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NANOFIBERS: ADVANCED FORMAT OF ORGANIC POLYMER-BASED MATERIALS FOR SAMPLE PREPARATION IN HPLC

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Solid phase extraction (SPE) is one of the most popular sample preparation methods because it can significantly reduce the amount of interfering ballast compounds in the sample prior to HPLC analysis and matrix effects in MS detection. A large number of advanced sorbents suitable for SPE-HPLC and capable of purifying a variety of matrices includes among many other nanomaterials and, in particular, microfibers and nanofibers. Fibers made from synthetic polymers encompass a wide range of adsorption mechanisms due to their different chemistries, hydrophobicity/ hydrophilicity, acceptor/donor properties, dipole-dipole, and π-π interactions. Our micro- and nanofibers were prepared by simple meltblowing, a combination of meltblowing and electrospinning, as well as DC and AC electrospinning techniques. We tested fibers prepared from numerous fairly common polymers. Electrospun fibers have already been applied in both off-line and on-line sample preparation by SPE while treating different types of matrices. Their advantages include affordability, the wide variability in chemistries of available polymers, and high extraction efficiency. We also developed a composite material in which robust meltblown fibers were used as a scaffold for more fragile, smaller diameter electrospun nanofibers. This approach increased the overall surface area and extraction capacity while maintaining the desired robustness. Alternatively, we have introduced modifications allowing us to produce hybrid materials containing nanoparticles and coated fibers. For example, hybrid polymer fibers were prepared by dispersing particles, such as magnetic nanoparticles, graphene, activated carbon, and carbon black, into the polymer solution prior to electrospinning. Alternatively, small 10 mm diameter nanofiber discs were cut from a compact and mechanically stable 1–2 mm thick micro/nanofiber mat. The best mat was prepared by the AC electrospinning of poly(ε-caprolactone) solution containing graphene nanoplates. The off-line SPE using these discs was demonstrated with the extraction of typical contaminants of different polarities from local river water and its spiked counterpart.

The project “New Technologies for Translational Research in Pharmaceutical Sciences /NETPHARM” project ID CZ.02.01.01/00/22_008/0004607co-funded by the European Union, is gratefully acknowledged for support.

NEUROPROTECTIVE ACTIVITY OF NATURAL GREEN EXTRACTS AGAINST ALZHEIMER'S DISEASE INVESTIGATED BY FOODOMICS

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ABSTRACT

Microalgae and food by-products are promising sources of neuroprotective molecules. Previous studies from our laboratory have demonstrated the in vitro neuroprotective activity of a Dunaliella salina microalga (DS) extract obtained with supercritical fluids, and an orange juice by-products (ORB) extract obtained by pressurized liquids. The present work aims to evaluate the in vivo neuroprotective activity of these two extracts using an Alzheimer's disease model based on a transgenic Caenorhabditis elegans (strain CL4176), which expresses the human Aβ1–42 protein. A time and dose dependent paralysis assay was performed, and the transcriptomics and metabolomics changes after the treatment were evaluated by RNA-Seq and GC/HPLC-MS technologies, respectively. The in-vivo assay showed a dose-dependent protection against paralysis when the DS or ORB were used, being the paralysis of the worms reduced to 53% (for DS) and to 54% (for ORB) when 50 µg/mL of the extracts were used after 32 h of Aβ induction. At this concentration, the transcriptomics analysis revealed the significant alteration of 150 genes (120 up-regulated and 30 down-regulated) after DS extract treatment, while 294 genes were altered by ORB extract (186 up-regulated and 108 down-regulated). Moreover, the combination of the different advanced analytical techniques allowed the identification of more than 750 intracellular metabolites, of which more than 60 were significantly altered by DS extract, while 36 were altered by ORB extract. The integration of these and previous results provides with new evidences on the neuroprotection mechanisms of these promising extracts, representing a step forward on the valorization of microalgae and food by-products as valuable sources of neuroprotective compounds.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

This work was supported by grants PID2020-113050RB-I00 and PDC2021-120814-I00 funded by MCIN/AEI/10.13039/501100011033 (Spain) and European Union "NextGenerationEU"/PRTR".

