED OLIGODENDROGLIAL DEATH

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PPFF 10

Oligodendroglial death contributes to the development of multiple sclerosis (MS), the most common human demyelinating disease. Disturbances of the sphingomyelinase-ceramide pathway are implicated in apoptosis of human oligodendrocytes in MS [1] and C2-ceramide-induced cell death in MO3.13 cell line has been considered to model the oligodendroglial apoptotic changes in MS [2]. Therefore, novel therapeutic alternatives are needed directed towards oligodendrocyte protection [3]. Flavonoids isolated from various *Scutellaria* species have exhibited *in vitro* and *in vivo* neuroprotective activity, being proposed as potential therapeutic approaches for neurodegenerative disorders [4]. The Andean region is one of the greatest centres of *Scutellaria* species diversity [5] and Colombia harbours 18 species [6], but their chemistry and neuroprotective potential remains to be explored. In this study, we investigated the protective effect of five Colombian plants of the genus *Scutellaria* against C2-ceramide-induced cell death in MO3.13 cells. Ethanolic extracts of roots, stems and leaves of *S. incarnata* (*Si*), *S. pseudocoleus* (*Sp*), *S. racemosa* (*Sr*), *S. ventenatii* (*Sv*) and *S. ventenatii* var. *trianae* (*Svt*) were obtained by percolation. Preliminary phytochemistry assays detected flavonoids and terpenoids. MO3.3 cells were differentiated for 72-96 hours in DMEM without serum and containing 100nM PMA (4-β-Phorbol 12-myristate 13-acetate). Cell viability was measured by MTT (3-(3,4-dimethylthiazol-2-yl)-2,5-diphenyl-tetrazolium bromide) assay. Initially, cytotoxicity of increasing concentrations of C2-ceramide (25, 35, 50 and 100µM for 18 and 24 hours) and cytotoxicity of the extracts (25, 75, 125 and 250µg/mL for 24 hours) were evaluated in differentiated MO.13 cells. Subsequently, the protective effect of pre-treatment with 25, 75, 125 and 250µg/mL of the extracts for 24 hours were evaluated in differentiated MO3.13 cells upon exposure to 35µM of C2-ceramide for 18 hours. Cell viability was increased significantly by 75, 125 and 250µg/mL of *Sv* roots extract, compared to cells exposed to C2-ceramide alone (cell viability=49.3%); extracts of stems, leaves and roots of *Sr*, roots and leaves of *Si*, and roots of *Svt* were also protective. The results obtained indicate that *Sv* roots have a protective effect against C2-ceramide-induced cell death in the oligodendroglial human cell line MO3.13.

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Keywords: Oligodendrocytes, C2-Ceramide, Apoptosis, Neuroprotection, *Scutellaria*

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PRELIMINARY EVALUATION OF THE ANTITUSIVE ACTIVITY OF THE BRACTS OF *Bougainvillea glabra* CHOISY

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Bougainvillea glabra choisy is a plant native from Brazil and distributed in South America, which has a range of colors in its bracts ranging from white, pink, purple, yellow and orange, traditionally used in the ornamental field. In several studies have been determined its pharmacological activity to treat gastrointestinal and some of respiratory disease, but any investigation of antitussive activity has been performed.

To evaluate the antitussive activity of the alcoholic extracts of the bracts of purple and orange *Bougainvillea glabra choisy* by preclinical tests in albino mice of the CD1 strain.

The research was carried out at the "Planta Piloto de Farmacia", Research Laboratory and Biomodulo-Bioter- of the Universidad Tecnica de Machala, Ecuador. The study sample was collected in two areas of the City of Machala, washed and dried at room temperature for 48 hours and then stoved at 40 ° C for 48 hours, followed by milling to obtain particles up to 1mm diameter. The crude drug was subjected to quality controls such as: microscopic and macroscopic analysis; Physical-chemical analysis such as: moisture, total ash, soluble substances, phytochemical screening, thin layer chromatography, and quantification of secondary metabolites (phenols and alkaloids) and antioxidant activity. The ethanolic extract of the bracts of *Bougainvillea glabra choisy* was obtained by the maceration method, and its quality was evaluated by organoleptic and physical-chemical tests. The antitussive activity was evaluated by preclinical test, inducing the cough to the animal in experimentation by means of exposure of 25% ammonium solution, observing the frequency and latency of the cough within 5 minutes; for that were structured 7 groups of 5 animals having Group I as control to observe that the animals were without evidence of cough, to group II with induction of cough for validation and verification of the method. To group III, IV, V, VI, VII were applied the following pharmacological treatment: 30 mg/kg of Codeine, 250mg/kg extract orange *Bougainvillea glabra* , 500mg/kg orange *Bougainvillea glabra* , 250mg purple *Bougainvillea glabra* and 500mg purple *Bougainvillea glabra* respectively. Administration of pharmacological treatment was done 30 minutes before cough induction.

Pharmacological results were expressed as mean ± standard error of the mean. The statistical analysis used was the analysis of the variance of one path followed by the Dunnet test, using the group that did not receive any type of treatment as a control group. * P <0.05 were considered statistically significant differences. GraphPad Prism 5 software, version 5.03 for Windows was used. The values of humidity oscillate between 6-7% and total ashes between 6.5-7%, total solids in the purple bract (1.61%), were greater than the orange one (1.42%). Alkaloids (+++) phenols (+++) antioxidant (+++). The preclinical test of the dried extract obtained from *Bougainvillea glabra choisy* bracts suspended in 5% Tween 80 showed antitussive activity in doses of 250mg and 500mg.

The bracts of *Bougainvillea glabra choisy* have antitussive activity and can be used to continue research for the development of phytopharmaceuticals.

Keywords: Antitussive, Bracts, *Bougainvillea*, Preclinical test.

IN VITRO EVALUATION OF INTERACTION OF ANTI-INFLAMMATORY, WOUND HEALING AND ANTI-LEISHMANIAL ACTIVITIES. AN USEFUL STRATEGY TO IDENTIFY HIT COMPOUNDS FOR DRUG DEVELOPMENT TO TREAT CUTANEOUS LEISHMANIASIS

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Cutaneous leishmaniasis is a disease caused by infection with *Leishmania* parasite. Up to now, there is no effective vaccine for prevention of disease, and treatment options have important drawbacks mainly related to toxic effects that force patients to interrupt treatment and development of resistance by the parasite. The use of combined therapies is a strategy aimed to reduce doses of compounds and duration of treatment in order to reduce side effects caused by high doses of toxic compounds. On the other hand, combining properties among compounds could enhance the desired effect. In this study, we evaluated *in vitro* the effect on the anti-leishmanial effectiveness when compounds with anti-leishmanial activity are combined with compounds that have immunomodulatory (anti-inflammatory and healing) properties.

Compounds with anti-inflammatory and wound healing properties were identified *in silico* by bioinformatics tools. The selected compounds were tested *in vitro* for cytotoxicity and anti-leishmanial activity in intracellular amastigotes of *L. (V) pananensis*. The effect of interactions between drugs was predicted by bioinformatic methods. Potential interactions were detected using the CDK (Chemistry Development Kit) software. Interactions were scored in the range of 0 to 1, and similarity values ??were defined as > 0.7. The *in silico* predicted drug interaction was validated in intracellular amastigotes of *L. (V) panamensis*. Compound mixtures were evaluated at three different concentrations. Data were analyzed using Compusyn program, according to Dose Reduction Index (DRI), Combination Index (CI) and Isobologram. Interactions were defined as synergy, additivity, or antagonism.

Bioinformatic analysis showed that all mixtures could be made, except for the mixture of Alendronate and Phenylbotazone, when used together it could cause gastric toxicitySeven mixtures of compounds with anti-inflammatory, wound healing and anti-leishmanial properties were assessed for effectiveness against *Leishmania* parasites: phenylbutazone / azelaic acid, phenylbutazone / salicylhydroxamic acid, phenylbutazone / propanteline bromide, propanteline bromide / azelaic acid, propylamine bromide / salicylhydroxamic acid, propanteline bromide / alendronate, adapalene / alendronate. The most representative association was that observed between adapalene and alendronate, but also phenylbutazone with salicylhydroxamic acid and propanteline bromide with salicylhydroxamic acid. These combinations allowed a reduction of required doses to produce an anti-leishmanial activity *in vitro.*

The combination of compounds is a useful methodology to reduce side effects without sacrificing the effectiveness of the compounds, and even as in the case of the Adapalene / Alendronate blend, their action can be enhanced and achieved the desired effect over longer periods Short of time and using smaller doses. The use of drug combinations is a strategy that has been widely used, because it decreases the dose required for the activity, the dose-related adverse effects and the resistance phenomena are frequent

Keywords: Interaction, Bioinformatic, Leishmaniasis, Anti-inflammatory, Wound healing

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PHARMACOGNOSTIC CARACTERIZATION AND MINERAL COMPOSITION STUDY OF ALGARROBO (*Prosopis pallida*)

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The algarrobo (*Prosopis*) is one of the Ecuadorian plant species considered ancestral, particularly for the communities of the south of the country. It is used for fodder in field animals, fertilizer in agriculture, as well as food consumed as a drink or prepared from carob syrup. Although some varieties of the *Prosopis* species are reported worldwide, ther are not enough studies of the two cultivated in Ecuador, *P. pallida* and *P. juliflora* [1] are available. The species has been associated with certain benefits in preventing anemia, maintaining healthy muscles, improving brain activity, reducing constipation symptoms [2]. In addition, it is attributed to energizing and nutritional properties [3], which would be associated with its mineral content. In the present work, the pharmacognostic characterization of the species *Prosopis pallida* is performed, considering the study of the bark, leaves and the fruit of the species. And the mineral contents are correlated in each of the analyzed parts by the application of inductive coupling plasma spectroscopy (ICP) technique. The results have been satisfactory and corroborate the previously described medicinal uses for the species, properly by their detected mineral content.

Keywords: Algarrobo, Carob Tree, *Prosopis pallida*, Mineral Composition, ICP, Pharmacognostic study.

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SCREENING OF COLOMBIAN MEDICINAL PLANTS AND ANTIMALARIAL ACTIVITY OF *Leandra subsidiaria*

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Tropical parasitic diseases, such as malaria, blight the lives of hundreds of millions of people worldwide. Most of the drugs available to treat these diseases have serious drawbacks. Hence, new drugs are urgently needed. Natural products (NPs) play a dominant role in drug discovery for the treatment of human diseases. Particularly, several well-established antimalarial drugs such as quinine and artemisinin have their origins in nature and ethnopharmacological knowledge [1,2].

The aim of this work was to perform a screening of antiplasmodial activity in plants with popular use related to malaria. Four species were selected and collected, *Miconia aeruginosa*, *Leandra subseriata*, *Austroeupatorium inulifolium* and *Miconia theaezans*. From each one of the collected plants, a whole ethanolic extract was prepared. Separately, three successive extractions with increased polarity solvents hexane, dichloromethane, and methanol, were prepared [3].

Eighteen extracts were tested *in vitro* to assess their antiplasmodial activity. The inhibition of development of *Plasmodium falciparum* FCR-3 strain was performed. The most active extracts were chloroformic from *M. theaezans* (IC50 2,0µg/mL), chloroformic from *A. inulifolium* (IC50 2,3µg/mL), and methanolic from *L. subseriata* (IC50 13,2µg/mL). From *A. inulifolium* there were already reports about isolation of active compounds. As a result, we chose to investigate the *M. theaezans* and *L. subseriata* extracts. We present in here the preliminary results obtained for the latest.

Regarding the phytochemical research on *L. subseriata*, a preliminar phytochemical analysis was performed to find out the presence of secondary metabolites. Additionally, an open column fractionation was performed, as a first step to isolate the active compounds present in the extract.

Alkaloids, flavonoids, tannins, saponins, and triterpens/steroids were found in the ethanolic extract. The fractions obtained by open column chromatography are rich in flavonoids. We already started a separation process by semi-preparative HPLC chromatography to purify and isolate them.

Keywords: *Leandra subseriata*, *Plasmodium falciparum*, Anti-plasmodial activity.

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IN VITRO ANTINEOPLASTIC EFFECT OF PLANT EXTRACTS USED IN THE COLOMBIAN TRADICIONAL MEDICINE AGAINST TWO CANCER CELL LINES

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Breast and cervical cancer are common types of cancer affecting Hispanic women [1]. In 2013, about 220.000 cases of breast cancer were diagnosed and 40.000 cases were fatal. With regard to cervical cancer, 12.820 new cases and 4.210 deaths were estimated for 2017 by the American cancer society. Although trends are alarming for Hispanic women, this type of cancer also affect any woman who is or has been sexually active, mainly those which have or have had human papillomavirus (HPV) [2]. Hence, an effective management and treatment for cancer is undoubtedly crucial. In this context, the ethnopharmacology research of botanical species has proved to be a useful approach to find potential antineoplastic agents. In this work, we evaluated the growth inhibitory effect of extracts obtained of ten Colombian Caribbean medicinal plants, against two cancer cell lines, MDA-MB-231 (breast) and HeLa (cervical), employing the methyl-tetrazolium bromide colorimetric method (MTT) [3].The extracts were classified into three categories as: active (IC50≤20 µg/ml), moderately active (20

Among the extracts tested, four showed inhibitory effect on the growth of cell lines. The *Mammea americana* extract was active on both cell lines (IC50 MDA-MB-231=9.62µg/mL and IC50 HeLa=6.89µg/mL). *Thevetia peruviana* extract was active on MDA-MB-231 (IC50=9.44µg/mL) and moderately active on HeLa (IC50=26.30µg/mL). Others extracts as *Tabernaemontana cymosa* and *Momordica charantia* affect the cell lines growth in a moderately form. Regarding the SI, with exception of *T. cymosa* and *M. charantia* (SI<2), all the active extracts exhibits a high degree of selectivity for both cell lines.

These extracts represent a promising source of cytotoxic compounds that should be further explored, aiming to obtain new active molecules that improve the therapeutic arsenal available for breast and cervical cancer treatments.

Keywords: Cytotoxic activity, Cervical cancer, Breast cancer, MTT.

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ANTI-NEOPLASTIC POTENTIAL OF THE A PRIMARY FRACTION FROM THE CALYCES OF *Physalis angulata* L.

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Colorectal cancer (CRC) is a life-threatening disease that historically has affected the population of highly developed countries. Nevertheless, its presence in developing Latin-American countries is rising, to the point that it was the fourth cause of death by cancer in Colombian men and the fifth in women back in 2011 [1]. *Physalis angulata* L. (Solanaceae) is a plant used in Colombian folk medicine due to a wide range of biological activities like antibacterial, antimalarial, antianemic, antipyretic and anti-inflammatory [2]. In this work, we evaluated in deep the anti-neoplastic potential of a fraction (F0-2) of the calyces of *P. angulata*, previously found active on the HT-29 colon cancer cell line (IC50=13.8µg/mL) at our lab.

F0-2 was obtained from the total ethanolic extract of the *P. angulata* calyces by liquid-liquid partition. The cytotoxicity of F0-2 on a HT-29 cell line 3D culture was evaluated using the hanging drop technique and the MTT method, the inhibitory concentration 50 (IC50) was calculated. The effect of F0-2 on cell migration was assessed using the wound healing method with the Ibidi µDish 35mm,high tool and ImageJ. Flow cytometry was employed to evaluate the cell cycle progression and apoptosis induction when cells were treated with F0-2.

The wound healing assay showed that the non-toxic concentrations of F0-2 did not affect significantly the migration ratio of CRC cells. At 72 hours the wound closure corresponded to 71.66% (control), 82.78% (F0-2 12.5µg/mL) and 75.49% (F0-2 6.25µg/mL). Interestingly, in the 3D cytotoxicity assay F0-2 showed a similar cytotoxic potential compared to the 2D model, with IC50=12.86±2.73µg/mL, which suggest that the effect of F0-2 is not diminished in hypoxic metabolic conditions. Previous reports of extracts and compounds from *P. angulata* demonstrate its ability to perturb the cell cycle and the apoptotic process [3,4]. In agreement, our findings showed that F0-2 induced arrest in G2/M phase (9.75%) and increased significantly the proportion of apoptotic cells (50%).

Our results indicate the therapeutic potential of *P. angulata* calyces as an alternative treatment for CRC. Further investigation is warranted for the identification of the bioactive components of F0-2 and the specific molecular mechanisms responsible for its effect.

Keywords: *Physalis angulata*, HT-29, Cytotoxicity, Colorectal cancer.

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ANTI-INFLAMMATORY ACTIVITY OF ESSENTIAL OILS AND EXTRACTS OBTAINED FROM COLOMBIAN PLANTS

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Inflammation is a complex process of events that occurs in response to harmful stimuli, trauma or infection. Although this response is helpful for the host, persistent inflammation leads to the development of several diseases such as arthritis, cancer, obesity, osteoarthritis and neurodegenerative disorders. Many drugs are currently used to treat inflammatory processes such as Non-steroidal anti-inflammatory drugs, however, these drugs are associated with adverse reactions such as gastritis and the development of thrombotic events [1]. Natural products, specially plant extracts and essential oils (EOs), have been used in the traditional medicine for the treatment of inflammatory diseases and some of their components such as coumarins, terpenoids, and flavonoids among others [2], have anti-inflammatory activity both *in vitro* and i*n vivo*. In order to determine the *in vitro* anti-inflammatory activity of plants from the Colombian biodiversity, we did evaluate 43 essential oils (EOs) and 57 supercritical fluid extracts obtained from different plant species. The effect of EOs and plant extracts on the LPS-induced production of Nitric Oxide (NO), Prostaglandin E2 (PGE2), Interleukin 1b (IL-1b), Tumor Necrosis Factor (TNF-a), and Interleukin 10 (IL-10) as well as on the expression of the corresponding genes were determined in RAW 264.7 macrophages. None of the extracts affected cell viability at a final concentration of 2,5mg/mL, NO and PGE2 production was strongly inhibited by EO from *Turnera diffusa* (74.5%, 86.3%), *Calycolpus moritzianus* (81.0%, 67.4%), *Ageratina aff. Popayanensis* (60.7%, 100%) and by the extracts from *Piper cumanense* (93.5%, 90%), *Achyrocline satureioides* (96.6%, 90.0%), *Ageratina aff. Popayanensis* (99.6%, 90%), *Piper eriopodon* (90%, 100%), *Piper subflavum* (90%, 100%), *Lippia origanoides* (90%, 100%), *Astronium graveolens* (100%, 63%) and *Piper aff peltatum* (92.8%, 63%). The EO of *Lippia origanoides* completely inhibited PGE2 production. The extracts obtained from *Piper eriopodon* and *Piper subflavum* did inhibit IL-6 production (48% and 37%, respectively). None of the extracts had effect on TNF-a production. The EO from *T. diffusa, A. popayanensis* and *C. moritzianus* inhibited at least in 2 fold the mRNA expression of COX-2. Extracts from *P. eriopodon* and *P. subflavum* did inhibit in 1.7 and 1.8 fold the mRNA expression of IL-6, respectively. The EO from *L. origanoides* did inhibit in 1.4, 1.5 and 2.0 fold the mRNA expression of COX-2, IL-6 and IL-10, respectively. The results suggest that the anti-inflammatory effect of *L. origanoides* and *T. diffusa* is due to the inhibition of NO, PGE2 and IL-6 production as well as a downregulation in the mRNA expression of iNOS, COX-2 and IL-6. The anti-inflammatory effect of *P. subflavum* is explained by the downregulation of mRNA expression for iNOS, COX-2, IL-6 and IL-10. The results indicate that extracts obtained from *L. origanoides, P. eriopodon, P. subflavum* as well as the EO obtained *T. diffusa* are a potential source of natural anti-inflammatory agents. **Acknowledgements:** Patrimonio Autónomo Fondo Nacional de Financiamiento para la Ciencia, la Tecnología y la Innovación, Francisco José de Caldas, Contrato RC-0572-2012-Bio-Red-Co-CENIVAM, Vicerrectoría de Investigaciones Innovación y Extensión Universidad Tecnológica de Pereira for financial support.

Keywords: Anti-inflammatory, Essential oil, Plant extracts, Supercritical fluid**References**

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TRYPANOCIDAL ACTIVITY OF COUMARINS ISOLATED FROM *Calophyllum brasiliense* LEAVES

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The current treatments for Chagas disease caused by the protozoan *Trypanosoma cruzi* show limited therapeutic potential and are associated with serious side effects. In recent years, the use of natural products has led to developing new chemotherapeutic agents. The mammea type coumarins isolated from the leaves of tropical tree *Calophyllum brasiliense* have shown significant activity against *T. cruzi* and *Leishmania* and low toxicity in a murine model; however, their mode of action and organelle targets are unknown. The aim of this study was to make a deep characterization of the trypanocidal activity of mammea type coumarins on three Mexican strains of *T. cruzi*, belonging to DTUs TcI (Ninoa and Querétaro) and TcVI (Ver6) genotypes. A mixture of mammea type coumarins A/BA+A/BB+A/BD (6:3:1), and pure mammea A/BA, were isolated from the leaves of *Calophyllum brasiliense* and identified by 1H NMR. The *in vitro* effects on mobility, growth recovery, morphology, ultrastructure, and infectivity were evaluated. The coumarins showed trypanocidal activity affecting the parasite ability to replicate and produced a significant reduction in infection *in vitro* on epithelial cells. Transmission electron microscopy showed that these compounds cause severe alterations on nuclear envelope, plasma membrane, as well as, mitochondrial swelling that produce the death of the parasites. Our results confirm that mammea type coumarins could be an important resource of trypanocidal drugs, since they showed low toxicity on mammalian cells, and were four times more potent than Benznidazole.

EFFECT OF POLYPHENOLIC COMPOUNDS: CAFFEIC ACID AND CHLOROGENIC ACID ON THE PLATELET AGGREGATION INDUCED BY THE LIPOPOLYSACCHARIDE OF *P. gingivalis*

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Different epidemiological studies have demonstrated the association between periodontitis and cardiovascular disease mainly in atherosclerotic processes [1], lipopolysaccharide (LPS) of periodontopathogens such as *P. gingivalis* induces the production of proinflammatory cytokines that activate mechanisms that stimulate the production of platelet pro-aggregating factors such as the Von Willebrand factor and thromboxane A2 [2, 3]. Many cardiovascular patients with active periodontal disease because of their condition cannot receive conventional treatments, so it is necessary to look for new therapeutic alternatives that can be used for cardiovascular treatment in patients with periodontitis; Previous studies have shown that polyphenols: caffeic and chlorogenic acid have antiplatelet effect, the objective of this study was to evaluate the effect of polyphenols on the aggregation induced by the lipopolysaccharide of *P. gingivalis* W83 in human platelets.

Platelet-rich plasma (PRP) was obtained from healthy volunteer donors with prior informed consent from the Hematologic Foundation Colombia. PRP was stimulated with LPS of *P. gingivalis* W83 (3.5, 7, 15, 30.60, 120 ?g/mL) at 37 °C for 30 minutes, followed by polyphenols: caffeic and chlorogenic acid (100-1µg/ mL). We used the spectrophotometric technique of platelet aggregation in which the inducing agent: ADP (10 ?M), collagen (10 ?g/mL), AA (150 ?g/mL) and U46619 (10 ?M; thromboxane A2 analog) were added remained in contact with the platelets for 5 to 10 minutes. As a positive control, acetylsalicylic acid and negative control, DMSO 1% were used. Treatment concentration curves against percentage of platelet aggregation were performed a $P < 0.05$ was assumed as significant. This study was approved by the Institutional Committee for Ethics in Research of the University El Bosque with No of act 011-2014.

The LPS of *P. gingivalis* W83 induces a platelet proaggregant effect *in vitro* in human platelets being its maximum magnitude (Emax) of 82%, in turn increases the effect in the presence of the agonist U46619 (Emax: 93%) and collagen (Emax: 110%) in relation to the control. Polyphenols; Caffeic and chlorogenic acid may possibly inhibit the effect induced by the LPS of *P. gingivalis* because it has been observed to have an antiplatelet effect on U46619 and its possible mechanism to be related to inhibition of thromboxane synthetase, blockade Of TXA-2 receptors, or by the inhibition of some of the second messengers linked to the TXA-2 pathway.

Keywords: Lipopolysaccharide, *P. gingivalis*, Platelet aggregation, Periodontitis, Polyphenols

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ANTI-INFLAMMATORY INTESTINAL ACTIVITY OF THE STANDARDIZED LEAVES INFUSION EXTRACT OF *Copaifera malmei* HARMS IN TRINITROBENZENE SULFONIC ACID COLITIS MODEL

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Copaifera malmei, Fabaceae, known as “copaíba-mirim”, is a native and endemic shrub of the Brazilian Cerrado, found in the states of Mato Grosso and Goiás. The leaves infusion of this plant is popularly used by riverine communities from the North Araguaia microregion, Mato Grosso, Brazil, for the treatment of gastric ulcers and inflammatory diseases of the respiratory tract. Ulcerative colitis is a chronic inflammatory bowel disease (IBD) related to a number of conditions involving inflammation (sometimes damage) of the large intestine. The objective of the study was to evaluate the activity of the standardized leaves infusion extract of *C. malmei* (SIECm) on the IBD, intestinal motility and secretion. The SIECm was prepared by infusion of 40g of dry leaf powder into 1L boiled distilled water for 15 min. To evaluate the activity of SIECm (25, 100 and 400mg/kg p.o.) on intestinal motility, the intestinal transit tests were carried out on Swiss female mice. The effect of the SIECm on the accumulation of intestinal fluid was evaluated by the castor oil-induced enteropooling test in Wistar rats. The effect of SIECm on intestinal inflammation was evaluated by the trinitrobenzene sulfonic acid (TNBS) induced acute ulcerative colitis model. The SIECm decreased intestinal transit at doses of 100 (63.4%, $p < 0.05$) and 400mg/kg (69.3%, $p < 0.01$) respectively, and the accumulation of intestinal fluid at the highest dose tested (56.9%, $p < 0.001$). In the TNBS-induced ulcerative colitis model, SIECm reduced macroscopic inflammatory damage at doses of 25 (40%, $p < 0.05$) and 400mg/kg (80%, $p < 0.01$), as well as reducing the myeloperoxidase (MPO) activity in the homogenate at three doses tested (73.7%, 66.0% and 90.5%, $p < 0.001$) respectively, whereas the treatment with SIECm did not alter the concentration of glutathione (GSH) in any dose. Histopathological analysis demonstrated that SIECm was able to reduce ($p < 0.05$) muscle (73.3% and 91.2%) and mucosal (50.0% and 58.5%) layers damage, as well as edema (56.2% and 75.0%) and cellular infiltration (50.0% and 75.0%) at doses of 100 and 400mg/kg, respectively, and increased the number of mucus secretory cells (200%) at the dose of 400mg/kg ($p < 0.05$). The data indicate that SIECm prevent the inflammatory bowel intestinal that may involve reduction of neutrophil infiltration and stimulation of mucus production. SIECm reduction of the motility and accumulation of intestinal fluids indicate that SIECm might be used in cases of ulcerative colitis where diarrhoea is a predominant symptom.

Keywords: *Copaifera malmei*, Ulcerative colitis, Intestinal motility, Intestinal secretion.

CHEMICAL COMPOSITION AND ANTIOXIDANT PROPERTIES OF INFUSIONS AND ESSENTIAL OILS OF MOROCCAN *Mentha* SPECIES

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The genus Mentha L. is represented in Morocco by 10 species including hybrids. Some members of this genus are also used as herbal teas and condiments both in fresh and dried form due to their distinct aroma. In this study, infusions obtained from the fresh aerial parts of three Mentha species commonly cultivated and used in Morocco's famous mint tea were evaluated for phenolic contents and antioxidant activity.

Total antioxidant capacity was assessed by three tests: scavenger activity by DPPH (1,1-diphenyl-2-pycril-hydrasil radical) method, FRAP (Ferric Reducing Antioxidant Power) method and β-carotene bleaching method. Infusions of *Mentha piperita* possess the best ability to reduce DPPH and chelate iron (IC50 =7.50±0.195 and 5.84±0.362µg/ml, respectively), while *Mentha spicata* (cultivated in Tiznit region) shows great efficiency on inhibiting β-carotene bleaching method (IC50 = 62.67 ± 0.002µg/ml). The antioxidant capacity was significantly correlated with the total phenolic content; TLC and HPLC chromatographic analyses showed the predominance of flavonoids and phenolic acids, specially rosmarinic acid.

Furthermore, a GC-MS analysis was carried out on Mentha spp. essential oils, for the determination of the volatile fingerprints. In general, predominant components resulted to be eucalyptol, cis-p-menth-2-en-1-ol, carvone and 4-thujanol.

Keywords: *Mentha spp*., polyphenols, TLC and HPLC, infusion, antioxidant activity

DEVELOPMENT OF AN ANALYTICAL METHODOLOGY FOR DETERMINING THE ORIGIN OF ENDOGENOUS ANDROGENIC ANABOLIC STEROIDS (AAS) BY GC-C-IRMS PRIOR L/L EXTRACTION AND FRACTIONATION BY HPLC/DAD AND IDENTIFICATION BY GC-MS/EI

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It is well known that athletes can use AAS to increase their performance, which has resulted in the prohibition of these drugs by WADA. Some of them are found naturally in the body, which make it difficult to interpret a result. GC-C-IRMS analysis is so far, the best tool to determine the origin of these substances. However, due to the low sensitivity and resolution of this technique, is necessary to carry out a previous purification of the sample using HPLC-DAD with posterior identification by GC-MS/EI. Consequently, the aim to the present study was development an analytical methodology for determining the origin of endogenous AAS by GC-C-IRMS after L/L extraction and fractionation by HPLC/DAD and identification by GC-MS/EI.

Urine spiked with standard AAS solution was hydrolyzed with beta-glucuronidase and extracted with 3mL of MTBE. Purification and fractionation of the extract was carried out using two HPLC-DAD methodologies with a C18 column at 254 nm and water – acetonitrile mobile phase in gradient elution. Each fraction was fully identified after acetylation with pyridine and acetic anhydride at 65°C by GC-MS/EI employed a 30mx0,25mm x 0.15µm column. Six fractions were collected as follows: F1: From 0.1 to 4.49 min, F2: From 4.5 to 7.9 min, F3: From 7.91 to 9.1 min, F4: From 9.11 to 10.6 min, F5: From 10.61 to 12.5 min, F6: 12.51 to 13.5 min. The fractions for the second method looking for a extra cleaning, were collected each 3 minutes. Fractions with the AAS of interest were finally analyzed by GC-C-IRMS with the same conditions of GC-MS/EI and the reactor of combustion at 940°C.

In the first method the following analytes were obtained: F1 any AAS, F2 11-OH-Androsterone, F3 Epitestosterone, Testoterone, 5B, 5a-Adiol, F4 Etiocholanolone, Androsterone, F5 Pregnandiol and F6 any AAS. In order to improve the purification fractions a second method was employed. The analytes obtained were: F1: 11 OH Androsterone, F2 Epitestosterone, Testosterone, F3 5BAdiol and 5aAdiol, F4 Etiocholanolone and Androsterone and F5 Pregnandiol.

According to literature, we can observe that the application of the two consecutive methods of cleaning, allows obtaining cleaner fractions, which increase GC-C-IRMS selectivity and therefore facilitate the analysis for determine the origin of the substances under analysis. The definition of these methods with the verification of their reproducibility is the initial stage to carry out the correspondent validation. A cleansing and fractionation methodology was developed for the analysis of endogenous AAS employed HPLC-DAD, GC-MS/EI and GC-C-IRMS, which allowed their unequivocal identification and differentiation between exogenous and endogenous substances.

Keywords: HPLC, Steroids, IRMS, Doping

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SECONDARY METABOLITES WITH QUORUM-QUENCHING EFFECT, A STRATEGY FOR CONTROL OF *Klebsiella* PATHOGEN.

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Quorum sensing (QS) is a bacterial communication mechanism, which allows colonies to sync genetic expression of some virulence factors. Subsequently, finding secondary metabolites that can inhibit this mechanism, results in a great strategy to control the bacterial pathogenicity [1,2,3]. Moreover, *Klebsiella pneumoniae* is a pathogenic agent causative of a high percentage of nosocomial infections, which, habitually elevates mortality rates; for this reason, World Health Organization (WHO) has ranked it as a bacteria that urgently necessitates new antibiotic agents in order to be controlled [4].

In search of secondary metabolites that can control the pathogenic bacteria by non-biocides methods, 30 molecules that belong to five substance groups were analyzed. Among these were: furans derivate, C6C3 and C6C2 type compounds, flavonoids, cinnamates, among others. Due to QS being a sequence of biochemical events involved in pathogenicity, the effect of the substances on the QS mechanism of *K. pneumoniae* were analyzed- through its effect on bacterial growing, the synthesis of homoserine lactones by biosensor, biofilm formation and finally the biofilm on urethral catheters.

It was observed that some compounds had QS inhibitory effects between 17% and 65% and the reduction in the capacity of biofilm formation of *K. pneumoniae* between 25% and 30%. The compounds also decreased the natural penicillin resistance of this bacteria.

Keywords: Quorum sensing, *Klebsiella*, Virulence factors, Secondary metabolites

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FEATURES AND POTENTIAL APPLICATION OF THE *Passiflora vitifolia* FRUIT COLLECTED IN TOLIMA

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Colombia has 170 species of Passiflora, 81 percent of which are in the Andean region [2], including the department of Tolima. To the best of our knowledge, from literature survey, several studies have mentioned to *Passiflora vitifolia*, but still there is no data available regarding the biological and chemical activities of its seeds and peel. The present work recognized and also evaluated those characteristics in order to stablish its potential use in the medical or industrial field. The fruits were harvested at the botanic garden Alejandro Von Humboldt at the University of Tolima in Ibagué (1285 masl, 27 °C). A plant voucher is deposited in the National University herbarium (No. COL 592024). Ethyl acetate and ethanolic extracts were obtained from the seeds and peel; moreover, a phytochemical screening and a bromatological composition and mineral content were determined. The antioxidant potential of each extract using 1,1-diphenyl-2-picrylhydrazyl (DPPH), 2,2'-azino-bis- 3-ethylbenzthiazoline-6-sulfonic acid (ABTS) radicals [3] was also determined. The Antidiabetic effect was analysed using two in vitro assays: glucose diffusion and alpha amylase inhibitory activity (Mendoza-Meza & Loza-Rosas, 2014). Furthermore, the physical and chemical characteristics of the crude oils from the seeds and peel were determined. *P. vitifolia* is native from the Amazon region. The flowers are strongly scented and red intense, and the fruit as well as the seeds have shown variation in size and mass (indehiscent berry). For instance, the seeds number varies by a factor of 20 to 60 among fruits. The bromatological analysis of the seeds showed higher values of protein (16%), crude fat (26%) crude fiber (53%) and minerals, such as P, Na, Mg, Cu and Zn. It was found that the seeds and pericarp of *P. vitifolia* contain reducing sugars, steroids, triterpenes and alkaloids and a high abundance of tannins and flavonoids. The ethanolic extract from the seeds appears to have the highest antioxidant properties [DPPH* (IC_{50} 9,5mg/L) and ABTS*(IC50 4,6mg/L)], with an inhibitory effect of 70% on the glucose movement towards the external solution across dialysis; the percent inhibition of enzyme alpha amylase was over 50%. Those physical and chemical characteristics determined to the plant oil insinuate a high content of unsaturated fatty acids; features that give good prospects to the species as a complementary material of other vegetable oils.

Keywords: *Passiflora vitifolia*, Antioxidant, Antidiabetic, Extracts.

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EXTRACTS FROM *Hyptis* SPECIES AS STARTING POINTS FOR RESEARCH ON ANTIVIRALS AND IMMUNOSUPPRESSANT DRUGS FOR DENGUE

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There are not effective drugs available to the treatment of dengue patients. Extracts (EXTs) from medicinal plants could serve as starting points for research on antivirals and immunosuppressant drugs.

This study aims to evaluate the inhibitory effect *in vitro* of EXTs from plants of Colombia on dengue virus (DENV) and cytokines implicated in its pathogenesis.

Supercritical fluid (CO2) extraction was carried out to obtain EXTs, which were collected at 40 (fraction 1) and 80 (fraction 2) bar. Ten samples from six plant species were profiled for cytotoxicity using MTT [3-(4,5-dimetil-tiazol-2-il)-2,5-difenil-tetrazolio] screening on four cell lines from organs targets of toxicity. Inhibitory effect on dengue virus (DENV) was evaluated using area fraction output method (with ImageJ freeware). Active EXTs on DENV were screened for skin sensitization by using the *THP-1*-derived *IL-8 (Interleukin-8) test, and for reduction of proinflammatory cytokines in stimulated-LPS p*eripheral blood mononuclear *cells* (LPS-PBMC).

Fractions 2 of all EXTs showed lower toxicity than fractions 1. EXTs from *Hyptis* species were the less toxic, and their fractions 2 reduced (40–51%) cell death caused by DENV. EXTs from *Cordia curassavica*, *Turnera diffusa* and *Wedelia cf. stuebelii* were inactive on DENV. All fractions of EXTs from *Hyptis* species did not increased IL-8 in treated THP-1 culture cells suggesting lack of *skin sensitization. In* LPS-PBMC, these EXTs reduced cytokines between 49– 62% respect to 100% control (untreated): *H. suaveolens* (fraction 1) was the most active on RANTES (Regulated on Activation, Normal T Cell Expressed and Secreted) (648 ± 430.0 *vs* 2388 ± 108.1 pg/mL); *H. brachiata (*fraction 2*)* on INF-γ (Interferon gamma) (153 ± 126.4 *vs* 773 ± 127.6pg/mL); and *H. pectinata* (fraction 1) on IL-8 (960 ± 48.6 *vs* 1644 ± 50.6pg/mL).

Fractioned EXTs from *Hyptis* species could serve as starting points for discovering of antivirals and immunosuppressant drugs for treatment of dengue.

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Chiliotrichum diffusum (ASTERACEAE): NEW CONTRIBUTIONS TO PHARMACOGNOSTIC KNOWLEDGE IN RELATION TO THE TRADITIONAL USE OF ONAS AND YAMANES

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Chiliotrichum diffusum (G.F.) K. is a shrub with alternating coriaceous leaves; dimorphous flowers corresponding to radiated chapters; glandular achenes, and papus formed by 2-3 sets of rigid hairs. In Argentina it inhabits since south of the 45° parallel to Tierra del Fuego. It has been described in traditional medicine Ona and Yamane for its medicinal and ritual uses.

In previous studies we demonstrated the chemical composition and pharmacological activity [1-3]. In this work we show the analysis of volatile components and bioautography studies related to traditional use. Aerial parts (pa) and flowers (f) were collected in summer of 2017 in 28 de Noviembre town, Santa Cruz, Argentina; these were dried at room temperature under roof, ground, sieved (20 mesh) and extracted with ethanol at 96° (pa) and with water at 100°C (f) [1,2]. Both extracts were analyzed by bioautography in a planar chromatographic system on Silicagel G60 with ethyl acetate - formic acid - acetic acid - water (100:11:11:26), in duplicate; one chromatogram was developed with DPPH and the other with NP-PEG. Another dry sample was extracted with chloroform (10 min, room temperature); the extracts were analyzed on Silicagel G60 with toluene-ethyl acetate (93:7) (developed with vanillin sulfuric), and GC-MS. Another sample of flowers was steam stripped off and also analyzed by TLC and GC-MS. Bioautography showed the presence of several zones with antioxidant activity in both extracts, it was more important in decoct of flowers. These zones coincided with quercetin, kaempferol-3-*O*-rhamnoside, quercitrin, apigenin-7-*O*-glucoside, chlorogenic acid, kaempferol-3-*O*-gentiobioside. The chloroform extracts showed spathulenol, bisabolol, azulene, farnesene and others terpenic derivatives; these compounds were corroborated by CG-MS; the composition of *C. diffusum* flowers with similar extracts of *Matricaria chamomilla* was similar. The volatile extract also showed bisabolol. The flavonoids and terpenes determined have anti-inflammatory, antioxidant, analgesic and anti-tumor activity [1,2,3]. It is directly related to the traditional uses of *C. diffusum;* these results being a new contribution for its validation.

Keywords: Flavonoids, Terpens, Asteraceae, Bioautography, Ona and Yamane traditional medicine

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CHEMICAL AND ENANTIOMERIC COMPOSITION OF THE ESSENTIAL OIL DISTILLED FROM *Niphogeton dissecta* (BENTH.) J.F. MACBR. (APIACEAE) COLLECTED IN ECUADOR

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Niphogeton dissecta (Benth.) J.F. Macbr. is a plant spread all around the andean region, as it has been recorded in Bolivia, Colombia, Ecuador, Peru and Venezuela [1]. In southern Ecuador, where our specimens were collected, the species is known with the common name *culantrillo de cerro*. *N. dissecta* has been observed in a wide altitude range, having been recorded between 2255 and 4500 m [1]. In this communication we are presenting, for the first time, the chemical and enantiomeric composition analysis of the essential oil, distilled from aerial parts of *N. dissecta*. The volatile fraction was analyzed qualitatively and quantitatively by GC-MS and GC-FID respectively. GC-MS analysis was performed with a 30 m DB-5ms column, with internal diameter of 0.25 mm and stationary phase thickness of 0.25 µm. The injector was operated in split mode (30:1), with He as carrier gas (flow: 1 ml/min). The injections (1µl) were carried out at the concentration of 1 µl/ml in cyclohexane, with the oven operating in thermal gradient, according to the following program: 60° for 5', from 60° to 180° at 3°/min, from 180° to 250° at 15°/min, 250° for 5'. The MS was set in SCAN mode, with a mass detection range of 45-350 amu. The identification of constituents was obtained by comparing each EIMS spectrum (70eV) and linear retention index (C8-C22 n-alkane series) with literature2. Forty components were identified in the essential oil, representing 98.31% of the total. Among the most representative components are acorenone B (41.01%) and (E)-β-ocimene (29.64%). The enantiomeric analysis permitted to determine β-pinene and sabinene as a mixture of enantiomers, being 80.90% and 19.10% the respective e.e. of (+)-β-pinene and (+)-sabinene. The rare major compound acorenone B was also isolated by preparative CC and characterized by NMR. An AChE (IC50 = 40µg/ml) and BChE (IC50 = 10.9µg/ml) inhibitory activity was observed for acorenone B.

Keywords: *Niphogeton dissecta*, Acorenone B, Essential oil, GC-MS, Ecuador

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EVALUATION OF ACUTE TOXICITY OF *Abuta grandifolia* AND *Curarea toxicofera*

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Tropical parasitic diseases, such as malaria, blight the lives of hundreds of millions of people worldwide. Most of the drugs available to treat these diseases have serious drawbacks. Hence, new drugs are urgently needed. Natural products (NPs) play a dominant role in drug discovery for the treatment of human diseases. Particularly, several well-established antimalarial drugs such as quinine and artemisinin have their origins in nature and ethnopharmacological knowledge.

The aim of this work was to test the acute toxicity of two plants used in the Amazonian rainforest to treat malaria. *Abuta grandofolia* and *Curarea toxicofera* belong to the Menispermaceae family. Both of them are used by local indigenous communities to combat malaria. Additionally, there are reports of bisbenzylisoquinoline alkaloids with antiplasmodial activity *in vitro*. The plants were collected, classified, and processed to obtain ethanolic, aqueous, and alkaloidal extracts. The antimalarial activity of those extracts was tested, showing promising results. The active extracts were both the ethanolic and the alkaloidal. As a result, they were chosen to perform the evaluation of their acute toxicity [1,2,3].

The methodology used to evaluate the acute toxicity of the extract was described in the OECD guideline No. 423. Healthy young adult mice for *A. grandifolia* and rats for *C. toxicofera* were employed. Animals were between 8 and 12 weeks old and their weight falled in an interval within 20 % of the mean weight. Test substances were administered orally in a constant volume over the range of tested doses. During 14 days, once each day, animals were observed and weighed. On the 14th day, a gross necropsy was performed and main potential target organs sent to microscopy examination [4].

For *A. grandifolia*, none of the extracts, ethanolic, aqueous, and alkaloidal, exhibited significative acute toxicity, according to the classification of the literature. The ethanolic and aqueous extracts showed 100% survival without showing toxicity signs at the highest tested dose (2000mg/Kg). The alkaloid extract had no mortality at 2000mg/Kg. However, it displayed some toxic effects at 500mg/Kg evident in the necropsy. The evaluation of the *C. toxicofera* is still in progress.

Keywords: *Abuta grandifolia*, *Curarea toxicofera*, Acute toxicity, Anti-malarial activity.

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ANTIMICROBIAL ACTIVITY OF LEAVES EXTRACTS FROM *Rhoeo discolor*

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Rhoeo discolor (Commelinaceae) commonly known as purple maguey is a plant used in traditional Mexican medicine. It has been attributed properties as antiparasitic, antimicrobial, anticancer, anti-inflammatory, antigenotoxic and antioxidant. However, the major secondary metabolites and/or compounds responsible for antimicrobial activity and the minimal inhibitory concentration for applying said extracts are unknown. The aim of this work was to evaluate the antimicrobial activity of leaves extracts of *R. discolor* against human pathogenic microorganisms, using the microdilution technique and TLC-Bioautography. Five *R. discolor* extracts were obtained and the antimicrobial activity was evaluated. The methanolic and aqueous extracts showed high activity (≥50% of inhibition) against 6 bacteria and 4 yeasts. Both extracts showed high sensitivity with MIC values of 0.8mg/mL against *S. tiphi* and 3.2mg/mL against *C. glabrata*. TLC-Bioautography analysis of the methanolic and aqueous extracts revealed at least nine antibacterial components and five antifungal components with different zones of inhibition. Given the solubility properties of the active extracts, the phenols may comprise most of the active R. *discolor* antimicrobial compounds, which were quantified by colorimetry and HPLC. This work demonstrated systemically the antimicrobial activity of leaves extracts of *R. discolor*.