NEW SUSTAINABLE EXTRACTION METHODS INVOLVING THE USE OF BIOBASED SOLVENTS AT HIGH PRESSURE

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ABSTRACT

During the last decades, chemical laboratories have focused their efforts on the development of analytical environmentally friendly alternatives based on the Green Analytical Chemistry Principles (GAC); being a key step in the whole analytical methodology, extraction has become one of the most important aspects to improve. Therefore, greener solvents and techniques are required in accordance with a sustainable procedure, reducing energy, reagents, and increasing the security of the applied analytical methodology.

In the present work, the solid residue from almond-based milk production has been employed in order to recover its fat content (rich in monounsaturated fatty acids and bioactive compounds such as α-tocopherol and vitamin A) by using a completely new approach consisting on the combination of supercritical CO2 extraction (advanced technique) and a hydrophobic deep eutectic solvent (HDES) (bio-based solvent) as a co-solvent. An HDES (eucalyptol-menthol of molar ratio 1:1) was chosen based on preliminary tests to be used as a co-solvent in supercritical extraction. Moreover, for the first time, the phase equilibrium of the selected HDES plus SC-CO2 was studied to determine the miscibility and phase behavior under the extraction conditions.

Results demonstrate that, under the selected conditions (15% HDES as a co-solvent, 50C and 200 bar), HDES was completely miscible with CO2 and the extraction took place under a single phase; the use of HDES accelerated the extraction of hydrophobic compounds from almond waste.

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USE AND ABUSE OF RETENTION INDICES IN GAS CHROMATOGRAPHY

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ABSTRACT

Retention indices (RI) were developed and successfully applied by Kováts [1] for the identification of compounds separated by gas chromatography (GC). Posteriorly, van den Dool and Kratz adapted the Kováts indices to temperature-programmed analyses [2]. Since then, the hyphenation of GC to mass spectrometry (MS) lead to a considerable amount of information to help structural identification, which made GC-MS one of the most (if not *the most*) applied technique to the analysis of volatiles [3]. But, and there is always a "but", GC-MS does not solve all problems, particularly in the analysis of natural products, as samples frequently contain many structurally related compounds, several of them with diastereomeric relations amidst each other. RI are quite valuable then, as they do provide a useful tentative indication of the possible molecule(s), provided their limitations are recognized. An author has a responsibility to correctly calculate the index and then use the values for (tentative) identification. Tables of reference RI values are useful in this respect, but finding an 'exact match' RI value does not confirm the identity. Unfortunately, cases of misuse and, sometimes, of clearly abuse on the application of RI persist in the literature. These wrong data, once published, are used by other authors and, therefore, the errors are compounded. Hence, it is necessary to understand how the RI value may be incorrectly used. It must be emphasized that both authors and reviewers of written research are responsible for ensuring the index values are applied in a rigorous manner. Some case studies from our own work and from the literature are presented, reinforcing that care that must be exercised when reporting RI values [4].

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EL ESTUDIO DE PRECURSORES GLICOSILADOS DE AROMAS EN PLANTAS AROMÁTICAS Y SU IMPORTANCIA ECOLÓGICA

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Los precursores glicosilados de aromas son compuestos donde una molécula de un compuesto orgánico volátil se encuentra unida a uno o más azucares, lo que los hace inactivos desde el punto de vista olfativo. Su liberación se produce mediante procesos enzimáticos o químicos que transforman los precursores en compuestos volátiles. Estos volátiles son importantes tanto para la ecología de las plantas como en sus propiedades organolépticas, siendo responsables de la percepción de los aromas y sabores característicos de muchas frutas.

En el contexto ecológico, los aromas liberados a partir de estos precursores tienen un papel fundamental en las interacciones de las plantas con su entorno.

En el ámbito productivo, el estudio de los precursores glicosilados de aromas en frutas tiene una gran relevancia, ya que estos compuestos son clave para el desarrollo de los sabores y aromas durante la maduración y postcosecha, influyendo directamente en la calidad y aceptabilidad de las frutas y sus derivados por parte de los consumidores.

El estudio de los precursores glicosilados de aromas en plantas, frutas y sus derivados no solo tiene importancia influyendo en las interacciones planta-entorno, sino también un impacto ignificativo en la industria alimentaria y agrícola, abriendo nuevas oportunidades para mejorar la calidad y el valor de los productos naturales.

En esta presentación se mostrarán resultados demostrativos del impacto de los compuestos volátiles glicosidados en casos de estudio vinculados a la producción de aceites esenciales, valorización de frutos nativos e impacto en el aroma de derivados cannábicos.

PLANT VOLATILES: A GREAT FUTURE BEHIND THEM

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ABSTRACT

Essential oils (EO) are products obtained from plants or a specific part of them with a rather homogeneous composition in terms of molecular mass and polarity of their components, (the latter is a distinctive trait often underestimated) mainly due to the isolation technique based on steam distillation or hydrodistillation (with the exception of citrus EO). This characteristic places EOs and their chemistry at a nodal crossroads between agronomy, biology, botany and biochemistry and their applications in innumerable fields, in particular food, cosmetics and pharmaceuticals. Modern research in the EOs field is a clear example of the ever-increasing integration of chemistry and biology and thus involves the synergic contribution of the expertise of industry, regulatory organisations and universities with their technologists, lawyers, biologists and toxicologists, pharmacologists and medical doctors, agronomists and botanists, and analytical and synthetic chemists. The misuse of the magic word 'essential oil', sometimes (indeed often) without knowledge, therefore hides a multidisciplinary entity that 'marries' research subjects and skills of a very different nature. The above concepts will be illustrated with some examples from the author's day-to-day experience.

NEW SUSTAINABLE TRENDS FOR PASSIVE MICROEXTRACTION TECHNIQUES

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ABSTRACT

Static or passive microextraction techniques have played a significant role over the last thirty years, emerging as modern and highly effective approaches to sample preparation. Notable examples of liquid-based microextraction techniques include dispersive liquid-liquid microextraction (DLLME), single-drop microextraction (SDME), and hollow fibre liquid-phase microextraction (HF-LPME). On the other hand, solid-based microextraction techniques such as solid phase microextraction (SPME), stir bar sorption extraction (SBSE), and, more recently, bar adsorptive microextraction (BAμE) [1], have been widely used with enormous success. These analytical approaches are characterized by the use of miniaturized devices, significant simplification, easy handling, substantial reduction or elimination of toxic solvents or ecologically undesirable materials, reduced sample volume, improved selectivity and sensitivity for trace analysis, and compatibility with common chromatographic and hyphenated systems. However, in the future, in addition to new trends for passive microextraction techniques being proposed or developed to be as simple as possible, considering scope, ease of use, automation, and cost, they should always be designed with complete sustainability in mind. Regarding this aspect, any future alternative development must take into account not only the principles of green chemistry but also the sustainable development goals proposed by the United Nations [2]. Thus, even though the main microextraction technologies mentioned above have demonstrated great effectiveness, some still have limitations that need to be reviewed or improved to be considered viable future alternatives.

This contribution will discuss various innovative advances and future trends in the field of passive microextraction technologies, with a particular focus on BAμE and related techniques. We will propose straightforward concepts that fundamentally aim to achieve not only the best analytical performance but also the best practices and strategies to guarantee full sustainability.