Keywords: Medicinal plant, *Rhoeo discolor*, Microdilution assay, TLC-bioautography

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POTENTIAL APPLICATION OF *Passiflora vitifolia*

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Colombia has 170 species of Passiflora, 81 percent of which are in the Andean region [2], including the department of Tolima. To the best of our knowledge, from literature survey, several studies have mentioned to *Passiflora vitifolia*, but still there is no data available regarding the biological and chemical activities of its seeds and peel. The present work recognized and also evaluated those characteristics in order to stablish its potential use in the medical or industrial field. The fruits were harvested at the botanic garden Alejandro Von Humboldt at the University of Tolima in Ibagué (1285 masl, 27 °C). A plant voucher is deposited in the National University herbarium (No. COL 592024). Ethyl acetate and ethanolic extracts were obtained from the seeds and peel; moreover, a phytochemical screening and a bromatological composition and mineral content were determined. The antioxidant potential of each extract using 1,1-diphenyl-2-picrylhydrazyl (DPPH), 2,2'-azino-bis- 3-ethylbenzthiazoline-6-sulfonic acid (ABTS) radicals [3] was also determined. The antidiabetic effect was analysed using two *in vitro* assays: glucose diffusion and alpha amylase inhibitory activity [1]. Furthermore, the physical and chemical characteristics of the crude oils from the seeds and peel were determined. *P. vitifolia* is native from the Amazon region. The flowers are strongly scented and red intense, and the fruit as well as the seeds have shown variation in size and mass (indehiscent berry). For instance, the seeds number varies by a factor of 20 to 60 among fruits. The bromatological analysis of the seeds showed higher values of protein (16%), crude fat (26%) crude fiber (53%) and minerals, such as P, Na, Mg, Cu and Zn. It was found that the seeds and pericarp of *P. vitifolia* contain reducing sugars, steroids, triterpenes and alkaloids and a high abundance of tannins and flavonoids. The ethanolic extract from the seeds appears to have the highest antioxidant properties [DPPH* (IC50 9,5mg/L) and ABTS*(IC50 4,6mg/L)], with an inhibitory effect of 70% on the glucose movement towards the external solution across dialysis; the percent inhibition of enzyme alpha amylase was over 50%. Those physical and chemical characteristics determined to the plant oil insinuate a high content of unsaturated fatty acids; features that give good prospects to the species as a complementary material of other vegetable oils.

Keywords: *Passiflora vitifolia*, Antioxidant, Antidiabetic, Extracts.

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EXTRACTS OF *Trichilia hirta* AND *Hyptis capitata* EXHIBITED ANTIOXIDANT AND ANTI-INFLAMMATORY ACTIVITY *IN VITRO*

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Inflammatory diseases such as gout, asthma, osteoarthritis, rheumatoid arthritis, degenerative disorders, cancer and allergies; have become a major cause of morbidity worldwide [1]. Many of the medications used to treat inflammatory diseases, including steroidal anti-inflammatory and nonsteroidal anti-inflammatory drugs (NSAIDs), have numerous adverse effects [2]. On the other hand, despite our dependence on modern medicine and great advances in synthetic drugs, approximately 80% of the world's population makes use of traditional medicine, which is derived mainly from plant material. Natural products have always contributed to the development of drugs, resulting in the discovery of antibiotics, anticancer agents, anti-inflammatory compounds and analgesics [3]. In this sense, the discovery of drugs based on the study of medicinal plants remains an important area to search compounds with potential pharmacological activity. In this work, we evaluated the antioxidant and anti-inflammatory potential of four vegetable species (*Trichilia hirta*, *Hyptis capitata*, *Crataeva tapia* and *Annona squamosa*) of Colombian Caribbean region, used in the folk medicine. Total extracts were obtained with ethanol by maceration at room temperature. Secondary metabolites were identified by preliminary phytochemical screening. The content of phenols and flavonoids was determined by the methods of Folin-Ciocalteu and aluminum trichloride, respectively. The antioxidant potential of the extract was determined using the free radical scavenging DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS+ (2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)) spectrophotometric methods. Finally, anti-inflammatory activity of the extracts was evaluated determining their activity on the production of TNF-α, IL-1β and IL-6, in LPS-stimulated RAW 264.7 macrophages, quantified on the obtained supernatants using commercial enzymelinked immunosorbent assay (ELISA) kits, following the manufacturer's protocol. The results obtained show that *Hyptis capitata* had the highest content of phenolic compounds (96,8±0,8mg gallic acid/g extract) and flavonoids (69,4±2,3mg catechin/g extract), while the other extracts showed a low content of phenolic compounds and flavonoids. As for the antioxidant potential, the extracts of *Hyptis capitata* (seed and leaves) showed a potent scavenging effect of DPPH? with IC50 values of 127,9µg/mL (119,9-136,1µg/mL) and 202,4µg/mL (194,1-210,7µg/mL), respectively, and ABTS?+ with IC50 values of 37,1µg/mL (35,0-39,3µg/mL) and 167,1µg/mL (157,7-77,0µg/mL), respectively; while the other extracts showed a moderate scavenging effect. In the evaluation of the proinflammatory cytokines, the extract of *Trichilia hirta* had a potent inhibitory effect on cytokine IL-6, while the other extracts showed lower inhibition, but significant, compared with the LPS group. The extracts of *Trichilia hirta* and *Hyptis capitata* showed a potent inhibitory effect on cytokine TNF-α, the rest of the extracts had a moderate inhibitory effect. The extracts evaluated did not present significant inhibition of IL-1β. This study provides evidence that the extracts of *Trichilia hirta* and *Hyptis capitata* are a source of metabolites with potential to modulate the inflammatory response.

Keywords: Inflammation, Cytokines, Free radical.

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IN SILICO EVALUATION OF CELASTRACEAE SESQUITERPENOIDS ON ACETYLCHOLINESTERASE FROM *Drosophila melanogaster*

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Celastraceae is a family of plants known for its use in traditional medicine and agriculture as stimulant, sedative, purgative, memory restorative, antitumor, antibacterial, insecticidal, insect repellent activities among others. These properties are due to a large family of oxygenated sesquiterpenoids based on a tricyclic dihydroagarofuran skeleton [1].

The principal purpose of this investigation is the study of some molecules derived from Celastraceae family (oxygenated agarofuran derivates) as inhibitors of the enzyme Acetylcholinesterase from *Drosophila melanogaster* (*Dm*AChE, 1DX4 PDB).

The target-based in silico screening was carried out in Molegro Virtual Docker (6.0), with the finality to predict the bioactivity of 128 molecules isolated from Celastraceae species against *Dm*ACHe, in that way they could be used to design more efficient inhibitors.

The results obtained showed the top-five molecules with the lower MolDock scores, all with typical agarofuran skeletons, with interesting oxygenation patterns. A detailed analysis of ligand-enzyme complexes revealed molecular interactions of poses with important interactions between the amino acids His480, Trp83, Gly150, Thr154 and Ser238 which are part of the active site and gorge of the active site of *Dm*AChE2. Also was found a group of molecules that are until seven times more selective for DmAChE than human Acetylcholinesterase (hAChE, 4Ey7 PDB).

Acetylcholinesterase is involved in the termination of impulse transmission by rapid hydrolysis of the neurotransmitter acetylcholine in numerous cholinergic pathways in the central and peripheral nervous systems. The inhibition of the activity of DmAChe is a viable way for the development of new selective insecticides forms with lower bad impact for the environment and also expands the field for fighting the insect's resistance to carbamate and organophosphate pesticides [3].

Keywords: *Acetylcholinesterase, Celastraceae, Drosophila melanogaster,* Interactions, Insecticides.

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PHYTOCHEMICAL AND ANTIPLASMODIAL ACTIVITY OF COLOMBIAN PLANTS WITH ETHNOPHARMACOLOGICAL BACKGROUND

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Searching for new species with antimalarial medicinal potential through the research of the Colombian biological and cultural diversity, there were developed pharmacological and phytochemical studies of native plants with ethnopharmacological uses related to malaria. For such purpose, leaves of *Cecropia metensis* Cuatrec and *Cecropia membranacea* Trécul, aerial parts of *Verbena littoralis* Kunth. and the stems (lianas) of *Ambelania duckey* Mark and *Curarea toxicofera* (Wedd.) Barneby & Krukoff were selected and collected. The ethanolic extracts were prepared by discontinuous percolation and tested in an *in vitro* screening for antiplasmodial activity. Bisbenzyisoquinolinic alkaloids are reported in *C. toxicofera* [1], so we proceed to a pH-dependent fractionation. The ethanolic extracts of the five species and the fractions of *C. toxicofera* were characterized by TLC and HPLC [2]. The *in vitro* pharmacological screening was performed by the developmental inhibition assay, using *Plasmodium falciparum* FCR-3 strain (chloroquine resistant) [3]. The hemolytic activity of the ethanolic extracts was developed following the adaptation to the protocol described by Rocha [4]. The presence of polyphenols, flavonoids, steroids and terpenes was detected in the five ethanolic extracts. It was recorded the absence of cardiac glycosides, anthracene derivatives and saponins in all species. *C. toxicofera* was the only species that presented alkaloids; there were detected in its ethanolic extract and in several of its fractions. In the chromatographic profiles by HPLC, of the ethanolic extracts of *Ambelania duckey* and *Curarea toxicofera*, groups of compounds of high and medium polarity were evidenced. For *C. toxicofera* the signals with greater area eluted between 2-10 min and possibly correspond to phenolic carboxylic acids, flavonoid glycosides or bisbenzylisoquinolinic alkaloids. For *C. metensis*, *C. membranacea* and *V. littoralis*, compounds of low, medium and high polarity were observed. The ethanolic extracts of *A. duckey*, *C. metensis*, *C. membranacea* and *V. littoralis* showed IC50 higher than the maximum evaluated (100µg/mL) and they were classified as inactive. The ethanolic extract of *C. toxicofera* exhibited moderately active, with IC50 of 22.3µg/mL. This activity may be associated with bisbenzylisoquinolinic alkaloids [2,5]. None of the extracts generated damage to the host cell membrane (CH50> 1000µg/mL). From the five studied species, *C. toxicofera* presented the major *in vitro* antiplamodial activity so it was selected to confirm the *in vivo* antimalarial activity and to deepen the phytochemical studies.

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Keywords: Traditional medicinal plants, Malaria, Antiplasmodial activity, *Curarea toxicofera*

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VOLATILES PROFILE ON PIPERACEAE SPECIES FROM CAQUETA

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Three Piperaceae species, *P. aduncum*, *P. peltatum* and *P. tuberculatum*, were studied by hydrodistillation in a Clevenger-type apparatus and HS-SPME alllowing compare their volatiles profile by GC-MS.

Dill apiol, (*E*)-β-ocimene and (*E*)-cariophyllene were the main constituents of *P. aduncum*, (*Z*)-β-ocimene, germacrene-D and β-bisabolene of *P. tuberculatum* and (*E*)-cariophyllene and l-limonene of *P. peltatum*. Some differences between the two techniques in the volatiles profile were observed, but the main compounds were similar.

Keywords: Piperaceae, Hydrodistillation, HS-SPME, GC-MS

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IN VITRO EVALUATION OF THE ANTIOXIDANT ACTIVITY OF COMPOUNDS ISOLATED FROM THE INNER BARK OF *Tabebuia rosea* (Bertol) DC.

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Plants are an important source of biologically active natural products and many of them have been used for the synthesis of numerous drugs. The genus *Tabebuia* includes about 100 species and is the largest genus from the Bignoniaceae family. Several compounds with pharmacological potential have been isolated from the inner bar of some species of this genus [1,2]. The aim of this study was to evaluate the Nrf2 mediated antioxidant activity of two compounds isolated from the *n*-butanol extract obtained from the inner bark of *Tabebuia rosea*, using the HepG2 cell line. The extract was obtained by maceration with methanol and liquid-liquid extraction with *n*-butanol. Two compounds (Specioside and Catalposide) were isolated and characterized from the n-butanol extract. The evaluation of the antioxidant activity of Specioside and Catalposide using the ORAC and DPPH assays in a concentration range of 0.25-2 µg/mL indicated that the antioxidant activity increases at low concentrations, as observed with controls compounds such as α-lipoic acid (ALA), curcumin (CUR) and quercetin (QUER). The ORAC assay showed that both, Specioside and Catalposide displayed the highest antioxidant activity (85.7 and 72.3 mmoles Eq Trolox/g sample, respectively), at a concentration of 0.25µg/mL. Significant differences ($p<0.05$) were observed when the activity was compared with ALA control. The same results were observed with the DPPH method. Specioside and Catalposide did show an antioxidant activity similar to CUR and QUER controls. To determine the effect of Specioside and Catalposide on HepG2 cell proliferation, cell viability was determined using the MTT assay. The results indicated that the isolated compounds did not affect the viability of HepG2 cells, since viability was greater than 90% after 24 hours of exposure. Based on these results, experiments are in progress in order to evaluate the effect of the isolated compounds on the Nrf2-mediated antioxidant system in HepG2 cells.

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Keywords: Specioside, Catalposide, Antioxidant activity, *Tabebuia rosea*.

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SEASONAL INVESTIGATION OF BETULINIC ACID IN BRAZILIAN *Eugenia florida* RAW EXTRACTS USING HPLC-UV-DAD

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Betulinic acid (BA) is a lupane triterpene widely distributed throughout the plant kingdom and it is investigated to have a variety of pharmacological properties, including immunomodulatory, anti-inflammatory, anticancer, anti-bacterial and antimalarial activities [1]. In Brazil, the Myrtaceae family have more than a thousand of species distributed in 20 genus. Many of them, produce BA and are used in the traditional medicine such as *Eugenia florida* (EF) [2]. Considering the natural variation in secondary metabolites content in a plant, it was important to monitorate the BA content in EF leaves during different harvest periods. Thus, EF leaves were collected from Botanical Garden of Rio de Janeiro (‘Jardim Botânico do Rio de Janeiro –JBRJ’ - 22 ° 58 '2:45' 'S, 43 ° 13'2467' 'W; 16msnm altitude) in summer, winter and autumn and were extracted with ethanol by dynamic maceration, in a shaker, at room temperature for 7 days. The obtained raw extracts were analyzed by HPLC-UV-DAD using methodology developed to decrease the time of the analysis of the triterpenic acids. Analytical HPLC was performed on a LC 20ADXR system, an autosampler, and a SPD-M20A diode array detector using a Sulpelcosil-LC 18 column (250mmx4.6mm i.d.; 5µm particle size). The gradient mobile phase was carried acetonitrile and water acidified with TFA (0.05% v/v) the flow rate was 1.0mL/min-1 in methanol. Each determination was carried out in triplicate. According the literature data, the Rt between 18.68 and 18.73min and the UV absorbance are compatible with the BA in all three raw extracts samples. The major BA content (5.5%) was observed in the EFREA (from the leaves collected during autumn), 5.2% in the EFRES, from summer and the minor content in the EFREW (1.9%), from the winter sample. This study contributed to determine the best harvest period to the development of a standardized extract from EF leaves based on BA content.

Keywords: Betulinic acid, *Eugenia florida*, Triterpenes

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CHEMICAL STUDY OF GREEN AND RIPE FRUIT SEED OIL OF *Manilkara bindetata* subesp. *surimanensis* (Miq), T.D.Penn.

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Manilkara is a genus grown in tropical and subtropical areas belonging to the family of Sapotaceae. The most known species of this genus are: M zapota or M. chicle (acacia, chicle) and Manilkara bindetata (balatá), these species are widely used for their large latex production that was used in the food industry in chewing gum, the fruit has great nutritional value [1,2,3]. Objective: Extract and characterize the seed oil of the green and ripe fruit of *Manilkara bindetata subesp. surimanensis (Miq), T.D.Penn*., that grows in Ecuador.

Green and ripe fruits of M. bidentata ssp surimanensis, collected at the Botanic Garden of the City of Guayaquil, Ecuador and identified at the Guay Herbarium, Faculty of Natural Sciences - University of Guayaquil, Ecuador, were used. The extraction of the oil from the seeds was carried out by Soxhlet, with hexane as solvent. The oils obtained were saponified to separate the saponifiable (fatty acid) and unsaponifiable fractions. The saponifiable fractions were methylated for characterization by gas chromatography coupled to mass spectrometry. These fractions as well as the unsaponifiables compounds were analyzed on an Agilent 6890 gas chromatograph coupled to mass spectrometer 5973N: Ultra 2 column 12 mx 0.20 mm x 0.33 microns, initial temperature: 60° C for 3 Minutes increasing 10°C/min to 300°C for 5 min. Spectrometer operated at 70eV in full scan mode from 50 to 600 units of mass. Temperature source 230 ° C, quadrupole temperature 150 ° C. Injector temperature: 280°C, injection volume 2µL, carrier gas helium 1mL/min.

The yield obtained for the fixed oils was 0,86% (green) and 1.25% (ripe). For both fractions the major component was 10-octadecenoic acid 54.55% (ripe fruits) and 47.34% (green fruits). In the fraction of unsaponifiable compounds, methyleugenol (39.63%), α-amirin (9.91%), estragol (7.84%) and β-amirine (5.75%); For the mature fruits, were α-amirine (27.11%), β-amyrin (16.31%) and 9,19-cyclolaniost-3-ol-24-methylene- (3β) (12, 56%).

The saponifiable and unsaponifiable fractions of the endosperm oil of the seeds of the green and mature fruits of *Manilkara bindetata* subsp. *surimanensis* (Miq), T.D. Penn., which grows in Ecuador were characterized. Differences in chemical composition attributable to the ripening process were found.

Keywords: *Manilkara bindetata subesp. surimanensis (Miq),* Seed oil yield, Chemical composition

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STUDY OF CHEMICAL COMPOSITION, CYTOTOXIC AND ANTITUMOR ACTIVITIES OF *Croton discolor*

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Croton discolor, commonly known as "lechecillo", is a plant that belongs to the family of *Euphorbiaceae.* This native plant can be found in tropical systems such as in Puerto Rico. In previous studies, *this plant* has shown a growth inhibition (> 84%) against two cancer cell lines, MCF-7 and T47D.1. Two aporfine alcaoides have been isolated from this plant, characterized by an amine group and a group of carbon rings.

Based on the cancer growth inhibition studies, we decided to isolate and identify the chemical compounds in the cortex of *Croton discolor* responsible for this biological activity. The plant was collected, dried and extracted with a mixture of CH2Cl2-MeOH (1:1). The resulting crude extract was suspended in water and extracted with solvents of different polarities. These extracts were analyzed by proton - nuclear magnetic resonance (1H- NMR) and cytotoxic activity against breast and prostate cancer cell lines. The preliminary data shows, that ethyl acetate and chloroform extracts are the most promising to isolate the compounds of interest.

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Keywords: Natural Products, Drug discovery, Cytotoxic activity

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EFFECT OF *Citrus aurantium* ESSENTIAL OIL ON CASTOR OIL-INDUCED EXPERIMENTAL DIARRHEA

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Citrus aurantium L. (Rutaceae), known as “laranja amarga” ou “laranja azeda”, is popularly used for the treatment of gastrointestinal disorders besides diuretic, antispasmodic and antitachycardic action. This study investigated the antidiarrheal effect of *Citrus aurantium* essential oil (CAEO) in male Swiss mice (n=7-9, 7-8 weeks). The CAEO was given orally in three doses (50, 100 or 200mg/kg). Morphine (5mg/kg subcutaneous route) or loperamide (10mg/kg) were used as a positive control and Tween 80™ 8% as vehicle. Diarrhea was induced experimentally by oral administration of castor oil (0.2mL/animal) [1, 2]. Activated charcoal (10%) was used to evaluate intestinal motility [3] and also to determinate the intestinal fluid accumulation induced by castor oil [4, 5]. All procedures were approved by the institution's ethics committee. The results are expressed as mean ± S.E.M. and statistical significance was determined by ANOVA followed by Dunnett's or Kruskal-Wallis’ test (p<0.05). After administration of castor oil, CAEO-treated mice (200mg/kg) had the onset of liquid feces significantly delayed compared to the vehicle-treated group (173.3 ±21.2 and 91.75 ±10.5 minutes, respectively). Also in this model, administration of *C. aurantium* oil reduced the evacuation of liquid feces (1.71 ± 0.68 number of stools) when compared to the vehicle group (5.43 ±0.65). CAEO (200mg/kg) also inhibited intestinal motility significantly when compared to the vehicle group (0.79 ± 0.03 g and 0.99 ± 0.01 g, respectively). In the castor oil-induced enteropooling model, CAEO (200mg/kg) inhibited the volume of intestinal contents by 39.4%, indicating that both the reduction of motility and inhibition of accumulation of intestinal fluid are involved in the mechanism of antidiarrheal action of *Citrus aurantium* oil. However, other investigations are necessary to elucidate mechanisms involved in this activity. In conclusion, the essential oil of *Citrus aurantium* presents promising antidiarrheal activity, confirming its indication for gastrointestinal disorders.

Keywords: *Citrus aurantium*, Diarrhea, Essential oil, Intestinal motility

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ANTIDEPRESSANT LIKE ACTIVITY OF A METHANOLIC EXTRACT OF *Hypericum juniperinum*

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Depressive disorders affect 350 million persons worldwide and is increasing [1]. In Colombia 4,7% of the population suffers of this disease [2]. Depression is characterized by feelings of misery, guilt, suicidal thoughts, and lack of appetite and sexual desire. The treatment of this ailment involves the use of tricyclic antidepressants, serotonin selective reuptake inhibitors (SSRIs) and monoamine oxidase inhibitors (iMAO), among others. However, these therapies have pronounced side effects [1]. To avoid this inconvenient an alternative option are botanical origin products. *Hypericum perforatum*, an European species, is traditionally used for the treatment of anxiety and depression. *In vitro* and *in vivo* assays have proved that methanolic and ethanolic extracts of *H. perforatum* are active as antidepressants, with a mechanism similar to the SSRIs. This effect has been mainly attributed to flavonoids and anthraquinones [3]. In this work, we assessed the antidepressant like effect of a methanolic extract obtained from aerial parts of *Hypericum juniperinum*, a Colombian native species with no chemical nor biological studies. The activity was evaluated in the pharmacological models of forced swim (FS) and tail suspension (TS). ICR mice males of 7 to 10 weeks were used. Three different doses of extract (150, 300 y 500 mg/kg) were orally administrated one hour previous to the test. For the control group (N=6 per treatment) a vehicle composed by polypropileneglycol 10%, glicerin 10%, and polysorbate 2%, was used. Reference drug was imipramine (30mg/kg, p.o). As a result, the methanol extract of *Hypericum juniperinum* (500mg/kg) reduced the time of immobility in the FS and TS experiments. Preliminary phytochemical analysis of the methanolic extract of *Hypericum juniperinum* revealed the presence of saponins, flavonoids and terpenes. These results show the potential of this plant as a possible antidepressant. However, further studies are necessary to confirm this activity.

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Keywords: *Hypericum juniperinum*, Flavonoids, Antidepressant activity, Forced swim test, Tail suspension test.

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EXTRACTS OF EPICARP AND SEEDS FROM AVOCADO WITH ANTIMICROBIAL ACTIVITY AGAINST STRAINS OF *Staphylococcus spp*

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Staphylococcus spp is responsible of systematic diseases and opportunistic infections that can affect skin, soft tissues, bones, genitourinary tract and other organs. *Staphylococcus aureus* is associated with hospital-acquired infections of difficult treatment due to its multidrug resistance [1]. On the other hand, *Staphylococcus epidermidis* can be an opportunistic pathogen causing nosocomial infections together with *S. aureus* [2]. The increased incidence of these infectious encourages the search for new antibacterial agents, being plants and fruits an invaluable source. Avocado [*Persea Americana* Mill *(*Lauraceae)] is an exotic tropical fruit which pulp is widely used in the traditional Latin America cuisine, whereas the epicarp and seed are considered waste materials. Recently, the antimicrobial properties of ethanol and water extracts from these fruit parts were described [3]. In this work, we evaluated the antibacterial activity of total and polyphenol-enriched extracts and fractions obtained from the epicarp and seed of avocado against two strains of *Staphylococcus* (*S. aureus* ATCC 25923 and *S. epidermidis* ATCC 12228).

Ground epicarp (E) and seeds (S) from ripped avocados were extracted with acetone (EC, SC); ethyl acetate (EA, SA); or water (EH, SH). A polyphenol-enriched extract was obtained using amberlite XAD-7 polymeric resin (ER, SR), which was further fractionated using Sephadex exclusion (E1-3, S1-3). The bacterial sensibility was calculated using the microdilution method following the CLSI guidelines. Given the results, the extracts and fractions that inhibited more than 90% of bacterial growth at 1000µg/mL, were selected to calculate their minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC). Gentamicin (16µg/mL) was employed as positive control.

Two extracts obtained from epicarp (EA and ER) were strongly active against *S. aureus* with MIC and MBC values of 500µg/mL. Remarkably, all the extracts from this part showed bioactivity against *S. epidermidis*, with MIC and MBC values of 1000 and 500µg/mL, respectively. In the case of the seed, only the SR extract inhibited significantly the growth of *S aureus* (MIC=250µg/mL and MBC=1000µg/mL), whereas *S. epidermidis* was susceptible to the treatment with SC (MIC and MBC=1000 µg/mL) and SA (MIC=1000 and MBC >1000 µg/mL). The fractionation allowed us to identify two enriched-polyphenolic fractions from epicarp (E3) and seeds (S2) that significantly affected *S. epidermidis*, both with MIC=125µg/mL and MBC=250µg/mL.

These findings provide a scientific support for the folk employment of avocado epicarp and seed to treat skin infections related to *Staphylococcus* spp, in part due to the presence of polyphenolic compounds with antibacterial activity. Further studies to isolate the bioactive metabolites and test their effect using animal models are warranted.

Keywords: Antibacterial activity, Folk medicine, Avocado, *Staphilococcus spp*.

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LICHENS: BIOPOTENTIAL SYMBIOTIC ASSOCIATION

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Currently, there is a growing scientific and technological interest in obtaining new potential products from the medicinal and industrial point of view, so the research has focused on the search for novel substances mainly of natural origin, however they are still found Natural products that may be an important source of bioactive compounds, but which remain anonymous without being exploited. An example of this are lichens, this is the association between a mycobionte organism (fungus) and another photoautotroph (alga or cyanobacteria); traditionally used in the treatment of severe pathologies such as: mental disorders, epilepsy, diabetes, cancer, respiratory diseases [1]. Among the biological functionalities exhibited by these organisms can be mentioned: antimicrobial, antioxidant, antiviral, antiproliferative, anti-inflammatory, analgesic, anti-mitotic, cytotoxic, etc [2].

In Colombia, exist approximately 1500 lichen species [3], on which the growing interest in determining its taxonomic profile is recognized, although in terms of its chemical composition and biological functionality, much remains to be done, and interest of this research focused on characterizing chemically and determining the biological potential of extracts and fractions of *Usnea angulata* and *Parmotrema robustum*, collected in Tolima.

A phytochemical screening on hydroalcoholic extract was performed to establish the presence of some of the main nuclei of secondary metabolites and, in turn, allowed to visualize these organisms as promising reservoirs of metabolites of phenolic nature; result ratified by the quantification of total flavonoids and phenols. Was posible to demonstrate several nuclei that confer different polarity, so the extracts were fractionated by vacum liquid chromatography with solvents of increasing polarity in order, to obtain fractions with organics chemical groups of similar polarity.

The biological potential activity of extracts and fractions was established *in vitro* by antioxidant assays using colorimetric methods [4]: ABTS•+ (λ 754nm) radical cation inhibitory activity; Ferric reducing power measurement, FRAP (λ 700nm); Total watersoluble antioxidant capacity, TAC (λ 695 nm); evaluation of stabilization DPPH• radical (λ 517nm). The results showed a decrease in the media Inhibitory concentration (IC50) of the fractions to stabilize of the radicals in comparison to extracts, so it can be said that separating the groups of compounds the bioactivity is increased up to 3 times. In addition to this, the cytotoxic effect was evaluated by the colorimetric technique based on the metabolic reduction of the MTT salt to formazan [5], thereby establishing the mitochondrial viability of the treated cells in order to recognize the safety of the extracts and/or fractions. The results of this research constitute a contribution to the chemical knowledge of lichen organisms. The biopotentialities evidenced make it possible to consolidate them as a source of bioactive compounds that may be useful in the food, textile, cosmetological or pharmacological industry, among others.

Keywords: Bioactivity, Lichens, *Parmotrema robustum, Usnea angulata*

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Vernonia scorpioides: MORPHO-ANATOMICAL AND PHYTOCHEMICAL STUDY

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Vernonia scorpioides (Lam.) Pers. (Asteraceae) is a plant used in popular therapy in the form of fluid extracts to treat a variety of skin conditions. The objective of this work was to define parameters for verifying the authenticity, integrity and purity of the leaves of *V. scorpioides* and its extract in order to guarantee criteria for evaluating the quality of leaves and products derived from the species.

Leaves of *V. scorpioides* were collected in March 2009 in São Luís, Maranhão, Brazil. With the fresh leaves the macroscopic and microscopic characteristics were evaluated. A part of the leaves was dried, ground and used for analysis of the microbiological quality and to obtain the extract, which was prepared by maceration with 70% ethanol, the extractive solution was filtered and concentrated in a rotavaporator to obtain the hydroalcoholic extract. With the extract the dry residue, phytochemical screening and the chromatographic profile by HPLC were determined.

In the morphoanatomical evaluation, the following characteristics were observed: whole leaves, with bright appearance, of membranaceous consistency, dark green on the adaxial face and light green on the abaxial face. Leaf blade with oval outline, acute apex, rounded base, serrated margin and symmetrical shape. The surface of the leaf blade appeared rough on both faces and hirsute. The petiole has straight aspect, marginal insertion, concave-convex cross-section and hairy surface. The leaves have characteristic aromatic odor and pungent taste. The anatomical study revealed sinuosities in the cell walls, stomata of the anomocytic type, tector and glandular bristles. It was evidenced the count of aerobic microorganisms and fungi within the acceptable limits. The phytochemical profile was positive for tannins, flavonoids, alkaloids, saponins and coumarins.

The results indicate parameters for the evaluation of *V. scorpioides* leaves quality, allowing the monitoring of samples available in the market.

Financial support: FAPEMA

Keywords: *Vernonia scorpioides*, Medicinal plant, Quality control, Pharmacognosy

ANTI-INFLAMMATORY AND ANTI-OXIDANT POTENTIAL OF SEED EXTRACTS OF *Ambrosia cumanensis*

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The inflammatory response is a basic biochemical process that is activated to eliminate stimuli that injure the body, however, when it occurs abruptly or in a chronic way may cause tissue damage, which leads to the appearance of various diseases, such as arthritis. Macrophages constitute one of the most important effector cells in the inflammatory response, while they play a critical role in developing diseases related to chronic inflammation. When these are activated, they have the ability to release reactive oxygen species (ROS) and pro-inflammatory cytokines, including TNF-α, IL-1β and IL-6 [1]. The drugs currently used for the treatment of inflammation are mostly of synthetic origin, with diverse related side effects. It is estimated that between 25 and 50% of the drugs currently marketed are of natural origin. In addition, because of their chemical diversity, plants are an important source of new compounds that potentially may be used to make new drugs. In this work, we evaluated the antioxidant and anti-inflammatory potential of ethanolic extract of *Ambrosia cumanensis* seed. Total extract was obtained with ethanol by maceration at room temperature. Secondary metabolites were identified by preliminary phytochemical screening. The content of phenols and flavonoids was determined by the methods of Folin-Ciocalteu and aluminum trichloride, respectively [2]. The antioxidant potential of the extract was determined using the free radical scavenging DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS+ (2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)) spectrophotometric methods [3,4]. The anti-inflammatory activity of the extract was evaluated determining their activity on the production of TNF-α, IL-1β and IL-6, in supernatants of LPS-stimulated RAW 264.7 macrophages, using commercial enzymelinked immunosorbent assay [ELISA] kits, following the manufacturer's protocol. The results showed that the extract of *Ambrosia cumanensis* had a moderate content of phenolic compounds (23,27±0,50mg of gallic acid/g extract) and flavonoids (9,13±0,44mg of catechin/g extract). As for the antioxidant potential, the extract of *Ambrosia cumanensis* showed a potent scavenging effect of DPPH and ABTS+ free radicals, in a concentration-dependent manner, with IC50 values of 772,6µg/mL (CI95% =735,3–810,2) and 271,3µg/mL (CI95% = 225,8–316,1) respectively, this activity may be associated with the content of phenolic compounds and/or flavonoids presents in this extract; which are recognized for their antioxidant activity. About anti-inflammatory activity, the extract of *Ambrosia cumanensis* decreased the production of IL-6 (96%), IL-1β (86%) and TNF-α (78%). In conclusion, *Ambrosia cumanensis* seed are a promising source for the search of new compounds with potential antioxidant and anti-inflammatory activity, it could contribute to the development of new natural anti-inflammatory drugs to treat inflammatory diseases.

Keywords: Inflammation, Natural products, *Ambrosia cumanensis.*

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CHANGES IN THE CHROMATOGRAPHIC PROFILE OF EXTRACTS OF TOMATOES EXPOSED TO 1,8-CINEOLE VAPORS DURING POST-HARVEST TREATMENT

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Natural products and especially essential oils have been deeply studied as pesticides to control plant pathogens, specifically bacteria and fungi, as well as food preservatives [1], but until now, post-harvest effects are not well known, especially those most related to their effect on plant biochemistry, such as maturation processes and metabolic profiles [2].

In this work, we observed that exposure of unripe tomato fruits to 1,8-cineole vapors modifies several biochemical processes involving flavonoids and lycopene levels; respect to normal ripening fruit, flavonoid concentration is hardly modified whereas lycopene production was delayed after 120h of exposure. On the other hand, a ripening deferred is observed in fruits treated with this essential oil. Additionally, biotransformation of 1,8-cineole to 2-hydroxy derivative is detected [3].

The results of this study provide evidence to establish that the exposure of green tomato fruits to 1.8-cineol vapors can be used as a tool to improve storage life, which is very short naturally, and maintains high levels of nutritionally important substances such as flavonoids [3].

Acknowledgements. Authors thank to Universidad de Antioquia (Colombia) for financial support through Sustainability Program

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ANXIOLYTIC AND ANTIDEPRESSANT LIKE EFFECT OF THE ETHANOL EXTRACT OF *Valeriana pilosa* IN MICE

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Mental disorders, such as depression and anxiety, affect millions of people around the world [1]. Alternative treatments for these disorders can be obtained from natural sources. Species of the genus *Valeriana* have been used traditionally and contemporaneously as mild sedatives and anxiolytics. Iridoids, known as valepotriates, sesquiterpenes and flavonoids are found as their main active metabolites [2].

In this work, the EtOH extract (96%) obtained from roots of *Valeriana pilosa* was used to evaluate its effect on the central nervous system in ICR mice (150, 300 and 600 mg/Kg v.o.) using the following tests: elevated plus maze, forced swimming, hole-board and pentobarbital induced sleeping-time. Clonazepam (0.3mg/kg; v.o) and imipramine (30mg/Kg; v.o) were used as reference agents.

V. pilosa ethanolic extract displayed significant effect in the elevated plus maze and behavioural despair test (300mg/Kg, v.o.), suggesting anxiolytic and antidepressant properties. These effects could be related to valepotriates and flavonoids detected in this species. Our results may provide support to the use of *V. pilosa* as anxiolytic and tranquilizer. Further studies are necessary to confirm these activities and establish the responsible metabolites.

Keywords: Valeriana pilosa, Anxiolytic, Antidepressant, Sedative

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ANTIMICROBIAL ACTIVITY OF *Senna reticulata* (TOTAL EXTRACT AND FRACTIONS)

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Senna reticulata is used by the indigenous community for its therapeutic effects. Some studies carried out on this plant have determined that it has activity against pathologies of type hypoglycaemic, rheumatic and against topical diseases such as fungal infections, scabies, rashes, and warts. The present work evaluated the antimicrobial activity of the extract and its fractions from the aerial parts (leaves, flowers, and stems) of *Senna reticulate* against *Bacillus cereus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Lactobacillus acidophilus*, *Lactobacillus casei*, *Staphylococcus aureus* and *Streptococcus mutans. Senna reticulate* was collected in the municipality of Viotá (Cundinamarca, Colombia) and a voucher is found in the National Herbarium of Colombia for taxonomic classification. Ultrasonic-assisted extraction was used to obtain the total extract in ethanol (Total ext.). Then solid-liquid fractionation was performed using petroleum ether (Fr. Pe), ethyl acetate (Fr. EtOAc), and dichloromethane (Fr. DCM). The evaluation of antimicrobial activity was performed by the agar diffusion method using disks and wells. Antimicrobial activity was determined as relative percentage of inhibition (RPI) and as minimal inhibitory concentration (MIC). Amoxiciline (30mg) was used as positive control [2, 3]. Only activity by the well diffusion method was observed for the four treatments (Total ext., Fr. Pe, Fr. EtOAc, and Fr. DCM). At a concentration of 100µg/µL, the RPI was 156.5±13.2% against *Lactobacillus acidophilus* (Fr. DCM), 128.1±9.6% against *Streptococcus mutans* (Fr. Pe), 125.6±10.2% against *Lactobacillus casei* (Fr. EtOAc) and 120.3±12.9% against *Lactobacillus casei* (Total Ext.). The MIC against *Bacillus cereus* was 80mg/mL of total extract (49.3±9.8%), *Lactobacillus acidophilus* was 40 mg/mL of total extract (79.6±7.3%), *Lactobacillus casei* was 10 mg/mL of Fr. DCM (92.5±8.7%), *Pseudomonas aeruginosa* was 100mg/mL of Fr. DCM (60.8±9.9%), *Staphylococcus aureus* was 10mg/mL of Fr. DCM (58.6±5.6%) and *Streptococcus mutans* was 10 mg/mL of Fr. DCM (86.1±7.8%). In conclusion, the total extract and fractions of *Senna reticulate* shown antimicrobial activity against pathogenic and cariogenic microorganisms.

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Keywords: Antimicrobial, *Senna reticulata*, *Bacillus cereus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Lactobacillus acidophilus*, *Lactobacillus casei*, *Staphylococcus aureus*, *Streptococcus mutans.*

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SYNTHESIS OF CHOLESTEROL DERIVATIVES AND THEIR POTENTIAL ACTIVITY AS INSECTICIDES

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Nowadays insecticides have been a controversial topic in society, they are known for their efficiency in decreasing the population of insects in crops, however they have been given a bad reputation due to the elevated number of deaths worldwide that have been caused due to a prolonged exposition to insecticides, and have been the central topic of several arguments regarding the safety in their use [3].

The main advantages of using pesticides are reflected mainly in the economical aspect in the increase of profits, saving money on labor costs, among other advantages, however, several disadvantages have been found in the use of pesticides when they are not properly used since they can also injure living beings such as human beings, and animals which are non-targeted pests, they can also cause negative environmental effects such as a disruption of the balance of an ecosystem, and pest resistance to certain inseticides. Therefore, the need to design new selective compounds that have a pesticide activity has risen after these discoveries were made. Several derivatives have been proposed, designed, and tested in other articles, however one approach we want to use is throughout the design of several cholesterol derivatives, mainly cholesterol esters with saturated fatty acids of short and long length in their carbon chain that havea selective insecticide activity only towards insects and don´t affect human beings or any other animal species [1].

In a reaction mixture that contains 100 miligrams of cholesterol, 25 miligrams of iodine, we added 1 mililiter of acetyc acid anhydride to synthesize the cholesteryl acetate, and for the other derivatives we added 1 mililiter of any other organic acid chloride, then the reaction mixture was stirred for 5 minutes, after the reaction time concluded, we added 5 mililiters of a saturated solution of sodium thiosulfate to stop the reaction with iodine, and the reaction product was recovered throughout a vacuum filtration, the dry solid was crystallized using acetone [2].

The results obtained in the *in silico* evaluation of the cholesterol derivatives show that cholesterol butyrate has one of the lowest values in the MolDock score against acetylcholinesterase from *Drosophila melanogaster* due to the interaction between the cholesterol butyrate with the following aminoacids: Glycine-150, Glycine-151, and Alanine-239, all of the previously mentioned aminoacids are components of the oxyanion hole inside the active site of the enzyme.

Keywords: Cholesterol, Acetylcholinesterase, Insecticide, *D. melanogaster*.

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CYTOTOXIC EFFECT OF THE n-BUTANOL EXTRACT OBTAINED FROM THE STEM BARK OF *Tabebuia rosea* (Bertol) DC. ON HUMAN LEUKEMIC CELLS

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Cancer is a public health problem because of its high incidence and mortality. Leukemia's are among the most common types of cancer in children and adolescents, however, therapies used to control cancer cell proliferation are also toxic to normal cells. For this reason, natural products are considered as an important alternative in the search of new drugs with anti-cancer activity [1,2]. *Tabebuia rosea* (Bertol) DC is a tropical tree that belongs to the Bignoniaceae family, it is widely distributed in South America, and is used in traditional medicine as anti-inflammatory and antimicrobial. In addition, molecules isolated from different species of this family such as iridoids, naphtoquinones and flavonoids have cytotoxic effects on tumor cells both in vitro and in vivo. For this reason, it is important to demonstrate the antiproliferative effect of the n-butanol extract obtained from the stem bark of *Tabebuia rosea* (Bertol) DC on THP-1 leukemic cells. The extract was obtained by maceration with methanol and liquid-liquid extraction with *n*-butanol. The cytotoxic effect of the extracts on THP-1 cells was evaluated using the MTT colorimetric method (3-4,5dimethylthiazol-2-yl -2,5-diphenyltetrazolium), 20,000 cells were seeded in 96-well flat bottom plates and exposed to different concentrations of the extract (1, 10, 50, 100 and 200µg/mL) during 12, 24 and 48 hours. As a control, cells were exposed to culture medium with 0.1% DMSO. Doxorubicin, a reference drug currently employed for leukemia treatment, was used as a positive control. All experiments were performed three times in triplicate. At each evaluated time, culture medium was replaced with 100 µL of MTT and incubated at 36°C in darkness during 4 hours, then the MTT was removed and 200 µL of DMSO were added to dissolve formazan crystals and the absorbance was read at 570 nm in a microplate reader. The results were expressed as percentage of cell viability compared to control cells. In addition, the cellular morphology of THP-1 cells after 24 h treatment with 325,7 nM doxorubicin was evaluated by fluorescence microscopy after the addition of propidium iodide (1mg/mL).

A dose response effect was observed in the three evaluated times. The n-butanol extract significantly decreased the viability of THP-1 cells at 10, 50, 100 and 200 µg/mL, compared with the control ($p<0.05$). The IC50 values for the extract and doxorubicin at 12, 24 and 48 hours were 35.30, 44.7, 36.44µg/mL and 2183.9nM, 325.7nM and 8.1nM, respectively. When comparing the IC50 values of the extract, no significant difference was observed ($p<0.05$). However, the IC50 of doxorubicin at 12 hours was significantly different with respect to the values obtained at 24 and 48 hours ($p<0.05$). The results indicate that the *n*-butanol extract has a cytotoxic effect on THP-1 cells. Doxorubicin has a cytotoxic effect on THP-1 cells and changes its morphology.

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Keywords: Leukemia, *Tabebuia rosea*, Cytotoxicity, Apoptosis.

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CARDIOVASCULAR AND CARDIOPROTECTIVE EFFECTS OF *Gomphrena perennis* L. (AMARANTHACEAE) DYE TINCTURE IN RATS

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Gomphrena perennis L. (Amaranthaceae) is a South American plant. In Argentine it is widely used as emollient, diuretic, hypotensive and for cardiac diseases. We previously demonstrated its antispasmodic effect on rat duodenum. This work evaluated the effects of Gomphrena tincture (GphT) on the contractile and energetic recovery of isolated rat hearts exposed to a model of stunning due to ischemia and reperfusion (I/R) as well as on the blood pressure of normotensive rats. GphT was prepared by aceration of leaves at 20% in ethanol 70°. Rats were anesthetized with 1.5g/kg urethane via i.p. and placed in a supine position with tracheal cannulation. Blood pressure (BP) was directly measured through an heparinized cannula in the internal carotid artery connected to a pressure transducer. To evaluate whether the GphT have a direct effect on hearts by an ischemic insult, isolated rat hearts were perfused at 37°C with control Krebs (C) in the chamber of a flow-calorimeter. After a 30-min equilibration period, the following protocols were done on each heart: perfusion with 0.1, 0.3 and 0.5% v/v GphT, followed by exposition to no-flow ischemia (I) during 20 min and to R with Krebs during 45 min. The contractility was evaluated from the left intraventricular pressure (P) which was measured simultaneously with the total heat rate (Ht) released by the heart. Basal BP of normotensive rats was 70.2 ± 15.2 mm Hg (n=4). GphT induced a dose-dependent hypotension (ΔBP: -13.6 ± 6.0 and -28.2 ± 11.6 mmHg respectively for 0.5% and 2% GphT, n=4). ΔBP was significantly reversed by the pre-treatment with L-NAME. Heart rate (HR) was not significantly modified by GphT at any dose, as neither after L-NAME. Perfusion of GphT in hearts produced a concentration-dependent positive inotropism. Nevertheless, 0.1% GphT significantly reduced cardiac contractility (P) and total muscle economy (Eco = P/Ht), as well as induced a diastolic contracture during R. The results suggest that: 1- The i.p. administration of GphT produced a dose dependent transitory hypotension and this effect was mediated by release of NO from the NO-synthase; 2- GphT induced a positive inotropism but increased the stunning of hearts exposed to I/R.