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TRANSDISCIPLINARY STUDY OF THE DURAZNO RIVER BASIN (COSTA RICA): THE ROL OF ANALYTICAL CHEMISTRY

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ABSTRACT

The Durazno River micro-basin, spanning 12 km^2, is a part of the Río Grande de Tárcoles Basin in Costa Rica and a water source for human consumption. However, the potential presence of emerging contaminants such as antibiotics and AMR genes has raised severe concerns about microbiological contamination and the physicochemical quality of the water. The implications for public health are grave, and immediate action is necessary. As the Durazno River basin is located near urban areas and has multiple land uses, it is important to take a multidisciplinary approach to evaluate its water quality. The project aims to assess the Durazno micro-basin's water quality through physicochemical and microbiological analysis. It will involve the detection of emerging contaminants, such as antibiotics and resistance genes, and environmental risk assessment. Our research here started in 2021 and has yielded significant findings. While the water quality, based on physicochemical parameters, is acceptable overall, we have observed variations between the dry and wet seasons and between different sampling points. These differences may be due to variations in land use or soil types. From a microbiological perspective, the water is unsuitable for human consumption. Our tests have also revealed the presence of doxycycline (DC) and cefotaxime (CT) in concentrations ranging from 2.13-11.74 ng L-1 and 0.68-1.20 ng L-1, respectively. Notably, this is the first time cefotaxime has been detected in Costa Rican water. Since 2022, we have detected the presence of E. coli bacteria that are resistant to multiple drugs, including tetracycline, beta-lactams, and sulfas. In some cases, the bacteria were also resistant to aminopenicillins and quinolones. This poses a significant environmental risk, as the contamination can impact the resistome of the river's surface waters. We plan to continue researching and incorporating additional geological and environmental information.

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PLANTAS AROMÁTICAS: ALTERNATIVA PARA LA INDUSTRIA DE INGREDIENTES NATURALES EN COLOMBIA

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ABSTRACT

Colombian farmers face a difficult reality marked by limited purchasing power, low economic returns and productivity, and a lack of technical expertise in rural operations and processes. The standard of living of rural workers and the impact on their health due to the conditions in which they work, motivated the development of projects for the implementation and development of the agroindustry of essential oils and plant extracts, to add value to the harvest of aromatic plants and diversify both the rural economy and the professional performance spaces of young workers. Several sites for the rural distillation of essential oils were installed in Santander. A process for obtaining extracts by dispersion of the matrix in a solid phase was developed on a pilot scale. Good agricultural practices and the circular economy were used to achieve the comprehensive use of plant mass and eliminate waste. Bioprospecting studies of Colombian biodiversity have resulted in an information base and in the development of prototypes based on natural ingredients, which can be converted into commercial products. The joint work of different research groups, chemical characterization with high-resolution tools, the development of stability and functionality tests, and the participation of trained scientific and technical personnel have allowed the development of several bioproduct prototypes, all of them incorporating natural products as active ingredients. Their technological development levels are between 4 and 7. They include surface disinfectant, deodorant cream, lip balm, hand conditioning cream, microemulsion for the treatment of cutaneous leishmaniasis, disinfectant for the fertile egg chain, photoprotective face powders, and encapsulated repellent air freshener, among others. All these developments had as a fundamental pillar the instrumental chemical characterization (GC, GCxGC, HRMS, UHPLC) for the identification of active components, quality control, and process optimization.

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CROMATOGRAFÍA Y ESPECTROMETRÍA DE MASAS EN EL ANÁLISIS DE SUSTANCIAS PSICOTRÓPICAS NATURALES Y SINTÉTICAS

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ABSTRACT

The analysis of psychoactive substances poses several challenges due to their wide range of chemical structures, their presence at low concentrations in complex matrices, their different ionization efficiencies, and the scarcity of reference standards. The combination of highly efficient isolation techniques such as matrix solid-phase dispersion, or solid-phase microextraction, with high-resolution chromatography and high-resolution mass spectrometry have been employed to successfully address these barriers to identification and quantification of natural and synthetic psychoactive substances. Studies of the transfer of tropane alkaloids from flowers to visiting bees revealed cocaine concentration levels of 10 μg/g in the coca flower and 0.013 μg/g in visiting bees. Analogously, caffeine was found at concentrations of 614 μg/g in coffee flowers and 0.5 μg/g in visiting bees. Solid-phase microextraction with previous loading of an internal standard was employed in the GC/MS analysis of the headspace of 73 different commercial cannabis products. A total of 414 substances were distinguished at concentrations above 0.1%, 153 of which were not common to several products, but were present in just one product