Keywords: *Gomphrena perennis* L, Blood pressure, Ischemic reperfusion, Calorimetry

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Hydrocotyle bonariensis LAM. (ARALIACEAE): CHROMATOGRAPHYC ANALYSIS OF CARBOHYDRATES FROM AERIAL PARTS

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Hydrocotyle bonariensis Lam. (Araliaceae) is an herbaceous plant commonly known as "redondita de agua" or "paragüita", widely distributed in South America. In Argentina inhabits the Northwest, Northeast and Central region. Infusion from aerial parts is used as anti-inflammatory against erythema and psoriasis, and diuretic among other properties. In previous work we reported the anti-inflammatory activity [1]. In this study, carbohydrates were extracted by infusion from aerial parts [2]. This aqueous extract was fractionated by dialysis (cutoff 6,000-8,000). The dialyzed fraction was dissolved in 0.2 M NaCl, and it was sub-fractionated by anion exchange chromatography on DEAE A-50 / Sephadex G100. Elution was carried out by stepwise addition on increasing concentrations of NaCl until 4 M. The main products, after hydrolysis with TFA 2 M (121 °C, 90 min), were analyzed as their corresponding aldononitrile acetates by GC-MS [3].

Sugar composition analysis showed that polysaccharides from *H. bonariensis* consisted primarily of galactose, rhamnose, glucose and uronic acids (glucuronic and galacturonic acid). The main fractions were obtained with 0, 0.2 and 0.7M NaCl (this fractions represents › 90 % of its weight). The minor fractions were obtained with 3.5 and 4 M NaCl (1 %).

Fraction from 0.2M NaCl contained the main proportions of neutral polysaccharides containing galactose and rhamnose (rhamnogalactans). The main polysaccharides from 0.7M NaCl fraction were galactorhamnans and galacturonans. Fractions from 1.5 - 2M NaCl showed uronic acids and sulfated galactose, this suggests the presence of rhamnogalacturonans and sulfated galactans.

The chromatographyc methodology used in this work allowed to optimize this analysis. These are the first results describing the polysaccharides of *H. bonariensis*. These carbohydrates are in relation with anti-inflammatory and inmunomoduladore activity of this specie.

Keywords: *Hydrocotyle bonariensis*, Araliaceae, *P*olysaccharides, Chromatography

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ANTI-RADICAL ACTIVITY AND TOTAL PHENOLIC CONTENT OF THE FRESH LEAVES ETHANOLIC EXTRACT OF *Annona purpurea*

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The pursuit for new antoxidants of plant origin has been one of the most attractive areas during the last years [1]. In this sense, the objective of this research was to evaluate *in vitro* the antioxidant activity of the fresh leaves ethanolic extract of *Annona purpurea*. For this purpose, the effect of the extract on DPPH and ABTS radicals and on the discoloration of β-carotene were evaluated. In addition to this, the phenols total content was determined by the Folin-Ciocalteu assay. The results showed high percentages of DPPH entrapment [2], distributed as follows: at concentrations of 1.5, 2.4 and 8µg/mL, 53.1, 70.8 and 93.36% of entrapment were obtained, respectively. The extract had a similar behavior with the ABTS radical where at concentrations of 0.50, 1.0 and 2.0µg/mL were obtained percentage entrapment of 31.95, 36.7 and 77.06, respectively. On the other hand, it was possible to determine that the extract prevents the discoloration of β-carotene at concentrations of 3.9, 7.8 and 15.6µg/mL with inhibition rates of 34.8, 57.5 and 76.14, correspondingly. The EC50 of the extract in every one of the applied techniques was calculated, yielding data of 1.55, 1.22 and 7.27µg/mL for DPPH, ABTS and β-carotene, respectively. When comparing these results with the standards (ascorbic acid for the first two, 3.09 and 1.03µg/mL, and α-tocopherol for the third, 6.96µg/mL), we can see that the antiradical effect is similar, and in the case of DPPH is greater in the extract than in the standard that is 99% pure, contrary to what happens in the extract, which is made up of many substances and compounds that act in synergism. The total phenol quantification test yielded a concentration of 4.4µg equivalents of gallic acid/20µg plant sample of these substances, which is in accordance with the results obtained in the antioxidant evaluation. These results convert *A. purpurea* leaf extract into a candidate for the isolation of active substances as antioxidants. So far, the evaluation of the antioxidant capacity of fresh leaves *A. purpurea* is not defined so this study contributes to enrich the knowledge about this family especially of the species under study.

Keywords: *Annona purpurea*, Antioxidant, DPPH, ABTS.

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VIRTUAL SCREENING OF AGAROFURAN COMPOUNDS FOR THE DEVELOPMENT OF MULTI-TARGET DRUGS, USEFUL IN THE TREATMENT OF ALZHEIMER´S DISEASE

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Alzheimer's disease (AD) is characterized by cognitive impairment and behavioral disorders. It occurs most frequently in people over 65 years old, although it is becoming more common in younger people. The current treatment includes a set of active principles capable of inhibiting the enzyme acetylcholinesterase (*h*AChE). Also, butyrylcholinesterase (*h*BuChE) increases its levels during the disease, reason why it becomes a possible molecular target for the treatment of AD [2]. In this project, we perform a virtual screening of a set of natural occurring compounds, to determine their potential as simultaneous inhibitors of both enzymes (*h*AChE, 4YE7 PDB; *h*BuChE, 5DYW PDB) with the purpose to develop multi-target inhibitors. The molecules used proceed in the majority from Celastraceae family, which comprises by around 100 genders and 1300 species, distributed mainly in the tropical and subtropical zones of the world. Some species are known in traditional medicine for various purposes such as sedative, antibacterial, stimulant, antitumoral among others. It is known that medicinal properties are attributed to the sesquiterpenoids, mainly with a tricyclic dihydro-agarofuran skeleton [1]. The results show several dihydro-agarofuran molecules with highest theoretical affinities, and several combinations of selectivity. One group of molecules showed better theoretical affinity to *h*AChE than *h*BuChE, while other group of molecules showed the opposite effect. However, some molecules showed high theoretical affinities against both enzymes, demonstrating at least in a *in silico* study, the possibility to design multi-target inhibitors for the treatment of AD from dihydro-agarofuranes.

Keywords: Alzheimer's disease; Dihydro-agarofuran; Celastraceae; AChE; BuChE.

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TRPA1 RECEPTOR AGONISTS ON THE CONTROL OF GLUCOSE HOMEOSTASIS

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Pre-clinical study of TRPA1 channels on targets for glucose homeostasis by using three different agonists: cinnamaldehyde (CINNA), allyl isothiocyanate (AITC) and carvacrol (CARV) [1]. Fasted male *Wistar* rats (180–200g) were divided into groups of 5 animals for glucose tolerance test (GTT): 1) Hyperglycemic control (4g/kg of glucose body weight intraperitoneally (i.p.); 2) hyperglycemic plus CINNA (5, 10 and 20mg / kg, i.p.); or 3) AITC (5, 10 and 20mg / kg i.p.) or 4) CARV (25, 100, 300 and 600mg / kg i.p.) The glycaemia was measured before any treatment (zero time) and at 15, 30, 60 and 180 min after glucose overload. The serum insulin and GLP-1 was measured by ELISA. Isolated pancreatic islets were used to measure insulin and calcium influx. Intestinal disaccharidases activity was evaluated *ex vivo* (Protocol CEUA/UFSC/PP00398/749). CINNA and AITC reduced glycaemia *in vivo* and increased insulin levels *in vivo* and *in vitro*. CARV was not able to induce serum glucose lowering. The mechanism of calcium influx caused by CINNA in isolated pancreatic islets depends on K+ -ATP channels and voltage-dependent calcium channels. In addition, CINNA and AITC increased serum GLP-1 *in vivo*, and CINNA was able to raise GLP-1 *in vitro* as well. CINNA and AITC were inhibited the activity of intestinal disaccharidases. TRPA1 channels represent a promising pharmacological target for the treatment of diabetes.

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ANALYSIS OF ESSENTIAL OILS IN TWO SPECIES OF GINGER GROWN IN ECUADOR

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Ginger is one of the most used species in traditional and ancestral medicine in different countries as it contains certain chemical constituents such as gingerol and shogaol that possess scientifically proven pharmacological and nutritional actions. The useful part of the plant is the rhizome and contains the essential oil composed by: Monoterpenes: camphene, neral, citronellol, 1,8-cineol, β-felandren, camphor, geranial, borneol, linalool and sesquiterpenes: (zingiberene, zingiberol, β-eudesmol, α-curcumene, β-bisabolene, β-bisabolone, (EE) -α-farnesene, elemol, β-sesquifelandren, furanogermenone, being responsible for the aroma sesquiterpenes [1,2]. Objective: Extract and characterize the essential oils of two species: sweet ginger and spicy ginger, grown in Ecuador.

The rhizomes of the collected species were used. The samples were collected in the province of Esmeralda, Ecuador and identified in the Guay Herbarium, Faculty of Natural Sciences-University of Guayaquil, Ecuador. The extraction of essential oils was carried out by hydrodistillation cohobation. The essentials oils were analyzed by using Agilent Technologies gas chromatography mass spectrometry equipment (7890A GC system and 5975C inert XL MSD with triple axis detector). A capillary column DB-5ms UI (30m x 0.25mm x 0.25µm) and helium as the carrier gas (1.1ml/min). The injection of 1.0µL of sample diluted in hexane was done at a temperature of 250°C with split mode, split ratio 25:1, the detector temperature was 230°C and the oven temperature was maintained at 60°C for 1.0 minutes, then it was increased to 240°C at 2°C/min. The electron ionization to 70eV and 230°C was used as ion source and the data compounds were collect with the full scan mode (40-1000 µ ma). Finally, the compounds were identified by comparison of their mass spectra and mass reference of Wiley 9th with NIST 2011 MS Library [3].

An essential oil yield of 0.5% was obtained for sweet ginger and 0.2% for spicy ginger. A total of 62 compounds were identified for sweet ginger and 82 for spicy, which showed a chemical composition with abundance of sesquiterpenes: sesquifelandreno (8.53%); zingiberene (8.18%) and farnesene (7.99%); which corresponds to that reported for *Zingiber officinalis* R. In sweet ginger the major component was 1.8-cineol (34.4%), in addition to methyl eugenol and β-pinene.

The joint analysis of the botanical characteristics and chemical composition enabled us to confirm that the so-called sweet ginger, despite its macromorphological similarity, does not correspond to a Zingiberacea.

Keywords: Sweet ginger, *S*picy ginger, Essential oils, Chemical composition

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HYPOGLUCEMIENT EFFECT OF THE PLANT *Cecropia peltata* L. (YAGRUMO) IN VIVO AND IN VITRO

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The plant yagrumo or guarumbo (*Cecropia peltata* L.) as is commonly known, is a specie of the genus *Cecropia* from the family *Cecropeaceae*, and from the popular knowledge are attributed medicinal properties (hypotensor, spasmolytic, bronchodilator and hypoglycemic), is used by communities as a therapeutic alternative in the treatment of diabetes mellitus. The objective of this work was to verify the hypoglycemic effect of plant *C. peltata* assayed *in vivo* with normoglycemic rabbits, New Zealand breed, and using human leukocytes *in vitro* in normoglycemic media. The type study is experimental. Rabbits were grouped into 6 groups of 5 animals, giving 3 cc of aqueous suspension of the plant at different concentrations from 0.8% to 6.4%. *In vitro* assay was performed with aqueous suspension of the plant at different concentrations from 3.2% to 9.6%, placing them in normoglycemic media with human blood cells, using Humulin® insulin as a control. A phytochemical screening was performed with ethanolic extract of the plant, evidencing the presence of saponins, cardiotonic glycosides, triterpenes and cyanogenic glycosides. Subsequently, the active substance β-sitosterol was isolated for *in vitro* assay at various concentrations, using Humulin® insulin as a control. In the in *vivo test*, the results were statistically homogeneous, even though there was no marked decrease in glycemia concentration; while in the *in vitro* assay of the aqueous suspension of the plant there was a slight tendency to decrease the glucose levels in the medium. As for the *in vitro* assay with β-sitosterol, a sustained hypoglycemic effect was observed over time with no variation in concentration×time interaction. Based on the analysis of the results obtained both *in vivo* and *in vitro* assays, it was concluded that aqueous suspension of the plant *C. peltata* had a lower hypoglycemic effect than shown by the isolated active ingredient β-sitosterol in the *in vitro* test.

Keywords: Hypoglycemic, *Cecropiapeltata*, Yagrumo, β-sitosterol.

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PHARMACOGNOSY OF *Ulva rigida* (ULVACEAE): A GREEN SEAWEED USED IN TEHUELCHE TRADITIONAL MEDICINE

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San Jorge Gulf (Patagonia Argentina) has an important algal diversity. Original people, Tehuelches and Mapuches, had used *Ulva* ("lúa", "luga-luga") for the treatment of internal inflammations. In previous studies we showed results of chemistry and primary bioactivity in *Ulva rigida* [1]. In this work we analysis of carbohydrate composition in *U. rigida* collected in spring, and its relation to anti-inflammatory activity. Metabolites were extracted from dried powder of the fronds with water at 100°C for 20 minutes (decoction) [2]. One fraction of aqueous extract was fractionated by dialysis (cutoff 6,000-8,000). Other fraction of decoction was fractionated with urea 7M and EDTA. Dialyzed fraction (Dd) and water from dialysis (Dwd) were analyzed for carbohydrate, proteins, sulfate, uronic acid and total phenols content by usual methods [3]. One portion of Dd, after hydrolysis with TFA 2M (121 °C, 90 min), was analyzed as their corresponding aldononitrile acetates by GC-MS [3]. Anti-inflammatory activity was analyzed with auricular edema by tetradecanoylphorbol acetate (TPA) in mice and carrageenan induced paw edema in rats.

Decoction showed oligosaccharides and polysaccharides enriched in rhamnose, xylose and/or arabinose, galactose residues with heavily sulfated suggesting presence of the sulfated xylorhamnans, glucuronoxylorhamnans and/or glucuronorhamnans, with galactose and/or glucose or arabinose residues, proteins and phenols.

The dialysate was enriched in rhamnose with arabinose and xylose residues, proteins and polyphenols. Waters dialysis showed oligosaccharides and peptides. The exhaustive sequence using 7M urea and EDTA corroborated the data previously obtained.

Anti-inflammatory activity was shown 57.9 % after 3 hours of carragenan-induced leg edema in rats but auricular edema by TPA didn't show activity. That bioactivity explains the use of this algae by original peoples from Patagonia. Among the compounds responsible for this activity, they are highlighted sulfated polysaccharides. Sulfated polysaccharides and their lower molecular weight oligosaccharide derivatives from marine macroalgae have been shown to possess a variety of biological activities.

Keywords: Polysaccharides, Green seaweeds, Anti-inflammatory activity, Tehuelche traditional medicine

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ANTIFUNGAL ACTIVITY OF BRANCHES METHANOLIC EXTRACT PHASES FROM *Minquartia guianensis* Aubl. (OLACACEAE)

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The wide spread of resistant microorganisms is a major threat to treat human diseases successfully. Many studies have been developed and directed to the discovery of new antimicrobial agents from plants extracts and other natural products [1]. Plants contain thousand metabolites and are valuable sources of molecules having antimicrobial properties [2]. In the search of these metabolites, we focus this work on *Minquartia guianensis* (Olacaceae) which is popularly known as Acariquara and huacapu, being found in several countries such as Colombia, Venezuela, Peru, Bolivia and Brazil [3]. The branches of *Minquartia guianensis* were collected in Reserva A. Ducke/INPA, Manaus-AM, dried and extracted with hexane and methanol. The branches methanolic extract was liquid-liquid partitioned afforded three phases: dichloromethane, ethyl acetate and hydromethanolic. The phases were assayed against the fungal strains: *Cryptococcus neoformans* and *Cryptococcus gattii* obtained from patients infected from Manaus (Brazil) and *Candida albicans* (ATCC 36231), to determine the minimum inhibitory concentration (MIC) by the Clinical and Laboratory Standards Institute (CSLI) method. Samples were dissolved in DMSO 10% and serial dilutions of each phase were performed with Roswell Park Memorial Institute (RPMI) medium to achieve concentrations from 800 to 6.25mg/mL. The 96-well plates were filled and incubated at 35 °C for 24 h for *Candida albicans* and 72h for *Cryptococcus gattii* and *Cryptococcus neoformans*. Amphotericin B (64mg/mL) was used as positive control. After incubation time, it was observed that the hydromethanolic phase showed MIC of 200 µg/mL and 800µg/mL against *Cryptococcus neoformans* and *Candida albicans*, respectively. The ethyl acetate phase showed MIC of 400 µg/mL against *C. albicans*. The dichloromethane phase do not showed activity against any tested strain. According to the results it was possible observed, that the hydromethanolic phase showed the best antifungal activity against *Cryptococcus neoformans*, followed by the ethyl acetate phase against *Candida albicans*. It is important to highlight that *Cryptococcus neoformans* and *Candida albicans* are two of the most important human-pathogenic fungi, being the main responsible cause of mortality in AIDS-patients [4]. All these results are being described for the first time.

Acknowledgements: To CT-Agro/CNPq, Pro-Amazônia/CAPES, FAPEAM and PPBio/CNPq for the financial support.

Keywords: *Cryptococcus neoformans, Cryptococcus gatti, Candida albicans*

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Ibervillea sonorae A MEXICAN MEDICINAL PLANT WITH ANTI-INFLAMMATORY AND ANTIPROLIFERATIVE PROPERTIES

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The high incidence and mortality due to cancer together with the problems that exist in its treatment are the main reasons that make it necessary to search for new treatments [1]. Plants represent a resource for obtaining new pharmacological principles [2]. Ethnics groups use *Ibervillea sonorae* medicinally in northwest of Mexico as topical antibiotic, antiarthritic, antirheumatic, antidiabetes, anti-inflammatory and anticancer [3]. In a previous work we demonstrated the antiproliferative activity of *I. sonorae* [4]. In the present work, we demonstrated for first time that the methanolic extract (ME) from *I. sonorae* inhibit the NO and TNF-α production in LPS-activated RAW 264.7 cells as a signal of its anti-inflammatory effect. NO levels were notably reduced by the ME from unripe fruits (MFU) and ripe fruits (MFR) with IC50 values of 20.4 and 23.1µg/ml respectively without affecting cell viability, while the ME from root (MR) decreased the NO production with IC50 value of 40.5µg/ml. Only MR showed cytotoxic effect at 200µg/ml decreasing cell viability to 79 %. In addition, TNF-α levels were reduced by 30 % with MFU and MFR at the maximum concentration tested (50 µg/ml). Additionally, both extracts showed great growth inhibition effect on HeLa, RAW 264.7 and A549 cell lines. MFU and MFR were the most active on HeLa with an IC50 of 3.1 and 3.6µg/ml, respectively. However, no effect by MFU and MFR on the inhibition of the non-cancerous L-929 cell line at 100µg/ml. Therefore, our data suggest that the antiproliferative capacity is of a selective type.

Keywords: NO, TNF-α, Cytotoxic effect, Antiproliferative effect.

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ANTINOCICEPTIVE ACTIVITY OF METHANOLIC EXTRACT FROM THE LEAVES OF *Byrsonima intermedia* A. JUSS (MALPHIGHIACEAE).

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Byrsonima intermedia popularly known as “murici pequeno”, is a Cerrado bush considered medicinal due to its astringent property in diarrheas and dysenteries, antimicrobial, anti-inflammatory and antiulcerogenic action. The present work aimed to evaluate the antinociceptive activity of the methanolic extract from the leaves of *B. intermedia* (MEBI) in experimental models with Swiss mice (n=7-10, 4-6 weeks old). The antinociceptive activity of MEBI was evaluated with the formalin test [1]. Male Swiss mice received MEBI (125, 250 and 500mg/kg) and vehicle (10mL/kg) orally as a control. The antinociceptive mechanism of action from MEBI related to acid-sensing ion channels (ASIC) and transient receptor potential (TRP) ion channels were investigated. The time (seconds) animals spent licking their right hind paw was used as the nociception indicator. Statistical significance ($p<0.05$) was determined by one-way ANOVA followed by Dunnett's test or by Student´s t test (protocol nº 1021 was approved by ethics committee). The formalin test in mice is a reliable model of nociception sensitive for various classes of analgesic drugs. The treatment with MEBI 250 mg/kg decreased the time animals spent licking their paw in both neurogenic (36.6%) and inflammatory (44.1%) phases when compared to vehicle-treated group. ASIC and TRP channels are involved in several aspects of nociception making them valuable targets in nociception studies. The investigation of these receptors revealed that MEBI only acts on ASIC (55.6%) decreasing the licking time of the MEBI-treated group when compared to the control group. These results indicate antinoceptive activity of the leaves of *Byrsonima intermedia*, which acts on ASIC receptors.

Keywords: *Byrsonima intermedia*, Pain, Formalin test, Malphighiaceae.

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ALKALOIDS OF *Zephyranthes fosteri, Habranthus concolor* (AMARYLLIDACEAE) AND THEIR HYBRID

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Zephyranthes fosteri, *Habranthus concolor* and *Habranthus* aff. *concolor* (Amaryllidaceae) were studied chemically in order to support or refute the hypothesis that the last one is a hybrid derived from the two former species. These three taxa grow at the Ecological Reserve (REPSA) located at the National Autonomous University of Mexico (UNAM). We identified the alkaloids present in the methanol extract and the alkaloid fraction of the bulbs and the leaves. The extracts were analyzed by gas chromatography coupled to mass spectrometry. The three taxa showed different chemical profiles. The major alkaloid of *Z. fosteri* was licorine, followed by an alkaloid whose mass spectrum had a base peak and a molecular ion in m/z 189 (261). This compound was isolated by chromatographic methods, and analyzed by 1H y 13C nuclear magnetic resonance finding that it is a novel compound, which was named as 3'-demetoximesembranol. In the case of *H. concolor* the major alkaloids were galantamine, and chlidantine. In the case of the hybrid were licorine, and an alkaloid whose mass spectrum had a base peak and a molecular ion in m/z 175 (247), respectively. We also evaluated the ability of the methanol extracts to inhibit the enzyme acetylcholinesterase and determine their potential as phytodrugs for the treatment of Alzheimer's disease. The methanol extract of the bulbs showed the highest inhibitory activity, *Z. fosteri* being the most potent, then *H. concolor*, and finally the hybrid. Our results allowed to conclude that there are chemical differences between the three taxa, and therefore support the existence of the hybrid.

BIOACTIVITY AND HISTOCHEMISTRY OF *Euphorbia tithymaloides, Cnidoscolus chayamansa, Jatropha curcas, Jatropha gossypifolia* and *Croton conduplicatus* Kunth (Euphorbiaceae)

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The Euphorbiaceae family possesses a wide botanical and chemical diversity, covering a wide range of applications such as nutritional, poisonous, medicinal, industrial, among others. The main secondary metabolites detected were triterpenes, followed by flavonoids and alkaloids [1]; They are usually aporphine's type, pyridine, indole, quinoline or tropane; these compounds mentioned have varied biological activities such as amoebicide, antispasmodic, antihypertensive, antineoplastic, diuretic, hypoglycaemic and anti-inflammatory; Within the family, the most outstanding genera are: *Euphorbia, Croton, Jatropha, Phyllanthus* [1]. In this family the *Euphorbia tithymaloides* specie is distinguished in which the ethyl acetate fraction of their leaves is active against *Bacillus cereus, Staphylococcus aureus* and *Pseudomona aeruginosa*. The dichloromethane fraction of fresh leaves is active against *Fusarum oxysporum* at the concentration of 10mg/mL and showed an LC50 of 378,997 ppm against *Artemia salina* [2]. The chloroform subfraction extracted of the leaves of *Cnidoscolus chayamansa* showed low toxicity to nauplii of *Artemia salina*. This fraction, at a concentration of 2 µg / mL, presented a 78.5% antioxidant activity in the linoleic-β-carotene complex compared to 55.1% presented by the vitamin C standard at the same concentration [3]. Ethanol's extracts of the dry leaves of *Jatropha curcas* and *Jatropha gossypifolia* do not present acute toxicity or anti-inflammatory effect against *Wistar* rats, respectively, in these species both phytochemical and histochemical screening corroborate the chemical diversity reported in the literature for the Family Euphorbiaceae [4]. *Croton conduplicatus* kunth (Euphorbiaceae) reported for the department of Sucre-Colombia for the first time. Gas chromatography coupled to mass spectrometry showed the presence of Amuronin, the majority aporphinic alkaloid, potentially useful for the control of *Aedes aegypti* larvae; Vector of the Yellow Fever virus, Dengue, Chikunguya and Zika, with a mean lethal concentration (LC50) of 320,995 µg/mL [5].

Keywords: *Euphorbiaceae, Jatropha, Croton, Cnidoscolus.*

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HISTOCHEMISTRY AND GAS CHROMATOGRAPHIC PROFILE COUPLED TO MASSES OF THE ETHYL ETHER FRACTION FROM FRESH LEAVES EXTRACT OF *Cnidoscolus acontifolius* (EUPHORBIACEAE)

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The histochemistry of *Cnidoscolus acontifolius´s* leaves showed the presence of calcium oxalate crystals, flavonoids, lignans, saponins, tannins and alkaloids [1]. The ethyl ether fraction of the aqueous extract of C. acontifolius leaves showed low toxicity against *Artemia saline* [2].

The gas chromatographic profile of the fraction shows two peaks (8 and 13) with percentages of areas of 7,711 and 30,251; Retention times of 68,184 and 86,589 minutes respectively; they were analyzed with a mass selective detector (MS), operating in full scanning mode to perform a comparative analysis between fragmentation patterns with their mass specters and the databases NIST, Wiley and Adams; In the peak (8) the molecular ion at m/z 429.3 (2.38%) was registered and peaks at m / z 355.1 (4.76%) [M+-74.2], 309,3 (1.9%) [M+-120], 281 (24.76%) [M+-148.3], 239 (2.38%) [M+-190], 207 (55,23%) [M+- 222.3], 178 (1,90%) [M+-251.3], 169(3.33%) [M+- 260], 141,2(6,66%) [M+-288.1], 113,2(10%) [M+-316.1], 85,2(56,19%) [M+-344.1], 70,2(66,19%) [M+-359.1], 57,2(100%) [M+-372.1]. The base peak of 57.2, characteristic for isoquinoline alkaloids referenced in the family Euphorbiaceae; Molecular formula C27H27NO4, derived from the Hemiargyrine [3]. For the peak (13) the molecular ion at m / z 429 (2.38%) and peaks at m / z 408,4(11.02) [M+-20,6], 355.2 (9,48%) [M+-73.8], 325,2 (5,17%)[M+- 103,8], 281 (50,00%) [M+-148], 249 (12.06%)[M+-180] , 207 (100%)[M+-222], 190 (95,68%)[M+-239], 175(26,72%)[M+- 254] , 148(22,41%) [M+-281], 121(58,62%) [M+-308], 81,2(60,34%)[M+-347,8], 53,1(9,48%) [M+-375,9]. The base peak of 207.1 is characteristic for benzophenanthridical alkaloids referenced in the family [4,5], molecular formula C22H23NO8, corresponding to an angina derivative [6].

Keywords: Histochemistry, *Cnidoscolus acontifolius*, Alkaloids

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ESSENTIAL OIL OF *Chrysopogon zizanioides* (L.) ROOTS: TLC/GC-MS ANALYSIS, ACUTE TOXICITY AND ANTIMICROBIAL ACTIVITY AGAINST MULTIDRUG RESISTANCE MICROORGANISMS

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Chrysopogon zizanioides (L.) commonly known as vetiver, is a perennial grass native to India, belonging to Poaceae family. Essential oil from *C. zizanioides* (L.) root (CZR-EO) was analyzed to determinate its chemical composition, *in vitro* antimicrobial activity and *in vivo* acute toxicity. The CZR-EO was obtained by steam distillation process. Methicillin resistant *Staphylococcus aureus* ATCC 43300 (MRSA), resistant to vancomycin *Enterococcus faecalis* ATCC 51299 (VREF), TEM-1 β-lactamase producer *Escherichia coli* (BLEC), inducible AmpC β-lactamase *Pseudomonas aeruginosa* ATCC 27853 (iAmpC-BLPA) and MDR *Candida albicans* ATCC 10231 (MDRCA) were used as target microorganisms. Adapted microdilution protocols M07-A9 and M27-A2 from Clinical and Laboratory Standards Institute (CLSI) were used to determine minimal inhibition concentration (MIC) of bacteria and yeast, respectively [1,2]. For direct bioautography test, silica gel was used as stationary phase and ethyl acetate-toluene (1:1) and toluene were used as mobile phases in two-dimensional thin-layer chromatography (TLC). Muller Hinton broth/agar (9:1) was used as media culture layer. The compounds belonging to the fraction presenting antimicrobial effect were preliminary identified through accoupled TLC–Gas chromatography/Mass spectrometry (GC/MS) [3]. *In vivo* acute toxicity of essential oil, expressed as lethal concentration 50 (LC50) was assessed using *Caenorhabditis elegans* Bristol strain (N2 line) [4]. The MICs of CZR-EO for MRSA and VREF were 0,25µL/mL and 0,50µL/mL respectively using microdilution test. There was no effect against gram-negative bacteria and MDRCA. MRSA and VREF were also inhibited in direct bioautographic assay with 0,16µL/mL applied on TLC plaque. Fraction 6 (F6) was identified in bioassay as the causative of antimicrobial effect through two-dimensional TLC with retention factors of 0,70 and 0,08. GC/MS analysis of F6 revealed eleven identical compounds of those identified in unfractionated essential oil, representing 84% of total compounds in the fraction. The major compounds characterized from F6 (55,8% of total fraction) were: 4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane, 8-Cedren-13-ol, and 3,8-Dimethyl-4-(1-methylethylidene)-2,4,6,7,8,8a-hexahydro-5(1H)-azulenone. The LC50 of CZR-EO —determined through Probit analysis— was 4,1 mg/mL. In conclusion, volatile compounds of *C. zizanioides* root have a great potential to be used as a source of antibacterial molecules. Although deep research to determinate specifically the compound(s) causing antibacterial activity of CZR-EO is necessary, the present study represents an important contribution in this way.

Keywords: Antimicrobial activity, *Chrysopogon zizanioides*, Multidrug resistance, Essential oils, Bioautography, *Caenorhabditis elegans*, Acute toxicity.

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5.

CHEMOSYSTEMATIC STUDY OF POLYISOPRENYLATED BENZOPHENONES OF *Clusia* GENUS

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Benzophenone derivatives are special metabolites that arouse great scientific interest. The Clusiaceae family is known for producing large amounts of benzophenone derivatives with several isoprene residues on their structures, which are responsible for the observed complexity and structural variety in this class of substances, and also contribute for their biological activities. The genus *Clusia* comprises species of neotropical distribution and many species are used in folk medicine to treat health problems such as hypertension, cardiovascular disorders, headaches rheumatism and syphilis. *Clusia* represents an important genus of Clusiaceae, with 55 different polyisoprenylated benzophenones identified so far. These substances were analyzed from biosynthetic and chemosystematic points of view, allowing the determination of characteristics regarding their production, accumulation and distribution within this genus. Polyisoprenylated benzophenones found in *Clusia* showed a high prenylation degree, with 2 to 5 isoprene units and a greater occurrence in flowers and fruits. Section *Cordylandra* showed a very similar occurrence of 2,4,6-trihydroxybenzophenone derivatives and bicyclo[3.3.1]nonane-2,4,9-trione derivatives, the majority of them with 4 isoprene units. In section *Anandrogyne* there is a predominance of simple 2,4,6-trihydroxy-benzophenone derivatives, with 2 isoprene units, and in *Chlamydoclusia* predominates bicyclo[3.3.1]nonane-2,4,9-trione derivatives with 4 isoprene units. Although highly prenylated, these substances showed low oxidation indexes, which from an evolutionary perspective corroborates the fact that Clusiaceae is a family in transition, with some common aspects with both basal and derived botanical families. This fact can justifies the changes in the taxonomic position of the family Clusiaceae in recent years.

Keywords: Chemosystematics, *Clusia*, Clusiaceae, Polyisoprenylated benzophenones

BIOLOGICAL ACTIVITIES OF *Phaedranassa carmioli* ALKALOID EXTRACT: ACETYLCHOLINESTERASE INHIBITION IN RAT HIPPOCAMPUS HOMOGENATE AND ANTI-INFLAMMATORY ACTIVITY IN MOUSE AND RAT MODEL

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Phaedranassa carmioli (Amaryllidaceae) is an endemic species of Costa Rica. With the exception of P.carmioli described from Costa Rica, the genus Phaedranassa is restricted to the northern Andes on open moist slopes and xeric valleys in Colombia and Ecuador.

The bulbs of *P. carmioli* were recolected in Santa María de Dota (9º 38' 41,07''N, 83º 58' 00,36'' W, 1550 m) in January. The plant identification were done by the botanist Luis Poveda and a sample was deposited in the Juvenal Valerio Rodríguez Herbary of the Universidad Nacional. The recollection were endorsed by the Biodiversity Institutional Commission with the MINAET/SINAC agree.

The alkaloid extract of the bulbs, realized according to Iannello *et al.* [1] and analized by GC-MS, contained as major compound lycorine (70%) and other minor alkaloids like deacetylcantabricine (5.4%), sternbergine (3.2%) and galantamine (0.4%).

The antiacetylcholinesterase activity was assessed with an *ex vivo* model using a rat hippocampus homogenate as source of the enzyme. The alkaloid extract showed a significant enzyme inhibition ($p<0.001$) in a concentration range between 18.8 and 600 µg/mL (IC50: 87.1±4.0 µg/mL). For determination of the Ki constant, three different alkaloid extract concentrations were used, and acetylthiocoline was used as a substrate at five different concentrations. The inhibition type of this alkaloid extract was determined as mixed inhibition.

In order to assess the anti-inflammatory activity two models wer adopted: auricular edema, induced by 12-O-tetradecanoylphorbol acetate (TPA) in the mouse and the carrageenan-induced edema of the hind paw of the rats. In the mouse model, the extract did not reduce significantly the edema but on the carrageenan model the alkaloid extract (60%, 16mg/kg) demonstrated a significant ($P<0.001$) inflammatory inhibition between 2-4 hours after the inflammation induction similar to indomethacin (65%, 50mg/kg,). These procedures were approved by the Institutional Committee for Care and Handling of Experimental Animals of the University of Costa Rica (CICUA #1713).

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Keywords: *Phaedranassa*, Antioxidant, Antinflammatory, Antiacetylcholinesterase, Amaryllidaceae.

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SEMIQUANTITATIVE ANALYSIS OF LINALOOL AND LINALYL ACETATE CONTENT IN TWO LAVANDULA ESSENTIAL OIL COMMERCIAL SAMPLES BY CG-MS

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Lavender oils are used and known around the world, either by its aroma or by its relaxing effect on smooth muscle, as an spasmolytic activity because they cause they open potassium channels and hyperpolarise the cells. [1,4]. This sedative action is also reported and has been investigated in several species including man, due to its vapour effect [2]. Preparations concerning lavender oils are used at a dilution, in body massages, mainly to produce muscle relaxing effects, and these therapeutic effects are atributed to the monoterpenes linalool (L) and linalyl acetate (LA) which are responsible by reduction in overall activity cause they stimulate olfactory sense organs. Linalool are also described to produces a fall in blood pressure, due to peripheral vasodilatation [3]. Considering that linalool can be converted in linalyl acetate in plant tissues and the linalyl acetate can be converted in the linalool, by the humans enzymes, by plasmatic esterases, we performed the quantification of these two monoterpenes together. According literature data, there are diferent possible route of administration, exposure to the aroma of an essential oil and the application of the diluted oil on skin. In this work, we would to estimate the semiquantitative content of two monoterpenes metabolites, linalool (L) and linalyl acetate (LA) from two diferent commercial samples of the *Lavandula officinalis* essential oils by two CG-MS methodologies, to estimate the [L+LA] content of two commercial *Lavandula* essential oil samples used diluted on skin, in body massage to relieve pain. In the first analysis by the Methodology A, the LEO1 showed 38 signals, 23 substances were identified on it and 66,34% of [L+LA] were present. The LEO2 analysis by the same methodology (A) shows 29 signals, with 23 identified substances and 85,06% of [L+LA] content. In the second methodology (B), the LEO1 sample presented 53 signals, 23 identified substances and 74,49% of [L+LA] content and the LEO2, presented 28 signals, 24 identified substances and 90,18% of [L+LA] content. In both methodologies analysis, the chemical profile and the [L+LA] content were compatible with the literature. This semiquantitative results are importante to determine the dose-related effect of the lavender oil comercial sample, the comercial lavender essential oils that present the compatible [L+LA] content and to define the essential oil concentration could be used therapeutically to relieve pain in public health care.

Keywords: Lavender, Essential oil, Linalool, Linalyl acetate, Therapeutic uses

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ANTIOXIDANT AND ANTIBACTERIAL SCREENING OF SIX AMAZONIAN PLANTS

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The Amazon state located in northern Brazil has a large variety of plant species with a rich metabolic production due to the characteristic conditions of environmental stress the Amazon region where they are located [1]. Therefore, in order to find out their biological potential, it is necessary to use fast, inexpensive and efficient methods to perform a good screening [2]. The present study aimed to investigate the *in vitro* bioactive potential of vines, bark, leaves and branches extracts of six plants of the Amazonas state (*Diplotropis purpurea*, *Bauhinia* sp, *Pricramnia selowii*, *Ormosia excelsa*, *Acacia altiscandens* and *Parkia igneida*) and evaluate its antioxidant and antibacterial activities (table 1). Dichloromethane and methanol extracts were prepared and as well the dichloromethane and ethyl acetate phases of the methanol extract partition from *P. selowi.* To evaluate the antioxidant capacity, we used DPPH and Fe3+/Phenanthroline methods, and the determination of antibacterial activity was made by agar diffusion method against *Bacillus cereus* (ATCC 14579 T), *Klebsiella pneumoniae* (ATCC 13883 T), *Nocardia* brasiliensis (ATCC 19296 T), *Pseudomonas fluorescens* (ATCC 13525), *Serratia marcescens* (ATCC 6919). In DPPH and Fe3+/Phenanthroline, *Bauhinia sp.* (vines) extracts possessed higher antioxidant potential (1.6/ 0.6). The promising antioxidant efficacy was also detected for *O. excelsa* leaves (1.7/ 0.6), *D. purpurea* leaves and branches (1.8/2.0 and 1.9/2.1, respectively). The extracts were evaluated against some bacteria and the best results were found to methanolic extracts from branches from *D. purpurea*, methanolic extract of leaves of *O. excelsa,* and AcOEt phase of the methanolic extract from leaves of *P. sellowii.* Theses extracts were active for all bacteria tested. The high antioxidant, antibacterial activity of the *D. purpurea* and *Bauhinia* sp. extracts and antibacterial activity of the *P. selowii* extracts and phases encourage the chemical fractionation to find out the active substances.

Acknowledgements: To CT-Agro/CNPq, Pro-Amazônia/CAPES and PPBio/CNPq for the financial support.

Keywords: Bioactivity, Amazonian plants, Antioxidant activity, Antibacterial activity.

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PHARMACOGNOSTIC AND PHYTOCHEMICAL EVALUATION OF OREGANO (*Origanum vulgare* L.)

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Oregano *(Origanum vulgare L.)* is an aromatic plant, commonly used for culinary purposes, which is attributed to the antispasmodic effects, being effective in the treatment of asthma and with a greater demand for its application in the perfumery industry. The essential oil obtained from its distillation, shows antimicrobial, antiparasitic, and antioxidants properties, depending on its composition by the presence of chemical substances characteristic of the species. In this work, the pharmacognostic and phytochemical properties of the oregano leaves cultivated on the Ecuadorian coast were evaluated; and thereafter the essential oil obtained therefrom, as well as its antimicrobial and antifungal activity. The results obtained in the physicochemical parameters presented an average value of 19% as percentage of total ash, which differs from the amount established by Codex Alimentarius [1] for dried oregano in a maximum of 10% total ash; this can be associated with the characteristics of the cropland. In the phytochemical screening, the aqueous, ethereal and alcoholic extracts determined the presence of metabolites such as: alkaloids, quinones, triterpenes, reducing sugars, flavonoids and phenols, with results similar to those obtained in *Ocimun gratissimum L.* (Oregano cimarron) according to the literature [2]. The analysis of oregano oil by gas chromatography coupled to mass spectrometry (GC-MS) reported a concentration of 42.83% of carvacrol, followed by 18.38% of 4-terpinenol, and 3.98% of thymol, as the most abundant compounds between all detected. The antimicrobial activity was demonstrated against *Escherichia coli, Sthaphylococcus aureus, Salmonella typhimurium* and *Candida albicans*, with sensitivity in all cases to a concentration of 300 ul of the essential oil, this is attributed to the presence of phenols such as thymol and carvacrol.

Keywords: *Origanum vulgare L.*, Oregano, Thymol, Carvacrol, Oregano oil.

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METABOLITE PROFILING AND IDENTIFICATION OF THE CHEMICAL MARKERS FROM FOUR DIFFERENT BRAZILIAN

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Many Asteraceae medicinal plants in Brazil are popularly known as “arnica” and they are used in substitution of the exotic species Arnica montana, which has ceased to be used for its oral toxicity and because this is a European species threatened with extinction. They are *Solidago chilensis*, *Chromolaena odorata*, *Wedelia paludosa*, *Tithonia diversifolia*, *Porophyllum ruderale* and *Lychnophora ericoides*. However, many of these species, as *A. montana*, couldn’t be used as medicinal plants cause their oral toxicity, as Lychnophora ericoides and *Arnica montana* itself. These “arnica” species are widely distributed in tropical and subtropical regions of Brazil and they are described as anti-inflammatory, anti-hyperalgesic, antinociceptive, antispasmodic, diuretic and used topically to treat edema and healing [3] AGRA, 2008. In this work, we investigated four “brazilian arnica” species: S*olidago chilensis*, *Chromolaena odorata*, *Wedelia paludosa* and *Tithonia diversifolia* to compare their therapeutic uses and their chemical profile using GC-MS and HPLC-UV-DAD with the literature data and *A. montana*. The essential oil of leaves and inflorescences were carried out by hydrodistillation and analyzed through CG-MS [1]. These analyzes showed sesquiterpenes as germacrene-D and B, (+)-spathulenol, caryophyllene oxide, β-caryophyllene and d-cadinene as their major compounds. The aerial parts of the species studied were dried, pulverized and extracted through dynamic maceration. The obtained extract were reduced pressure, and fractionated with increasing polarity solvents. Hexane, ethylacetate, dichloromethane and buthanol fractions of the aerial parts were performed through TLC, CLC, GC-MS and HPLC-UV-DAD chromatographic techniques according with their polarity characteristic in order to separate and identify the major substances present. The main compounds of these “Brazilian arnica” extracts were terpenoids, such solidagenone, from *S. chilensis* inflorescences and rhizomes, kaurenoic acid, from Wedelia paludosa leaves and stems, d-cadinene, from *Chromolaena odorata* leaves, steroids and sesquiterpenelactones from *Tithonia diversifolia* leaves and flowers. Phenolic compounds are also present in the analyzed extracts and they are mainly quercetin flavonoids derivatives known for their anti-inflammatory activities. The characterized compounds may be therefore responsible to the activities described for these species.

Keywords: Arnica, CG-MS, HPLC-UV-DAD.

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ANALYTICAL MICROSCOPY OF *Bixa orellana* L., SUBSTITUENT OF *Crocus sativus* L. AND *Capsicum annuum* L.

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Bixa orellana "rucu", "urucu", "achiote", "bija" is a species originated in tropical America, probably in the southwest of the Amazon region. It extends from Mexico to Brazil and Argentina (Chaco, Córdoba, Formosa, Salta) and in the Caribbean. Nowadays, it is distributed in tropical countries from the old and new world.

The seeds which are used by indigenous communities to paint their bodies

in religious rituals produce a dye, which is the main adulterant and/or total substituent for saffron and pepper.

In this study, we will present the histological elements of diagnosis corresponding to each drug with the purpose of detecting a substitution or alteration when presented in powder form, fragmented or as a manufactured product.

Bixa orellana fruit: it is a coffee colored ovoid capsule which is covered with soft thorns and several seeds coated with a reddish-orange pulp (aril).

Histological elements of diagnosis: Outer layers of the seed, amiliferous parenchyma.

Crocus sativus flower: the trifid stigmas are the drug.

Histological elements of diagnosis: pollen grains, parenchyma cells of the stigma with extended buds, libero-ligneous bundles remains, epidermal cells with buds.

Capsicum annum fruit: it is a berry with a reduced mesocarp.

Histological elements of diagnosis: strongly cuticularized epidermis, layers of sub epidermal collenchyma. On the border of the mesocarp: large cells were observed with sclerosed cells of the inner epidermis underneath them. Seed: testa, very sinuous cells (encephaloid cells).

Microphotographs and designs of each drug will be presented. A dichotomous key will be created to distinguish each of the species when they are fragmented or in powdered form.

Keywords*: Bixa orellana, Crocus sativus, Capsicum annuum*

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ISOLATION AND CHARACTERIZATION OF TWO INUSUAL SESQUITERPENE LACTONES FROM THE METHANOLIC EXTRACT OF *Hedyosmum racemosum* (Chloranthaceae)

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The genus *Hedyosmum* (Chloranthaceae) comprises approximately 45 species distributed throughout the tropical and subtropical regions of America. Sixteen of them have been reported in Ecuador. *Hedyosmum racemosum* (Ruiz & Pav.) G. Don, is known by the indigenous population as, "guayusa", "guayusa de monte", and "jicamilla". The species is widely used under the folk medicine to treat inflammations together with *Bixa orellana.* It is also used with *Cordia* to treat snakebites. Studies of other species of *Hedyosmum* genus indicate the isolation of guainolides, sesteterpenes, and lindenalolides. Sesquiterpenlactones are also isolated from species of Brazil [1] and flavonoids glycosylated from Colombian species [2]. Although the folk use, of "guayusa" there is not data about chemical and pharmacological studies of this species. With the purpose of identify the major metabolites present in the organic extracts, and evaluate their potential biological activity, the study of *Hedyosmum racemosum* was undertaken. Dry leaves of plant (500g) were macerated with solvents of increasing polarity, n-hexane, ethyl acetate and methanol. Each one of these extracts were submitted to column chromatography according to the best conditions found by TLC. From the methanolic extract were isolated two unusual lactones bolivianine (**1**) previously isolated from *Hedyosmum angustifolium* [3] and onoseriolide (**2**) isolated from *Hedyosmum brasilensis* [4].

Keywords: *Hedyosmum racemosum*, Bolivianine, Onoseriolide, Antimicrobial

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QUALITY ASSESSMENT OF COMMERCIAL SAMPLES OF ESPINHEIRA-SANTA

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Maytenus ilicifolia Reiss. (Celastraceae) is included in "Formulário de Fitoterápicos da Farmacopeia Brasileira" under the vernacular name espinheira-santa, and the preparation of its dry leaves by infusion in water is associated with therapeutic indications such as anti-dyspeptic, anti-acid and gastroprotective [1], regarded as medicinal tea in Brazil by Resolução das Diretorias Colegiadas (RDC) of Agência Nacional de Vigilância Sanitária (ANVISA) no. 26, of May 13, 2014. The leaves displaying spiny teeth along the margin of *M. ilicifolia* are similar to those of other botanical species, leading to adulterations and falsifications [2]. Under those circumstances, the objectives of this work were to analyse the labels and evaluate authenticity of commercial samples of espinheira-santa by macro and microscopic morphological study of the leaves. Nine samples of espinheira-santa were obtained from supermarkets, newsstands and herbalist's shops in the state of Rio de Janeiro, Brazil. The labels were analysed according to RDC 26/2014, which provides for registration and notification of phytotherapeutic products. Leaves and foreign matter were separated, weighed and the measurements compared to the ones reported on the labels. Dried and fragmented leaves were submitted to diaphanization and cross-sectioned on the petiole and midrib, following usual techniques for the preparation of semi-permanent slides. Photomicrographs were taken and analysed using cameras fitted to stereomicroscope and light field optical microscope. The labels were inconsistent with RDC 26/2014, including mentions to legislation of exemption from product registration related to food categories, although medicinal teas must be notified in the category of traditional phytotherapeutic product. Weight measurements showed significant variations in relation to data reported on the labels. In the leaves of samples 1, 2, 3, 5 and 7, the venation pattern is semicraspedodromous and the midrib and petiole are concave-convex with vascular bundles arranged as an arc opened towards the adaxial surface. In the leaves of samples 4, 6, 8 and 9, the venation pattern is simple craspedodromous, the midrib is biconvex with a cylindrical to flattened vascular bundle and the petiole is also biconvex, with two projections facing the adaxial region and cylindrical vascular bundle. Morphological descriptions were compared to literature data [2], suggesting the identification of samples 4, 6, 8 and 9 as *M. ilicifolia* and 1, 2, 3, 5 and 7 as *Sorocea bonplandii* (Baill.) W.C. Burger et al. (Moraceae), for which there are no clinical studies assuring its effective and safe use.

Keywords: Medicinal plants, Plant anatomy, *Maytenus ilicifolia*, *Sorocea bonplandii*

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SEROTONERGIC LIKE PROFILE OF 4-PROPYL-2H-BENZO[H]-CHROMEN-2-ONE (FCS-304) IN MICE AND RATS

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The aim of this work was to assess the serotonergic like profile of 4-propyl-2H-benzo[h]-chromen-2-one (FCS-304) in L-5-hydroxytryptophan (L-5-HTP) test in ICR mice as well as in behavioral despair and reserpine tests in Wistar rats. Previous works shown that FCS-304, a semisynthetic coumarin, displays MAO-A inhibitory properties.

FCS-304 (50-75-150 mg/Kg, p.o.) significantly potentiated L-5HTP signs in mice in a dose dependent manner. In rats, FCS-304 was effective to decrease the immobility time in behavioral despair induced for forced swimming and to antagonize reserpine induced signs. Imipramine (30mg/kg, p.o.) was the reference agent used.

These results add support to propose that FCS-304 could elicit antidepressant effects related to MAO-A inhibitory activity.

Keywords: Antidepressant, Coumarin, L-5-hydroxytryptophan, MAO-A, Reserpine.

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EVALUATION OF SOME PHYSICOCHEMICAL PROPERTIES AND STABILITY OF RUTIN IN A EXTRACT FROM CALYCES OF *Physalis peruviana*

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Physalis peruviana is a plant used in traditional medicine for its antioxidant properties which are attributed to its phenolic compounds. The calyx of *P. peruviana* is widely used in folk medicine for its properties as anticancer, antimicrobial, antipyretic, diuretic, and anti-inflammatory.

Rutin is the major flavonoid of the ethanolic extract from calyces of *P. peruviana* [1], this flavonol has antioxidant properties, it has been used in the treatment of a number of diseases [2], but a big limitation associated with rutin is its poor aqueous solubility which leads low oral bioavailability.

The aim of this study was to evaluate the aqueous solubility, partition coefficient and stability of rutin in the ethanolic extract from calyces of *P. peruviana* and isolated rutin in order to generate information for the development of herbal formulations with this extract.

The solubility of isolated rutin and rutin in the extract from calyces of *P. peruviana* was evaluated in different aqueous mediums like phosphate buffer pH 6.8, phosphate buffer pH 7.4 and water at 25 and 37°C. Partition coefficient was determinate between octanol and buffer pH 7.4 at 25 and 37ºC. Finally, stability study was carried out under stress conditions such as acid, alkaline, neutral hydrolysis and oxidation.

Based on the solubility data it was possible to conclude that isolated rutin is very slightly soluble in aqueous media (1,000 - 10,000mL of media to dissolve 1g of rutin) while rutin in the extract was classifying as slightly soluble (100 - 1,000mL of media to dissolve 1g of rutin). In same way, partition coefficient for rutin in the extract was higher that the isolated rutin. Regards to the stability, isolated rutin showed higher degradation under neutral hydrolysis, acid hydrolysis and oxidation conditions than the rutin in the extract. The results suggested that the extract from calyces of *P. peruviana* is a promising rutin source with advantages for pharmaceutical formulation since it increases the solubility and partition coefficient of rutin and provides stability to this flavonoid.

Keywords: *Physalis peruviana* , Rutin, Solubility, Stability

Acknowledgments: DIB- UNAL and Colciencias for financing the project "Preclinical evaluation of a microencapsulated extract from *Physalis peruviana* calyces with potential use in the treatment of diabetes mellitus." 677-2014 contract.

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EVALUATION OF *Passiflora tripartita* var. *mollisima* SEEDS OIL AS POTENTIAL FUNCTIONAL INGREDIENT OF PHARMACEUTICAL NANOEMULSIONS

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Nanoemulsions are kinetically stable liquid-in-liquid dispersions with droplets in the range of 50-500nm with low polydispersity [1]. In the pharmaceutical field, nanoemulsions are employed for oral, topical and parenteral drug delivery systems, since it is possible to incorporate drugs with poor aqueous solubility, to improve the bioavailability of drugs and to promote the skin penetration, among others. In addition to water and surfactants, oil is the other important excipient for nanoemulsions development. Fruit seeds oils has been used for topical emulsions since they are sources of fatty acids with beneficial properties in health. *Passiflora tripartita var. mollisima* known as "curuba" or banana passion fruit is a wide distributed plant in Colombia. Its fruit is used for food proposes, especially for juices and desserts discarding the seeds. Previous investigations have reported antioxidant activity for *P. tripartita var. mollisima* seeds oil [2].

The aim of this work was to evaluate the viability of the seed oil of *P. tripartita var. mollisima* as oil phase in pharmaceutical oil in water (o/w) nanoemulsion development.

Initially, *P. tripartita var. mollisima* seeds oil was obtained and characterized in terms of its physicochemical properties (viscosity, density, refraction index, acid value, iodine value, saponification value, ester value and peroxide value). For nanoemulsion formation, at first it was determined the required hydrophilic-lipophilic balance (RHLB) for *P. tripartita* seed oil. For this, several emulsion was elaborated with different HLB (different mix of surfactants), doplet size and polydispersity was measured by a MasterSizer E3000 [3]. Once RHLB for *P. tripartita var. mollisima* seed oil was determinate, pseudo-ternary phase diagram for the oil, water and surfactant mixture system was constructed, in which it was possible to determine the region of existence of o/w nanoemulsion, droplet size and polysdispersity were measured by a zetasizer Nano ZS.

It was found a hydrophilic RHLB value *P. tripartita* seed oil since it was greater that 10, 54% of the elaborated emulsions were considered as stable nanoemulsions (droplet size less than 500 nm and polydispersity index less that 0.5). All the *P. tripartita* seed oil stable nanoemulsions were required more than 60% of water, less that 30% of oil and less that 30% of surfactant.

Based on the results, it was possible that conclude that seed oil of *P. tripartita* var. *mollisima* is a potential functional ingredient for development of o/w pharmaceutical nanoemulsions.

Keywords: Nanoemulsion, Curuba, *Passiflora tripartita* var. *mollisima*, Required hydrophilic-lipophilic balance, Pseudo-ternary diagram.

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OPTIMIZATION OF MACROPOROUS RESIN ADSORPTION FOR THE EXTRACTION OF FLAVONOIDS AND LIMONOIDS IN ORANGE JUICE OF OVALE CALABRESE (*Citrus sinensis*) BY DISPERSIVE SOLID-LIQUID EXTRACTION.

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In this study, the extraction of flavonoids and limonoids from orange juice by dispersive solid-liquid extraction, to different materials was investigated. Orange is a fruit that contain high amount of bioactive compounds especially flavonoids [1] and limonoids [2]. An adsorption procedure for the recovery of these compounds from juice of a particular cultivar of orange called “Ovale calabrese” (*Citrus sinensis*) was developed and evaluated. Three different resin adsorbents (XAD-2, XAD-4 XAD-16), chosen for their high affinity for polyphenolic compounds, were tested. The time of contact was fixed at 2 h on the basis of kinetic studies and after the adsorption, the efficiency of each resin to elute the analytes using an opportune solvent (recovery %) have been evaluated. The main parameters affecting on desorption of analytes (elution solvent composition, elution solvent volume, desorption time and pH) were carefully studied and optimized in order to improve the recovery % and reducing the analysis time. The result shows that the XAD-2 has low affinity for the target analytes whereas the other two resin XAD-4 and XAD16 proved to be very efficient in adsorbing flavonoids and limonoids. The highest adsorption efficiency for the target compounds in a short time was observed when, Amberlite XAD-16 was used. The use of a polymeric macropouros resin, to recovery bioactive compounds from orange juice, allowed the removal of almost the analytes contain into the juice. After the elution the DPPH test was carried out to evaluate the antioxidant activity of these extract. The orange extract concentrated on Amberlite XAD-16 resin exhibit high antioxidant activities for the high concentration of flavonoids and limonoids.

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PRE/PROBIOTIC WHEY POWDER: A NEW FUNCTIONAL AND ECO-FRIENDLY FOOD PRODUCT

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PPAF 02

Food waste is the single-largest component of the waste stream, in order to protect and safeguard the public health, useful and innovative recycling methods are investigated. The conversion of food wastes in value-added products is becoming a more economically viable and interesting practice.

The main goal of the study is to create new functional foods obtained from a dairy company waste: the whey.

The encouraging challenge is to produce a probiotic and prebiotic whey powder by spray drying.

According to WHO, probiotics are "live microorganisms which, when administered in adequate amounts, confer a health benefit to the host". *Lactobacilli* have been showed to exert health benefit both for human and animals in preventing or treating several disease caused by pathogens.

Probiotic drinks usually start from a milk-based matrix because the presence of proteins and lactose make up the best matrix for probiotics environment [5].

The survival of different lactobacilli cultures, in citrus juices, was previously investigated during drying and subsequent storage and compared with microorganisms powders obtained by freeze drying [1, 2]. Spray drying is a powerful tool to transform liquid food products into dry powder of high quality and at low cost.

In order to formulate novel probiotic drinks, whey, a diary waste provided by diary sicilian factory, was used. The probiotic cultures together with maltodextrin and the protein, obtained from whey, make the final product healthy and tasty. In response to the growing functional food demand on the international market, the promotion of this new functional powder, obtained from waste thanks to an innovative method based on low costs and short times, could lead to economic and substantial environmental and health benefits.

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MINERALS PROFILE IN NEW SWEET-POTATOES CULTIVARS (*Ipomoea batatas* L.Lam.)

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PPAF 03

The sweet potato (*Ipomoea batatas* (L.) Lam.) is a tuberous root largely cultivated throughout the world and has great importance in the diet of many people. The sweet potato is a source of energy and some cultivars are rich in biocompounds such as polyphenols, anthocyanins and carotenoids further nutrients like vitamin C and minerals. The objective of this study was to evaluate the mineral profile in new cultivars of sweet potatoes developed in Brazil by EPAGRI-EEI/SC. The mineral profile of three new sweet potatoes samples (SCS370 Luiza, SCS371 Katiy, SCS372 Marina) and Beauregard cultivar were determined according to the methodology described by Association of Official Analytical Chemistry-AOAC in official methods nº 975.03 and 965.09. The analysis were performed using atomic absorption spectrophotometry A300 (Analytik Jena AG) with air-acetylene flame (C2H2). The minerals analyzed were: Copper (Cu), Iron (Fe), Zinc (Zn), Manganese (Mn), Sodium (Na), Potassium (K), Calcium (Ca), Magnesium (Mg), Phosphorus (P), Cobalt (Co), Cadmium (Cd), Chromium (Cr), and Lead (Pb). The mineral content results (wet basis) of the samples SCS370 Luiza, SCS371 Katiy, SCS372 Marina and Beauregard was estimated in mg/100g and presented in the following order: ***Cu***: 0.56, 0.61, 0.58, 0.89; ***Fe***: 0.78, 1.00, 9.29, 1.24; ***Zn***: 0.77, 0.82, 1.00, 1.30; ***Mn***: 0.39, 0.27, 0.22, 2.74; ***Na***: 65.92, 58.17, 166.41, 290.73; ***K***: 1078.76, 989.42, 1037.25, 1087.83; ***Ca***: 164.12, 144.53, 18.71, 277.56; ***Mg***: 56.90, 119.05, 9.46, 189.00; ***P***: 13.12, 18.10, 57.35, 5.82; ***Co****Cd, Cr, Pb*

Keywords: Minerals, Sweet-potatoes, Composition, Nutrition

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INCIDENCE OF THE C/N RELATIONSHIP IN THE BIOTECHNOLOGICAL PRODUCTION OF *Pleurotus eryngii* USING CEREAL AND LEGUME FLOURS AS COMPONENT OF THE CULTURE MÉDIUM

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PPAF 04

Macromycetes fungi have within their constituents a wide variety of different secondary metabolites, responsable of various biological activity. For this reason, have been encouraged the study of the different process that allow stimulate the production of biomass with potential to be employed as functional food component, as submerged fermentation or liquid state fermentation (LSF).

LSF has been specially study using traditional carbon source, in contrast to the unusual ones. In the search of the increase the performance production, has been promoted the uses of non-traditionals carbon source (CS) as cereal and legume flours. The mayor component of these source are carbohydrates, those contributes the nitrogen and micronutrients necessary for the fungi growth. Is well know that the relation C/N is a important factor in the biomass production, reason for which in this research was evaluated the incidence that this relation have in the biotechnology production of Pleurotus eryngii , a medicinal and edible mushroom.

For this purpose, the LSF was performed using the standar methodology of the research group in Química de Hongos Macromicetos. Subsequently the biotechnological product was vacuum filtered and dried for 48 hours at 40 °C (all processes were performed in triplicate). The CS were: Bienestarina (BN), soybean milk (SYM), linseed (LI), flour of precooked yellow maize (YMp), yellow maize (YM), oats (OA), wheat (WH), barley (BR), soybean (SY), whole wheat (WW), chickpea (CH), rice (RC), sago (SO), seven grains (SG), rye (RY), Wheat bran (WB) and banana (BA). The C/N ratio was determined by elemental analysis. The results allowed to determine that doesn't relationship between C/N and biomass, consistent with previous reports, which suggest that this parameters wouldn't be applicable to the use of non-traditional source. The biomass obtained with Ymp and RC doesn’t present significant differences (7.7 and 8.03 g/L, respectively), although they have different C/N ratio (41,14 and 28,71 respectively). Similar case when using SG and YM, which have different C/N ratio (17.54 and 33.33 respectively) but the amount of biomass is similar (13.13 and 13.8 g/L respectively). On the other hand, with OA, SG and WH which have similar C/N ratios, the amount of biomass obtained is significantly different (16.55, 13.13 and 15.58 g/L respectively).

The above, can hypothesizes that the others components of the flours, as the fat acids or the differents metals, could play an important key in the biomass production, stimulating specific biosynthetic pathways and/or as enzimatic cofactor. For this reason, this components of the culture medium, would allow the obtention a higher biomass production and thus would be the first option in a biotechnological process for the obtention of P eryngii mycelium that could be incluid as component of a functional food.

MICROPROPAGATION OF TWO CULTIVARS BY STEVIA REBAUDIANA IN THREE TEMPORARY IMMERSION SYSTEMS TO INCURRATE IN AGRICULTURAL PRODUCTION

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Stevia rebaudiana (Asteraceae) produces in the leaves a sweetener, due to the presence of steviol glycosides (stevioside and rebaudioside), being attributed medicinal uses. Its commercial production requires high seed density and germination problems. The Temporary Immersion Systems (TIS) have the advantages of being semi-automated and lower cost systems. The objective of this study was the scaling in the *in vitro* production of two cultivars of *S. rebaudiana*; Morita II and Silvestre, using RITA®, BIT® and SETIS® and biomass production in the field for use like functional food. We were used Nodal segments with axillary shoots (2 to 3 cm) of the mother plants for the initiation of shoots cultures *in vitro*. We worked with half of the capacity of each system, at the density of 10 ml per explant, inoculated material maintained *in vitro* at one month of age. Explants of 0.5-1cm in length were introduced (not apical shoots).

The treatments produced vigorous plants, increased leaf numbers, shoots and multiplication rate compared to semi-solid medium. Both materials showed longer stem length in BIT compared to SETIS and RITA. Morita II in BIT produced on average eight shoots per plant, while in SETIS three. Silvestre, produced two outbreaks, with no significant differences between the systems, given the physical characteristics of the vessel, mainly. Regardless of SIT, the greenhouse survival was very similar, for both materials, as well as the production of foliage in the field. Morita II produced 260.7g and Wild 214.4g fresh weight. There were no statistically significant differences in the dry weight variable (80g dry matter / sample / material), so the selection of the material should be made based on the content of stevioside and on the adaptation of the material to the planting site. All the SITs evaluated allowed the scaling of plant production and both materials are promising for planting.

Keywords*:* Temporary Immersion Systems, *in vitro*, Biomass, Functional food

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TECHNOLOGICAL SURVEILLANCE STUDY: TRENDS OF ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY FOR FOOD INDUSTRY

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The accelerated growth of the pharmaceutical and food industries and their innovations in product development have increased the demand for versatile instrument analyses to ensure reliable results processed in the shortest time possible. Nowadays, many countries have promoted regulations that demand acceptable levels for individual chemical additives, residues and contaminants in food products, to ensure food safety and nutritional quality. Therefore, current industry needs fast and reliable results that allow determinations at very lower levels, greater specificity and greater facility in the detection of any alteration that can present a food. The High-Performance Liquid Chromatography (HPLC) has been proven to be an optimal technology for detecting and/or quantifying the great majority of food analytes, being largely applied in food analysis. In this study, a technological surveillance of the use of UHPLC technology for food analysis on the last five years was made. Systematic searches of scientific articles and patents were carried out. The data were systematized under InnoViTech technological surveillance methodology and processed using Microsoft Excel. In the period evaluated, a greater number of UHPLC related references were found in 2015 followed by 2016 and 2014. China leads the publications followed by Spain and the United States. Universities such as Almeria and Gent are pioneers but Thermo Fisher Scientific excels as a company in publications. Chemistry, agriculture and the biological sciences; biochemistry, genetics and molecular biology and medicine are the main subareas of approach. Concerning patents, a greater number of publications were registered in 2016 and 2013, being Solazyme Inc and Waters Technologies Corp, the most patent applicants. Some of the analyses carried out in foods using UHPLC are the determination and quantification of carotenoids and pigments, polyphenols, ascorbic acid, capsaicinoids, sterols, sugar profiles, sterols, aflatoxins, antibiotics such as 5-nitroimidazole and pesticides multiresidue analysis. Patents show information on the detection of poisons, pesticides, 2-methylimidazole, dioxide thiourea, L-carnitine, alpha glucosidase, endocrine disruptor chemicals. The information found provides an overview of progress and uses of this technology for the food industry.

Keywords: UHPLC, Innovitech, Instrumental method, laboratory

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RESISTANT STARCH (RS) FROM ANDEAN TUBERS AND TUBEROUS ROOTS: A PROMISING PREBIOTIC

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Studies related to ethnobotanical research and characterization of undervalued tubers and tuberous roots such as *Tropaeolum tuberosum*, *Ullucos tuberosus* and *Canna edulis*, have partially revealed their important nutritional and medicinal potential. However, the fact that the state has neglected this type of crops has resulted in: lack of resources for research and promotion, non-inclusion in rural or urban nutrition programs, absence in priority productive chains, systematic reduction of agrobiodiversity and disappearance of collective memory as to their cultivation, use and taste; said crops used to be part of the identity and culture of the indigenous people and peasants of the Andes [1]**.** Similarly, adequate bioprospecting to establish metabolites of interest present in each species is vital to be able to take advantage of all the natural competitive advantages of these resources still cultivated in small agricultural units of families of the Andes. Among these advantages are: adaptation to difficult climates and terrains, little or no requirements for agrochemicals and their resilience to climate change [2]. In this research, fifteen undervalued species of tubers and tuberous roots were evaluated in terms of their potential as raw material for native starch. Later physical and chemical processes were developed to obtain resistant starch RS: a type of modified starch whose chemical structure supports the attack of digestive enzymes [3,4]. RS percent obtained from three of the evaluated Andean resources was determined with Megazyme enzymatic kit K-AMYL based on ISO 6647:1987 and certified controls, SEM, DSC and TGA and AOAC methods were used to characterize the RS obtained. The starch obtained from the roots and tubers evaluated had a RS content between 5 and 30 percent. After a hydrothermal process the RS was increased between 50% and 65%, which means an important percentage available fiber [5]**.** Resistant starch RS is demanded by both the functional food industry and animal food industry since it is considered to be a prebiotic that provides beneficial properties to health such as: it improves bowel function, stimulates beneficial intestinal flora, increases fat oxidation, generates energy, promotes the intestinal immune system, lowers blood glucose level and promotes the loss of body weight [5]**.**

Keywords: Prebiotic, Resistant starch, Andean tubers, Andean roots

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PPAF 08

FEASIBILITY STUDY FOR DEVELOPMENT OF SPIRULINA BASED BAKERY SUPERFOODS

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Protein–energy malnutrition (PEM) or protein–calorie malnutrition refers to a form of malnutrition related to an inadequate calorie or protein intake in diet. PEM is fairly common worldwide in both children and adults and accounts for 6 million deaths annually. In the industrialized world, PEM is associated with diseases and predominantly seen in hospitals, and it is often found in the elderly. Protein energy malnutrition is common in low-income countries but also in children from higher-income countries including children from low socio-economic neighborhoods of large urban areas. Malnutrition may also be associated with other deficiencies related to the lack of microelements or essential fatty acids and amminoacids. Based on these considerations, the aim of the research team was to launch a research line focused on fortified and low-cost bakery products so that consumers in low-income or elderly people can be easily access as well as consumers with particular pathologies or adopting poor food regime. Thanks to the new and advanced technologies that deliver high quality products and cheaper than the past, attention has been focused on the use of microalgae ingredients.The microalga *Arthrospira maxima* (common name: *Spirulina*) is considered a "super-food" for its health promoting benefits and disease preventing properties over and above their usual nutritional value1. The interest in *Spirulina* is mainly due to its high concentration of phytonutrients and pigments useful in manufacture of functional food which include: oil rich in essential fatty acids and omega 3 and 6-fatty acids, high protein quality with good array of amino acids, sulphated polysaccharides, energy, minerals (Se, Zn, Ca, Fe, P), vitamins (vit C, E, folic acid, B 12) zinc and calcium, pigments (carotenoids and phycocyanin), flavonoids and phenolic acids2. The studies were conducted in collaboration with two companies in the sector (Dolciaria Monardo and Coacchio Foods). Spirulina extracts were supplied by Oil Fox Italia srl, located in Calabria (Italy), part of Oil Fox s.a. with headquarters in Buenos Aires (Argentina). A range of biscuits, sweets and bread-like products as well as pasta have been designed. Statistical delineates and response surface methodology were used to assess different formulations. The products were evaluated as compared to the technological, composition and sensory aspects comparing them with the standards. The results revealed in terms of texture, expansion coefficient, centesimal composition and sensory acceptance the feasibility of this enrichment without affected in a significant manner the typical characteristics of the products, including, with satisfactory sensory acceptance. The developed products presented appealing and stable colours, with added value in terms of health benefits, considering the antioxidant properties and PUFA-x3 content of the Spirulina, resulting in stable, attractive and healthier foods with enormous potential in the functional food market.

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Keywords: Microalgal, Bakery Products, Powered Food, Protein

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PRELIMINAR STUDY ON POLIPHENOLIC CONTENTS AND ANTIOXIDANT CAPACITY OF *Malus domestica* CULTIVATED IN COSTA RICA

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Malus domestica have been introduced in Costa Rica and adapted to its climatic conditions of altitude (2800 masl), being cultivated specifically in Los Santos region. These efforts have allowed to obtain fruits that are well accepted in the market because of their flavor, aroma and easiness of handling [1]. On the other hand, the advancement of biologic and chemical techniques has enabled more detailed research on polyphenols –abundant in these fruits- because of their bioactive properties such as antioxidant potential [2]. This scientific knowledge has in turn been an important factor in a higher consumption of fruits with high polyphenolic contents both fresh and in nutritional supplements. Hence, the present work focuses in the study of these high-altitude fruits cultivated in Costa Rica, regarding agro-ecologic improvement as well as determination of polyphenolic contents and antioxidant capacity. Two cultivars of *Malus domestica* were acquired, namely var. Anna and var. Jonas, which were processed to carry out analyses [3]. Also, work was performed in agro-ecologic conditions amelioration and biocontrol for soil protection. In this last, findings indicate adequate soils characteristics but some deficiencies in phosphorus and in biocontrol, *Trichoderma* spp and *Metarhizium* spp were isolated in leaves and branches as wells as a strain of Bacillus thuringiensis spp. Characterization of polyphenolic compounds through HPLC-MSQ lead to the identification of 28 compounds in the apple peel and pulp, including hydroxycinnamic acids, flavonoids, chalcones, and flavan-3-ols, including monomers, and procyanidin dimers and trimers(3). Regarding the in vitro antioxidant capacity evaluated through ORAC, results showed between 11.2 ±0.1µmol TE/mg extract and 16.8 ±0.3 µmol TE/mg extract for the samples of *M. domestica* var. Ana, and values ranging from 7.6 ± 0.1 µmol TE/mg extract and 10.2 ±0.2 µmol TE / mg extract for the var. Jonas [3,4].

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PECTIN PRODUCTION FROM *Manilkara surinamensis* MATURE FRUITS

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The mature fruits from *Manilkara surinamensis* were collected at the Guayaquil botanical garden and prior to their use were selected and physically characterized. As acid type and pH of extraction could influence the yield and type of pectin obtained [1], pectin extraction was carried out using the acid hydrolysis method with hydrochloric acid (HA) and glacial acetic acid (GAA). In each case, the pH values ??(2 and 3) and three extraction times (30, 60 and 90 minutes) were evaluated. Pectin was characterized using infrared spectroscopy (IR), for determining not only the characteristics of the bands but also the degree of methylation. Statistical analysis of pectin extraction indicated that HA yields were generally higher than those obtained with GAA and that the maximum yield (77.2%) was obtained with HA when pH was 3 and extraction time was 90 minutes. The IR analysis showed that the pectin obtained from this fruit has a percentage of methylation (45.06%) lower than 50% and therefore is classified as low methoxyl pectin, useful for the preparation of jams with low sugar levels.

Keywords: Pectin, *Manilkara surinamensis*, Acid extraction, Yield

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CHEMICAL CHARACTERIZATION OF NUTRACEUTICAL BIOACTIVE COMPOUNDS FROM A PARTICULAR C*itrus sinentis* CULTIVAR OVALE CALABRESE BY UHPLC-HRMSN/UV AND FEASIBILITY STUDY OF NUTRACEUTICAL DRINKS AND BEVERAGES

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Consumers are aware of diet related health problems and therefore are increasingly demanding natural ingredients that are expected to be safe and health-promoting. By-products of citrus fruits processing industries represent a serious problem, but they are also considering as a rich sources of bioactive constituents which may be used in the food industry for their nutraceutical properties. Phytochemicals of nutraceutical importance are bioactive constituents that have great health-protective benefits including natural antioxidants compounds that have been associated with protection from and/or treatment of chronic disease such as heart disease, cancer, diabetes, and hypertension as well as other medical physiological disorders [1]. These health benefits have been associated to some of the phytochemical constituents such as flavonoids, terpenoids, carotenoids, limonoids, anthocyanidins. In this study a chemical characterization of a typical cultivar of orange (*Citrus sinensis)* well known in south region of Italy as "Ovale Calabrese" have been done. To the best of our knowledge there are no scientific literature about nutritional and functional characteristics of this typical cultivar. Then, the aim of this paper was the development of an ultra high pressure liquid chromatography coupled with high resolution mass spectrometry and UV (UHPLC-HRMSn/UV) method for the identification of the main bioactive compounds of “Ovale Calabrese” in juice and its by-products and of a feasibility study on nutraceutical drinks and bevarages. The chemical composition and quantitative analysis of different parts of by-products industry and juice extract of "Ovale Calabrese” were carried out. The mass spectrometry analysis, obtained with an Orbitrap spectrometer, showed that these parts of “Ovale” fruit have similar chromatographic pattern with the identification of 29 compounds mainly belonging to flavonoids (naringin, naringenin, hesperedin and neohesperidin) and limonoids (limonin, nomilin and limonin glucoside), but with different quantitative distribution.

The results of this study indicate that the “Ovale Calabrese” contain low concentrations of bitter limonoinds aglycones (limonin and nomilin), compared to the other cultivars and moreover the high amount of bioactive compounds, allow its potential use in the juice industry for the formulation of nutraceutical beverages and drinks. The formulation of new functional drinks, based on “Ovale” juice, are being develop in collaboration with the project partner “DistillerieF.lliCaffo srl”.

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A THOROUGH CHEMICAL INVESTIGATION ON *Citrus limetta* Risso FROM AEOLIAN ISLANDS (ITALY)

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Citrus limetta Risso, known as sweet lemon or sweet lime, is a scarcely investigated species from the genus Citrus. The tree easily grows in the Mediterranean area, although it is underestimated as a useful source of food and pharmaceuticals. Numerous ethnobotanical reports testify its use in Mexico for treating a variety of ailments [1]. In this study, various analytical techniques have been applied to the investigation of both the juice and the essential oil. In particular, multidimensional gas chromatography (MDGC) with a chiral selector was used for the characterization of the volatile fingerprint and elucidation of the chiral distribution. The results showed that *C. limetta* is similar in part to bergamot, in part to bitter orange. The fruit juice was subjected to HPLC-MS/MS for elucidation of the polyphenolic fraction, evidencing a prevalence of syringaldehyde, 3,5-dimethoxy-4-hydroxycinnamic acid, caffeic acid, verbascoside, and eriocitrin. Finally, the application of nuclear magnetic resonance (NMR) spectroscopy allowed to determine the presence of sugars and aminoacids in the juice, both qualitatively and quantitatively. The most abundant sugar resulted to be glucose, followed by sucrose and xylose, whereas proline, asparagine and GABA were the prevalent aminoacids determined. All the results obtained suggest sweet lime to be a good source of raw materials to be employed in food and in cosmetic/pharmaceutical industry. At present, in Italy, this species is still ignored and considered solely as an ornamental tree.

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CHARACTERIZATION OF INSOLUBLE DIETARY FIBER IN THE BY PRODUCTS FRACTIONS OF COFFEE (*Coffea arabica* L. VAR. TYPICA) AND CACAO (*Theobroma cacao* L. VAR. COMPLEJO NACIONAL TRINITARIO)

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Large volumes of by-products are generated by the industries of cocoa and coffee grains causing an undesirable environmental impact. The major fraction in these by-products is insoluble fiber. With the objective of finding alternatives for their use, we studied, the techno - functional properties and their individual fiber components like hemicelluloses A and B, cellulose and lignin. By using gravimetric and enzymatic methods, insoluble fibers free of pectin were obtained, and from them the individual components were determined. By-products of crops from the provinces of Guayas, Loja and Zamora Chinchipe in Ecuador were evaluated. The hemicellulose found varied between 4.05 and 8.73 (g/100 g of dry matter) and hemicellulose B between 1.59 and 4.28 (g/100 g of dry matter). Cellulose was the major component in the cocoa shells and coffee parchment, shells, while the hemicellulose was in the coffee pulp. Cocoa shell presented high lignin content (11.86 and 13.97g/100 g of dry matter). All by-products showed high capacity of water retention (between 4.24 and 21.83 g water/g of dry sample), exceeding that of cereals, and low oil retention capacity (between 0.93. and 1.63 g oil/g of dry sample). Cocoa shell presented the best properties of hydration. It is concluded that the analyzed by-products are promising sources of insoluble dietary fiber with good functional properties. In particular, the shell of cocoa presented a content of cellulose and lignin exceeding foods traditionally considered as resources of these components.

Keywords: By-products, Coffee, Cocoa, Insoluble dietary fiber, Techno-functional properties

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IDENTIFICATION AND QUANTIFICATION OF ISOFLAVONES FROM A NUTRITIONAL COMPLEMENT BASED ON SOY PROTEIN ISOLATION

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Soy proteins are vegetable proteins with a protein quality equal to that of meat and eggs; in the food industry is found in three forms mainly, soy flour, soy protein concentrate and soy protein isolate, this last, has a significantly higher protein content than other products and it is used for the manufacture of infant formulas and nutritional supplements.

During the process of obtaining, together with the proteins, coprecipitate another type of compounds with biological activity as the glucosides and aglycones isoflavones. These are phytoestrogens that have been classified as endocrine disruptors because of their ability to bind to estrogen receptors. It is therefore necessary to quantify these compounds, to estimate the exposure of consumers and to study their possible effects on health.

The largest number of studies have focused on infant formulas, using different analytical techniques such as liquid chromatography, gas chromatography and ultimately liquid chromatography coupled to mass spectrometry, using internal standard methods and external calibration for their quantification.

The aim of this study was to simultaneously identify and quantify the content of glucosides and aglycones isoflavones in a commercial nutritional supplement based on soy protein isolate, by reverse phase liquid chromatography coupled to tandem mass spectrometry (LC/MS-MS), Using the standard addition method with variable volumes.

Three samples of different batch and flavor (strawberry, vanilla and chocolate) were taken from the nutritional supplement and an alcoholic extraction of the isoflavones was carried out, separated using a C18 column and an elution gradient with an acidified mobile phase, composed of Water/acetonitrile, the sample was ionized by electrospray in negative ion mode.

The isoflavones identified were the glucosides genistin, daidzin and the aglycones genistein, daidzein and glycitein. In the vanilla and strawberry flavor samples, the highest glucosides content was 80.62% and 57.67% respectively, with genistin being the highest concentration, followed by daidzin; In the chocolote flavor sample, a higher percentage of aglycones was found 62.76%, genistein in higher concentration, then daidzein and glycitein.

The distribution of aglycones showed, on average a similar pattern in all three samples, genistein 64.59%; Daidzein 29.09% and glycitein 6.31%. These percentages were within the range reported for these isoflavones, identified and quantified in infant formulas based on soy protein isolate.

The total content of isoflavones in the samples, expressed as the sum of glucosides and aglycones was among 78.9 µg/g and 98.0 µg/g, the variation between samples, was 10.14 µg/g, these variations were expected since factors such as the environmental conditions of the crop and the processing methods for obtaining the soy protein isolates, can modify the amount and the distribution of glucosides and aglycones.

In conclusion, the standard addition method with variable volumes using LC/MS-MS allowed the simultaneous identification and quantification of glucosides and aglycones isoflavones in soy protein isolates, with good linearity and precision for high concentration analytes. However, linear ranges of work concentration are very narrow because of the chemical effects of the matrix components, which may be a limitation for low concentration analytes.

Keywords: Soy protein isolate, Nutritional supplement, Isoflavones, Liquid chromatography, Mass spectrometry, Standard addition method

NUTRITIONAL VALUE OF COMMERCIAL PASSION FRUIT FLOUR

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The diversity of fruits produced in Brazil constitutes an alternative of consumption when industrialized and transformed in flour, becoming a source of bioactive compounds, dietary fibers and minerals. This study aimed at characterizing the physical chemical composition of passion fruit flour from Paraná State, Brazil. Three different lots of passion fruit flour were obtained from a local market in Francisco Beltrão city and were analyzed concerning physical chemical parameters according to methods described by Analytical Standards Methods of Adolfo Lutz Institute. The following analyses were accomplished in triplicate: pH, Aw, Humidity, Protein, Vitamin C, DPPH, ABTS and Mineral Residues. Dietary Fibers analysis was measured in duplicate. Mineral contents were determined by atomic absorption spectroscopy - Method 975.03 and 965.09 (AOAC) for Cu(copper), Fe(iron), Zn(zinc), Mn(manganese), Na (sodium), K(potassium), Ca(calcium), Mg(magnesium), P(phosphorus), Co(cobalt), Cd(cadmium), Cr(chromium) and Pb(lead). The evaluation of the antioxidant activity by the DPPH• (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assay showed that the passion fruit flour extract presented 0.921 ± 0.063 µm TE.g-1 and the antioxidant activity by ABTS (2,2'-azino-Bis-3-ethylbenzo-thiazoline-6-sulfonic acid) method showed 7.683 ± 0.946 µm trolox.g-1. Passion fruit flour presented distinguished results for physical chemical parameters, such as high protein content (6.59 ± 0.86 %) and low levels of dietary fiber (2.80 ±0.85 %), vitamin C (0.033 ±0.005 mg.g-1) and total anthocyanin (1.018 ±0.042 mg.g-1). For mineral composition, the samples presented high levels of potassium (752.59 ± 150.75 mg.g-1), calcium (127.84 ±48.21 mg.g-1), magnesium (86.09 ±29.57 mg.g-1) and sodium (41.7.79 ±36.40 mg.g-1). Concerning the results obtained in the present study and the values of recommended daily intake for adults, it is possible to consider these samples as alternative sources of many nutrients. Therefore, the passion fruit flour showed a great nutritional potential to be used as food supplement for industry and consumers.

Keywords: Quality nutritional, Processing, Chemical composition, Mineral levels

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HANDBOOK FOR CONDUCTING CLINICAL TRIALS WITH DIETARY SUPPLEMENTS OF NATURAL ORIGIN

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The clinical development of natural products, especially dietary supplements, is a field of research currently under development around the world and in Cuba. The clinical trials with dietary supplements used different methodologies which are sometimes inadequate, with inconclusive results. There is no methodology for clinical trials with these products, the scientific evidences, supporting health benefits, are insufficient and limited for their generalization. To prepare a handbook for conducting clinical trials with dietary supplements of natural origin. A study that classified as applied research was carried out. The current situation of clinical trials with dietary supplements, the theoretical and the methodological foundations and the methodology used in clinical trials with these natural products, were identified in the scientific literature; and was designed a handbook to conducting clinical trials with natural dietary-supplements. The dietary surveys, anthropometric, biochemical and hematological determinations are methodological aspects defended by specialists of nutrition and the handbook suggest, it have to take into account in the investigative practice with this type of natural product, that`s why that proposal suggest necessary the participation of the accredited specialist in nutrition and propose their functions. The handbook contains issues to be taken into account during the planning and execution of the clinical trial. The specialists who valued the proposal agree with more than 75% of the indicators and 76.92% with all the indicators to evaluate the guide. The handbook provides the necessary theoretical and methodological aspects while performing clinical trials with dietary supplements of natural origin.

Keywords: Natural products, Clinical trials, Dietary supplements

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CULTIVATION OF *Pleurotus tubarius* (Pat.) Pegler ON AGROINDUSTRIAL RESIDUES OF TOLIMA

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ice cultivation is one of the largest generators of by-products, such as husk and rice bran, however due to the high quantities produced and to their scarce use they end up accumulating in the environment. An alternative of recovery is through the use of white rot fungi, capable of degrading lignin, generating biomass of interest in animal and human food, and others biotechnological applications contributing to generation of added value [1,2]. This work first evaluated the growth of *Pleurotus tubarius* (Pat.)

Pegler on cascarilla and rice bran by measuring the relationship with the variables of the composition of the substrates, subsequently the best treatment for culture of *P. tubarius* by solid state fermentation (FES) was chosen, and evaluated the proximal composition of basidiomas biological efficiency in basidiomas production, composition of the spent residue and production of total polysaccharides and β-glucans. The growth rate of *P. tubarius* on rice brand was 2,53 cm/day, however a better mycelial growth rate on rice husks (4,84 cm/day) was obtained. In this treatment, *P. tubarius* reached a biological efficacy of 40% and protein content of 17.57 ±1.2%. The depleted residues presented higher protein, fiber and nitrogen values than the starting substrates, indicating their possible use as soil improvers and as a source of animal feed.

The content of polysaccharides and β-glucans was comparable to that reported with other higher fungal species [3]. These results suggest the possibility of using agricultural residues such as rice husks to produce by FES compounds of biological value that can be used as natural components for the substitution of additives in food matrices, the generation and elaboration of functional compounds, as well as the use of depleted materials for other applications.

Keywords: Macromycetes, β-glucans, Funcional foods, Agriculturals by-products.

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ANTIOXIDANT POTENTIAL OF FRUITS CULTIVATED IN COLOMBIA AND IDENTIFICATION OF PHENOLIC AND FLAVONOIDS COMPOUNDS

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Reactive oxygen species (ROS) are compounds derived from metabolism as a consequence of partial oxygen reduction. When the intracellular accumulation of ROS exceeds the antioxidant capacity of the cell, there are alterations in the processes of obtaining energy, cellular structure and function, mutation and/or cell death, generating a lot of diseases that have been related to stress oxidative and free radical production [1]. Therapies and diets enriched with antioxidants may reduce cellular deterioration caused by excess ROS [2]. Fruits have several bioactive substances among which are phenolic compounds such as flavonoids, with demonstrate antioxidant activity [3].

In this work was evaluated the antioxidant potential of Curuba (*Passiflora cumbalensis*), Chirimoya (*Annona cherimola*), Zapote (*Pouteria sapota*), Mamey (*Mammea americana*) and Nispero (*Manilkara zapota*); fruits grown in Colombia. The fruit pulps were lyophilized and a total ethanol extract was obtained by maceration. Phenolic compounds and flavonoids were quantified by Folin-Ciocalteu and aluminum trichloride methods respectively. The antioxidant potential of the extracts was determined using the free radical scavenging DPPH (2,2-diphenyl-1-picrylhydrazyl), ABTS+ (2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)), NO (nitric oxide) and hydrogen peroxide (H2O2) spectrophotometric methods. The results showed that the extract of Curuba had the highest content of phenolic compounds (2,50 ± 0,064 mg gallic acid/g of pulp) and flavonoids (1,84 ±0,071 mg quercetin/g of pulp). The extracts of Zapote, Nispero, Mamey and Chirimoya showed a low content of phenolic compounds and absence of flavonoids. As for the antioxidant potential, the extracts of Curuba and Zapote showed significant scavenging effects of DPPH, ABTS+, NO and H2O2 free radicals; the remaining extracts had a moderate antioxidant potential. In addition, the extracts of Nispero, Mamey and Chirimoya did not show scavenging effects of NO free radical.

In conclusion, our results provide evidence that the extracts of Curuba and Zapote are an important source of metabolites with antioxidant properties, whose activity may be related to the presence of phenolic compounds, to which this activity is attributed.

Keywords: Oxidative Stress, Antioxidant, Fruits.

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RP-HPLC-DAD-ESI-MSn AND NMR ANALYSES OF *Adansonia digitata* L. FRUITS

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PPAF 19

Adansonia digitata L. is a massive deciduous tree, growing in South-Africa and Madagascar, which can reach a height of 20m and 12m in diameter. Baobab fruit has an ovoid-shaped form, of about 15 cm long, with a woody shell covered by velvety hairs. It contains big seeds that are embedded in a powdery pulp and harvested in April and May [1]. In African tradition, the baobab fruit is exploited as food in daily diet and in medicine, too. In fact, in the scientific literature there are many papers that confirm the numerous heath properties of baobab. The pulp of baobab fruit show anti-inflammatory, analgesic, gastroprotective, and hypoglycemic properties, both *in vitro* and *in vivo* studies [2]. These properties are principally ascribed to the rich nutritional profile of baobab fruit, consisting in pectins, essential fatty acids, vitamins, especially a large amount of vitamin C, and mineral salts. To better understand the bioactive compounds which confer the nutraceutical properties of this fruit, we study the chemical profile of the baobab fruit pulp, using a RP-HPLC-PDA-ESI-MSn and a NMR.