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Optimization of SPME and Needle Trap Technologies for Fragrance Determinations

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The advent of microextraction techniques revolutionized sample preparation by combining clean-up, sampling, and sample preparation into a single step. Further adding to their appeal, microextraction methods are also sensitive, environmentally friendly, fast, portable, and rather inexpensive. It is estimated that approximately 10,000 volatiles are present in food, yet only a small fraction significantly contributes to the final aroma of food products. A major challenge arises from the fact that many of these aroma-active compounds exist in extremely low quantities, often at the ppt (part per trillion) level and are characterized by high polarity (logP < 1). The inherent difficulties in analyzing such compounds stem from the low sensitivity and affinity of sorbents or solvents towards polar analytes, rendering odorants analysis a complex and demanding process. Alcoholic beverages serve as an ideal model for investigating odorants due to their rich composition of volatiles with diverse physicochemical properties, coupled with the frequent occurrence of off-flavors in these products. Various methods advocate for developing Solid-Phase Microextraction (SPME), citing its efficiency, robustness, reliability, automation potential, and eco-friendly nature. However, a notable challenge in SPME for food samples, particularly those with a simple matrix composition and high concentration of hydrophobic compounds, is the displacement effect. This effect can impede the quantitation of analytes with low affinity towards the extraction phase. In the presentation the sequential extraction will be introduced to address this challenge. Of the various available microextraction techniques, needle-based methods are among the most intriguing. In needle-based methods, an extraction phase is immobilized/packed inside of a needle, which is then used for extraction and the subsequent desorption of analytes via direct injection into chromatographic instruments. The main difference between NTDs and other microextraction techniques is that NTDs enable exhaustive extraction if the breakthrough volume (BTV) is not reached. The importance of incorporating the particle filter as an additional packing material will be emphasized. This modification results in a Filter-Incorporated NTD (FI-NTD), which expands the potential areas of this technology including a free and total concentration measurement when combined with non-exhaustive SPME measurement as the active sampling mode of the NTDs are also suitable for trapping particle- and droplet-bound compounds. Such combination between SPME and NTD can be optimized to provide comprehensive characterization of the aromas originating from different sources.

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El papel de la química analítica en la política pública: el caso del plomo

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La química analítica, muchas veces percibida como una disciplina lejana a la toma de decisiones, puede, y debe ser utilizada como herramienta para diseñar o mejorar las políticas públicas dirigidas a garantizar el bienestar general de la población. Diversas investigaciones llevadas a cabo en los últimos años han mostrado niveles elevados de plomo en sangre de niños en varias poblaciones vulnerables del Caribe colombiano, comprometiendo su capacidad intelectual, crecimiento físico, sistema hematológico y elevando su susceptibilidad a infecciones, entre otros problemas detectados. Estos resultados de investigación, generados desde la academia, sentaron los pilares para elaborar una propuesta legislativa cuyo objetivo estuviese orientado a proteger a los ciudadanos, en especial niños y niñas, de la exposición al metal neurotóxico. Con los datos disponibles y el respaldo de iniciativas normativas de carácter internacional relacionadas con el tema, fue posible redactar la exposición de motivos y un articulado preliminar para someter la propuesta a consideración del Congreso de la República. Bajo el liderazgo de una legisladora regional, el proyecto cursó su trámite y hoy día es la Ley 2041 del 27 de Julio de 2020, por medio de la cual se garantiza el derecho de las personas a desarrollarse física e intelectualmente en un ambiente libre de plomo, fijando límites para su contenido en productos comercializados en el país y se dictan otras disposiciones. Este caso demuestra cómo las ciencias analíticas pueden emplearse para trascender, ofreciendo datos robustos para soportar normatividades. Queda claro que la ciencia, en particular bajo nuestro contexto, necesariamente debe pasar de la generación de conocimiento a participar de manera activa en la construcción de soluciones. En síntesis, los datos analíticos constituyen argumentos irrefutables para garantizar la salud de la actual y futuras generaciones, transformando el conocimiento en acciones que contribuyan al desarrollo sostenible de Colombia.