Keywords: Baobab fruit, *Adansonia digitata* L., RP-HPLC-DAD-ESI-MSn, NMR

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GLUCOSE, FRUCTOSE AND, SUCROSE CONTENT FROM THREE ECUADORIAN HIGHLANDS FRUITS AND GLUCOSIDASE INHIBITION FROM AQUEOUS EXTRACTS

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The Ecuadorian Highlands possess climatic and geographic conditions suitable for the development of fruit cultures, which integrates the food sovereignty of this region. Nutritional parameters and bioactivity evaluation from Andean fruits will provide useful information to appraise the culture and the functional food. The present work assess glucose, fructose and sucrose content in pulp and juice from tree tomato (*Solanum betaceum)*, golden berry (*Physallis peruviana* L.) and a local ecotype of apple (*Pyrus malus*). Sugars content was performed by Fourier Transform Infrared Spectroscopy (FTIR).

The aqueous extracts from the fruits under study were evaluated as inhibitors of alpha and beta glucosidases; key enzymes for Type 2 Diabetes mechanism. The fruits under study displayed promising bioactivity, evaluated in an "*in vitro*" spectrophotometric test. Our results highlight the importance of Andean fruits as functional foods, given its nutraceutical potential. Besides, sugars quantification by Infrared Spectroscopy presents several advantages compared with classic methods. This is a robust and reliable technique, with a minimum sample treatment and very good correlation with routine methods to assess sugars concentration in fruits.

Keywords: Andean fruits, Glucosidase inhibitors, Sugars content

SUPERFOODS INGREDIENTES: FEASIBILITY STUDY ON AROMATIC WATERS FROM SIX MEDICINAL PLANTS OF SARDINIA

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In recent years there has been an great increasing in of medicinal plant extracts consumption, probably due to the increased people attention to health and well-being.

Even if is well known that the plant secondary metabolites are responsible for pharmaceutical and pharmacological activities, the content of active principles could change non only from plant to plant but also within the same plant aside, balsamic time, habitat. Then the study of plant composition is therefore an extremely important step in assessing their safety and efficacy.

There are a lot of studies focused on medicinal plants that highlight the differences of composition between different origins but few on its by-products including residual aromatic waters (Hydrosol) that could be used as ingredients for soft drink or special food preparation with healthy effects.

The aromatic waters are waters enriched with both the essential oil and the water-soluble volatile components of plant. The diverse origin of these products caused a very diverse constituents and therapeutic activity. Although in some cases, these aromatic waters have a similar aroma to the pure essential oils they were co-distilled with because of essential oil is finely dispersed through the water in a low concentration, in many cases, they have different volatile constituents due to different water solubility of the volatile compounds and thus these have different properties. The water-soluble components in solution give to the aromatic water additional properties not possessed by the essential oil alone.

The aim of this work was the development of a feasibility study for testing the potential for use in healthy beverage industry.

In traditional medicine of many countries several hydrosol drinks obtained from different medicinal plants have been used for a range of health conditions. Different therapeutic effects have been cited for them such as antianxiety, sedative, anticonvulsant, antifatigue, analgesics for headaches, and so on.

Then six sardinian medicinal plant: *Cistus x incanus* L., 1753; *Helichrysum microphyllum* Cambess. subsp. tyrrhenicum Bacch., barren & Giusso; *Hypericum perforatum* L.; *Lavandula angustifolia* Mill., 1768; *Malva sylvestris* L., 1753 and *Salvia desoleana* Atzei & Picci, 1982, were steam distilled and essenzial oils and floral/leaf water characterized by gas chromatography-mass spectrometry.

With a special focus on their aromatic waters the study showed that, by blending different aromatic water it's possible to create tonic water and sophisticated soft drink with positive effect on health related to the plant species from which they are extracted.

EVALUACIÓN DE RASGOS FITOTÓXICOS Y BIOACUMULACIÓN DE PLOMO EN ACELGA (*Beta vulgaris*) Y LECHUGA (*Lactuca sativa* L.) Y SU EFECTO GENERADO EN LA INTERACCIÓN PLANTAS-MICROORGANISMOS RIZOSFÉRICOS.

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PPAF 22

Metals such as lead considered harmful to any living organism according to IARC can cause toxic effects on vital functions. Lead is present in soil and water naturally in trace concentrations, however, exploitation on an industrial scale has led to an increase in concentrations in the environment, accumulating in high concentrations. However, lead can be absorbed by plants and be bioaccumulated in concentrations that could generate toxic effects in the soil. Organisms through the chronic consumption of these. As objective, this work evaluated the acute and chronic effect of different doses of lead established as safe in the current legal norms of Colombia on seeds, plants and rhizospheric microorganisms such as Pseudomonas fluorescens, as well as bioaccumulation in plant tissue of plants Of chard and lettuce exposed during 45 in hydroponics and greenhouse tests to estimate toxic risk according to the exposure dose/Reference Dose (DREF) of JECFA - FAO, 2011. As results, it was observed that lead generated acute toxic effects on the germination of chard seeds with a percentage of germination of less than 90% and decrease in the length of radicle and hypocotyl, whereas in lettuce there was no significant statistical difference, Effects on bacterial growth were also observed at the exposure dose of 0.2 mgxL-1 lead relative to the control. On the other hand, in the tests of evaluation of chronic toxicity, toxic effects on the growth of plants of both species were evidenced, due to a decrease of the vegetal biomass in all the doses of exposure with respect to the control. Also, higher bioaccumulation of lead was observed in both plant species at the dose of 0.1 mgxL-1 in plants that had chelates as a treatment in fertilization compared to conventional fertilization.

ANTIOXIDANT AND CARDIOPROTECTIVE EFFECTS OF FERMENTED EXTRACTS OF *Theobroma grandiflorum* (COPOAZÚ)

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PPAF 23

Within the biological activities of some functional foods, the action against Reactive Oxygen Species (ROS) is highlighted, the own products of cellular reactions and indispensable in the regulation of different metabolic pathways. The significant increase of ROS produced by imbalances between their formation processes and the antioxidant defense system generates oxidative stress. This oxidative damage seems to be involved in aging, and in several degenerative diseases related to it, such as cardiovascular diseases (CVD), cataracts, cognitive dysfunctions and cancer [2]. To avoid this type of pathologies, the World Health Organization (WHO) recommends the regular practice of physical activity and consumption of a balanced diet, taking into account the properties of functional foods such as fruits and vegetables rich in polyphenols or other bioactive molecules [3]. The Cupuassu (*Theobroma grandiflorum*) is a fruit species belonging to the Amazon region, its beans have been used in a similar way to cocoa beans in chocolate or other derived products [1]. Phytochemical studies have shown that Cupuassu pulp and beans contain potent antioxidant polyphenols including flavones, flavan-3-ols and proanthocyanidins, related to positive health effects [4,5]. Considering the foregoing, the objective of this research was to evaluate the effect of Cupuassu fermented extracts with possible therapeutic potential.

The cupuassu beans were fermented for ten days, then an aqueous extraction was prepared for each sample taken at intervals of two days, it was frozen and lyophilized.

The qualitative and quantitative analysis of the chemical composition of the extracts of the fermented beans of cupuassu were carried out using colorimetric methods and HPLC. The evaluation of the antioxidant activity of the extracts was performed using colorimetric methods (DPPH, FRAP, superoxide radical and peroxynitrite anion) and electrochemical, using cyclic voltammetry. Also, the cardioprotective effect was assessed using the ischemia and reperfusion model of rat isolated heart using the Langendorff system. During the fermentation process of the cupuassu bean, changes in polyphenolic composition were observed, these variations were statistically correlated with changes in antioxidant activity. The polyphenolic content, and the antioxidant activity at day ten of the fermentation process, was lower than at the beginning of the fermentation process. The experimental results showed that the fermented, dry and roasted extract at day ten, reduces the post-ischemic alterations of myocardial function and oxidative damage generated by the process of ischemia and reperfusion. The cardioprotective mechanisms of the extract are dependent on the activity of the enzyme nitric oxide synthase. This study demonstrates for the first time, the cardioprotective action of an aqueous extract *T. grandiflorum* in a model of ischemia and reperfusion revealed in the decrease of the infarct size, the increasing post-ischemic recovery and decrease of oxidative damage observed in the isolated heart. For the reasons set out above, the data provided by this research indicate that the cupuassu extract at day ten, fermented, dry and roasted, has antioxidant and cardioprotective effects, this fact potentially converts this fermented, dried and roasted extract of *T. grandiflorum* in a dietary option at consumption.

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DETERMINATION OF VIRGIN OLIVE OIL SECOIRIDOIDS AND THE RELATED HEALTH CLAIM: AN INSIGHT ANALYSIS

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PPAF 24

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The properties of extra virgin olive oils (EVOOs) are attributed mainly to fatty acid composition and phenolic compounds. Phenolic compounds of EVOO, mainly hydroxytyrosol, tyrosol and secoiridoids, afford several desirable properties (protection of oil from oxidation, bitter-pungent taste) and health benefits (anti-in?ammatory, depletion of oxidized low density lipoprotein, and increase of plasmatic antioxidant capacity) to EVOOs.

Actually, European Union (regulation EUn.432/2012) allows to attribute the health claim "*Olive oil polyphenols contribute to the protection of blood lipids from oxidative stress*" to EVOOs containing contains at least 5 mg of hydroxytyrosol and its derivatives (e.g. oleuropein complex and tyrosol) per 20 g of olive oil. Thus, it is very important to have analytical tools to determine with accuracy the content of olive oil polyphenols and to give value to high quality EVOOs.

Nevertheless, nowadays there is no a standardized analytical method for the quantitative determination and the unambiguous identification of hydroxytyrosol/tyrosol and its derivatives (secoiridoids). The most widely adopted method is the one recommended by the International Olive Council (IOC).1 However, it has some advantages, mainly the incomplete separation of all phenolic secoiridoids and the lack of standards for accurate quantification. To address such a challenge, a simplified analytical protocol that involve the hydrolysis of the bound forms of hydroxytyrosol and tyrosol and quantification of their total free forms, was recently proposed.2

The aim of the present study was to enhance the insight into analysis of olive oil phenolic compounds. Firstly, high resolution mass spectrometry (HRMS) and high resolution tandem mass spectrometry (HRMS/MS), in positive and negative electrospray ionization (ESI) modes, coupled to fused-core reverse phase chromatography, were applied to determine the EVOO profile of IOC extracts, after the optimization of chromatographic conditions. Subsequently, the sample preparation (extraction and dissolution solvents) was carefully studied to avoid the hemiacetal formation from secoiridoids. Finally, the best quantitative method was investigated to obtain more accurate data. As result, an upgradated analytical procedure, easily available in most of the laboratories with an acceptable analysis time and improved resolution and accuracy, was proposed to assess the EU health claims and to characterize the secoiridoid profile of EVOOs.

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MSPD EXTRACTION OF THYMOL AND CARVACROL INCORPORATED INTO CHICKEN FEED AS POSSIBLE GROWTH PROMOTERS

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PPAF 25

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Essential oils (EO) obtained from aromatic plants, for example, *Lippia origanoides* H.B.K. and *Thymus vulgaris*, possess antibacterial activity against several microorganisms, this property is associated with the presence of phenylpropanoides, thymol and carvacrol, in the oil [1]. These natural products are a safe alternative for the control of infections in farm animals due to the antimicrobial resistance associated with the excessive use of synthetic antibiotics [2]. Due to the growing demand for food products for broilers, which contain EO as active ingredients, it is necessary to develop a reliable analytical technique for the quality control of the products supplied to the Colombian poultry industry. The present work describes the use of the solid phase matrix dispersion extraction technique (MSPD) for determine thymol and carvacrol in feeds for broiler chickens. A factorial experimental design, 24, was used to find the best extraction conditions. The variables were: sample-silica gel ratio, volume of dispersant solvent (1,4-dioxane), ultrasound time and volume of elution solvent (dichloromethane). The quantification of the extracts and the identification of the analytes was carried out by gas chromatography with flame ionization detector (GC-FID). Chromatographic data were obtained on a Hewlett-Packard HP 5890 Series II (HP, Palo Alto, California, USA) GC equipment with flame ionization detector (FID) equipped with split/splitless injection port. A fused silica capillary column, DB-5MS (J&W Scientific, Folsom, CA, USA) was used 60m×0.25mm×0.25µm. The oven temperature in the gas chromatograph was programmed from 45°C ramap from 4°C/min to 150°C, a ramp 5°C/min to 250°C, a ramp 10°C/min to 280°C/min. The best extraction conditions were 1: 2 dispersant sample ratio, 500 µL of 1,4-dioxane, 10 min of ultrasound and 30 mL of dichloromethane. The regression coefficients for the calibration and validation matrix were 0.90 and 0.88, respectively. Recovery rates were between 70-90%. It was concluded that the extraction by MSPD is a good alternative to the control of quality of natural products present in feed for broiler chickens, because it simplifies extraction and clean up in a single step, through the use of solid adsorbents decreasing significantly the amount of sample, interferences and solvents, as well as the time of the analysis.

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Keywords: MSPD, Thymol, Carvacrol, Food, Broiler chickens, GC-FID.

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MOLECULAR DESCRIPTORS A NEW WAY TO ASSESS TO THE POTENTIAL THEORETICAL TOXICOLOGY AND ENVIRONMENTAL EFFECTS OF ORGANIC COMPOUNDS IN vilchisS AND PERSONAL CARE PRODUCTS

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PPQV 01

In this research, we wanted to explore the chemical properties of several organic compounds found them in cosmetics and personal care products, using Datawarrior software to evaluate potential risk. In this study, we randomly selected 123 organic molecules from literature, which are presents in that kind of commercial products. Molecules were analysed through of Datawarrior software, elucidating it theoretical potential risk. Topological structure of organic compounds was related with its main physicochemical properties, molecular weight (MW), Log P, donors hydrogen groups (HD) and acceptors hydrogen groups (HA). We studied four potential risks of this molecular library, as none, low, and high-tumorigenic, mutagenic, irritant and reproductive effects. From our analysis, we found that only the 16.26 % have not any potential risk, eight of all molecules showed at least one effect with low risk. Six molecules were identified as highly toxic in all evaluated risks, including compounds like limonene and styrene. In the case of tumorigenic activity, 30.89 % were include in this category, highlighting, compounds like benzophenones, eugenol, EDTA, trichlosan, among others. About others risks, 50 compounds showed mutagenic potential risk, 56 showed reproductive effects and 85 could be show irritants properties. These risks could be used to complement several assays to describe biological properties of organic molecules includes into cosmetics and organic compounds.

Regarding to the Log P, 82.11 % of all compounds are water-soluble because it low Log P values, < 5.00. A low log P makes the compounds more bio-available to the aquatic life and eco-toxics effects can be more dangerous and efficient. At the same time, it result to be a big trouble because these molecules normally cannot be depurated in wastewater treatment plants. Others compounds like benzotriazoles (UV filters) which have lipophilic (Log P ≥ 5) properties can be releases to waters bodies like pools, beaches, lakes, among others; and become aerosol particles. At the same time, almost all selected molecules were classified as small molecules with molecular weight less than 500 g/mol. This property make molecules available for cellular environments. HA and HD properties also can describe solubility and acid-base properties, both were analysed to all compounds.

Keywords: cosmetics, personal care products, Datawarrior, molecular descriptors

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PRELIMINARY PHYTOCHEMICAL ANALYSIS OF THE ROOTS OF GALIC SACHA, *Mansoa alliceae*

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PPQV 02

The roots of Galic sacha (*Mansoa alliceae, Lam*), of the family Bignoniaceae, are used widely in the Peruvian Amazon for the treatment of rheumatism, respiratory diseases and inflammations of varicose veins, which is why the alcoholic extract, in tinctures, is one of the best selling products by Takiwasi laboratories (Tarapoto, San Martin Department).

The literature review on previous chemical studies on the roots of *Mansoa alliceae* provided only a phytochemical study performed with a plant cultivated in India [1], so we decided to carry out the phytochemical research of this plant grown in Tarapoto-Peru.

i. 1. 5g of dry and pulverized drug was soaked in metanol for 20 hours at room temperature, followed by reflux for 3 hours. The mixture were filtered.ii. 5 mL of the methanolic extract was concentrated under reduced pressure at 400C. (fraction for primary and/or secondary amino groups, free phenolic groups and tannins). iii. The solid obtained above was dissolved in 1% HCl at 50 ° C, filtered (2x10 mL). The filtrate was stored for further treatment. iv. The solid obtained from the previous step was dissolved with chloroform at 50 ° C and filtered. The chloroform phase was dried with anhydrous sodium sulfate, (fraction for testing of triterpenes, steroids, quinones and anthrones or anthranols). v. The previously stored acid solution was basified with 7.5 N NH3 (ca. 15 mL) to pH = 9, then extracted with chloroform (2 x 25 mL). vi. The chloroform phase was washed with distilled water (10 mL). It was then dried with anhydrous sodium sulfate, (fraction for alkaloid, triterpene and steroid tests). vii. The aqueous phase from the previous section (ca 25 mL) was extracted with chloroform: ethanol (3: 2) (2 x 25 mL). The aqueous phase was stored for further use. viii. The organic phase was washed with distilled water (10mL) (the aqueous phase was combined with the one already stored in the previous step). Finally, the organic phase was dried with anhydrous (fraction for tests of flavonoids, alkaloids, leucoanthocyanidins and catechins, triterpenes and steroids). ix. The aqueous phases stored in the previous stages (ca. 25 mL) are part of the fraction where the tests were performed for flavonoids, leucoanthocyanidins and catechins. x. Finally, 10 mL of distilled water was added to 1 g of dry and pulverized sample and heated for 15 minutes in "water bath", filtered and allowed to cool to room temperature (fraction for primary or secondary aminogroups tests and Saponins) [2].

Preliminary phytochemical analysis of the roots of galic sacha (*Mansoa alliceae)* of methanolic extract showed the presence of alkaloids, phenolic compounds, tannins, triterpenes and steroids.

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ALLELOPATHIC POTENTIAL OF SUNFLOWER (*Helianthus annuus* L.) LEAVES EXTRACTS OBTAINED BY HIGH PRESSURE SOLVENTS

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PPQV 03

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Supercritical fluid extraction that use carbon dioxide (CO2) as solvent has demonstrated to be an efficient technique to obtain *Helianthus annus* L. leaf extracts rich in bioactive molecules [1-3]. Nevertheless, the scientific community continues to deepen the study of sunflower extracts with potent allelopathic activities which would be useful to develop new natural herbicide models. In this way, the potential allelopathic of sunflower, (*Helianthus annuus* L. variety P64-LL-62) leaf extracts was evaluated by using hight-pressure solvents such as system mixtures of CO2 with 50% of polar co-solvents such as water, ethanol-water and ethanol. The extraction and fractionation process was carried out in a pilot-plant scale high pressure equipment from Thar Technology (Pittsburgh, PA, USA) model SF5000, which consists a vessel of 5L of capacity and three cyclonic separators with 1L of capacity, respectively. A pressure of 400 bar was fixed in the extractor vessel and the temperature was varied from 55 to 100°C. Different conditions of pressure and temperature were fixed in the separators in order to enhance the fractionation of the extract. The bioactivity and allelopathic potential of the fractions were determined according to coleoptile bioassay and phytotoxicity tests. The use of the hydroalcoholic co-solvent at 100ºC favored the obtaining of high extraction yields. As far as the fractionation of the extract is concerned, the increase of the percent of ethanol in the solvent system led to enhance the recovery in the third separator (S3). However, the fraction S3 obtained at 55ºC by using water and the hydroalcoholic mixture as co-solvent showed the best bioactivity profiles.

Keywords: *Helianthus annuus*, Extraction by high pressure solvents, Allelopathy, Bioactive molecules

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CHEMICAL COMPOSITION OF THE SPECIES *Pilocarpus alvaradoi* AND EVALUATION OF CATCHER CAPACITY OF FREE RADICALS.

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PPQV 04

Free radicals cause changes in cells, increasing the risk of cancer by genetic mutations, decreasing the functionality of cells and causing aging. When the level of free radicals exceeds the body's antioxidant defenses, oxidative stress occurs, generating the elimination of reactive oxygen species that cause degenerative diseases such as: Cancer, Alzheimer's, Diabetes Mellitus, among others [1]. Studies on plants especially on genera of the family Rutaceae, report the isolation of biologically active secondary metabolites to mitigate these diseases, effects attributed to polyphenolic compounds such as flavonoids, alkaloids and coumarins. Such as the species *Pilocarpus alvaradoi*, which reports the isolation of a-Benzoyl-g-valerolactone, two pentacyclic triterpenes: lupeol and epibetulin; and the furanocumarins, bergapten, psoralen and xantotoxin [2]; as well as the isolation of a flavonoid called 7-hydroxy-6-rutenflavanone that presented an antioxidant activity value of 1.55 mmol Trolox / g extract, expressed in units of Antioxidant Capacity Equivalent to Trolox - TEAC [3].

This research shows the production of secondary metabolites as well as the evaluation of the antioxidant activity of the extracts and subextracts of the species *Pilocarpus alvaradoi* (Rutaceae), where two coumarins were isolated and identified: Bergapten (1), Escopoletina (2), and a furofuranic lignan known as Sesamin (3). The compounds were isolated and purified by chromatographic techniques and identified by NMR (mono and two-dimensional) spectroscopic techniques. Antioxidant activity was assessed using the ABTS • +, DPPH • and FRAP methods; Ethanolic extract and ethyl acetate subextracts from the bark showed moderate antioxidant activity with IC50 values of 13.5 and 19.5 mg / L respectively, the inhibitory concentration 50 (IC50) was determined using linear regression.

The study shows the presence of secondary metabolites with antioxidant potential present in the extracts evaluated, which represents an alternative in the search for promising new molecules with antioxidant activity, thus reducing adverse effects caused by diseases caused by oxidative stress.

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ANALYSIS OF THE CONTENT OF TILIANIN IN VITRO CULTURES OF *Agastache mexicana*.

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PPQV 05

Tilianin is a non-toxic flavone type flavonoid. Its antihypertensive, antidiabetic, antihyperlipidemic and anti-inflammatory effects have been documented [1]. The current source of higher tilianin production is *Agastache mexicana* (Kunth) EF Linton and Epling [2], however this production is limited due to insufficient supply of plant material and seasonal variation. In the absence of a continuous and abundant supply of vegetable material producing tilianin a viable alternative is the cultivation of plant tissues and cells. This strategy also allows the study of the factors that affect the production of this and other molecules in the plant. Seeds obtained from plants of a wild population located in the State of Morelos, were sterilized and seeded in Murashige and Skoog culture medium. Once the seedlings were obtained they served as starting material for the tests carried out, including micropropagation of seedlings, induction of rhizogenic calli and friable callus. The latter were used for the establishment of suspension cell cultures. To obtain methanolic extracts from the pulverized samples, the methodology described by Hernández-Abreu *et al*. (2009) [1]. The profiles of the metabolites present in the extracts were visualized through thin layer chromatography. The determination and quantification of tilianin in different in vitro cultures was performed using high performance liquid chromatography [3]. In vitro cell and tissue culture is one of the alternatives for increasing the production of bioactive compounds of pharmaceutical interest. In the present project cultures of micropropagated seedlings, calli, adventitious roots and cells in suspension were established. Analytical techniques such as thin-layer chromatography and high-performance liquid chromatography have allowed the identification and discovery of natural compounds of pharmaceutical importance. In our case we observed in the in vitro cultures that the friable callus generated are able to maintain the production of tilianin at a concentration of 2.6 mg / g. In suspension cells and adventitious root cultures have also been identified the flavone tilianin. The highest production of tilianin was presented in the in vitro seedlings of 4 weeks of culture. Therefore, this project allows the development of strategies for the controlled production of bioactive compounds with antihypertensive activity such as tilianin, as well as an interesting opportunity for the study of the accumulation and production of phenylpropanoids in *A. mexicana*.

Keywords: Flavonoid, Tilianin, Toronjil, Vasorelaxant.

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A CONTRIBUTION TO CITRUS BIOREFINERY. POTENTIAL USE OF TANGELO AND MANDARIN BYPRODUCTS

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PPQV 06

Citrus is a seasonal crop. This causes an oversupply of fruit in certain times of the year and therefore, lower sale prices, becoming an unsustainable practice to harvest the fruit. This situation not only affects the farmer economically but also represents an environmental and phytosanitary problem for the crop, because of the generated residue [1].

Tangelo (*C. paradisi x reticulata*) and mandarin (*C. reticulata*) are two citrus fruits cultivated in Colombia, of great economic interest and widely studied, because they contain chemical compounds with antioxidant activity that may contribute to the prevention of diseases derived from oxidative processes that take place inside living organisms [2-4]. The present work is a contribution to the citrus biorefinery model, by giving more added-value to the production chains.

In the present study, the total contents of phenols (using Folin-Ciocalteu method), flavanones (by the dinitrophenylhydrazine method) and carotenoids (extraction with hexane) of tangelo and mandarin epicarps were determined from soxhlet extracts obtained with GRAS solvents of different polarity (ethyl acetate and ethanol) at vacuum pressure, obtaining yields of 4-6% for ethyl acetate extracts and 34-40% for ethanolic extracts.

The antioxidant capacity of the obtained extracts were measured by means of the DPPH radical scavenging assay and also, they were applied to an edible vegetable oil type RBD, for the evaluation of the extracts capacity to inhibit lipid peroxidation by the Rancimat test, in which the oxidative stability of the oil when applying the extract and the estimated time of conservation were determined.

Keywords: Citrus peels, Flavanones, Antioxidant Activity, Lipid Peroxidation.

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CHIRAL GC-MS IN THE ASYMMETRIC REDUCTION OF THIOKETALS WHEN USING VEGETABLES AS SOURCE OF CHIRALITY

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One of the greatest interests in organic synthesis is to obtain chiral compounds with a defined stereochemistry, since the configurations of the chiral centre in many cases determine the biological activity. Besides, the need of low cost alternatives or methodologies that diminish the negative impact on the environment and that allow the scientific community to obtain this kind of compounds has become very important in the last decades. One alternative is the use of whole cells as biocatalyst; particularly vegetables can be used as because of its high stereoselectivity. Therefore, this work aims to evaluate the potential of vegetables: *Daucus carota*, *Apium graveolens*, *Beta vulgaris*, *Arracacia xanthorriza*, *Zingiber officinale* in the production of chiral alcohols from thioketals (β-ketodithian) and the determination of enantiomeric excesses, using Chiral Gas Chromatography-Mass Spectrometry (Chiral GC-MS). Initially it was necessary to synthesize the thioketals from 1,3-propanedithiol and 4,4-dimethoxybutan-2-one with catalytic I2 in dichloromethane to room temperature for 3 hours (Yields 55-90%). Later, the bioreduction assay was realized with vegetables in distillate water mainly to room temperature for 48-96 hours (Yields 57-98%). The alcohols were characterized by 1H and 13C NMR. The analyses to determinate enantiomeric distributions were performed on a GC-MS QP2010S (Shimadzu, USA) using a Chiral column Hydrodex β-TBDAc (25m x 0,25 mm x 0,4 mm). Helium was used as the carrier gas at a constant flow of 1.0 mL/min, with an injection volume of 1.0 µL and split ratio of 1:10 and the electron multiplier were set at 70 eV. The results evidenced that *D. carota*, *A. graveolens and B. vulgaris* presents enantiomeric excesses >95%. Nevertheless *A. xanthorriza* afforded a racemic mixture and with *Z. officinale* the reaction did not proceed. We conclude that the proposed methodology is adequate for obtaining chiral centers with an environmentally friendly procedure.

Keywords: Chiral Center, Thioketals, Biocatalysts, Chiral GC-MS.

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QUANTIFICATION OF HEAVY METALS ABSORBED BY *Raphanus raphanistrum* L. IN HIGH BASIN OF THE BOGOTÁ RIVER (VILLAPINZÓN)

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The soils adjacent to the upper basin of the Bogotá river (Villapinzón Cundinamarca) are contaminated by anthropic use. An economical alternative to this problem is phytoremediation. The objective of this work was to evidence the accumulation of heavy metals in the organs of *Raphanus raphanistrum* L. using the atomic absorption technique to determine their phytoremediation potential. Digestion was obtained with nitric acid, hydrochloric acid 1:1, to obtain chlorides and nitrates, followed by atomic absorption analysis for the metals cadmium, lead, arsenic, chromium and cobalt. As a result, high concentrations of arsenic, lead, and chromium, cadmium and cobalt lows in mg of metal / kg of organ were collected from the species collected in Villapinzón compared to that collected in Bogotá. The results indicate a high contamination by heavy metals in soils of the upper basin of the Bogotá river and it is concluded that *Raphanus raphanistrum* L. is a species with potential of phytoremediation

Keywords: Heavy metals, Bogota river, High basin, Atomic absorption, Phytoremediation.

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BOTRICIDE ACTIVITY OF NEW PHENYLPROPANOIDS DERIVATES OF EUGENOL

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B. cinerea is a serious problem for the Chilean fruit industry. Chile is the main fruit exporter of the South Hemisphere and accounts for ~60% of the production of grapes, apples, blueberries, kiwis, avocados, nectarines, peaches and pears. The high economic costs associated to *Botrytis* represents a growing burden for agricola industry. This has led to the use of a variety of control methods, of which the most used are the chemical fungicides. In Chile the fungicides currently available to control *B. cinerea* on grapevines are hydroxianilides (Fenhexamid), anilinopyrimidines (Cyprodinil and pyrimenthanil), dicarboximide (Iprodione), carboxamides (boscalid), strobilurin, phenylpirroles (Fludioxonil) and some inhibitors of ergosterol synthesis [1]. Despite of numerous variety of fungicides mechanism of action, the magnitude of the fungicidal treatments against this fungus has induced the appearance of resistant isolates, necessitating the development of new molecules [2]. Eugenol (4-allyl-2-methoxyphenol) is a major component of essential oil isolated from the *Eugenia caryoplyllata*. Some studies on *B. cinerea* report the antifungal activity of eugenol or its essential oils on this phytopathogen. For example the activity of eugenol oil in vitro and in vivo against four apple pathogens namely *Phlyctema vagabunda*, *Penicillium expansum*, *Botrytis cinerea* and *Monilinia fructigena*. The minimum inhibitory concentration (MIC) of eugenol incorporated in malt extract agar medium was found to be 2 mg mL−1. Mycelial growth of the four test pathogens was completely inhibited when treated with 150 µl L−1 of volatile eugenol whether at 4 or 20 °C. Conidia of *P. vagabunda*, *P. expansum*, *M. fructigena* and *B. cinerea* suspended for 2 min in eugenol solution at 2 mg mL−1 heated to 50 °C germinated at rates of 19, 37, 38 and 39%, respectively [3]. Complementary to this, the in vitro activity of eugenol was tested on *B. cinerea*. The EC50 value of eugenol on mycelial radial growth of *B. cinerea* was 38.6 µg/mL; however, eugenol had no bioactivity against conidia germination [4].

Based on the previously mentioned antecedents, in this work we study the effect on the mycelial growth of a series of phenylpropanoids derivatives of eugenol. The results obtained, indicate that both eugenol as synthetic derivatives exhibit antifungal activity on *Botrytis cinerea*, with IC50 values in the range of 54-94 ppm. The determination of EC50 values of mycelial growth for B05.10 isolates in different conditions were analyzed through the PROBIT Test using the MINITAB V.16 program.

Our preliminary results show that all compounds tested inhibit mycelial growth of *B. cinerea*, so it is possible to suggest that these compounds could be an interesting candidate to design a new and effective natural control of this pathogen.

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ANTIFUNGAL ACTIVITY OF 3, 9-DIMETOXYPTEROCARPAN DERIVATIVES AGAINST PHYTOPATHOGEN FUNGI *Colletotrichum gloeosporioides*

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Pterocarpans have been involved in a series of investigations that have proposed relations between the structural geometry, the type of substituents in the pterocarpan nucleus and the biological activity. Some authors have confirmed the existence of these relationships and have proposed the possibility of increasing the activity of these nuclei, through the insertion of oxygenated groups in the extreme rings [1,2]. On the other hand, several naturally occurring pterocarpans have a high antifungal, antiviral, antibacterial, antitoxin and antiosteoporosis activity. Even, some pterocarpans have been reported as phytoalexins: antimicrobial compounds produced by plants in response to infection [1].

The 3,9-dimethoxypterocarpan (homopterocarpine) has been reported in 28 species of plants of different families, including *Platymiscium* [2]. Recently the homopterocarpine, reported in *P. gracile*, showed antifungal activity against *C. gloeosporioides* and *C. acutatum* (phytopathogenic fungi causing anthracnose in crops of commercial importance including citrus [3, 4]). Based on the above and with the purpose of obtaining derivatives with greater antifungal activity, the 3,9-dimethoxypterocarpan was submitted to reactions of bromination (Br2/AcOH and NBS), nitration (HNO3/H2SO4), reduction of the nitro group (Sn/HCl), among other. A series of homopterocarpine derivatives, including polynitrated, polybrominated and polyaminated derivatives was obtained. The derivatives were purified by conventional chromatographic techniques (CC on silica gel and Sephadex LH-20) and identified by spectroscopic methods (1H y 13C RMN, IR). The antifungal activity against *C. gloeosporioides* was evaluated with the radial mycelial growth technique in solid medium PDA, using 90 mm diameter petri dishes. The growth diameter of the fungus was determined every 24 hours and the percent inhibition was calculated [3]. All derivatives, along with homopterocarpine, was evaluated to 200 µg/mL.

The results of the mycelial growth inhibition of *C. gloeosporioides* showed that some of the derivatives have inhibition rates higher than those found for 3,9-dimethoxypterocarpan (55%). It is concluded that homopterocarpine can be used as structural template for the development of new antifungal agents for the control of *C. gloeosporioides*.

Keywords: pterocarpanos, *Colletotrichum gloeosporiodes*, nitration, bromination, reduction.

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DEVELOPMENT OF AN ULTRAFILTRATE PROTOTYPE ASSITED WITH DENDRIMERIC POLYMERS FOR REMEDIATION OF SEWAGE CONTAMINATED WITH HEAVY METALS

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Residual water is called all liquids used in the daily activities of a population. They are classified as municipal or industrial. Another denomination is according to its content of contaminants: residual water (coming from toilets ie which carry excrement), gray water (all domestic sewage less the toilets), industrial sewage (are all those that come from industry and in most cases have health effects). Water treatment involves a set of complex multi-step operations by the different types of impurities. Within that range of contaminants are the heavy metal ions that are usually eliminated in tertiary treatments of wastewater purification. Heavy metals are discharged from a variety of sources in everyday life and can readily oxidize into ions when dissolved in water. They don't degrade them naturally and have significant risks to human health and the environment.

The main objective of this project is to develop a micro-scale prototype to study the ultrafiltration of metal ions from residual water in the laboratory. The dendrimer PAMAM 3,3 '- ((3-hydroxypropyl) azanediyl) bis (N - ((Z) -2-aminovinyl) propanamide) is a macromolecule which, thanks to its chelating properties, is a promising heavy metal encapsulant in sewage treatment. Because the green chemistry is oriented to find new ways to synthesize chemicals to achieve a more amiable chemistry with health and the environment this project will generate information that will contribute to implement improvements for the cleaning of residual water

Keywords: Heavy metals, Residual water

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EXTRACTION, CHROMATOGRAPHIC EVALUATION AND ANTIOXIDANT ACTIVITY OF ESSENTIAL OIL OF *Origanum vulgare* L.

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Aromatic plants are the ones that make secondary typical metabolites and they can be either useful or toxic for an organism. In this research, essential oil was obtained by hydrodistillation assisted through microwave radiation (MWHD). The process was performed during three cycles (40, 50 and 60 minutes) with four cycles and two working power (700, 800 watts), where 300 grams samples of leaves obtained from the municipality of Vijes Valle del Cauca were used.

That place is located at 987 meters over sea level, with an average temperature of 24ºC and HR of 89%. The essential oil (EO) was evaluated in terms of relative density to 20ºC, index of refraction and solubility to the ethanol (70 % v/v). The chemical composition was evaluated using a gas chromatography-mass spectrometer (GC-MS). For the case, 10 µl of the sample was taken and dissolved in 990 µl of ethyl acetate, and vortexed. Subsequently, a second dilution was performed also, to have a final dilution of 10,000 fold. GC-EVOQ 456 was used with a BR-5ms column (30 mx 0.25 m, 0.25 µm) and helium as the entrainment gas.

Detection is performed using a MS-EVOQ-TQ Select system with a mass range of 40 - 500 amu. The EO oregano from Vijes shows evidence of 45.06 and 14.86% of carvacrol and thymol respectively. Its antioxidant activity was evaluated by the methods of DPPH*, ABTS*+ and ORAC. The performance of the process for power of 800 watt was of the order of 0,190 ± 0.00035 - 0,201 ± 0.00086; 0.211 ± 0.00012 - 0.229 ± 0.00057 and 0.213 ± 0.00032 - 0.231 ± 0.00043). The power of 800 watt had values between (0.182 ± 0.00067 - 0.195 ± 0.00089; 0.199 ± 0.00061 - 0.212 ± 0.00032 and 0.205 ± 0.00015 - 0.216 ± 0.00087); the major compounds were carvacrol (65.06%) and thymol (13.79%). Also, EO of oregano was found to have good antioxidant activity ranging from 318.8 ± 0.009-320.6 ± 0.003 (700 watt) and 310.8 ± 0.021-312.1 ± 0.014 (800 watt) µg / ML for DPPH •, and 23.852 ± 0.018-24.019 ± 0.011 (700 watt) and 23,128 ± 0,012-23,412 ± 0,009 (800 watt) µg / mL for ABTS • +. Finally, it is important to say that these natural resources are at our disposal for the benefit of humanity.

Keywords: Essential oil, Antioxidant capacity, Chromatography, HDMW

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EVALUATION OF THE ANTIOXIDANT AND ANTIFUNGAL ACTIVITY OF EXTRACTS OF *Stemmadenia littoralis*

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Commonly known as Azucene, it is a species of the Apocynaceae family native to Central and South America of shrub habit. Its scientific name is *Tabernaemontana litoralis*, but it is also known as *Stemmadenia littoralis*. They have milky latex, simple and opposite leaves, its flowers are white and its fruits are 2 short, fleshy and orange follicles with high presence of seeds. In the city of Medellín they are common as ornamental plants in buildings, pedestrian ways and antejardines [1]. Little or nothing has been reported on investigations of the phytochemical properties of this species, but a number of indole alkaloids and terpenes have been found in species of the same family, such as *Stemmadenia Donell-Smithii* [2] and *Stemmadenia grandiflora* [3]; Also in species such as *Tabernaemontana divaricate*, biological and antioxidant activity has been evaluated [4], which gives evidence of good results in species of the same family. Were obtained from leaves, stems and fruits of azuceno (*S. littoralis)* in the University of Antioquia. The taxonomic identification was carried out in the Herbarium of the University of Antioquia. The plant material was grinding and removal of metabolites with solvents of different polarity (ethanol, ethyl acetate, etc) and were monitored by thin layer chromatography CCD and revealed with specific reagents for alkaloids and terpenes. The crude extracts underwent evaluation of antioxidant activity by the test of DPPH. To evaluate the antifungal activity of these followed the method established by Canton, Marin and Espinel [5] for Fusarium sp and Rhizoctonia sp. For antifungal evaluation, it was found that the extract of leaves and stem had the best results, with an inhibition to the growth near 40% in Fusarium sp, compared with a commercial antifungal (mixture of azoxystrobin and difenconazole). For antioxidant activity, it was found that the best extracts were those of leaves and stems and fleshy fruit (area) with a total solution discoloration of 20mg/L of DPPH, using a concentration of extract of 62.5 ppm, these results were compared with a standard curve of Trolox, expressing the results in TEAC. These results demonstrate the significant antioxidant and antifungal activity of the plant *S. littoralis*. It is recommended to explore the structural characteristics of the compounds present in the extracts, using a fractionation bio guided by gas chromatography to isolate and purify metabolites that have a promising antioxidant and antifungal activity with the presence of bioactive substances such as tannins, flavonoids, alkaloids, sterols unsaturated and/or triterpenes that you can explore in more depth for a greater understanding of the potential of this plant.

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IDENTIFICATION OF AUTOINDUCTORS INVOLVED IN *Quorum sensing* MECHANISMS IN *Microcystis aeruginosa.*

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Cyanobacteria are a group of prokaryotic Gram-negative photosynthetic organisms; they represent a problem for water resource managers, the kind most commonly founded in water reservoirs is M*icrocystis aeruginosa* and it is recognized because it produces a wide variety of toxins. The conventional techniques for water purification are not effective for the total removal of these molecules [1]; for this reason, it is necessary to seek a system to reduce the presence of these compounds. One of these could be Quorum sensing, a bacterial chemical communication mechanism that regulates several biochemical functions and that could be involved in the production of these toxins. Therefore, the modulation of this mechanism would allow to control the concentration of these toxins in the matrix.

The signals used by Gram-negative bacteria to perceive cell density are Acyl-Homoserine Lactones (AHLs) molecules of different chain size. Once AHLs are produced, they diffuse in and out of cells through passive diffusion, as well as through active transport mechanisms. When the AHL concentration finally reaches a certain threshold or bacterial quorum, some biochemical processes are induced [2]. Therefore, it is important to identify the specific AHL to which that cyanobacteria respond by producing toxins, in order to regulate this biochemical process by the application of specific inhibitors.

In the present work, many types of lactones were evaluated (AHLs C4-C12) to determine their ability to induce toxins biosynthesis in M*icrocystis aeruginosa*. These results suggest that this phenomenon is only caused by AHL C6. In addition, some types of natural products are analyzed as inhibitors of toxins biosynthesis.

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Keywords: Cyanobacteria, Cyantoxins, Quorum sensing, Lactones.

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QUORUM SENSING EVALUATION OF MORA DE CASTILLA (*Rubus glaucus* Benth)

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The majority of infectious diseases caused by bacterial agents proliferates through a cellular communication mechanism known as *Quorum sensing* (QS), in this phenomena the more cellular density causes an increase in the concentration of signaling molecules, giving place to genetic expression changes, physiologic and the deployment of another collective behaviors. Some natural products or polyphenols, as Kalia, (2013) [1] and Truchado, (2015) [2] stated, has an antagonic effect against signaling molecules, interrupting bacterial communication as a result. Different cultivars of *Rubus* has a great diversity of polyphenolic compunds [3], but also antioxidant capacity at their different maturity stages. The aim of this study is oriented towards the obtention of *Rubus glaucus* Benth at their seix maturity stages and its further evaluation of QS inhibition.

The obtention of the above mentioned extracts from *Rubus glaucus* Benth fruits collected at the municipality of Belén de Umbría at coordinates N 05°11'02,61'' W 075°52'42,38'' (Risaralda-Colombia) was completed following the methodology (4) (acetone-water 31:69). These extracts were evaluated in a QS inhibition model considering agar diffusion assays [5] and [6] and using the reference strain *Chromobacterium violaceum* 026. This evaluation showed that the extract corresponding to maturity stage number five inhibited QS, based on the observation that this stage have the major polyphenolic content compared to others. In that sense, it can be considered that advanced maturity stages of *R. glaucus* could represent an affordable source with antimicrobial potential.

Keywords: *Quorum Sensing*, Rosaseae, Compuestos fenólicos, Antocianinas.

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NEW USES OF NATURAL PRODUCTS IN DESIGN AND FASHION

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The LANDESIGN ® Research Group (scientific managers Sabina Martusciello., Maria Dolores Morelli) has activated the section "ACTIVEMODESIGN" starting from the threefold meaning of habitus, (habit, way of life, living, dressing) is composed of various-fashion actions responding mainly to the "ecological" requirement in the sense of use of natural materials produced on site (e.g. use of hemp already cultivated and in the working land).

ACTIVEMODesign is a creative cosmetic activity that is oriented towards the Mediterranean territory offering a new lifestyle which perceives economy differently and progresses through "the culture of waste".

ACTIVEMODesign is the design of accessories, clothing, packages, aids and decors aimed at cosmo-ethics: it produces healthy products and actions related to people and environmental products, "reparative and reinforcing stem cells of the evolutionary processes." Actions and products coming from "culture" and "knowledge" of the territory, whose potential is to be optimized and become a subject of the project. This SOCIAL DESIGN COLLECTION is characterized from accessories, clothes, containers, supports and furniture for the" benessere" considered as " (da ben – essere = "stare bene" or "esistere bene"), (OMS, 1948): designed and prototyped in respecting the environment and the welfare of the people, aimed at the cosmo-ethics, actions and processes related benefits to people and the environment (ACTIVEMODesign). For example the FlavaAlba collection (LANDESIGN ® with Sefora Maria di Palo and Simona Cupido) uses the fabric from the family of Cannabinacee, with their breathable, hypoallergenic properties, produced locally, therefore economical, naturally colored with the Hyperic (Hypericum perforatum L.) and the coppered onion (Allium cepa) for a collection of natural garments for babies, or table (LANDESIGN ® with Lucia Uccello) that uses the same principles (colours and natural fabrics) with comfortable solutions for the clothes of teenagers. "Active" text clothes made with foods, fibres impregnated with natural essences, technical fabrics and smart in order to produce "beneficial processes" related to senses and communication, linked to the power of touch, as in the collection of the Synesthesia (LANDESIGN ® with Anna Candela).

EVALUATION OF PERINAPHTHENONE DERIVATIVES AS AN ALTERNATIVE DEFENSE AGAINST PHYTOPATHOGENIC FUNGI

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Phytoalexins are defined as low molecular weight antimicrobial secondary metabolites, which constitute the secondary defense mechanism in plants as a natural response to pathogen attack [1].Phenylphenalenones are derived from the peri-fused tricyclic ring system cyclized of phenalenone (perinaphthenone), which is the basis of more than 30 phytoalexins isolated from plants of the family Musaceae [2]. These compounds have been postulated as possible structural templates for the design of novel antifungal agents [3].

In the present study, the *in vitro* antifungal activity of perinafthenone and derivatives of nitration, bromination, epoxidation and reduction reactions, oximes and hydrazones were analyzed; as well as their metabolism against the phytopathogenic fungi *Botryodiplodia theobromae*, *Botrytis cinerea* and *Fusarium oxysporum* of citrus crops. The antifungal activity was determined by the "poisoned agar" method [2] and the metabolism was evaluated in Czapeck-Dox liquid stirred culture medium, whose monitoring on days 1, 3, 6, 9 and 12 of the biotransformation process was carried out by high performance liquid chromatography (HPLC).

Significant antifungal activity was found for perinaphthenone from 25 µg/mL with percentages of growth inhibition against the three phytopathogens around 30 to 80% at 100 µg/mL. Metabolic studies revealed that the microbial transformation of perinaphthenone by *Fusarium oxysporum* shows two major metabolic products, whose concentration increased progressively during the twelve days of the test. One of the products correspond to an reduction product of the α,β-unsaturated carbonyl system, characteristic of the original substrate, the second compound, is still in the identification process. The purification of compounds was carried out by conventional chromatographic techniques and structural elucidation was assessed by interpretation of nuclear magnetic resonance (NMR) spectra.

The presence of the α,β-unsaturated carbonyl system in perinaphthenone derivatives, led us to determine the relationship between this structural characteristic with the antifungal activity, showing a promising application against the phytopathogen *Botryodiplodia theobromae* and thus demonstrating qualitatively that the activity of these compounds can be attributed to the presence of this system.

Finally, it is concluded that perinaphthenone can be an important structural template for the development of new antifungal agents.

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EFFECTS OF *Caryocar brasiliense* OIL NANOEMULSIONS ON THE CELL VIABILITY OF THREE SPECIES OF LEISHMANIA AND *Trypanosoma cruzi*, IN VITRO

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Neglected diseases are concerning problems worldwide, especially in tropical and developing countries. Examples of them are the leishmaniasis and Chagas disease, caused by the protozoans of the genus *Leishmania* and *Trypanosoma cruzi*, respectively. Conventional chemotherapy for these infections (e.g. amphotericin B) presents expressive systemic toxicity for being of little specificity to their target and of high dosage. To overcome the adverse effects of conventional drugs, nanostructured bioactive compounds can be a promising strategy to treat infections due to the special properties of the nanometric scale and their capacity of delivering molecules, enhancing their bioavailability and decreasing the adverse effects. Making use of the nanobiotechnology, our group developed a nanoemulsion (NE) of pequi oil (*Caryocar brasiliense*, which is a Brazilian fruit presenting many pharmacological properties) in order to increase its solubility in the water-based biological environment, and tested its antiparasitic potential, in vitro, on *Leishmania infantum*, *L. braziliensis*, *L. amazonensis* and *Trypanosoma cruzi*. Parasitic cell viability was assessed by resazurin assay after 24 and 48 hours of incubation with the NEs at concentrations ranging between 22,5 - 360 µg/mL. The NE inhibited the cell proliferation up to 90%, approximately, on *L. infantum*, *L. braziliensis* e *L. amazonensis*, at 360 µg/mL past 48 hours. The NE functionalized with the biopolymer chitosan showed even greater inhibition of cell viability, reaching 95% of efficacy against Leishmania spp. In contrast, *T. cruzi* presented smaller vulnerability to the treatments with nanoemulsions (approximately 20% of inhibition). The control groups with free oil or DMSO did not show antiparasitic effect. Moreover, our nanoemulsions did not show cytotoxic effect against macrophages (J774). Based on our results, we concluded that the nanoemulsified pequi oil have expressive leishmanicidal activity on the tested species and may be a safer alternative for the treatment of leishmaniasis. Further studies should be conducted in vivo to further analyse their pharmacological and toxicological effects.

Keywords: nanobiotechnology, nanoemulsion, leishmania, trypanosoma, chitosan, Caryocar brasiliense

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PRELIMINARY STUDY OF USE PROFILE OF FOUR COLOMBIAN AMAZONIC FRUITS

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Biodiversity is one of the most important characteristics of the Amazonian region. More than two thousand species are referenced in the COAH, the herbarium collection of the Colombian Amazonia region. Fruits of Amazonian plants are a significant source of bioactive compounds used for the development of natural products with an economic and nutritional impact to the native communities of the Colombian Amazon. Phytochemical composition of different parts of fruits of Caimo (*Pouteria caimito*), Tucumá (*Astrocaryum vulgare*), Ucuye (*Macoubea guianensis*) and Umarí (*Poraqueiba serícea*) were characterized to identify possible use as natural ingredients sources for their technological development and commercialization by local indigenous communities. The principal bioactive compounds were polyphenols (tannins and flavonoids) in Caimo, Tucumá and Ucuye and endocarp of Umarí. Alkaloids were identified in Caimo, exocarp of Tucumá, exocarp and seeds of Ucuye and mesocarp of Umarí, these compounds are associated with cytotoxicity and/or antimicrobial activity. Carotenoids could only be quantified in mesocarp of Umarí (12.49 ± 0.85 mg of β-carotene/g of sample) but were also identify in seeds of Caimo and mesocarp of Tucumá. High levels of ether extract were found in Tucumá (26.30 ± 0.07 % in exocarp and 71.86 ± 4.34 % in mesocarp and 30.53 ± 1.62 % in seed) and Umarí (19.65 ± 2.60 % in exocarp and 43.70 ± 4.42 % in mesocarp). The highest level of fructose was determined in mesocarp and mucilage of Ucuye (2318.85 ± 268.12 and 8154.42 ± 339.02 mg of sugar/ 100 g of sample, respectively) follow by mesocarp of Umari (2273.08 ± 157.66 mg of sugar/ 100 g of sample) and mesocarp of Caimo (2187.65 ± 105.51 mg of sugar/ 100 g of sample). Mesocarp of Caimo presented el high content of sucrose (5365.03 ± 401.41 mg of sugar/ 100 g of sample) which is why it could be considered a fruit with a significant caloric contribution. This preliminary characterization revealed possibilities to Tucuma, Umarí and Caimo fruits as potential sources for the extraction of naturals oils for cosmetic and food uses, mainly by the presence of carotenoids in the mesocarp of Umarí. Likewise, Ucuye fruit can be considered for food products as natural sweetener.

Keywords: Phytochemical analysis, Bioactive compounds, Natural ingredients, Amazonian fruits

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GREEN SYNTHESIS OF NEW IMINES DERIVED FROM 4-BROMO-BENZALDEHYDE WITH CHIRAL AMINES

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Our research is based on the synthesis of chiral imines, also known as Schiff bases, employing the "Solvent-free" method from Green Chemistry, which allows developing processes that reduce or eliminate the use or generation of dangerous substances for human health and environment. On the other hand, chiral imines can be easily coordinated with metals and form metallic complexes with interesting structures and potential applications on different fields, like biology and catalysis, presenting thermic, magnetic and electric properties. In Pharmacology, chiral substances are very important due to the molecular docking done by cellular receptors in the organisms, meaning that they are able to differentiate similar molecules by their functional groups or distinguish stereoisomers with different configuration. In this work, we report the synthesis of chiral imines derived from: 4-bromo-benzaldehyde and the optically active aromatic amines: (S)-(-)-1-phenylethylamine, (S)-(-)-1-(4-methylphenyl)ethylamine, (S)-(-)-1-(1-naphthyl)ethylamine in absence of solvent. The structure of the products was assessed by spectroscopic methods (FT-IR, 1H and 13C NMR, and EI-MS). All the imines crystallized allowing to obtain a suitable monocrystal, and then the structures were fully confirmed by X-ray diffraction studies.

OBTAINING OF VEGETABLE OILS FROM AGRO-INDUSTRIAL WASTES

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Vegetable oils are a staple food, mainly in Latin American countries, where vegetable sources such as soy, olive, corn, sunflower, sesame, cotton and coconut are grown. In general, vegetable oil intake should be at least 15% of the food consumed to meet the basic energy requirements [1]. In addition to this, some oils contain unsaturated fatty acids, considered essential fats in the human diet since the body cannot synthesize them naturally and must be obtained through diet to fulfill important biological functions in the body. Essential fatty acids provide an important health benefit in protecting cardiovascular diseases [2], as well as in the prevention of arthritis, cancer, coronary diseases, diabetes, among others [3]. However, to obtain oil from some agricultural products, such as oilseeds, deforestation actions are carried out, which exert a strong influence on some of the factors driving the climate change [4]. Nevertheless, the problem of climate change is also a consequence of the large amount of waste generated daily. For example, the food industry generates more than 500 million tons of fruit residues worldwide; on average 70% of the fruit production becomes waste. Bearing this in mind, an efficient alternative to reduce this problem is to valorize the residues, obtaining oil from different seeds (blackberry, papaya, guava, lulo, tamarillo, soursop, passion fruit and mango). These oils were obtained by Soxhlet and supercritical fluids extraction methods. These extracts were characterized according to the total phenol content-TPC, total flavonoids content-TFC and fatty acid profile. The yields of extraction ranged from 8.54 to 23.97%, obtaining the highest yields for tamarillo seeds (23.97%) and passion fruit (23.21%). The TPC ranged from 69.03 to 292.38 mg-eq of gallic acid per gram of sample and the TFC ranged from 114.47 to 1074.73 mg-eq of quercetin per gram of sample. Linoleic acid was the predominant fatty acid in blackbery (52.00%), guava (52.14%), lulo (70.57%), tamarillo (68.31%) and passion fruit (68.14%). Considering the above, oils obtained from fruit seeds are promising for the food and its related industry.

Keywords: Agro-industrial wastes, oilseed, phenolic compounds, fatty acids

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DETERMINATION OF PLASTICISERS AND BPA IN TUNISIAN CULINARY HERBS AND SPICES BY GC/MS

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Introduction of organic contaminants into the agricultural system can be through atmospheric deposition pesticide application, irrigation and fertilisation with organic waste products. Many plasticisers and additives are groups of compounds of special interest. They are interesting classes of compounds from the environmental point of view due to their moderate persistence and the large world-wide production (1). In the present study 18 plasticisers and bisphenol A (BPA) in 10 different Tunisian culinary herbs and spices (black pepper, mint, caraway, coriander, oregano, rosemary, thyme, fennel, verbena and laurel) were determined by GC/MS. Di-(2-ethylhexyl)phthalate was the most abundant plasticiser in all 65 samples, reaching up 1,18±0,81 □g g^{-1} (black pepper and rosemary), whereas the concentrations of the other phthalates varied from not detectable to 2,17±1,02 □g g^{-1} (rosemary). Di-methyladipate was detected in all samples, whereas the concentrations of the other adipates varied from not detectable to 0,74±0,38 □g g^{-1} (caraway). Di-(2-ethylhexyl)sebacate was detected in only four spices with mean value of 1,24 (caraway, coriander, oregano and rosemary). Dioctylterephthalate was found in all samples, except in mint, reaching up 1,9±0,72 □g g^{-1}(black pepper); conversely benzyl benzoate was not detected in any samples. Trace levels of BPA was never found. Probably, as already observed for the other food (2,3), these contaminants could result from environmental pollution (air, water and/or soil) and /or agricultural practices (4).

Keywords: Plasticisers, Bisphenol A, Tunisian spices, GC/MS

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IDENTIFICATION OF THE VOLATILE COMPOUNDS OF OIL PALM FLOWERS THROUGH HEADSPACE SOLID-PHASE MICROEXTRACTION-GAS CHROMATOGRAPHY MASS SPECTROMETRY

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Effective pollination of oil palm flowers is an important step to achieve higher fruit set and oil to bunch (g/g). *Elaeidobius kamerunicus*, a weevil introduced in the African oil palm *Elaeis guineensis* plantations around 80's, was found to be the main pollinator of oil palm to address the poor natural pollination problem in Malaysia [1]. Whereas, *Elaeidobius subvittatus* and *Mystrops costaricensis* have been reported as the most common pollinator weevils for American oil palm *Elaeis oleifera* and their interspecific OxG hybrids [2]. However, the species and population of pollinator insects that visit the flowers, could vary among and within genetic backgrounds and inflorescence type (male or female) and could be related to the different compounds emitted by the flowers [3]. In this sense, the aim of this work was to identify and quantify the relative abundance of volatile compounds emitted by male and female inflorescences in different genetic backgrounds of *E. guineensis*, *E. oleifera* and OxG hybrids. Extraction of volatile compounds of the flowers was conducted using HS-SPME. Identification of compounds was made by GC-MS. The results showed that estragole is the main compound of male and female flowers for most accesions of *E. guineensis*. However; other compounds such as cis-anetole, trans-anetole and β-elemene were found. Flower extracts of *E. oleifera* and OxG hybrids showed lower percentage of estragole than extracts of *E. guineensis.* Variation in estragole percentage was found among cultivars of *E. guineensis* and cultivars of *E. oleifera*. These results help us to understand the relationship between volatile compounds emitted by flowers of *E. guineensis*, *E. oleifera* and OxG hybrids, and the variation on the population and species of pollinators associated to oil palm.

Keywords: Oil palm, *E. guineensis*, *E. oleifera*, Pollinators, Volatile compounds, Estragole.

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CHEMICAL COMPOSITION AND EVALUATION OF THE BIOLOGICAL POTENTIAL OF THREE VEGETABLE SPECIES OF THE CARIBBEAN REGION

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At present the search for molecules with biological activity represents a tool applicable in biomedicine, chemistry and industry, process based on the isolation and purification of secondary metabolites on plant extracts and the evaluation of the biological activity. The Rutaceae and Annonaceae families have a wide variety of genus and species distributed whole the world. Muñoz et al., 2016 [1], which report the isolation of compounds in different species with biological activities and with structural variability, which infuse versatility to the molecules to generate new compounds with improved properties and that can be used as new alternatives for therapeutic treatments against diverse diseases. From the leaves of *Pilocarpus spicatus* the extraction of the essential oil by steam trawl is reported, identifying 17 components: limonene (41,8%), 2-undecanone (11,0%) and sabinene (10,7%). This essential oil showed antibacterial activity aganist *Escherichia coli* and *Staphylococcus aureus* and also showed anticholinesterase activity [2]. The furoquinolines alkaloids: skimmianin, haplopine, kokusaginine, acronydine and acronycidine, asylums of *Geijera balansae* presented *in vitro* activity against *Plasmodium falciparum* and *Leishmania spp* [3]. This work shows the results of evaluation of the biological activity on isolated extracts and compounds of the species *Pilocarpus alvaradoi* (Rutaceae), *Esenbeckia litoralis* (Rutaceae) and *Rollinia pittieri* (Annonaceae). From *Pilocarpus alvaradoi* four compounds were isolated and identified: a coumarin known as escopoletine, an alkaloid named dictamine and two sterols: sitosterol and lupeol. The ethyl acetate extract of leaves and the ethanolic extract of *P. alvaradoi* bark showed moderate activity against intracellular amastigotes of the parasite *Leishmania panamensis*, with EC50 of 45,1 and 30,7 ug /ml respectively and with low cytotoxicity. From the ethyl acetate extract of the bark of *Esenbeckia litoralis* was isolated: 1-hydroxy-3-methoxy-N-methylacridone that showed activity against *Leishmania (Viannia) panamensis*, being able to inhibit the parasite load in 37,2% also presented low cytotoxicity compared to the reference drug Amphotericin B, this extract had a poor inhibitory capacity with 9,2%. The ethanolic extract of the root of the species *Rollinia pittieri* (Annonacea) showed activity against *Staphylococcus aureus*, and from which an aporfinic alkaloid named Anonaina was isolated. The compounds were isolated and purified by chromatographic techniques and identified by NMR (mono and two-dimensional) spectroscopic techniques. Extracts and compounds isolated from these species constitute a promising sample with a high biological potential, which motivate to continue searching for active molecules as candidates for future drugs.

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PHYTOREMEDIATING ACTIVITY OF *Baccharis latifolia* (Ruiz & Pav.) Per IN SOILS CONTAMINATED WITH HEAVY METALS IN THE UPPER BASIN OF THE BOGOTÁ RIVER. VILLAPINZÓN (CUNDINAMARCA)

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Phytoremediation is a technique with a lower impact on the environment than other economic alternatives. It uses species that accumulate metals in their organs during their development. This study tested the capacity of the species *Baccharis latifolia* (Ruiz & Pav.) *Per* to accumulate heavy metals like cadmium, chromium, lead, cobalt and arsenic in order to determine if it is a potentially useful species for phytoremediation. Samples of the species were collected in the vicinity of the municipality of Villapinzón (upper basin of the Bogotá river), a sector where waters and soils are highly contaminated by heavy metals produced, over decades, by the local tannery industries, which shed their wastes into the river without any type of treatment and have caused health problems for the inhabitants. The samples of the *Baccharis latifolia* (Ruiz & Pav.) *Per* species, along with the soil where it grows, were collected in Villapinzón (problem plant) and the control plants were gathered in the municipality of La Calera-Cundinamarca. Each of the organs (leaves, stem, root) and the soil were subjected to a digestion process with hydrochloric acid and nitric acid 1:1 to obtain chlorides and nitrates, with the subsequent quantification of the heavy metals by the atomic absorption technique. The analyzed metals were: cadmium, chromium, cobalt, lead and arsenic. We obtained high concentrations of arsenic in the leaves (103.91 mg / kg) and stems (480.45 mg / kg). The levels of chromium in the leaves were: 19.54 mg / kg and in the stems: 136.40 mg / kg. The highest levels of arsenic in the roots and soil were 491.97 mg / kg and 461.77 mg / kg; And for chromium: 185.09 mg / kg, 1,294.43 mg / kg respectively. The study shows that the plant has a strong potential for phytoremediation in the area.

Keywords: Phytoremediation, Heavy metals, *Baccharis latifolia* (Ruiz & Pav.) *Per*.

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MICROORGANISMS FROM THE COLOMBIAN CARIBBEAN SEA AS A SOURCE OF COMPOUNDS FOR PHYTOPATHOGEN CONTROL: EXPLORING CHEMICAL DIVERSITY IN MONO-CULTURES AND CO-CULTURES

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Marine natural products play an important role in the discovery of bioactive compounds [1]. Besides its pharmacological uses, some of them have potent insecticidal, antibacterial and antifungal activities, which make them excellent candidates for their use as agrochemicals. However, marine natural products are not usually obtained at large amounts (supply problem) [2]. Therefore, research for alternatives for bioactive compounds production have been developed, in this way, marine microorganisms allows to find a source of novel bioactive compounds, at the time that they are a sustainable source of these compounds. In addition, genomic studies have shown that some microorganism have secondary metabolite pathways that are not expressed under standard laboratory growth conditions. One approach to more fully access the metabolic potential of microbes is co-cultivation, where the presence of neighbouring microbes may induce the production of previously undetected metabolites due to activation of silent gene clusters [3].

In a previous work, we identify marine strains that can disrupt quorum systems of *Chromobacterium violaceum* ATCC31532 and control *Burkholderia glumae, B. plantarii* and *B. gladioli* (rice pathogen); *Fusarium oxysporum* f. sp. *dianthi* (carnation pathogen) and *Colletotrichum gloesporoides* (yam pathogen)[4]. Some of these microorganisms have been chemically studied leading to the discovery of some bioactive compounds.

In this work, 12 bacteria and 1 fungus were selected for co-culture in order to enhance the chemical diversity that could lead to discovery of new bioactive compounds or increase the production of bioactive ones. Four criteria were used for the selection of the microorganisms: strains with at least one of the aforementioned biological activities, strains isolated from the same marine sample, mycolic acid containing strains and bacteria from *Streptomyces* genre.

Initially, binary interspecies interactions between this set of microorganisms were established in solid and liquid culture media. Solid interaction assays allowed to look out for phenotypic changes that serve as sensors for the metabolic production of interacting strains. Liquid cultures were used for the assessment of biological activity as well as the metabolic profiling of the organic fraction using UHPLC-ELSD and NMR. Finally, based on bioactivity and chemical information, three co-cultures were selected for further chemical study and structure identification analysis of metabolites induced by co-culture.

The Ministerio de Ambiente y Desarrollo granted permission to collect samples and perform this research (Contrato de Acceso a Recurso Genético No. 108).

Keywords: Marine microorganisms, Co-culture, Phytopathogen.

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EFFECT OF ETHANOL PRETREATMENT IN COUMARIN CONTENT OF DRIED *Mikania glomerata/laevigata* LEAVES

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Mikania glomerata Sprengel and *Mikania laevigata* Sch. Beep. ex Baker are widely used to treat bronchitis, cough and asthma [1]. These species are one of 71 components from RENISUS - List of medicinal plants interesting for Brasilian Public Health System [2]. Coumarin content has been considered to be the main bioactive component, reported to be responsible for *M. glomerata* and *M. laevigata* pharmacological activity [3]. It is noteworthy that, as any secondary plant metabolite, coumarin content in guaco depends on cultivation, drying and storage conditions [4,5]. If any of those steps are not properly conducted, the quality of the pharmaceutical preparations and their therapeutic value may be compromised.

Given the importance of medicinal plants processing steps, this study evaluated the influence of ethanol pretreatment on coumarin content in guaco leaves. Using an experimental design with 2 factors (concentration of solvent and immersion time) on 3 different levels. The pretreatment consisted of immersing guaco leaves in ethanol in three different concentrations (40, 70% and 100%) for three different immersion times (5, 45, and 85 seconds) at room temperature. As a result, drying time was significantly reduced (20-40%) compared to non-treated leaves. Taking into account the results obtained in the drying kinetics, which the leaves treated with ethanol presented greater removal of the moisture content and less time of drying in comparison with the control, proven by Scanning electron microscopy.

These results agreed with the Mayor and Sereno (2004) [6] description for the shrinkage phenomenon. The treatment with ethanol 70% and immersion time of 45 seconds presented higher content of coumarin content (4.10 mg/g). The immersion time had a great influence on the content of coumarin. The optimum point calculated by STATISTICA 12 program was observed between the ethanol concentration of 60 and 100% and the immersion time of 20 to 40 seconds. This is an affordable and cost-effective method. We believe that with the appropriate adaptations, it could be extrapolated to other medicinal plants generating major repercussions for small producers and pharmaceutical industry.

Keywords: phytochemistry; herbal medicine; HPLC; experimental design; response surface; optimization

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MICROWAVE ASSISTED BIOSYNTHESIS OF SILVER NANOPARTICLES USING *Stevia rebaudiana* EXTRACT

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Antibacterial and antinflamatory properties of silver nanoparticles (AgNPs) have been widely exploited in several areas, including the biomedical field, where the classical methods of obtaining AgNPs with organic solvents have been replaced by green methods that produce more biocompatible materials [1]. In order to better parameterize nanoparticle preparation conditions, the use of microwaves as heat source has shown promise in the production of silver nanostructures, since it allows reduction on time of synthesis and better control of nanoparticles morphology as fast preparation [2]. In this context, one proposes in this work the use of *Stevia rebaudiana* Bertoni, a plant widely used in food industry and that has a reducing character regarding to polyphenols as tanin and flavonoid content, in the biosynthesis of AgNPs. *S. rebaudiana* raw material has water content of 8,62 ± 0,20 % and total ash content of 8,16 ± 1,08% [3]. The preparation of stevia extract itself was carried out employing a microwave reactor under pre-established conditions and the analysis of dry matter from these aqueous extract used was 1,05 ± 0,02 %. To optimized this synthesis, the study was carried out by means of the experimental design of Box-Behnken to determine the best reaction condition. The best condition was observed as 80°C for 25 minutes and proportion Stevia extract/AgNO3 solution 1:1. Ultraviolet/visible spectra confirms the formation of silver nanoparticles showing a surface plasmon resonance (SPR) band around 420 nm [4]. Also, it was observed that the increase of intensity of this band is associated with higher temperatures and longer reaction time. Furthermore, increasing the amount of Stevia extract in the synthesis impaired the formation of AgNPs. The X-ray diffraction (XRD) analysis showed that, depending on the synthesis conditions, further metallic silver, AgCl was also formed concomitantly. Transmission electron microscopy indicate that nanoparticles are approximately spherical with diameters ranging from 4 to 24 nm. Zeta potential measurements reveals that at pH = 5, ? ~ -20 mV, indicating that Stevia extract act as reducing agent and functionalizing molecules to stabilize nanoparticles into solution. Thus, in the present study it was developed and optimized a simple, fast and ecofriendly method for the silver nanoparticles microwave assisted synthesis employing Stevia extract as both the reducing and stabilizing agent. All steps, since the extract production, were controlled by a high performance microwave reactor, which ensures the reliability and repeatability of the process.

Keywords: Silver nanoparticles, Green synthesis, Microwave assisted, Extract.

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AVOCADO OIL OBTAINED BY SFE METHOD (SUPERCRITICAL FLUID EXTRACTION)

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To obtain supercritical CO2, it is necessary to subject this gas to high pressures and temperatures. There, it turns into a powerful solvent which acts in the analyte and extracting the oils and its nutrients. This method is known as supercritical fluids extraction (SFE). The avocado has some regenerative properties, a high vitamin E level and many other characteristics. The extraction of the avocado oil by the supercritical fluid extraction method has a high level of effectiveness (over the 90%); it is a clean technology which allows obtaining a product with high characteristics of purity. In Caldas (Colombia), the SFE technology has a specific use for research in the universities. The objetive was to optimize the avocado oil extraction through the supercritical fluid method to increase its use and its productivity in the Caldas department. The specific objectives were: to design a SFE continuous system with recovery of CO2; to use the SFE continuous system with recovery of CO2 to improve the avocado oil extraction process; to create a manual explaining the operation of the machine and the extraction process. Enough literature review will be studied in order to carry out this research project, this will be helpful to know the state of the technique used; also data will be classified and a draft of different alternatives will be made which can generates a possible solution to the research problem. Then, a filter of the sketches will be carried out taking into account the best operating alternatives and the lowest impact in the environment. Finally, the 3D pre-designs will be elaborated by calculating the mechanical elements necessary to reach the final 3D design. When the 3D design will be defined, the lifting of the workshop plans, assembly plans, and the list of materials will be executed in order to design the budget in which a filter will be applied taking into account the cost, quality and reliability. Regarding that, a review of financing alternatives will be carried out for the construction of the machine and the proposal will be presented so that could be approved. At last, the period of building will be started; the construction phase of the machine, also, operating, calibration tests and some necessary adjustments shall be carried out. It will be helpful to begin writing the operations manual. Once the sample is defined in the project, in this case Hass variety avocado, an election of the preliminary processes will be carried out and these will be chosen to be applied to the sample. Subsequently, the variables to control the experimental process will be established, the quality of the obtained product will be evaluated through sensory, physical and chemical analysis, and finally the comparison of the obtained results with those found on the literature review will be analyzed. The expected results were: to develop the SFE continuous system with recovery of CO2; to obtain avocado oil with greater production per hour in relation to the found data; to publish the operation manual of the continuous SFE method with recovery of CO2.

Keywords: Avocado, Extraction, Carbon Dioxide (CO2), Supercritical.

EVALUATION OF ORGANIC POLLUTANTS PRESENT IN HONEYS AND SOILS NEAR BEEHIVES THROUGH THE TECHNIQUES OF u-ECD AND DSA-TOF-MS

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Honey is a food with a high added value, whose composition depends on its botanical origin and physicochemical characteristics of the soil near the hives. Soils may contain both organic and inorganic contaminants depending on the anthropogenic activities in them. It has been described that contaminants can be transported to hives through the interaction of bees with water and plants in contact with the soil, or by transporting soil particles to hives. Identification of the geographical origin of honey is information that can help both consumers and producers to prevent bees from being exposed to pollutants that may be present in foraging areas or to select honey from areas with less risk of contamination. Through the development of new analytical methodologies it is possible to identify and quantify contaminants present in soils and to relate this information to the content of contaminants present in honey. For this study a sampling of soils and honeys was carried out in southern Chile, an area characterized by a high and varied honey productivity. Samples were characterized by standardized methods (pH, organic carbon content, metal content, etc.). For the extraction of organic pollutants from the soil an ultrasound methodology was evaluated. The identification and quantification of contaminants was performed by GC-µECD. The contaminants were confirmed by direct sample - time of flight - mass spectrometry technique (DSA-TOF-MS), the same technique used for honey analysis. For the GC-µECD analyzes the soil samples were subjected to ultrasonic extraction for 30 minutes, using acetone as the extraction solvent in a 1:2 soil: acetone ratio, then the supernatant was removed by centrifugation and filtration1. The obtained extracts were brought to dryness at 35°C with a stream of nitrogen. For DSA-TOF-MS analysis, aqueous extracts were obtained using a soil: water ratio of 1:2.5; In the case of the honey, aqueous extracts were obtained in a 1:1 ratio. The soil characterization results showed a pH in water that fluctuated between 4.56 and 6.57, with high organic carbon content. The m/z spectra obtained through the DSA-TOF-MS technique of aqueous extracts reported the presence of organic pollutants of the organophosphorus type in at least three sampling sectors. Limits of detection and quantification for 8 PCB congeners (8, 20, 28, 52, 101, 118, 138 and 180) were determined for GC-µECD, which were 0.04 and 0.1µg/L, respectively. Likewise, the limits of detection and quantification of organophosphorus compounds were determined, which for chlorpyrifos were 2 and 3.73 µg/L, respectively. From the results obtained it is possible to conclude that the DSA-TOF-MS technique allows to show the presence and origin of contaminants in the honey of the sampled sectors, and that the method of extraction with ultrasound is a simple and low cost technique, Which allows the quantification of organic pollutants by GC-µECD.

Keywords: GC-µECD, Soil, Honey, Organic pollutants

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PRODUCTION OF URSOLIC AND OLEANOLIC ACID IN CALLUS CULTURES OF *Lepechinia caulescens*

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Lepechinia caulescens (Ortega) Epling (Lamiaceae) is commonly known as “bretonica” and has been used in traditional Mexican medicine for the treatment of diabetes, diarrhea, vomit and hypertension [1]. This plant is rich in substances with biological potential, including terpenoids and sterols [2]. Among the triterpenoids reported in *L. caulescens*, ursolic acid (UA, 3ß-hydroxyurs-12-en-28-oic acid) and its isomer, oleanolic acid (OA) stand out. These triterpenoids are believed to be responsible for many of its medicinal properties [3]. However strategies are needed to enhanced and standardize the production of metabolites as Plant cell cultures. In this work a callus culture system was established for the production of these compounds, leaf explants were exposed for the induction of calli at different concentrations and combinations of plant growth regulators, 2,4-dichlorophenoxyacetic acid (2,4-D) and 6-benzylaminopurine (BAP). HPLC method was used to quantify ursolic and oleanolic acid content in each treatment. Treatment with 3.0 mg/L of 2,4-D and 0.1 mg/L of BAP produced the best results for calli induction and production of ursolic (1.57 mg/g DW) and oleanolic acid (1.13 mg/g DW). The combination of auxins and cytokinins showed favorable results for the induction of calli. Variation concerning the accumulation of ursolic and oleanolic acid was observed between treatments. There is a greater accumulation of ursolic (16.58 mg/g DW) and oleanolic acid (1.94 mg/g DW) in leaves of wild plants. This is the first work reported for this species *in vitro* culture, being this system the base to establish a production of these terpenes, increasing the levels of accumulation with the help of elicitors

Keywords: *Lepechinia caulescens*, plant growth regulators, triterpenes, calli.

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FABRICATION OF *Vaccinium meridionale* Swartz EXTRACT SENSITIZED TiO2 PHOTOELECTRODES

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Since Michael Grätzel reported DSSC's (Dye Sensitized Solar Cells), this kind of technology has been deeply investigated as economic and efficiently alternative to conventional silicon solar cells [1]. Currently, highest confirmed efficiency for this kind of cell is 11.9% (+/- 0.4), to reach this values, DSSC's includes ruthenium(II) polypyridyl complexes as sensitizer of TiO2 photoanode [2], however, these sensitizers are expensive and they are hazardous to environment. Furthermore, a variety of transition-metal complexes and organic dyes have been successfully employed as sensitizers in DSSC's; in last year extracts from natural dyes (e.g. *grapes*, *spinach*, *Raspberries*, Rosa xanthina) have been used as inexpensive and no toxic sensitizers in DSSC's [3], requirements for photosensitizers to function in DSSCs are the absorption in the visible or near-infrared regions of the solar spectrum and the binding to the semiconductor and different natural dyes accomplishment them [4]. In Colombia there are a variety of native plants that have a high antioxidant capacity and properties for being use in photovoltaic application as sensitizers. In this work we determined the potential of the extract of the shell of a Colombian species Agraz silvestre (*Vaccinium meridionale Swartz*) as a possible natural sensitizer for titanium dioxide (TiO2) electrodes for photovoltaic application. We obtained methanolic extract from *Vaccinium meridionale Swartz* through percolation method; extract was characterized by UV-Vis spectrophotometry and HPLC method. We deposited TiO2 thin films through doctor blade method and sensitization process was carried out by chemisorption. Properties of TiO2 and sensitized-TiO2 thin films were studied by X-ray diffraction (XRD), infrared spectroscopy (IR) and absorption diffuse reflectance assays. Extract was composed by anthocyanin, furthermore, the XRD patterns indicated that sensitization did not affect the crystalline phases radio of the TiO2 films; furthermore, the optical analysis showed sensitization process improved TiO2 photophysical properties in visible region of electromagnetic spectrum.

Keywords: Dye sensitized solar cells, TiO2, Sensitizer, Natural dyes, *Vaccinium meridionale Swartz.*

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RETRIEVAL OF METABOLITES FROM SEED KERNELS OF FOUR VARIETIES OF MANGO (*Mangifera indica*) GROWN IN THE DEPARTMENT OF TOLIMA

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Currently there exists a growing issue regarding the final disposal of agricultural waste linked to fruit production. For the year, 2014 in Tolima were produced 77.321 tons of mango, estimating that disposed mango seeds represent approximately 40% of total weight of the fruit, tantamount to 46.338,6 tons of residual biomass wasted. Mango varieties Mariquiteño, Manzano, Common and Yulima are widely cultivated in Tolima department. In this study, hexane and ethanol extracts of the seed kernel from the four mango varieties were evaluated and characterized. The extraction was performed using Soxhlet with n-hexane. Extraction yields and physicochemical properties of fats (index of: acidity, saponification, iodine, peroxide) were determinated. Antiradical capacity of ethanol extracts were measured towards ABTS and DPPH radicals. Fats yields from the varieties ranged from 7 to 11%. Physicochemical properties were similar, with iodine and saponification indexes oscillating values between 256 - 338 mg I2/g and 176 – 230, respectively. Opposite case occurred with peroxid and acidity indexes, showing major values in Yulima variety with 416 meq O2/Kg and 34 % (oleic acid), respectively. The other varieties showed values between 188 - 228 meq O2/ Kg and 25 - 26 % (oleic acid).Ethanol extracts had yields between 6,5% and 19%, being higher in Yulima variety, however, IC50 values for ABTS and DPPH radicals were similar overall 3 ppm to 3,4 for ABTS and 12 to 14 ppm for DPPH.

Results show important yields, around 30% for joint extraction from seed kernel of the studied varieties, leading to potential use of these residues in the obtaining of added value products for cosmetic or food industries, which must be strenghtened in posterior studies that delve into the characterization of present compounds and their possible industrial uses.

Keywords: Mangovarieties, Residual biomass, Seed kernel, Added value

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SUPERCRITICAL FLUID EXTRACTION OF CANNABINOIDS WITH FORENSIC PURPOSE

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Currently there is an important interest in cannabis and their therapeutic uses. This plant is one of the oldest medicinal plants known [1]. *Cannabis* contains more than 500 known compounds that include 80 cannabinoids, which are unique in those species. The major compound from cannabis THC has been registered for medical application in several countries but is also known for its psychotropic properties. It is too difficult to isolate pure cannabinoids in order to develop drugs for pharmacological studies or reference substances with forensic purposes. For this reason, the main objective of this study was apply a supercritical fluid extraction procedure for to obtain cannabinoids extracts. CBD, CBN and THC were quantified by GC-FID. A supercritical fluid extraction was selected because the non-use of solvents in this methodology makes it an extremely powerful green tool and small changes of pressures achieve more selectivity [2].

Extraction experiments were carried out with a central composite designed. The highest pressure and temperature were 330 bar and 80ºC and the lowest 150 bar and 40ºC. EtOH was used as cosolvent. The combination of CO2-cosolvent was from 0% to 5%. The flow was 5 L/min and the extraction time was 4 h. Characterization and quantification of the different extracts and their respective wastes were performed with a validated technical of GC-MS and GC-FID analysis. The calibration curve was developed with standard solutions of THC, CBD and CBN 100 ppm and tetracosane as internal standard at the same concentration. The analytical capillary column was an Rtx ® (30 m x 0, 25 mm x 0, 25 µm). The injector and detector temperatures were maintained at 290ºC and 300ºC, respectively. The injection split ratio was 1-20.

The best yield of the CO2 supercritical extraction was 26% (330 bar, 80 ºC, 5%EtOH) but it had a low cannabinoid content (18%). Otherwise the major cannabinoid content was 42% (330 bar, 60°C, 2%EtOH) and it had 16% of extraction yield. Finally it is worth highlighting an extract with a 34% of cannabinoids (150 bar, 40°C, 5%EtOH) which had a 23% of extraction yield, the extraction wastes analysis of this extract determined that it was THC free.

The extraction wastes analysis showed about half of the extractions could pulling out THC between the 90-100%. This is the first study related with colombian *Cannabis* performed by supercritical fluid extraction with co-solvent. We found some ways to extract large quantities of THC in order to obtain a processed vegetable material THC free.

Keywords: *Cannabis sativa*, Cannabinoids, Supercritical fluid extraction, GC- MS - GC-FID

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EXTRACTION OF HYPOGLUCEMIC TRITERPENES FROM *Eucalyptus tereticornis* BY SUPERCRITICAL FLUIDS

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Diabetes is a chronic disease that affects millions of people; it is generated when the pancreas does not produce enough insulin or it is not used effectively, thus that high circulating levels of glucose (hyperglycemia) damage tissues. This disease is usually controlled with medicines that are not always effective or have adverse reactions [1]. It is therefore necessary to expand the therapeutic options with new and better drugs or adjuvants.

Eucalyptus extracts have demonstrated hypoglycemic effects on in vitro models on C2C12 and HepG2 cells, and on in vivo model of diabetic mice [2]. And we have identified three bioactive triterpenes derived from ursolic acid whose activity seems to be synergistic when there is a mixture of them.

As a contribution to the application of environmentally friendly methods to discover and design new extraction processes with reduced energy requirements, resorting to non-hazardous alternative solvents, while ensuring safe and high quality extracts. The extraction with supercritical fluids was evaluated modifying variables such as temperature and flow to obtain an extract rich in triterpenes and compared with an already validated analytical method that the extraction by supercritical fluids allows obtaining triterpenes of interest in a time of 120 minutes with a higher yield (6%) than solvent extraction (2%).

Keywords: Hypoglucemic, Triterpenes, Supercritical fluids.

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NEW METHOD BY DIFFERENTIAL SCANNING CALORIMETRY (DSC) FOR CHARACTERIZATION OF ORGANIC EXTRA VIRGIN OLIVE OILS (EVOOS) FROM DIFFERENT INTERCONTINENTAL GEOGRAPHICAL AREAS

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The thermal properties of many organic extra Virgin Olive Oils (eVOOs) coming from different Intercontinental areas of the world were investigated by Differential Scanning Calorimetry (DSC). Different studies have shown that DSC provides significant information about the authenticity of an oil, its cultivars, its changes and its geographical origin [1]. DSC applications include the measurement of the melting point of vegetable oils [2], the determination of thermally oxidized olive oil, the determination of quality of frying oil [3], the detection of adulterated extra-virgin olive oil [4] and of seasonal changes. In this paper, we report the results obtained by using an improved methodology concerning DSC in combination with an unsupervised multivariate statistical analysis such as the Principal Component Analysis (PCA). This technique, through a series of heating and cooling cycles, provides a specific curve, i.e., a thermogram, which represents the fingerprint of each eVOO sample. In fact, variations due to the different cultivars, geographical origin or chemical composition can be highlighted because they produce changes in the corresponding thermogram. In particular, we apply the PCA to the melting thermogram characterizing the fusion temperatures of fatty acids and Triacylglycerols (TAGs) after proper cycles of crystallization.

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COAGULATING ACTIVITY OF THE SEED OF *Psidium guajava* L AND THE EPISPERM OF PERSEA AMERICANA IN SAMPLES OF WATER FROM THE BOGOTÁ RIVER, CHOCONTÁ & VILLAPINZÓN

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The objective of this study was to evaluate the reduction of turbidity in water samples from the Bogotá river, using the guava seed, *Psidium guajva* L, and the avocado seed episperm *Persea americana*, as natural coagulants. Three extracts were made from each seed, in water, with 10% ethanol and 10% acetic acid. Three tannins were used as an organic control: *quebracho* (*Schinopsis balansae*), mimosa (*Acacia dealbata*) and chestnut *(Castanea sativa*), with aluminum sulfate, Al2(S04)3 as the inorganic control. The samples of water were taken from the upper basin of the Bogotá river in the Chocontá - Villapinzón route to La Marinilla. A reduction in turbidity levels was observed in all cases, using the 10% acetic acid extract of *Psidium guajava* L, with an effectiveness of 94.95%, and of 93.71% using the extract of this same seed in water. Likewise, the episperm of the *Persea americana* avocado seed showed reduced levels of turbidity. The extract in 10% acetic acid was the most effective, with a percentage of 80.85%. The chestnut one showed the best yield of the three tannins with a maximum effectiveness of 91.75%.

Keywords: Coagulant activity, *Psidium guajava* L. *Persea americana*

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MARINE OCTOCORALS AS SOURCE OF PEST CONTROL COMPOUNDS

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Agriculture is susceptible to insect plagues. Currently, there are several approaches to control plagues such as physical, biological and mechanical control. Chemical control approach uses compounds to eradicate plagues and is recognized as the most effective approach [1]. There are some commercial insecticides based on terrestrial natural products such as limonoids, pyrethrins and some essential oils [2]. On the other hand, compounds from marine natural sources, which exhibit a wide range of bioactive effects, represent an interesting alternative to get new insecticides Furthermore, compounds isolated from marine organisms (e.g. briantenins, calicin, destruxins and telfairins) have shown insecticidal activity [3]. In this work, the potential of marine natural diterpenes as insecticides was explored. In this research we selected two insects: *Sitophilus zeamais* is an insect that attacks standing maize crops before harvesting. It infests raw or processed cereals such as wheat, oats, barley, sorghum and rye [4]. *Aedes aegypti* is a vector involved in the transmission of several tropical diseases such as dengue, yellow fever, chikungunya epidemic arthritis, Zika fever and Mayaro virus [5].

We tested organic extracts from seven Caribbean soft corals as antifeedant against *Sitophilus zeamais* and as acetylcholinesterase inhibitors. The most active extracts belong to *Pseudoplexaura flagellosa* and *Plexaura porosa.* Compounds form these two extracts were separated on chromatographic methods and analyzed by NMR and MS. In this way, *P. flagellosa* extract yielded compounds (8*S*)-plexaurolone (**1**), (8*S*)-dihydroplexaurolone (**2**), (8*R*)-dihydroplexaurolone (**3**), (8*R*)-dehydroxyiplexaurolone (**4**), (8*S*)-dehydroplexaurolone (**5**), (8*R*)-dehydroplexaurolone (**6**), and (1*R*, 3*R*, 4*R*, 8*S*, 11*R*, 12*R*)-3,6-dioxa-cembra-15(17)-en-6,11-diol (**7**). On the other hand, crassine acetate **8** was isolated as the major component in the *P. porosa* extract. Pure compounds were evaluated in the following bioassays: antifeedant activity (DA) against the insect *Sitophilus zeamais*; larvicidal activity against the vector of viral diseases *Aedes aegypti* (LA); lethality against shrimp *Artemia salina* as an indicator of ecotoxicity (ET) and finally acetylcholinesterase inhibition (AChEI) as mechanism study approach. Compounds **2**, **5** and **6** showed a high antifeedant activity against the insect *S. zeamais*, while compounds **5** and **6** strong larvicidal activity against *Ae. aegypti* larvae. These compounds were neither strongly ecotoxic nor inhibitor acetylcholinesterase. The obtained results suggest the potential of cembranes diterpenes from marine sources as insecticide compounds.