MULTIRESIDUE DETERMINATION OF 176 PESTICIDES IN BEE SAMPLES BY MINI-QuEChERS AND UHPLC-MS/MS

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ABSTRACT

Pesticides are widely used in agriculture, but after application, they are distributed in plants, soil, water or air and can also affect non-target organisms, such as honey bees, one of the most important pollinators. Bees can be contaminated in different ways, both while foraging from contaminated nectar and/or pollen and by ingesting irrigation water, and inside the hive. Studies show that the synergistic effects of multiple exposures to pesticides can contribute to the disappearance of bees, a worldwide phenomenon known as colony collapse disorder. The loss of these pollinators has a negative impact on agricultural production, as well as on the maintenance of plant biodiversity. In this context, the aim of this study was to develop and validate a comprehensive method for the multiclass determination of 176 pesticides in honey bees using ultra-high performance liquid chromatography with tandem mass spectrometry (UHPLC-MS/MS). For sample preparation, modifications to the QuEChERS method were tested in relation to different extraction conditions, partition salts, sorbents for cleaning the extracts and miniaturization of the extraction step, considering the difficulty of obtaining samples in adequate quantities. The method developed consisted of homogenizing the bee samples direct in a Falcon tube with ultrapure water, followed by extraction with acetonitrile containing formic acid, partitioning with anhydrous magnesium sulphate and sodium chloride, and cleaning the extract with PSA and C18. The extract obtained was analyzed on a Waters Xevo® TQ-XS UHPLC-MS/MS using an Acquity UPLC® HSS T3 column (2.1×100 mm; 1.8 μm). The proposed QuEChERS method proved to be effective for the multiclass determination of pesticides in bee samples, with quantification limits of 5 μg kg^{-1} for most compounds. The validated procedure was applied to 32 samples of honey bees from different states in Brazil, detecting 11 insecticides, 10 fungicides and 5 herbicides. The insecticide fipronil, which is highly toxic to bees, occurred most frequently.

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NEEDLE-BASED MICROEXTRACTION DEVICES COUPLED TO MASS SPECTROMETRY

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ABSTRACT

The systematic consideration of sustainability and affordability is a clear and established trend in sample preparation. The introduction of novel, green, low-cost supports and sorbents, combined with miniaturised extraction equipment, is key to reducing the environmental and economic impact of the entire analytical process. Together with sustainability, we have deepened the affordability of extraction devices by using commercially available low-cost elements. Their added value is increased by their market availability, which also has a positive impact on the reproducibility of the extraction equipment. With these trends in mind, we have explored the potential of hypodermic needles (HNs) as sorbent holders and electrospray (ESI) emitters, integrating extraction and analysis in a single device. The sorbent phase can be either packed into the hub/needle body or in the form of a thin film over the inner wall of the needle. When the configuration includes their use as electrospray emitters, on-line elution of the analytes is possible, resulting in efficient transfer to the MS inlet. This communication discusses the evolution of this line of research started by our group in 2021. The improved designs have increased the amount of sorbent that can be allocated within the needle, thus increasing the sensitivity of the measurements, while making HNs of different geometries and diameters compatible with direct elution of the analytes into the mass spectrometer by designing dedicated interfaces. HNs can also be integrated with miniaturised techniques such as miniaturised stir bar sorptive extraction, increasing their versatility in sample preparation.

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HOW EFFICIENT CAN THE DECOMPOSITION OF DIFFICULT SAMPLES USING DILUTED SOLUTIONS BE?