Keywords: Octocorals, Diterpenes, Insecticides, Antifeedant

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SENSITIZATION OF TiO2 THIN FILMS BY EXTRACT *Bactris Guineensis* TO BE USED IN PHOTOCATALYSIS

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Treatment of recalcitrant compound and solar recovery of polluted water is an intensive field of research around world laboratories. Currently, titanium dioxide (TiO2) is one of the most important photocatalytic materials for environmental purification; this material is inexpensive, it is available in abundance on earth surface, it is environmental safe, however, TiO2 has high band gap value (3.2 eV), for that, it is only photocatalytic active under UV irradiation, this drawback limit its practical applications [1,2]; TiO2 sensitization for absorption of naturals and/or synthetics organic dyes is an important research subject in the photocatalysis field, and it is an efficient method to develop practical application in waste treatment [3]. Natural dyes are an inexpensive and nontoxic option to sensitization process; in Colombia there are a variety of native plants that have a high antioxidant capacity and properties for using in photocatalytic application as sensitizers. In this work we sinsetized TiO2 thin films for using extract of the shell of a Caribean species Corozo (*Bactris Guineensis*) and we tested photocatalytic activity of the natural dye/TiO2 thin films. We obtained methanolic extract from *Bactris Guineensis* through percolation method; extract was characterized by UV-Vis spectrophotometry. We deposited TiO2 thin films through doctor blade method and sensitization process was carried out by chemisorption. Properties of TiO2 and sensitized-TiO2 thin films were studied by X-ray diffraction (XRD), infrared spectroscopy (IR) and absorption diffuse reflectance assays. Extract was composed by anthocyanin, furthermore, the XRD patterns indicated that sensitization did not affect the crystalline phases radio of the TiO2 films; and besides the optical analysis showed sensitization process improved TiO2 photocatalytic activity in visible range; finally, photocatalytic test showed that *Bactris Guineensis*/TiO2 thin films were effective in photocatalytic degradation of alizarin red.

Keywords: Photocatalysis, TiO2, Sensitizer, Natural dyes.

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SEMI-SYNTHESIS OF DIHYDROCHALCONES DERIVATES NATURAL ALTERNATIVE TO CONTROL SAPROLEGNIA INFECTION

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We describe the semi-synthesis of dihydrochalcone derivatives and their *in vitro* antioomycete activities. These compounds were prepared by modifying naturally occurring antimicrobial dihydrochalcone, 2',4'-dihydroxydihydrochalcone [1], isolated by us from *Adesmia balsamica*. The structures of the compounds were assigned on the basis of spectroscopic evidence and by comparing their physical and spectroscopic data with those reported in the literature. All the compounds were subjected to two pathogenic strains of the genus *Saprolegnia*, including *Saprolegnia parasitica and S. australis*. The antioomycete efficacies of this class of compounds were established by correlating the activity profile of each compound with its structure and by comparing the activities of all the compounds with each other based on their structure [2]. This should enable the development of other derivatives of the dihydrochalcone family that would serve as more potent antioomycete agents against *Saprolegnia* species.

Keywords: 2',4'-dihydroxydihydrochalcone, Dihydrochalcone derivatives, *Saprolegnia*, A*desmia balsamica*,

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VALIDATION OF THE CHROMATOGRAPHIC METHOD HPLC DAD AND UV VIS FOR THE QUANTIFICATION AND IDENTIFICATION OF HARPAGOSIDO PRESENT IN THE SECONDARY ROOT OF *Harpagophytum procumbens* (BURCH.) DC

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The presence of plant metabolites that help to control inflammatory processes caused by various sources has been reported at literature. These compounds may have effects on the expression of proinflammatory cytokines (interleukins and necrosis factor Tumor TNF alpha), mediating enzymes (COX-2 cyclooxygenase-2) and catabolites (NO nitrous oxide and prostaglandins E2). *Harpagophytum procumbens* (Burch.) DC has as active principles monoterpenic heterosides of the group of iridoids (harpagoside, harpagide, procumboside), mainly inhibiting the inflammatory process at the joint level.

Studies of harpagoside have focused on HPLC UV-Vis analysis, where the most common conditions were a C18 column (250mm, 4.6mm and 5 µm) with an ACN:H2O mobile phase at 278 nm [1], extraction time 20 min, and the molecule is found in concentrations of 1.51 mg mL-1 of harpagoside present *Radix scrophulariae* [2]. These conditions allowed to be a reference to make the analyzes in the plant of interest (*H. procumbens* (Burch.) DC), where its optimal parameters were established for the extraction, identification and quantification of the metabolites.

The analyzes for the identification and quantification of the analytes were performed using HPLC-DAD and UV Vis with a C18 column (150mm, 4.6mm and 5µm), the standardized working conditions are a mobile phase conformed by ACN: H2O (1% acetic acid) with a flow of 1mL min-1 in the initial gradient (20:80) and final (50:50) gradients for a run time of 10 min, with a retention time of 5.92 min, these parameters were optimized.

The standardization process established a detection limit of 0.01 µg g-1, the linear range was set from 5 µg g-1 to 70 µg g-1, which presented the following equation $y = 0.6043x + 3.2229$ with a correlation coefficient of $R^2 = 0.9983$. The repeatability parameters were evaluated with a % RSD of 0,10% and reproducibility with a% RDS of 3.80%; finally, a resolution higher than 1.5 is obtained. Additionally, the extraction process was evaluated comparing four techniques; Soxhlet, DSASE (Dynamic Solvent Assisted Sonication Extraction), RSDE (Rotatoring Disk Sorptive Extraction method), ESL-US (Solid-Liquid Extraction Assisted with Ultrasound). As a result, the most efficient technique was ESL-US, for which its working conditions were optimized: Sample weight of 0.5 g, sonication time of 30 min and type of solvent used (Ethanol: H2O 50:50).

Keywords: Harpagoside, ESL-US extraction, HPLC DAD and UV-Vis.

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PRODUCTION OF PARTHENOLIDE AND PHENOLIC COMPOUNDS FROM ROOT SUSPENSION CULTURE AND PLANTLETS OF *Tanacetum parthenium*

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Tanacetum parthenium has gained attention for drug development due to its production of bioactive secondary metabolites, such as phenolic compounds and parthenolide. Parthenolide is a sesquiterpene lactone having antitumor activity. It has been determined that some phenolic compounds are promising anti-cancer agents. The biosynthesis of secondary metabolites in plants growing in the open field shows variations in their content due to environmental and genotypic factors, so that the plant tissue culture, having controlled conditions can serve as a tool for their production. In the present work, differences in the production of these metabolites between *in vitro* cultures (organs from plantlets and root cultures in suspension) of *T. parthenium* were determinate. Results showed that the *in vitro* cultures produced phenolic compounds and parthenolide which depended on the type of culture and the incubation time. The content of the secondary metabolites was higher in shoots of plantlets, followed by root cultures in suspension and roots of plantlets. phenolic compounds and parthenolide production as well as morphogenesis and growth was enhanced in the plantlets by applying a combination of plant growth regulators: α-naphthaleneacetic acid 0.27 µM and kinetin 2.32 µM.

NAA (16.2 µM) promoted direct rhizogenesis (89.2 ± 5.2%). When root growth was characterized over time, two phases were observed: the exponential phase up to day 20, and the stationary phase from day 20 to 32. A maximum amount of 8.1 g/L of Dry biomass at day 32, a growth rate of 0.348 g/L per day, a doubling time (td) of 11.56 ± 0.62 days, a specific maximum growth rate (µm) of 0.0601 d-1. Glucose concentration at day 32 of culture was 17.5 g/L. Significant differences in the content of total phenols over time were determined, with the highest production being found at day 32; parthenolide production at a concentration of 0.0292 mg/g root, as well as caffeic acid (0.8529 mg/g), p-coumaric acid (1.8638 mg/g), chlorogenic acid (1.3448 mg/g) and salicylic acid (0.1905 mg/g). In plantlets, plant growth regulators increased the development of new shoots and leaves, as well as the length of apical shoots and the amount of biomass of roots and shoots.

GREEN SYNTHESIS OF (E)-2-BENZYLIDENE-1,1-DIPHENYLHYDRAZINE

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PPQV 43

Cancer is not a single disease but a collection of related diseases, related to the uncontrolled growth of cells that spread into the surrounding tissues. Cancer is the second leading cause of death globally. Depending on the type of cancer, a specific treatment regimen is required that encompasses one or more modalities such as surgery, radiotherapy, and chemotherapy, being surgery the oldest form of treatment and also the most effective [1].

In spite of the many tests found nowadays to find and diagnose any type of cancer, it is made imperative to do research in new synthesis methodologies of compounds with higher activity and selectivity but less harmful side effects.

Hydrazones and hydrazones derivatives have a very promising anticancer activity, which is the purpose of this project: to synthesize, to purify and to characterize compounds of the hydrazine type with new structures to evaluate their activity in specific cell lines.

In this research paper the synthesis of a hydrazone with a particular structure is developed through a method that allows saving time and costs, reducing wastes and harmful subproducts as a main challenge. The methodology takes place through Green Chemistry because the reactants are used in equimolar quantities, (atomic economy), green solvent and no heating (diminishing energy resources). Furthermore, since the products are crystals, the use of chromatographic columns is avoided, preventing the use of large quantities of solvents, reactants and energy consumption to achieve their separation and purification and instead using simple recrystalizations [2].

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GREEN SYNTHESIS OF A NEW CHIRAL LIGAND DERIVED FROM 2-THIOPHENCARBOXALDEHYDE AND ITS Pd(II) COMPLEX

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The aim of this report was to synthesize a new Pd(II) complex from the imine derived from 2-thiophenecarboxaldehyde and the chiral amine (S)-(-)-phenylethylamine using the Green "solvent-free" approach. The Green Chemistry, which consists in the design, development and implementation of products and processes that reduce or eliminate the use or generation of dangerous substances for the human health and the environment, allows to obtain compounds in a straighforward, cost-effective and gram-scale manner. Nowdays, one of the biggest challenges for chemists is the development of less pollutant and no-conventional synthetics methods gor the the design of cleaner chemical transformations. Such practice has been developed with good results due to the advantages: high yields, reduction of reaction time, elimination of harmful solvents, higher reactivity and simplification of the process. The structure of the products was established by spectroscopic methods (FT-IR, 1H and 13C NMR, and EI-MS). The structures were fully confirmed by X-ray diffraction studies.The interest on coordinating ligands with metals has grown since the discovery of the antitumor activity of Cisplatin; numerous analogous compounds with general formula ML2X2 have been synthesized (where M corresponds to Pt or Pd, L corresponds to an organic ligand and X is an halogen), and it has been observed that the bioactivity varies according to the metal and the ligands employed, hence the importance of this work, as we obtained a Pd(II) complex from a chiral imine. As antecedent, our working group has synthesized several Pd(II) complexes with anticancer activity.

NATURAL DYE SENSITIZATION OF TiO2 THIN FILMS WITH *Syzigium Cumini* EXTRACT FOR PHOTOCATALYTIC APPLICATIONS

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PPQV 45

Currently, advances oxidation process for water treatment is one the most researching topics and one of the most promising water clean technology around the world [1]. Several semiconductors have reported photocatalytic activity or water splitting (e.g., Fe2O3, CdS, Cu2O, WO3, SnO2, ZnO [2-3]), currently more than 190 semiconductors have been assayed as suitable photocatalysts; TiO2 has higher photocatalytic yields, this semiconductor is resistant to photocorrosion, innocuous to the nature, and inexpensive [4], However, due to its high band gap value (3.2 eV) TiO2 has one drawback for practical application, this material is active only under UV irradiation. Synthetic and natural dye sensitization is one of the strategies to improve photoactivity of TiO2 in visible range of electromagnetic spectrum. Requirements for photosensitizers to function in photocatalytic application are: (a) high absorption in the visible or near-infrared regions of the solar spectrum, (b) high photostability and (c) the binding to the semiconductor and different natural dyes accomplishment them [5]. In Colombia there are a variety of native plants that have a high antioxidant capacity and properties for being use in photocatalytic application as sensitizers. In this work we determined the potential of the extract of a Caribbean specie *Syzigium Cumini* as a possible natural sensitizer for titanium dioxide (TiO2) electrodes to photocatalytic application. We obtained methanolic extract from *Syzigium Cumini* through percolation method; extract was characterized by UV-Vis spectrophotometry and HPLC method. We deposited TiO2 thin films through doctor blade method and sensitization process was carried out by chemisorption. Properties of TiO2 and sensitized-TiO2 thin films were studied by X-ray diffraction (XRD), and absorption diffuse reflectance assays. Results indicated that extract was composed by anthocyanin, furthermore, the optical analysis showed sensitization process improved TiO2 photophysical properties in visible region of electromagnetic spectrum; finally, photocatalytic test showed *Syzigium Cumini* sensitized TiO2 films were effective in photodegradation of Blue methylene under visible light irradiation.

Keywords: Advances oxidation process, TiO2, sensitizer, Natural dyes, *Syzigium Cumini*.

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EXTRACTION OF METFORMIN FROM EXPIRED DRUGS AND EVALUATION OF ITS ANTICORROSIVE PROPERTIES

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Demographic increase are bringing to us several troubles related with wastes management. One of the must concern about waste generation has been lead to the dangerous ones, that can be generated from biomedical, batteries, flammable substances, expired drugs, among others [1]. Due to the misuse of drugs, wastes associated to this practice are increasing as interest to it management. Recently have been emerged some proposal to reuse expired drugs and therefore reaching the waste volume reduction [2]. In our research, we collect household expired drugs and select the metformin as potential organic anticorrosive looking to replace conventional toxics pigments [3].

Metformin hydrochloride expired medicament was milled, dissolved in water, filtered through of silica gel pad and vacuum concentrated. It was elucidate using IR and 1H NMR techniques to check purity and structure, comparing with literature reports. After metformin isolation, it was using as green anticorrosive organic compound in electrochemical impedance spectroscopy (ESI) and Potentiodynamic Polarization tests. Green corrosion inhibitor metformin was tested to different concentration (50, 100, 200 and 300 ppm) on AISI 1020 carbon steel in 1 M HCl medium to room temperature. Preliminary results showed that metformin reach high inhibitory corrosion effects obtaining inhibition efficiency of 90 % to room temperature and 6 h of immersion time.

Keywords: Green corrosion inhibitors, Expired drugs, Metformin.

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DEVELOPMENT OF A METHOD FOR QUANTIFICATION AND IDENTIFICATION OF TOTAL QUERCETIN BY HPLC-DAD AND UV VIS IN THE EXTRACT OF ALCOHOLIC *Bidens Pilosa* LINNÉ OBTAINED BY MINIATURIZED EXTRACTION

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PPQV 47

Research on new alternatives for phytochemical purposes allows the identification of plants with pharmaceutical potential related to the great diversity of secondary metabolites. Being of relevance for our community those of South American origin, such as *Bidens pilosa*, its great variety of secondary metabolites potentiate the great phytopharmacological use [1]. One of the metabolites present in the plant is quercetin a type of flavonol being a natural pigment that protects the plant tissue from damage caused by oxidizing substances or elements such as ultraviolet gray and environmental pollution. Provides the man with antioxidant activities, anti-inflammatory, antithrombotic, anti-microbial, anti-allergic, anti-tumor and antiasthmatic actions [2]. It is important to highlight the work of Muñoz [3] in *Calendula officinalis* as a reference and its subsequent analysis by HPLC.

The chromatographic separation was performed in a HPLC-DAD and UV Vis system with a C18 column (150mm, 4.6mm and 5um), the mobile phase was used methanol: water in initial ratio (40:60) to (60 : 40) for a running time of 10 min at a flow of 1 ml min-1; With a wavelength of 373 nm, and a 20 µl injection volume, obtaining a detection limit of 10 ng g -1. This research is based on the extraction of total quercetin from the aerial parts of the plant of *Bidens pilosa Linné* using the exhaustive technique of DSASE [4] (Dynamic extraction with solvent assisted by sonication), obtaining an alcoholic extract which is subjected to acid hydrolysis [3] and A subsequent concentration by means of a RapidVac together with reconstitution to perform the analysis. Extraction of different parts of the plant (stem, leaves, and flowers) shows that the flowers have higher quercetin content Linearity under gravimetric control between 1500 - 3700 ng / g (range in which the concentration of the samples is expected to be found), RSD% oscillates between 2.2 and 7.0, spectral analysis of the standard signal was performed using HPLC-DAD.

The process of hydrolysis with 3.5 M HCl is fundamental for the evaluation of quercetin in the different aerial parts of the plant, since the presence of quercetin in free form is not evident, as well as three extraction techniques such as Soxhlet , ESL-US and DSASE being the most efficient to evaluate quercetin obtaining a retention time of 6.41 min along with a resolution of 1, finally the antioxidant evaluation was done by the ORAC method, Using as a comparison method the trolox curve, evaluating extracts of leaves, stems and flowers of the plant in solvents like methanol and ethanol obtaining better results the flower extract with methanol.

Keywords: *Bidens pilosa* Linne, quercetin, DSASE, HPLC-DAD y UV Vis

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COUMARINS FROM LIME TAHITI AND THEIR ACCUMULATION IN RESPONSE TO DIFFERENT ELICITORS

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PPQV 48

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Citrus fruits are the main fruit trees crop cultivated around the world. Two of the most produced citrus fruits are limes and lemons, which have increased their production by about 11.4% in the last five years, according to the United States Department of Agriculture (USDA). The limes are remarkable in comparison with other citrus fruits because of their acids and sugars contents, flavor, aroma, constitution of the bark layer and their annual production [1]. However, one of the principal citrus yield loss are due to post-harvest diseases, particularly during storage and transportation processes. According to what is mentioned before, there are published studies that exhibit several fungal pathogens like responsibles for the decomposition in harvested fruits, being *Alternaria alternata* pv. Citri, *Penicillium italicum* Wehmer and *Penicillium digitatum* Sacc. the most important ones [2].

Traditionally, the most common way to control diseases has been the application of synthetic fungicides. However, these have adverse effects on human health and the environment. Additionally, the development of resistance to fungicides by pathogens can increase the production cost. Therefore, it is necessary to generate alternative methods to fungal diseases control. A potential option is the induction of natural resistance in plants by the use of elicitors, which are compounds that activate the plants defense responses, including the accumulation of fungitoxic compounds called phytoalexins. In citrus, coumarins have been reported as antimicrobial compounds produced in response to infection, which acting as a chemical barrier to avoid the disease development [3].

The present work describes the isolation of six known coumarins from Tahiti lime fruit (*Citrus latifolia*). These compounds were isolated using standard chromatographic techniques (column chromatography) and were identified by 1D and 2D NMR spectroscopic methods. Furthermore was evaluated the ability of some polysaccharides to induce plant defence responses, using a high-performance liquid chromatography (HPLC) method. The results showed that the chromatographic profile depended on the applied inducers. A significative increase was found in the amounts of coumarin compounds compared to blank (water-treated lime fruit). In conclusion, the coumarin-mediated defensive response of Tahiti lime fruit can be modulated by the application of elicitors. In addition, the greatest accumulation of coumarins was shown when gum arabic polysaccharide was used.

Keywords: *Citrus latifolia*, Elicitors, Phytoalexins, Coumarins

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DEVOLOPEMENT OF A CASCADE FRACTIONATION PROCESS OF *M. indica* LEAF EXTRACT WITH POTENTIAL ANTIOXIDANT AND ANTIBACTERIAL ACTIVITY

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PPQV 49

M. indica leaves are a great source of phenolic compounds with functional properties including antioxidant and antibacterial activities [1,2]. The innovative and green high pressure technique known as Enhanced Solvent Extraction (ESE) has demonstrated to be highly efficient to recover phenolic compounds from this by-product. It combines the advantages of carbon dioxide (CO2) and liquid solvents at high pressure and temperature. The high proportion of CO2 (> 20%) enhances mass transfer phenomena including an easier penetration of the solvent through the matrix. Besides, the use of water and ethanol increases the polarity of the solvent system favouring the recovery of polar molecules [2]. The present study proposed a green extraction and fractionation process in order to obtained fractions from mango leaves with strong antioxidant and antibacterial activities. Tests were carried out on a high-pressure pilot-plant scale equipment which comprises a vessel (5000 mL capacity) and three cyclonic separators (1000 mL). The solvent system consisted on a mixture of CO2 + 50% of polar cosolvent, the latter varying from 0 to 100% ethanol in water. As operation conditions a pressure (P) of 200 bar and a temperature (T) of 90 ºC were kept constant in the extractor vessel while different conditions of P and T were fixed in the separators in order to develop a cascade fractionation process. Fractions were evaluated according to the extraction yield, antioxidant activity determined by the DPPH assay, and the antibacterial activity against *E.coli*, *S. aureus*, *P. mirabilis*, *Pseudomona*, *Salmonella* and *E. aerogene*s that was analyzed by the agar diffusion method and the minimal inhibitory and bactericidal concentration was determined. The addition of ethanol in the solvent system increased the yield in the third separator (S3) and favored the obtaining of fractions with higher antioxidant activities than those obtained with water or the hydroalcoholic mixture as cosolvents. However, fractions with superior antibacterial activity were obtained with CO2-ethanol-water 50:25:25. Nevertheless, when the hydroalcoholic mixture was used as cosolvent the fractionation of the extract was not successful. The fractions presented similar antioxidant and antibacterial activities. The fractionation of the crude extract was observed only when pure ethanol or water were used as cosolvent.

Keywords: *M. indica*, antibacterial activity, phenolic compounds, high-pressure technique, enhanced solvent extraction.

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STUDY OF CYTOTOXICITY OF PLANT EXTRACTS ON CANCER CELL LINES AND EVALUATION OF ACTIVITY ENHANCEMENT BY ENTRAPMENT INTO POLYMER MICELLES

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PPQM 01

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The application of medicinal plants in the treatment of cancer is a matter of current interest [1], mainly because a large number of drugs with anticancer activity has been obtained from natural products [2]. Our research group has been engaged for long time in the study of Leptocarpha rivularis, more commonly known as “palo negro”, an autochthonous plant that grows at the southern zone of Chile. *L. rivularis* belongs to the family of Asteraceae, and it has been shown that contains a high percentage of sesquiterpene lactones (SQL), with leptocarpin (LTC) as major component [3].

In previous work, we have shown that LTC exhibits a significant cytotoxic effect, induces an apoptotic process on several cancer cell lines, and it is an effective inhibitor of nuclear factor kappa B (NF-κB) [4]. The latter is a very interesting effect because it has been shown that NF-κB is involved in the tumor initiation, progression, and therapeutic resistance in most of the major forms of human cancer [5]. On the other hand, the poor water-solubility of natural products is the main drawback in their potential clinical development as chemotherapeutics drugs. To overcome this difficulty the incorporation of them into polymer micelles as delivery vehicles for anti-cancer drugs has been extensively studied in the last two decades [6]. In this work we have evaluated the in vitro cytotoxicity of ethyl acetate and methanol extracts of L. rivularis on different cancer cell lines. The extracts are applied in homogeneous solution and entrapped into polymer micelles of Pluronic F127.

The results indicate that both extracts exhibit activity on HT29, MCF7 and PC-3 cell lines, with IC50 values in the range of 11−16 mg/mL. Interestingly, the cytotoxicity is enhanced by physical entrapment of both extracts into polymeric micelles formed by Pluronic F 127. This effect is especially important in the case of the ethyl acetate extract, where the IC50 values are almost 200 times lower than those measured with its free form. These results suggest that polymer micelles enhance the apoptotic process induced by active non-polar components.

Finally, it is also noteworthy that neither of both extracts shows activity on non-tumoral cancer line, suggesting that extracts from L. rivularis act selectively on tumor cells. Thus, these extracts could be considered as an interesting target for future action in vivo studies.

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SYNTHESIS OF TWO NEW ANANDAMIDE ANALYSES A P-HYDROXYBENZOIC ACID WITH POSSIBLE CAPACITY OF COUPLING TO CB1 BIOLOGICAL RECEPTORS AND MOLECULAR DOCKING STUDIES

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PPQM 02

The Medicinal Chemistry combines the knowledge of chemistry and pharmacology, among others, in order to propose molecules with biological activity, which serve as the standard for the development of new drugs. Nowadays, endocannabinoids constitute axes over any major part of the work of medical medicine, given their involvement in multiple physiological processes.

This project aims to design and synthesize new anandamide analogs with possible coupling of CB1 receptors from two starting reagents (gallic acid and P-hydroxybenzoic acid.) Recent studies have shown that these receptors have allo-galic binding sites that convert them into objects The research is based on the knowledge of the physiological functions of endocannabinoids, as well as on the work that has been reported on the coupling of Δ9-THC and anandamide to CB1 receptors. The proposed molecules are also based on the Molecular Pharmacology criteria, which do not indicate what type of biological activity the chemical groups are selected, and which product groups are provided.

These compounds were designed with Molecular Pharmacology criteria, and their ability to couple to CB1 receptors was optimized by molecular coupling techniques. For the synthesis of the compounds on different reactions such as the preparation of the Grignard reagent for the chain extension at the position of the initial carboxylic acid, the amidation and orthoacylation of the phenolic oxide. The control of the advantage of the reactions involved in the mentioned series is fixed using thin layer chromatography (TLC) and thereafter, the compounds are purified and applied to run the UV, IR, H-NMR and 13C-NMR and if necessary, MS, and determining the physical properties of each.

IDENTIFICATION OF POTENTIAL PANCREATIC LIPASE INHIBITORS BY STRUCTURE-BASED VIRTUAL SCREENING AND CONSENSUS SCORING FROM THE TRADITIONAL CHINESE MEDICINE DATABASE (TCM)

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PPQM 03

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Worldwide, the number of obese or overweight people has reached an incredible number of 2100 million people, which has then become a pandemic of the XXI century. Obesity is a risk factor to develop other illnesses such, hypertension, mellitus diabetes, cardiovascular diseases, dyslipidaemias and cancer, among others [1]. The enzyme pancreatic lipase (LP) is key for digestion of triglycerides, hence, it is a suitable target for the treatment of obesity. The inhibition of this enzyme avoids fat absorption into the body. Natural products are source of compounds with potential inhibitor activity for LP [2]. For instance, the Traditional Chinese Medicine database (TCM) contain thousands of chemical structures which have been isolated and identified from different natural sources.

In this work, structure-based virtual screening (SBVS) was performed in order to identify potential inhibitors of PL [3]. The TCM database was used as a source of natural products compounds and the LP 3D structure (PDB ID: 1LPB) was downloaded from the Protein Data Bank (PDB, http://www.rcsb.org). Three different molecular docking software (AutoDock 4.2, AutoDock Vina 1.1.2 y Dock6 v6.7) were utilised in order to identify compound with either high docking score or high binding energy into the LP catalytic site. The candidate compounds were selected by a consensus scoring method [4].

The five compounds with the top highest consensus score and different scaffold diversity were identified as ZINC04098621, ZINC85542831, ZINC85511097, ZINC27628528, ZINC1526032. The binding mode analysis of the top compounds into the catalytic site of LP show that all of them make hydrogen bond interactions with Ser152 and His263, residues involved in the catalytic triad. Another important interactions are π–π with Phe77 and Tyr 114 and, no less important, the multiple hydrophobic interactions with residues forming the hydrophobic pocket that drives and stabilize the carbon chain of the triglycerides during the hydrolysis process.

The compounds selected are expected to be active in *in vitro* assays against LP and serve to develop a pharmacophore model.

Keywords: Pancreatic lipase, Molecular docking, Obesity, TCM

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NOVEL ANTIFUNGAL STEROIDAL OXIMES

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PPQM 04

Most of the nitrogenous steroids possess interesting biological activities. Recently, some marine steroids have been isolated from marine sponges *Cinachyrella alloclada* and *C. apion.* From those species, two steroidal oximes were extracted [1] and their biological evaluation showed excellent inhibitory activity in several cancer cell lines (P-388, A-549, HT-29, MEL-28) [2]. Other synthesized steroidal derivatives acts as 5α-reductase inhibitors [3]. In this work, we report the synthesis of 4 new cholestane oximes, derived from diosgenin, and their antifungal activity. The synthetic route involved a regioselective opening of the diosgenin spiroketal using boron trifluoride etherate to obtain a 22-oxocholestane framework. Further oxidation produced an aldehyde group at C-26 position, and this compound was a key intermediary to access to oxime derivatives. The new steroidal oximes were evaluated in different strains of *Candida albicans.* Under low concentration of 0.2 mg/mL, the strain growth achieved 90% of inhibition.

The characterization of the steroidal compounds was carried out by physical and spectroscopic techniques.

Keywords: Steroids, Oximes, Antifungal Activity, *Candida albicans*

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ANTIOXIDANT AND CYTOTOXIC ACTIVITY OF FOUR FLAVONOIDS ISOLATED FROM LEAVES OF *Chromolaena tacotana* (Klatt) R.M. King & H. Rob.

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PPQM 05

Chromolaena tacotana is a species belonging to the Asteraceae family. This species has been used in the traditional medicine as an antineoplastic drug [1]. Previous chemical studies have reported the presence of flavonoids in extracts among other species of the same genus [2]. Furthermore in those studies it was observed a cytotoxic activity, of the compounds, on various cancer cell lines. In view of the above, here we isolated four flavonoids from the dichloromethane (CH2Cl2) extract of *Chromolaena tacotana* leaves. These compounds were extracted through column chromatography (Si gel G 60-200 microns 4x60cm) eluted with CHCl3, Mixtures of CHCl3:MeOH and MeOH). The compounds were identified as 3,5,4'-trihydroxy-7-methoxyflavone (named Ct1), 3,5,8-trihydroxy-7,4'dimethoxyflavone (named Ct2), 4',5-Dihydroxy-7- Methoxyflavanonol (named Ct3) and 5,7,3',4'-tetrahydroxy-3-methoxyflavone (named Ct4). Molecular structures were elucidated by spectroscopical methods: UV with displacement reagents and 1H-NMR, 13C-NMR 1D and 2D. In each flavonoid was evaluated its antioxidant activities by the methods DPPH? and ABTS?+ and the obtained values of IC50 were: for (Ct4) 2.51 mg / L; (Ct 2), and (Ct 1), 4.85 and 6.46 mg / L respectively, flavanonol Ct3) had no antioxidant activity. The cytotoxic activity of the flavonoids obtained from the leaves of Chromolaena tacotana were evaluated on cell lines A549, PC3, SiHa, MDA-MB-231 and MRC5 by the MTT method. According to the results, the Ct2 flavonoid showed the highest effect on the MDA-MB-231 cell line with IC50 values between 5 µg / mL and 15 µg / mL. Ct3 had its greatest effect on MRC5 with IC50 between 15 µg / mL and 30 µg / mL.Ct4 on MDA-MB-231 with IC50 between 17 µg / mL- 45 µg / mL. The Ct1 flavonoid had the lowest effect on tumor and non-tumor cells, with IC50 values between 39.266 µg / mL and 121.540 µg / mL.

Keywords. *Chromolaena tacotana*. Flavonoids, Antioxidant Activity, Cytotoxic Activity, Cancer Cell.

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STRUCTURAL ELUCIDATION AND ABSOLUTE CONFIGURATION STUDY OF LIGNANS ISOLATED FROM *Piper pseudochurumanyu* (Poepp ex Steud) AND *Piper subscutatum* (C.DC.)

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PPQM 06

The leaves of *Piper pseudochurumanyu* and *Piper subscutatum* were collected in a rain forest habitat in the Zamora Province-Ecuador, in 2007 and 2010, respectively. *P. subscutatum*, after drying, was extracted with ethyl acetate (EtOAc), followed by methanol (MeOH) and methanol-water (7:3). *P. pseudochurumanyu*, after drying, was extracted only with methanol. The fractionation of the EtOAc extract from leaves of *P. subscutatum* and the MeOH extract from leaves of *P. pseudochurumanyu*, afforded a crystalline compound named grandisin**.** X-ray diffraction and polarimetric experiments, performed on both crystalline compounds, showed that in the case of *P. subscutatum*, (-)-grandisin was obtained. In the case of P. *pseudochurumanyu*, the compound was racemic (±)-grandisin. The formation of this lignan in P. *pseudochurumanyu* is not stereoselective. From *P. subscutatum*, in addition to (-)-grandisin**,** four already know lignans were isolated:

- (-)-(*7S,8S,7'S,8'S*)-3',4'-methylenedioxy-3,4,5-trimethoxy-7,7'-epoxylignan1**,**
- (-)-(*7S,8S,7'S,8'S*)-3',4'-methylenedioxy-3,4,5,5'-tetramethoxy-7,7'-epoxylignan2,3,
- (-)-(*7S,8S,7'S,8'S*)-3,4,3',4'-dimethylenedioxy-5,5'-dimethoxy-7,7'-epoxylignan2**,**
- (-)-beilschminol B4.

The absolute configuration of these lignans was determined by circular dichroism experiments.

Keywords: *Piper subscutatum*, *Piper pseudochurumanyu*, Grandisin, *Lignans*, *X-Ray diffraction*.

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ANTIMICROBIAL ACTIVITY OF ESSENTIAL OILS AND ANTIBIOTICS ON MICROORGANISM OF IMPORTANCE IN BOVINE MASTITIS

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PPQM 07

Milk production in Colombia is a very competitive sector that ranks fourth place in Latin America, but requires the implementation of strategies that optimize its quality [1], aimed at reducing antibiotics traces and performing actions towards an organic production that guarantee its innocuity [2]. Specifically, for the case of bovine mastitis, *in vitro* studies have been carried out evaluating the antimicrobial activity of different essential oils showing interesting results as an alternative to conventional treatment [3,4]. Due to recurrence in cases of bovine mastitis and resistance to antibiotics, the *Staphylococcus spp* represents a greater interest as the main cause of chronic clinic mastitis, cases of recidivism and contagion [5].

The objective is to evaluate the antimicrobial activity of three essential oils and conventional antibiotics against isolated strains *Staphylococcus spp* of bovine mastitis and to find significant differences in the growth of these strains against the antimicrobial ones. The susceptibility of isolated strains of *Staphylococcus spp* (n = 80) was evaluated against essential oils of *Thymus vulgaris* (L), *Lippia Alba* (Mill) and *Aloysia citriodora* (L'He ' R.), as well as the antibiotics Oxacillin, Gentamicin, Clindamycin, Chloramphenicol, Amoxicillin, Enrofloxacin and Erythromycin by the *Kirby-Bauer* method. For statistical analysis, the sample size was calculated with GRANMO® 7.12 and the IBM SPSS statistical package was used. The growth inhibition diameter was measured against the essential oils and the descriptive statistic was calculated. From these values a sensitivity was defined for disks larger than 20 mm and resistance for disks smaller than this value.

The evaluated essential oils present antimicrobial activity with the following percentages of inhibition of strains: *Aloysia citriodora* (85%), *Thymus vulgaris* (83.5%) and *Lippia Alba* (50.6%). The highest sensitivity was presented against Chloramphenicol with 92.6% of sensitive strains, whereas the antibiotic in which the greater resistance of the Clindamycin was originated with a sensitivity in only 25% of the strains. For the other antibiotics the sensitivity was not conclusive: Amoxicillin with 50.1%, Enrofloxacin with 46% and Oxacillin with 60.1% of the strains.

It is concluded that there are significant differences in the sensitivity of the isolated strains compared to the essential oils of *Aloysia citriodora* and *Thymus vulgaris* showing an antimicrobial activity ($p < 0.05$), as well as a sensitivity of these strains against Chloramphenicol and a resistance to Clindamycin ($P < 0.05$).

Keywords: Bovine mastitis, antibiotic resistance, essential oils.

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Petiveria alliacea L. MEDICINAL REMEDY FOR ABDOMINAL PAIN

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Petiveria alliacea L., is a perennial herb which belongs to the family Phytolaccacea, is widely distributed in Mexico, mainly in the states of Yucatan, Chiapas, Campeche and Veracruz, commonly know as “hierba de zorrillo”, “mapurite” or “anamú”. In Veracruz the traditional healers use it as anti-spasmodic, anti-cancer, anti-inflammatory, wound healing and anti-amebic. Recent studies have shown its anti-amebic effect on the protozoan *Entamoeba histolytica* [1] due to its potential against this protozoan and to abdominal pain that is a symptom associated with this disease, which is one of the most frequent problems in medicinal practice and not there is an effective and harmless treatment for the people who suffer it [2], the need to seek new treatments arise, so, the aim of this work was evaluate the antinociceptive effect of *Petiveria alliacea*. The leaves were colected in Catemaco, Veracruz, Mexico, a herbarium specimen was deposited in the National Herbarium of Mexico (MEXU) with voucher number 1414464. For the extraction of the aqueous extract and methanol, the dried and crushed leaves were macerated in distilled water and methanol respectively. Subsequently the methanol extract was fractionated with n-hexane, ethyl acetate and methanol. The antinociceptive effect of the extracts and fractions were evaluated by “Writhing” model, male CD-1 mice were administered by oral dose of 30 mg/kg, the nociceptive behavior evaluated was the frequency of abdominal stretching performed every 5 minutes for 30 minutes. The pharmacological evaluation of the extracts and fractions showed a statistically significant antinociceptive effect with respect to the control (saline solution); however, the n-hexane fraction exhibited a higher activity, because reduces the number of abdominal stretches similary to the reference drug (ketorolac), for this reason, the extract was fractionated by column chromatography and a triterpene identified as isoarborinol, was isolated and purified, which showed statistically significant antinociceptive effect with respect to the control at doses 1, 10 y 30 mg/kg intraperitoneal, the latter dose showed better activity. The results obtained indicate that isoarborinol isolated from the leaves of *Petivera alliacea* is one of compounds responsible for antinociceptive activity.

Keywords: Antinociception, Isoarborinol, *Petiveria alliacea*, Chromatography

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IDENTIFICATION OF POTENTIAL PANCREATIC LIPASE INHIBITORS FROM *Piper* GENUS COMPOUNDS AND SOME OF THEIR DERIVATIVES USING COMPUTATIONAL METHODS

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PPQM 09

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Obesity is a chronic disease with a growing incidence in the last decades in both adult and child population. That is why recent research is focusing on mitigating its advance by the influence it has on other diseases, in the same category or even worse as diabetes [1]. The inhibition of the pancreatic lipase (PL) enzyme, responsible for hydrolyzing triglycerides in monoglycerides and free fatty acid, is the most common strategy to face it. Natural products is a source of compounds with potential inhibitor activity of LP [2]. For instance, compounds from *Piper nigrum* have activity on the reduction of blood lipid and lipoproteins levels by modulating the enzymes involved in lipid metabolism [3].

In the present work, a virtual screening was done at the catalytic site of PL in conjunction with an in-house library of 69 compounds from genus *Piper*, including some derivatives. The in-house library was created from all the investigation reports of our research group. Two different molecular docking software were used (AutoDock 4.2 and AutoDock Vina 1.1.2) and the LP 3D structure (PDB ID: 3LPB) was downloaded from the Protein Data Bank (PDB, http://www.rcsb.org). The potential *Piper* compounds were selected by a consensus method [4]. Pymol and Free Maestro® software were used for visualization and analysis.

It was found that the binding energies of the top consensus compounds are better than the crystallographic ligand and the drug used for the treatment of obesity, i.e. orlistat. It is worth to mention about the high scaffold diversity of the top consensus compounds. The most promising *Piper* compounds are: 24-ethylcholest-4,22-dien-3,6-dione and (E) -1- (4-fluorophenyl) -3- (3- (3- (nitrophenyl) acryloyl) -benzyl) -urea (ketoesteroid and chalcone, respectively); 5,7-dihydroxyflavanone (flavanone). All compounds bind into the catalytic site and make close contacts with catalytic triad residues (Ser152, Asp176 and His263). Considering that the active site of LP has abundant aromatic and polar residues, the most common molecular interactions are either π-π or hydrogen bond with Phe77.

Keywords: Obesity, Pancreatic lipase, Molecular docking, Natural products, Virtual screening.

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4-AMINOQUINOLINE-HEDERAGENIN BASED HYBRIDS: HEMISYNTHESIS OF POTENTIAL ANTI-MALARIAL AGENTS

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PPQM 10

Malaria is one of the greatest relevant infectious disease in our days, there were 0,7 million deaths a year, with 214 million people infected, mainly located in tropical and subtropical regions [1]. *Plasmodium falciparium* is the most virulent kind of malaria parasite [2].

The 4-aminoquinoline is the first choice to combat against malaria for decades of drug development labors. This pharmacophore is extensively used because has a well know clinical efficacy and low toxicity [3]. However lately strains has been found resistance to modern therapeutics in Cambodia, Southeast Asia, which has led to ignite the alarms of the global health organization system to seek alternatives to malaria treatment [2].

In the development of new therapeutic agents, it has been demonstrated that the making of hybrids of active substances is a valid and effective strategy to deal with resistant strains of different infectious diseases [3]. This methodology consists of linking two different substances that has a good reported activity and binding covalently them through linkers, improving the pharmacological properties of known drugs with multiple pharmacophores.

In our research used the antiprotozoal triterpenic acid hederagenin [4], which was coupled with a different series of 4-aminoquinoline analogues by linkers kind diamine alkanes; NH2-R-NH2, with R is a diverse length of a simple carbon chain. The synthesis of the hybrids is performed by means of an acid chloride formation on the hederagenin and making nucleophilic additions on the activated compound with the sequence of 4-aminoquinolines previously formed, obtaining a 4-aminoquinoline-hederagenin hybrid with a hydrolysable amide type linker.

The antiplasmodial activity in vitro of the compounds against strains FCR3 (cloroquine resistant) and citotoxical activity of HepG2 cell line were evaluated by radioisotopic methods. The 4-aminoquinoline-hederagenin hybrids obtained presents better activity than the native molecules, results of importance for its potential use against resistant strains.

Keywords: Antimalarial Hybrids, 4-Aminoquinoline, Hederagenin, Malaria , *Plasmodium falciparium.*

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CHARACTERIZATION BY MEANS OF GAS CHROMATOGRAPHY / MASS SPECTROMETRY (GC / MS) AND EVALUATION OF THE ANTIBACTERIAL ACTIVITY OF THE ESSENTIAL OIL OF THE BARK FROM *Astronium graveolens*

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Astronium graveolens is abundant arboreal specie in the mounts of Maria, on the Caribbean coast of Colombia; it has traditionally been for diseases such as diarrhea and inflammation. In recent years it has been given a pharmacological approach given that the essential oil of its aerial parts is rich in monoterpenes and sesquiterpenes that have reported antibacterial, antifungal activity etc, among these compounds we have β-Caryophyllene and Germacreno D [1]. One of the major health problems at present is resistance which presents great diversity of bacteria both Gram positive and Gram negative compared to the wide range of existing medications. In addition the toxicity of some of these drugs is potentially serious and its occurrence is unacceptable if the patient did not need the drug [2]. Due to this, it is sought using different pharmaceutical strategies that products of topical use of organic type or that in their formulation contain products of natural origin generate less bacterial resistance and greater benefit for the patient. Colombia is one of the most biodiverse countries in the world; among the genera that exist in our territory we have the genus *Astronium*. Literature reports that the extracts and oils of the leaves of these plants are rich in compounds such as terpenes, sesquiterpenes and monoterpenes [3]. These have been reported to have biological activities against bacteria, most of which are highly positive in the genera *Staphylococcus* and *Enterococcus*, reporting even greater activity than some antibiotics known in the market. The methodology used consisted, first of all in collecting of plant material, the bark was obtained from the *Astronium* tree collected in the mounts of Maria, Bolívar-Colombia, then it was chopped and washed with distilled water, then, the essential oil was obtained by the microwave assisted hydrodistillation method. The radiation time is 1 hour and a half, performing 3 cycles of half an hour to complete an extraction. The equipment used for the analysis by gas chromatography / Mass Spectrometer was an Agilent technologies 7890A GC System, column: 30m x 250mm x o,25mm, conditions: flow: 1,2mL/min, pressure: 14,493 psi, temperature: initial 50°C, maximum 325°C. Finally the essential oil was evaluated against strains of *Strafilococcus* sp. The results for the analysis of the essential oil were 56 chromatographic peaks corresponding to different compounds detected by the equipment. From this set, the most important ones were selected, taking into account the parameters of area under the curve percentage (% ABC) and similarity. Obtaining Caryophyllene (11, 46%), Germacrene D (13,80%) and γ-Muurolene (5,33%) as major compounds. These substances are known for their antibacterial activity [1]. The essential oil presents promissory antibacterial activity against *Strafilococcus* sp.

Keywords: Gas chromatography, Antibacterial activity, Essential oil, Terpenes.

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CHLOROFORMIC FRACTION ENRICHED IN DITERPENES FROM *Ageratina vacciniaefolia* EXHIBITS A HIGH ANTIINFLAMMATORY ACTIVITY IN AN ANIMAL MODEL

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PPQM 12

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Inflammation is a complex process that can be induced by physical damage, chemical precursors, microbial invasion, primary immune response or by combination of these. The study of medicinal flora allows the search for new therapeutic alternatives for the treatment of inflammation. Among these species are those belonging to the genus *Ageratina* (Asteraceae), a genus widely distributed in Central and South America. In the present study the antiinflammatory activity of extracts obtained from the aerial parts of *Ageratina vacciniaefolia* (Benth.) R.M.King & H.Rob.was evaluated *in vivo*. *A. vacciniaefolia* (leaves, stems and flowers) was collected in Páramo de Cruz Verde, Cundinamarca, Colombia. The plant was dried, ground and extracted with ethanol by Soxhlet, after the ethanolic extract was fractionated with solvents of different polarity. The treatments were evaluated using female albino Swiss Wistar rats, in a λ-carrageenan-induced edema model. The ethanolic extract, the low polarity fractions (chloroform -Cav - and ethyl ether - EEAv) and the hydroalcoholic residue (HAv) inhibited inflammation during the first hour of experimentation with percentages greater than 60%, however, only with the Fractions CAv and EEAv remained the effect during the 7 h evaluation. These results were confirmed by histopathological analysis by evaluating edema, vascular response and cellular infiltrate versus controls. In the CAv fraction, four diterpenes derived from dihydroxykaur-16-en-19-oic acid and its β-D-glucopyranosyl ester, were identified by HPLC-DAD-MS analysis. The CAV fraction had the highest percentages of inhibition of inflammation over the follow-up period (68.94%) associated with a histopathological profile with moderate edema and cellular infiltrate and incipient vascular response. The dihydroxykaur-16-en-19-oic acid derivatives, identified in the CAv fraction may be responsible for the anti-inflammatory activity.

Keywords: Inflammation, Carrageenan, *Ageratina vacciniaefolia*, Plants, Medicinal.

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CHEMICAL ANALYSIS AQUEOUS, METHANOLIC AND HEXANIC EXTRACTS OF *Jathropha dioica* ROOT

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PPQM 13

The study of medicinal plants, in order to demonstrate their therapeutic effects designated by tradition for the treatment of diseases, in many cases has been very useful for the development of new pharmaceutical products. *Jatropha dioica*, also known in Spanish as Sangre de Drago is endemic in different areas of Hidalgo State, México. It has been used for many ailments such as periodontal disease, hair loss, skin infections and cancer, but there is little evidence about its chemical composition.

Aqueous, hexanic and methanolic extracts from the root of *Jatropha dioica*, were analysed by Dragendorff test. In all the extracts was demonstrated the presence of alkaloids that can be related with some physiological activities as has been reported previously in other species of *Jatropha* by Can and Villareal [1,2].

The yield of hexanic extract was the most abundant followed for methanolic one. This fact indicates that not polar compounds are the main chemicals presents in the root. In a quantitative analysis of yield, hexanic extract, tripleted the amount when compared with the aqueous extract.

Fractions of the aqueous extract from the root of *Jatropha dioica* were obtained by column chromatography. The solid fraction eluted with the polarity 80:20 hexane:ethyl acetate were analyzed by 1H-NMR and 13C-NMR. The NMR showed multiple signals for this fraction which corresponds to a tricyclic diterpene structure that was previously described as citlalitrione [3]. In the methanolic extract we obtained a solid compound on fractions named 115-121. The spectrum for 1H-NMR and 13C-NMR founded for these fractions corresponds to a polioxigenated compound characteristic of a disaccharide not reported at literature. In a comparative test versus Eberhard Breitmainer and Wolfgang Voelter data [4] this compound appear to correspond to a sucrose or cellobiose. The fraction 89 of methanolic extract was distinguishable by many signals detected in 1H-NMR and 13C-NMR, they match for a sesquiterpene with some methyl branches united to de basic structure, which has not been yet elucidated.

In conclusion *Jatropha dioica* has many chemical compounds with a potential effects in health based on the partial results of this study.

Keywords: *Jattropha dioica*, Citlalitrlione, Column chromatography, Extracts

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SYNTHESIS AND TRYPANOCIDE ACTIVITY OF CHLORO AND BROMO L-TYROSINE DERIVATIVES

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PPQM 14

Chagas disease is a parasitemia caused by *Trypanosoma cruzi*, one of the major health problems in the Americas, with incidence around 21 countries in the region. Reports from the WHO estimate that there are approximately 6 to 7 million people infected around the world, were American continent has the highest percentage of infection. Annual cases increase in the region is approximately 56,000, leading to an average of 12,000 deaths annually [1].

Chemotherapeutic options for the control and treatment of these protozoa infections, are limited to few drugs, which in many cases are associated with severe toxicity and variable efficiency [2]. These options, associated with emerging resistance against current drugs, encourage the discovery and development of new, safer and more effective anti-protozoal agents. Bromotyrosines are L-tyrosine derivatives isolated from marine sponges of *Verongida* genus with selective trypanocide activity [3]. In this work, it reported synthesis of twenty-two Bromo and Chloro derivatives with different *N*-methylation levels of L-tyrosine and its anti-protozoal and cytotoxic evaluations *in vitro*.

Compounds 2, 9, 11-13, 20 and 21 were the most active against *T. cruzi.* Compounds 7, 13 and 18 had the highest SI (Selectivity index), determinated by LD50/ED50, where compound 20 is the most selective against *T. cruzi*. It results can be considered very significant such as trypanoside agents.

Keywords: Trypanocide, L-tyrosine derivatives, Chagas desease

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STUDY AND ANALYSIS OF CHEMICAL COMPOSITION AND CYTOTOXIC ACTIVITY OF CHLOROFORM EXTRACT *Guaiacum sanctum* LEAVES

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PPQM 15

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The goal of this study is to detect potential sources of cytotoxic and antitumor compounds from endemic and native plants of Puerto Rico. In a preliminary study, other species of this genus, known as *Guaiacum officinale*, were analyzed. The chloroform and ethyl acetate extracts showed strong activity with values below 10µg/mL of lethality against *Artemia salina* and growth inhibition of breast cancer cell lines [1]. Due to these results, the study with another species known as *Guaiacum sanctum* in order to isolate compounds with biological activity against cancer cells was performed. The leaves were collected, dried and extracted with a mixture of CH2Cl2-MeOH **(1:1).** The resulting crude extract was suspended in water and extracted with solvents of different polarities. The cytotoxic activity of all extracts were tested against different cell lines derived from solid tumors including ovarian (A2780, SKOV3), breast (MCF-7, MDA-MB-435), prostate (PC-3, LNCAP), and mammary epithelial cells (MCF-10A). Additionally, the chloroform extract was purified using column chromatography in order to isolate the active compounds.

Keywords: Puerto Rican plants, column chromatography, antitumor activity

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EVALUATION OF NEUROPROTECTIVE EFFECT OF METHANOL EXTRACT OF *Tovomita guianensis* (Clusiaceae) AGAINST ROTENONE-INDUCED TOXICITY OVER *Drosophila melanogaster*

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PPQM 16

Drosophila melanogaster has been widely used in pathogenesis studies of Parkinson's disease and in the discovery of new strategies in the treatment of neurodegenerative diseases. On the other hand, therapeutic properties of natural products have been investigated in different plant and animal models and the results derived from such studies have served as the basis for development of new drugs [1].

Previous studies performed at the Biotechnology – Natural Products Laboratory ascribed to the Universidad Tecnológica de Pereira reports that methanol extract of *Tovomita guianensis* belonging to *Clusiaceae* possess strong antioxidant capacity [2]. Based on that, the aim of this study was to evaluate the neuroprotective effect of methanol extract of such specie over *in vivo* model of *Drosophila melanogaster*.

The methanol extract was obtained through maceration and phytochemical characterization was performed by thin layer chromatography and HPLC techniques. Additionally, modulation effect of the mentioned extract was evaluated by supplementing the *D. melanogaster* food at concentrations of 0.05, 0.1 and 0.2%. Negative geotaxis was used in order to evaluate locomotive modulation capacity of two populations (males and females), showing a locomotion effect at concentrations of 0.2 and 0.1% for females and males, respectively. Also neuroprotective effect against rotenone-induced toxicity over *D. melanogaster*, thus, contributing towards bioprospection of plants belonging to coffee eco-region and to the use of the Colombian biodiversity.

Keywords: Neurodegenerative Diseases, Antioxidant, Neuroprotection, Bioprospection.

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SYNTHETIC DERIVATIVES OF THE DUBAMINE ALKALOID AS POTENTIAL ANTIBACTERIAL AGENTS

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PPQM 17

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The family of the Rutaceae is one of the most studied, due to the large number of alkaloids that they have already provided and the importance of them, in 1962 was isolated from the species Haplopillum Dubium (Rutaceae) the quinoline alkaloid known as Dubamine (2-(benzo[d][1,3]dioxol-5-yl)quinoline) (I) [1], which showed relevant antimicrobial activity. Although many strategies are known for the synthesis of this system employing coupling reactions, catalysed by different metals [2], these do not allow the (tetrahydro)quinoline (THQ) system functionalization previously synthesized.

The synthesis of new THQ derivatives of Dubamine analogues was performed using the multicomponent imino-Diels-Alder (iDA) methodology [3] and their antibacterial activity was evaluated against the following strains: Methicillin resistant *Staphylococcus aureus* (SAMr) ATCC 43300, *Klebsiella pneumoniae* ATCC 1705, *Staphylococcus aureus* wild type ATCC 25923, *Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 27853, *Enterococcus faecalis* ATCC 27853. The inhibition percentage obtained suggests promissory antibacterial activities of the analysed compounds specially against the Methicillin resistant *Sthaphilococcus aereus* and *Klebsiella pneumoniae* strain.

Keywords: Dubamine, imine-Diels-Alder, tetrahydroquinoline, Antibacterial activity.

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PEQUI OIL NANOEMULSIONS: PHISICO-CHEMICAL CHARACTERIZATION AND EVALUATION OF THEIR EFFECTS ON NORMAL AND TUMORAL BREAST CELLS, IN VITRO.

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Oil obtained from the pequi fruit (*Caryocar brasiliense*), representative of the Brazilian Cerrado biome, contains vitamins, fatty acids, phenolic compounds, and other biomolecules with antioxidant properties. Breast cancer is the most diagnosed and leading cause of cancer death among women in the world. Its treatment involves varied adverse effects affecting the quality of life of the patient and making it necessary to search for alternative and complementary therapies. Therefore, the aim of the present work was to develop and characterize pequi oil nanoemulsions as well as to evaluate their effects on mammary carcinoma cells (MCF-7) and healthy mammary epithelial cells (MCF-10A), *in vitro*. It was possible to characterize physico-chemically the pequi oil nanoemulsions coated or not with chitosan polymers, which presented hydrodynamic diameters >200 nm and PDI >0.25. Moreover, they were stable for 120 days after storage at 4°C. Cell viability was tested by incubating cells with 90, 180 or 360 µg/mL of nanoemulsions without chitosan (NE-) as well as with chitosan (NE + CH). The viability of MCF-7 cells demonstrated a reduction of 46% and 39% after 24 and 72 hours of treatment in the highest concentration, respectively. In contrast, no significant reduction in cell viability of healthy mammary epithelial cells was observed ($p<0.05$) even in the highest concentration suggesting selectivity of this nanoemultions against tumoral . Gene expression studies are under evaluation in order to better understand the mechanisms involved in cell viability reduction of MCF-7 cells.

Keywords: Nanomedicine, Antineoplastic Agents, Breast Carcinoma *In Situ*, Plant Oils.

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EVALUATION OF THE ANTINOCICEPTIVE EFFECT OF THE ETHYL ACETATE EXTRACT OF *Salvia circinata* CAV.

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Salvia circinata Cav. (Lamiaceae) is an endemic species of Mexico, commonly known as “bretónica”, it is widely used as an herbal remedy in tradicional medicine of Santiago Huauclilla, Oaxaca, for diseases of the gastrointestinal tract involving pain. The aim of the present study was to evaluate the antinociceptive activity of ethyl acetate extract of *Salvia circinata* and an active metabolite in a murine model of abdominal pain. The extract was obtained by maceration of aerial parts, previously degreased with n-hexane. The ethyl acetate extract was partitioned using three solvents of increasing polarity (n-hexane, ethyl acetate and methanol). The pharmacological evaluation was performed in the writhing test using male CD-1 mice. Animals were intraperitoneally (i.p.) administrated with the crude extract at doses of 1, 10, 30, 100 and 300 mg/kg; the isolated compound at 1, 5 and 10 mg/kg, i.p. and the reference drug (ketorolac, 1 mg/kg, i.p.). The fractionation of the ethyl acetate extract was performed by chromatographic column (CC), the identification of metabolites was done by high performance liquid chromatography (HPLC). The isolated pure compound was identified by H1-NMR. Results of the antinociceptive effect of the *Salvia circinata* crude extract showed a significant activity in a non dose-dependent manner in comparison with control. After HPLC profile of *Salvia circinata*, several bioactive compounds with recognized antinociceptive and anti-inflammatory activity were identified as follows: ursolic acid, β-amirine, oleanolic acid, ferulic acid, chlorogenic acid, caffeic acid, rutin, quercetin and florizine. The CC of the ethyl acetate fraction allowed the isolation of pure amarisolide, a diterpene that inhibited nociception for more than 50% at a dosage of 1 mg/kg. Our results give evidence of the potential of *Salvia circinata* and amarisolide for the treatment of abdominal pain.

Keywords: *Salvia circinata*, Amarisolide, Antinociceptive

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STRUCTURE-BASED VIRTUAL SCREENING OF AN IN-HOUSE ALKALOID COMPOUND LIBRARY TO IDENTIFY POTENTIAL ACETYLCHOLINESTERASE (ACHE) INHIBITORS

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Alzheimer's disease (AD) is a chronic neurodegenerative and irreversible disease that which usually starts slowly and gets worse over time. AD is the most common cause of dementia (60 % to 70 %). The AD early symptom is short-term memory loss and is the fourth leading cause of death in older adults worldwide. The current and standard medicines are based on the cholinergic hypothesis, which states that AD is caused by a deficiency of the neurotransmitter acetylcholine [1]. The acetylcholinesterase inhibitors reduce the rate at which the acetylcholinesterase (AChE) enzyme catalyzes the breakdown of acetylcholine, therefore AChE is one of the targets to face the AD. Natural products compounds have been an important source of bioactive compounds and have shown a widespread window of biological activities [2]. For instance, the sesquiterpene alkaloid huperzine, isolated from *Huperzia reflexa*, is a potent inhibitor of AChE [3].

In this work, we created an in-house alkaloid compound library (75 alkaloid compounds) generated from all the investigation reports of our research group and carried out a structure-based virtual screening (SBVS) against AChE to identify potential alkaloid inhibitors. All the alkaloids used in the library belong to the families Rutaceae, Lauraceae, Magnoliaceae and Solanaceae. The AChE 3D structure (PDB ID: 4M0E) was downloaded from the Protein Data Bank (PDB). Two different molecular docking software (AutoDock 4.2, AutoDock Vina 1.1.2) were used to carry out a SBVS and the alkaloid compounds, with high *in-silico* affinity to the binding site of AChE, were selected by a consensus scoring method [4]. Pymol and Free Maestro® software were used for visualization and analysis.

Results from the SBVS and the consensus scoring show that alkaloids compounds bind next to the catalytic site, blocking the entrance of acetylcholine. The four-top alkaloids with different scaffolds are sanginarine, rutaecarpine, (S)-3-methoxy-nordomesticine and N-methyl-benzofuran (2,3-b)quinolin-4(1H)-one. The main molecular interactions are: π-π with Tyr124, Trp286 and Tyr341; cation-π with Tyr341; and hydrogen bonds with Ser293 and Thr75. It is expected that those compounds show *in-vitro* activity in further studies.

Keywords: Alzheimer disease, Acetylcholinesterase (AChE), Molecular docking, Virtual screening.

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LEISHMANICIDAL AND CITOTOXIC ACTIVITY OF BENZOTHIOPYRANS. STRUCTURE-ACTIVITY RELATIONSHIP

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Leishmaniasis is a series of anthropozoonotic diseases; it is caused by parasites of the genus *Leishmania* and transmitted through the bite of female insects of the genus *Phlebotomus* and *Lutzomyia* [1]. According to the World Health Organization (WHO) [2] Colombia is one of the three countries with the highest occurrence of leishmaniasis. Although in the majority of cases does not become deadly the disease produce severe lesions in skin that significantly decrease the quality of life to whom suffer from it. In Colombia the treatment for leishmaniasis is performed mainly with pentavalent antimonials [3,4], which by their side effects generate a low adhesion of the patients to the treatment, also these pentavalent antimonials due to its high toxicity cannot be used in pregnant women or in patients with cardiac, liver, kidney or pancreatic issues. These problems highlight the needs of search for alternatives treatments for leishmaniasis that may have different mechanisms of action. In our recent work the benzothiopyran core (thiochroman) [5,6] was explored as a potential source of leishmanicidal agents, during our research more than 80 compounds with structural changes in different parts of the benzothiopyran moiety were obtained; the leishmanicidal and toxicity activity were tested with EC50 values lower than 10 µM and low citotoxicity which led to selective index higher than 100, even better than the Amphotericin B. Herein we report the Structure-Activity Relationships and recognized that the α-β-unsaturated moiety is key for the maximization of the antileishmanial activity.

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Keywords: Leishmaniasis, Benzothiopyran, Thiochroman, Structure-Activity Relationship.

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CHEMICAL COMPOSITION, ANTIOXIDANT ACTIVITY, ANTIMICROBIAL AND ANTIPROTOZOAL PROPERTIES OF ETHANOL PROPOLIS EXTRACTS OF BOLIVIA

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Propolis has important pharmacological properties and because of its broad spectrum of biological activities and uses in health food as well as in folk medicine, there is a renewed interest in the composition of propolis and its biological activities. In Bolivia, propolis alcohol extract is popular as a homemade remedy in Bolivian Traditional Medicine as an antimicrobial agent to treat respiratory illnesses, skin and gastric infections. The antimicrobial activity of two Bolivian propolis ethanolic extracts was tested against ten bacterial strains, both pathogenic and non-pathogenic. Both extracts ECEPCC and ECEPNC showed a higher inhibition in the disc diffusion assay inhibiting only to the strains *Staphylococcus aureus* ATCC 25923 (sensible) and *Staphylococcus aureus* ATCC 29213 (resistant) and no other tested strains of bacteria were susceptible. The antioxidant activity of the propolis ethanolic extracts EEPCC and EEPNC was measured using ABTS, DPPH and FC in vitro assays. Both propolis were able to act against ABTS, DPPH radical, and FC reagent. Because LC50 of the two propolis was lower than 100 mg/mL, they can be considered as highly cytotoxic. According to the results, the two propolis have good IS in *P. falciparum.* ECEPNC has good IS against *L. panamensis*. In sample ECEPNC were identified Kaempferol 3-methyl ether, Quercetin dimethyl ether, Kaempferol 7-*O*-methyl ether and ellagic acid methyl ether and in sample PCC were identified 3-Phenyl-4-methoxy cinnamic acid, Kaempferol dimethyl ether, Pinobanksin methyl ether, Kaempferol 7-*O*-methyl ether and Quercetin.

Keywords: Propolis, Antibacterial, Antioxidant, Antiparasite.

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LEISHMANICIDAL ACTIVITY AND CYTOTOXICITY IN VITRO OF STYRYLQUINOLINES

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Leishmaniasis is an infectious disease caused by a flagellate protozoan of the genus Leishmania, transmitted by the bite of a hematophagous insect. This disease is distributed worldwide in tropical and subtropical areas, such as South America, Africa, part of Europe and Asia; and is endemic in almost all Colombian territory. It is estimated that in the country there are about 11 million people at risk of contracting this disease [1].

In the search for new therapeutic alternatives in the treatment of infectious diseases, we have highlighted the discovery of organic molecules with a quinoline nucleus of natural and synthetic origin; Which are currently part of many active ingredients of a large number of medicines; Such as quinine, an alkaloid isolated from the bark of a quina tree Rubiaceae; Was employed for a long time in the treatment of malaria; Chloroquine and amodiaquine as antimalarial drugs and sitamaquine a synthetic drug used to treat leishmaniasis [1].

Recently quinolines have been developed by organic synthesis in order to find new alternatives for the treatment of leishmaniasis, because the parasite has created chemo-resistance to the drugs that are currently used in addition to the adverse effects that cause over the patient [2]. In the present work, quinoline analogs were synthesized by the Perkin type condensation reaction and their leishmanicidal potential and in vitro cytotoxicity were evaluated.

The synthesis of the styrylquinolines was performed from hydroxyquinaldine and aromatic aldehydes; the structures of the synthesis products were corroborated by one and two-dimensional NMR spectroscopic analyzes.The leishmanicidal activity of the synthesized compounds was evaluated against intracellular amastigotes of the Leishmania (Viannia) panamensis strain UA140-pIReGFP and cytotoxicity was determined using the MTT enzymatic micromethod on the U-937 cell line in vitro, having as reference Amphotericin B [4]. Four styrylquinolines were obtained: 2-[(E)-2-(3-methoxyphenyl)ethenyl] quinoline (Q1), 2-[(E)-2-(4- methoxyphenyl)ethenyl] quinoline (Q2), 2-[(E)-2-(4-methoxyphenyl)ethenyl] quinolin -8-ol (Q3), 2-[(E)-2-(2-acetyloxy-5-nitrophenyl)ethenyl] quinoline (Q4). The compound Q4 showed activity against intracellular amastigotes (EC50 = 2.50 ?g/ml) and moderate cytotoxicity (LC50 = 5.90 ?g/ml), in addition a remarkable leishmanicidal activity, which is reflected in its selectivity index (IS) of 2.4, taking into account this result, it is recommended to determine leishmanicidal potential in vivo to validate its therapeutic potential for the treatment of leishmaniasis.

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ANTILEISHMANIAL ACTIVITY OF RICH FRACTIONS IN ALKALOID AND FLAVONOID TO DESIGN AND DEVELOP A NEW LOW COST TOPICAL PHYTOMEDICINE PRODUCT FROM MEDICINAL PLANTS IN THE NORTHERN COAST OF COLOMBIA

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Products derived from medicinal plants have an important role in the treatment of some neglected tropical diseases [1]. In the Northern Colombian Coast, communities from endemic areas depend of popular and traditional treatments to heal some symptoms of these diseases. Consequently, new strategies to transform the popular knowledge into a tangible and secure product for the communities is particularly relevant nowadays [2].

This study evaluated the antileishmanial activity of rich fractions in alkaloid and flavonoid from *Cordia dentata* Poir (Cd) and *Heliotropium indicum* Linn (Hi) to design and develop a new low cost topic phytomedicine from medicinal plants in the Northern Colombian Coast. *Hi* and *Cd* were collected using structured interviews and through observations and conversations with local communities and a total of 500 participants from south of Bolivar were involved.

This study aims to evaluate in vitro cytotoxic activity on human promonocytic cell line U937 and leishmanicidal activity against intracellular amastigotes of *Leishmania* (V) *panamensis* (MHOM/CO/87/UA140-EpiR-GFP strain), as positive controls were used Doxorubicin and Amphotericin B. In the preformulation stage were studied the physicochemical and microbiological properties of the excipients and active fractions with the best EC50 and SI values. Samples were prepared based on the best formulation, where stability studies were realized during six months using accelerated temperature of 40 ± 3 °C and environment temperature of 30 ± 3 °C with 70 % ± 5 of relative humid.

Results were expressed as fifty cytotoxic concentrations (CC50), concentration necessary to kill 50% of cells, and fifty effective concentrations (EC50) calculated by Probit analysis (Parametric method of linear regression that permits doses-response analysis); it was similarly determined the Selectivity Index (SI). *H. indicum* and *C. dentata* fractions against cell line U937 were cytotoxic with a concentration of 131.58 ± 9.9 µg/mL and 425.53 ± 24.4 µg/mL. Besides, the fractions got a good result in the inhibition of intracellular amastigotes growth, with an effective concentration of 26.61 ± 5.3 µg/mL and 67.26 ± 34.3 µg/mL. The selectivity index of the acid fraction from Hi was 4.94 while the SI of the alkaloid rich fraction was 6.33. In these preformulation and formulation studies were achieved to get two products with HI which showed good physical, chemical, and microbiology stability. Two stables and low cost formulations were got using nitrogenous fractions from HI, which are going to be evaluated i*n vivo* against murine models infected with *Leishmania panamensis* amastigotes.These results contribute to search new therapeutic agents to treat Leishmaniasis disease, basically in the cutaneous form. These studies also reaffirm that the natural resources could be an important option to increase the current treatment. This Research was supported by a grants from the University of Cartagena and Colciencias-Colombia, Project No. 512-2012.

Keywords: Alkaloids, Flavonoids, Leishmaniasis, Phytomedicine, folk medical.

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TWO FLAVONOIDS ISOLATED FROM *Conyza trihecatactis* EXHIBIT HIGH SPECIFIC CYTOTOXIC EFFECT ON HUMAN BREAST ADENOCARCINOMA CELL LINE (MCF-7)

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For the evaluation of the cytotoxic activity of the species *Conyza trihecatactis* and *Ageratina vacciniae-folia* (Asteareaceae), from the aerial parts of the species the complete ethanolic extracts and fractions were obtained with solvents in order of increasing polarity. The evaluation of the cytotoxic activity was performed by the MTT method on tumor cell lines of human and murine breast cancer, and additionally, on a line non-tumorigenic fibroblast of murine origin. The dichloromethane fraction of *C. trihecatactis* (CD) showed the highest cytotoxic activity with an IC50 of 36,23 µg/mL for 4T1, 47,81 µg/mL for TSA, 46,05 µg/mL for MCF-7 and 70,67 µg/mL in 3T3 fibroblasts. From this fraction a mixture of flavonoids (CMF) was obtained, identi-fied as apigenin and hispidulina, which presented a marked cytotoxic effect on MCF-7 with an IC50 of 23,50 µg/mL. Fractions obtained from *A. vacciniaefolia* showed IC50 greater than 150 µg/mL on the tumoral cell lines evaluated and greater than 180 µg/mL on line 3T3 fibroblast. In the chloroform fraction from *A. vac-ciniaefolia* (AC) four terpenoid compounds were identified, which showed similarity in the retention time (tret) and the mass spectrum, comparing to the compounds isolated and determined in other studies for this species.

Keywords: Cytotoxicity, HPLC-MS, Flavonoids, Breast Cancer.

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ANTI-DERMATOMYCOSIS POTENTIAL OF ESSENTIAL OILS EXTRACTED FROM ECUADORIAN ENDEMIC MEDICINAL SPECIES: *Ocotea quixos, Clinopodium nubigenum, Piperomia inaequifolia* AND *Psidium guayava*

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This study was carried out to characterize chemical components by Gas chromatography-Mass spectrometry (GC-MS) of essential oils extracted from four endemic plants of Ecuador (*Ocotea quixos, Clinopodium nubigenum, Piperomia inaequifolia* and *Psidium guayava*) in order to evaluate its biological antifungal activities, against dermatomycosis causative dermatophytes fungi (*Trichophyton rubrum*, *Trichophyton mentagrophytes*, *Microsporum canis*) and cutaneous candidiasis yeasts (*Candida tropicalis*, *Candida albicans*). It was tested the minimal inhibitory concentration (MIC) *in vitro* following disk diffusion method. Then the essential oils were incorporated in cosmetic formulations (creams) and efficacy evaluation were measure by statistical analysis and MIC. Cromatographic results revealed that essential oils from these plants possess interesting chemical-toxicological profiles: *O. quixos* (trans-cinnamaldehyde >25%), *C. nubigenum* (carvacrol acetate >40%), *P. inaequifolia* (myristicin >50%) and *P. guayava* (limonene >25%) as the majority compounds. The antifungal activities were expressed in a high inhibition capacity over the fungal growth, being *O. quixos* (bark) essential oil and formulations which showed the most significative biological activity compared to the natural referent *T. vulgaris*, fluconazole and nystatin as positive controls, denoting a promising medicinal potential.

Keywords: *Ocotea quixos, Clinopodium nubigenum, Piperomia inaequifolia*, *Psidium guayaba*, GC-MS, dermatomycosis fungi, MIC, cosmetic formulation.

POTENTIAL ALPHA-AMYLASE INHIBITORS BY STRUCTURE-BASED VIRTUAL SCREENING FROM AN IN-HOUSE *Piper´*s NATURAL COMPOUND LIBRARY

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PPQM 27

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Diabetes type 2 (DTII) is a metabolic disorder characterized by high blood sugar, insulin resistance and relative low insulin levels. The common symptoms are increased thirst, frequent urination, and weight loss. This disease is considered by the OMS as a non-communicable epidemic which affects more than 415 million people worldwide and the cost to health systems is about US$ 825 billion annually. DTII along with obesity and cardiovascular diseases are the sixth leading cause of worldwide disability [1]. Alpha-amylase (α-amylase, αA) enzyme catalyses the hydrolysis of starch into sugar (disaccharides and trisaccharides) which are subsequently converted to glucose by other enzymes into the body. Therefore, αA is one of the therapeutic targets for decreasing the absorption of monochaccarides in the intestine. The search of natural or synthetic compounds that may inhibit the αA enzyme is a common strategy to face diabetes [2]. Some reports have shown that ethanolic and aqueous extracts of Piper nigrum (belonging to the Piperacea family) considerably decrease the activity of αA [3,4]. In this work, an in-house library of 68 natural compounds, belonging to genus *Piper*, was created from all the investigation reports of our research group. Then, a structural-based virtual screening was carried out in order to identify molecules with high affinity into the αA catalytic site. The αA 3D structure (PDB ID: 4GQR) was downloaded from the Protein Data Bank (PDB, http://www.rcsb.org). AutoDock 4.2 and AutoDock Vina 1.1.2 software were used to survey the binding affinity of the potential active compounds. The compounds were ranked by a consensus score method [5] and the top four compound with highest consensus score and different scaffolds were selected and analyzed. The binding modes were analyzed by using Pymol and Free Maestro® software.

About ten compounds were found with better binding affinity than the crystallographic compound myrecitin, which was taken as cutoff reference. The top four compounds with highest consensus score and different scaffolds (24-ethylcholesta-4,22-diene-3,6-dione; cumanensic acid; 3,5,7-triacetyl-flavone and 5-acetoxy-7-methoxyflavone) make hydrogen bond with Asn298, Ile235, Lys200, Trp59 and Arg195 residues. Other important interactions are π–π with His201, Trp58 and Trp59. Some of this molecular interactions are the same shown by myrecitin. The selected compounds are expected to be active in *in vitro* assays against the αA enzyme.

Keywords: α-amylase, Diabetes type II, Molecular docking, Virtual screening, Piperaceae,

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SYNTHESIS, LEISHMANICIDAL ACTIVITY AND CHIRAL RESOLUTION OF 4-OXOTHIOCHROMANE-2-CARBOXYLIC ACID AND ITS ESTERS AND AMIDES DERIVATIVES

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PPQM 28

Chromones are an abundant group of natural compounds which occur mainly in *Rutaceae, Asteraceae, Liliaceae, Piperaceae, and Clusiaceae* families, they display a wide range of biological activities and are frequently used as scaffold from drug design and development [1,2]. On the other hand, the sulfur analogues of chromones, the thiochromones or benzothiopyranes are absent in nature, however, this isosteric changes are frequently used in drug design to obtain compounds with higher activity or with better physicochemical properties, from a bioisosteric point of view the oxygen-sulfur interchange could led to important changes in the biological activities, there with the change in the oxidation state of sulfur atom, implies change in the polarity or membrane affinity [3]. Recent works suggest that compounds with the thiochroman core could be an important scaffold to be studied in the search for novel therapeutic targets against *Leishmania* parasites [4,5]. According to reports from the World Health Organization, 12 million people worldwide are affected [6]. Currently there are only few drugs to deal with this public health problematic, among the many difficulties, can be highlighted for example: availability, cost and resistance [7], which demonstrates the need for the development of new leishmanicidal drugs with novel mechanism of action. In the search for new leishmanicidal compounds our efforts are focused on the thiochromane derivatives as part of the molecular optimization process. Herein we report the synthesis and functionalization of 4-oxothiochromane-2-carboxylic acid which seeks to enhance the affinity and could led us to the identification of the pharmacophore. The synthesis of 4-oxothiochromane-2-carboxylic acid was carried out by one-pot reaction between thiophenol and maleic anhydride, after other methods were discarded. Chiral resolution of the racemic 4-oxothiochromane-2-carboxylic acid was performed by diastereomeric salt formation with brucine, leishmanicidal and citotoxic activity was tested on the levogyre and dextrogyre enantiomers and this allowed us to attribute the higher activity to the levogyre enantiomer, so far the former compound displayed the higher activity. Esters and amides were also prepared and tested for antileishmanial and citotoxic activity.

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Keywords: Leishmaniasis, Michel addition, Thiochroman, Chiral resolution

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LILLY OPEN INNOVATION DRUG DISCOVERY PROGRAM (OIDD): FOR SCIENTISTS, BY SCIENTISTS

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The Lilly Open Innovation Drug Discovery program (OIDD) was created to engage external investigators in a hypothesis-driven approach to early drug discovery. Program participants have the opportunity to contribute to the discovery of novel therapeutics that will improve patients' lives, and benefit by having access to cutting-edge research tools and data that can help them advance their own scientific work. The OIDD program is directed to investigators in academic/research institutions and small biotechs. Many of them encountered barriers to evaluate the therapeutic potential of their compounds and the OIDD platform was designed to minimize obstacles by offering:

• In-kind access to a panel of proprietary biological assays in the areas of Diabetes, Oncology, Pain, Neurodegeneration and Immunology, plus certain neglected and tropical diseases in collaboration with global leaders in the area,

• A variety of in silico tools to prioritize molecules with desirable drug-like properties,

• Opportunity to prepare compounds remotely in our Automated Synthesis Lab (ASL),

• Opportunity to have chemical samples selected for purchase through an algorithm applied to the molecular descriptor profile.

Affiliation is established at the institution level via a universal agreement that protects participant's intellectual contributions. Once the agreement is signed, investigators at the affiliated institution may create a user account that manage chemical structure selection, sample transfers, and biological data in a secure manner. The OIDD program is supported by a secure web-based interface that protects the confidentiality of proprietary information such as chemical structures. All Lilly-generated data is owned by the participating investigator and/or institution, and results are used to initiate collaboration discussions based on promising results and mutual interest of both parties. Otherwise, the investigator is free to publish and/or use the biological results in grant proposals. This poster will describe the scientific rationale behind OIDD, the business model, operational details and metrics illustrating the performance of the program. Detailed information can be found online (https://openinnovation.lilly.com/). The website provides details about the process, our offerings, sample logistics, biological screening and user account management. Our universal agreement is also available online. If you have questions, please feel free to contact openinnovation@lilly.com

BIOACTIVE POTENTIAL OF ARAZÁ SEEDS

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PPQM 30

Arazá (*Eugenia stipitata*), is a vegetable species mainly grown in the Amazon, with a lower appearence in some regions of Colombian center [1]. Its low commercial competitiveness is due to the short durability of its pulp compared with other tropical fruits. Some research shows its skin and pulp as an attractive natural resource with bioprospecting on the nutritional and pharmacological field [2], leaving a void concerning seed biological activity. This study was carried out using seeds from *E. stipitata* collected in the Department of Tolima. An ethanolic extract (EE) and a dichloromethanic fraction (DF), derived from EE, were the basis for determining the bioactive properties of the agroindustrial residue. A phytochemical screening showed a high content of polyphenols like tannins; less abundant were flavonoids, terpenes, saponins and non-reducing carbohydrates. The highest content of phenolic constituents was detected in EE (29.57±0.5 gGAE/100g), being the majority tannins (29.14±0.50 gGAE/100g); this high tannin content in EE in proportion to total phenols generate the need to investigate the antiparasitic potential effect of the extract, considering the sensitivity that have shown various species of gastrointestinal helminths to this metabolites [3]; even though the antioxidant activity of EE versus the ABTS radicals (acid 2,2'–azino–bis–(3–ethyllbenzothiazoline–6–sulfonic)) and DPPH (1,1-difeneil-2-picrilhydrazly) was lower (IC50 ABTS 4.22±0.02; IC50 DPPH 3.06±0.09) than in DF (IC50 ABTS 0.34 mg/L; IC50 DPPH 2.65 mg/L). Using *Escherichia coli* and *Salmonella typhi* strains together with *Rhizopus*, *Aspergillus*, *Fusarium* and *Penicillium* genus phytopathogen fungi, it was found that EE was more active against *E. coli*, inhibiting growth by 86.16±0.99 percent. The test additionally included physical, chemical and biological characterization of the raw fat from the seeds. This fat material is slightly yellow with a specific weight of 0.856±0.02 and a melting point between 68–73 °C. Iodine index (22.5 ±0.30 g I2/100 g), saponification (91.0±1.92 mg KOH/g) and esters (89±1.92 mg KOH/g), show a low-insaturation fat material formed by relatively big molecular size fatty acids, fairly esterified. Just the same, peroxide (4.8±0.20 meqO2/Kg) and acidity (1.9±0.02 mg KOH/g) indexes show fat with good preservation state; is added its low toxicity to human erythrocytes. This seems to be one of the few studies performed that shows the bioactive potential of *Eugenia stipitata* seeds and its bioprospection.

Keywords: *Eugenia stipitata*, bioprospecting, biological activity, Arazá

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EFFECT OF GINGER EXTRACT ON MEMBRANE POTENTIAL VARIATION AND AKT ACTIVATION ON A PEROXIDE-INDUCED OXIDATIVE STRESS CELL MODEL

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PPQM 31

Zingiber officinale is a kind of ginger used for the treatment of diseases associate to Reactive Oxidative Species (ROS). Reports show its use in cellular models such as pancreatic and intestinal tumor cells, however the biochemical bases of antitumor, anti-inflammatory and antioxidant activities are not fully elucidated yet. The aim of this study was to evaluate the effect of a ginger extract (GE) on the viability, ROS production, Akt activation and mitochondrial membrane potential (ΔΨm) on the H2O2-induced oxidative stress in HT1080 cells. The results revealed that cell viability significantly decrease with increasing concentration of the GE. ROS production and ΔΨm increased (200µg/ml) and a significant decrease of this potential (400µg/ml) of GE. Basal Akt activation was not observed in HT1080 cellsuntreated; however, its phosphorylation at ser473 was observed (750µM H2O2); treatment with GE (400µg/ml) decreased Akt activation. Literature reports biological activities of GEs; however, in this study it is shown a new way to investigate the intracellular changes afforded by GEs. In conclusion, this study indicates that GE inducesintracellular changes that lead to variations in ΔΨm and expression of signaling proteins such as AKT, which together promote early events associated with apoptotic and necrotic processes.

ANTINOCICEPTIVE ACTIVITY OF EXTRACTS OF *Salvia tilantonguensis* J.G. GONZÁLEZ & AGUILAR-SANT. (LAMIACEAE)

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PPQM 32

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The genus *Salvia* is one of the most widely distributed in the world and figures as a prominent element in the pharmacopoeias of many countries. The use of plants of the genus *Salvia* also stands out in the records of traditional medicine since ancient times and lasts until the present. Its wide geographical distribution has generated a diversity of species in constant growth, which allows the study of new species such as *Salvia tilantonguensis* J.G. González & Aguilar-Sant. (Lamiaceae) that was described in 2014, with an endemic distribution to the Mixteca Alta region, in Oaxaca, Mexico. Due to the background of the genus as plants that contain secondary metabolites with pharmacological potential, this plant is under study by our work group, from the chemical and pharmacological perspective. Extractions by maceration were performed to the aerial part of the plant, using hexane, chloroform, acetone and methanol. Extracts of hexane, chloroform and methanol were tested at the dose of 100 mg/kg in the murine model of writhing test, by intraperitoneal administration, with which their antinociceptive potential was measured. The methanol extract presented a greater antinociceptive effect in comparison to the other extracts, for which the doses of 1 and 10 mg/kg were evaluated. A negative control group was used, which induced pain without any treatment and a positive control group given ketorolac at 1 mg/kg as antinociceptive agent. An ANOVA was applied to the results obtained, followed by a Sidak test, to discriminate the statistically significant doses that had an effect with respect to the negative control. The methanol extract of *Salvia tilantonguensis* shows a statistically significant antinociceptive effect at doses of 10 and 100 mg/kg, with respect to the negative control. The trend of the results suggests a dose-dependent response of the methanol extract. This extract contains polar compounds, which due to the knowledge about predominant secondary metabolites in the genus, could be phenolic acids, flavonoids or some alkaloid, involved in the antinociceptive activity. A large number of useful metabolites have been isolated from sages, and the present study shows the potential to obtain new drugs, from the study of new species.

Keywords: *Salvia*, Writhing test, Nociception, Secondary Metabolites.

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STUDY OF THE AQUEOUS EXTRACT OF THE MEDICINAL PLANT *Bursera simaruba* AND ITS ANTIPROLIFERATIVE EFFECT ON CD4+ AND CD8+ HUMAN T-LYMPHOCYTES

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PPQM 33

Some medicinal plants are able to exhibit a pharmacological effect on the immune response-acting cellular components. Therefore, seeking for new medicinal plants compounds, we investigated the effect of an infusion obtained from Bursera simaruba on human CD4+ and CD8+ T-lymphocytes. Ten healthy individuals were selected and a daily intake of 5 g of the bark of *Bursera simaruba* was then administered, with prior informed consent. Subsequently, the amount of CD4+ and CD8+ T-lymphocytes were then determined by flow cytometry to five collected blood samples. In most cases, there was a decrease in the number of both CD4+ and CD8+ lymphocytes. The JF03 individual had the largest decrease in his CD4+ T-lymphocytes, from 564 to 174 per mm3, meanwhile, the DL07 individual had a greater decrease in his CD8+ T-lymphocytes, from 635 to 378 per mm3. This decrease in CD4+ and CD8+ T-lymphocytes indicates an immunomodulatory effect of Bursera simaruba aqueous extract, showing its therapeutic potential in the treatment of autoimmune diseases, transplants immunology, allergy or inflammatory diseases. It is pertinent to carry out a phytochemical study of the extract to identify the active principle(s) causing this decrease in CD4+ and CD8+ T-lymphocytes

EVALUATION OF THE ANTIINFLAMMATORY ACTIVITY OF LEAVES OF *Cavendishia Compacta* (Ericaceae)

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Cavendishia compacta is a neotropical species belonging to the Ericaceae family that is widely distributed in the Andes mountain range and in the Pacific slope of the Western Cordillera of Colombia is the area of greatest concentration. In the family Ericaceae, related studies have been reported for anti-inflammatory activity in several species such as *Arctostaphylos uva-ursi*, *Bejaria resinosa* [1], among others. The present work describes the results of the evaluation of the anti-inflammatory activity of the ethanolic extract of leaves of the plant species *Cavendishia compacta* classified in the Colombian National Herbarium under the collection number COL 574699. The evaluation of the antiinflammatory activity of the extract and of the fractions Obtained by the in vivo mouse ear induced edema assay [2,3] using 36 male albino mice from 32 to 38 g, from twelve to fourteen weeks of age.

The 13-acetate 12-tetradecanoylforbol (TPA, 2.5 µg / ear) irritant was administered along with 500 µg / ear indomethacin as the standard or substances to be evaluated (Ethanolic extract and hexane, dichloromethane and ethyl acetate 500 µg / ear fractions) Dissolved in Ethanol-acetone via topical on the right ear (total volume: 20µL / ear, 10µL / face). The left ear was used as a control. After 4 hours the animals were sacrificed by cervical dislocation and a sample of each atrial auger was obtained by punch (7 mm diameter).

The magnitude of the developed edema was measured by gravimetry and from the statistical analysis it was established that the ethanolic extract and the dichloromethane fraction exhibited moderate antiinflammatory activity with percentages of inhibition of 49.3% and 39.8% respectively, since reduced edema caused by TPA in the mouse ear with inhibition rates close to those of the reference drug, indomethacin.

Keywords: *Cavendishia compacta*, Ericaceae, Antiinflammatory Activity.

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POTENTIALS MECHANISM OF ACTION OF THE 18-(PHTHALIMID-2-YL) FERRUGINOL DURING DENGUE VIRUS INFECTION

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PPQM 35

RNA viruses, including Dengue virus, represent a challenge in the search for antivirals due to their high mutation rate and low genetic stability [1,2]. Recent studies demonstrate the importance of conducting antiviral research to find host-targeting antivirals, because do not induce selection of drug-resistant mutants, may show a broad-spectrum antiviral activity and would have mechanisms of action complementary to direct-acting antivirals [3]. Previously, we have reported that a ferruginol analogue named 18- (Phthalimid-2-yl) ferruginol, has relevant and selective anti-dengue activity in post-infectious stages, including a dramatic reduction in viral plaque-size [4]; these events are possibly involved in the alteration of cellular factors (organelles, proteins, and macromolecular complexes) essential to performing the viral replicative cycle [5]. The aim of this work was to determine the possible mechanisms of action of 18- (Phthalimid-2-yl) ferruginol compound during Dengue virus infection and its potential relation with host-targeting antivirals.

The effect of cell pre-treatment with 18- (Phthalimid-2-yl) ferruginol compound was investigated using a plaque forming units (PFU) assay. Alterations on cytoskeleton elements, such as actin filaments and microtubules, were predicted by molecular docking and subsequently was confirmed using advanced fluorescence microscopy techniques and image analysis. Changes in viral envelope protein (E) amounts were also evaluated under these treatment conditions. PFU assay revealed that 18- (Phthalimid-2-yl) ferruginol molecule had antiviral activity after the cells had been pre-treated during a period of 24 hours. Under these treatment conditions, this compound induced dramatic changes in actin filaments reorganization and slightly alterations on microtubules distribution, without nuclear fragmentation induction. Also, this compound reduced the E protein amount after 12 hours post infection.

Our findings suggest that 18- (Phthalimid-2-yl) ferruginol compound has a potential mechanism of action related to host-targeting antivirals, affecting the cytoskeleton remodelling and possibly, the E protein translation. However, additional experiments are necessary to confirm or refute these hypotheses.

Keywords: Dengue virus, Mechanism of action, Host-targeting antivirals, Ferruginols analogues.

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A COMBRETASTATIN-BASED HYBRID CONTROLS VIRUS DENGUE INFECTION

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PPQM 36

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An increasing number of investigations suggest that the cytoskeleton participates in the replicative cycle of several viruses and other infectious agents. In this research focused on the search for new synthesis molecules targeting the cytoskeleton. Therefore, combretastatin- based hybrids were proposed as compounds that potentially interact with the cytoskeleton and eventually control infection of dengue virus.

In order, we used computer tools to perform a screening of combretastatin- based hybrids that had interaction with the actin or tubulin cytoskeleton and those molecules that showed interaction affinity it would be carried out a biological validation. The above, in order to determine whether or not there is infection control.

We obtained that a combrestatin- based hybrid had an interaction affinity with the tubulin cytoskeleton with a scoring of -9.33 kcal/mol. Nevertheless, biological validation of our results showed mild infection control on epithelial cells at a concentration of 1.14 µg/mL.

Our results suggest that a combrestatin- based hybrid present mild control of dengue infection and that a possible mechanism of action of this molecule is subject to alterations on the tubulin cytoskeleton, an important cellular target for virus replication.

Keywords: Combretastatin- based hybrids 1, Dengue, Tubulin 3 and Antiviral 4

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