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Nowadays, techniques with high detection power for inorganic analytes are increasingly dependent on analyzing well-digested solutions with few interferences that could affect analytical results. This is an even greater concern in the case of decomposition of organic samples with high carbon content, since depending on the composition of the matrix it is sometimes very difficult to obtain efficient decomposition. It is known that analyses at low concentrations using some atomic spectrometry techniques (e.g., ICP-MS) or even chromatography (ion chromatography) and electroanalytical techniques (e.g., polarography) can be affected by the presence of organic compounds in high concentration, even after the matrix digestion stage. Normally, to obtain digests with low residual carbon content, it is necessary to use large volumes of concentrated oxidizing acids and relatively long reaction times. In this sense, even using methods based on microwave-heated closed vessels, some drawbacks may occur and incomplete decomposition and low analyte recoveries have been frequently reported. In this regard, the main trends for sample preparation for further halogen determination will be presented by using diluted solutions. Recent applications will be presented showing the advantages of methods using diluted reagents (MW-UV digestion, pressurized vessels with oxygen, etc.) for metals and non-metals determination using atomic spectrometry and chromatography techniques.

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THE POTENTIAL OF PLANAR SORPTIVE PHASES FROM A SUSTAINABLE PERSPECTIVE

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ABSTRACT

Planar sorptive phases (PSP) provide a high extraction performance thanks to their advantageous surface-to-volume ratio, thus allowing for a reduction of the amount of the material required for each extraction. If this resource reduction is combined with an environmentally benign synthesis, these phases can be considered sustainable solutions for sample preparation. In this communication, we will share our recent experience in the design and use of PSP in different fields of application, including bioanalysis, forensic, and environmental analysis. Our experience with PSP started in 2017 with the design of functional paper-based sorptive phases through the dip-coating technique. In this way, materials containing polymers (including molecularly imprinted ones) and nanocomposites have been synthesized. In theory, they can be tailored to solve a given analytical problem just by considering the chemical structure of the analytes. In recent developments, we have further developed the preparation of dual papers, their direct coupling with microextraction techniques, and the incorporation of particulate mixed-mode ion exchange sorbents for the selective extraction of drugs in biofluids. Simplicity, defined as the search for effective but affordable solutions, has been the driving force behind the evolution of this research line. Following this trend, sorbent phases have also been proposed using commercially available adhesive tapes that allow the arrangement of small quantities of particulate sorbents in a flat format, reducing material requirements while ensuring good extraction performance.

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SAMPLE PREPARATION STRATEGIES FOR THE SUBSEQUENT DETERMINATION OF HALOGENS AND THEIR SPECIES

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The determination of non-metals, particularly halogens, is essential for understanding their roles in fields such as nutrition, health, and toxicology. Despite advancements in instrumentation, sample preparation typically requires converting samples into a solution. Traditional digestion methods, often reliant on large volumes of concentrated reagents, are time-consuming and may necessitate dilution prior to analyte determination, potentially compromising detection limits. Even with microwave-assisted closed-vessel methods, challenges like incomplete digestion persist. Additionally, concerning halogen determination, volatile compounds can be lost in acidic mediums.

There is a growing emphasis on developing green analytical methods that minimize reagent use, reduce waste, improve the analytical processes, and achieve efficient digestion. Ensuring the suitability of digests for determination techniques is equally critical. This lecture will present the latest advancements in sample preparation for food and biological matrices, focusing on halogen determination and their species using inductively coupled plasma mass spectrometry and ion chromatography with mass spectrometry detection. Topics will include the use of diluted solutions, combustion systems, and recent technological innovations in this field.

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MICROPLASTICS IN AQUATIC ENVIRONMENTS: ADVANCES AND ANALYTICAL CHALENGES, SPECIALLY FOR DEVELOPING COUNTRIES

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ABSTRACT

The production and use of plastic materials have skyrocketed in recent decades, given the versatility and applicability of the various types of existing products. However, due to low recycling rates and poor waste management, a large portion of discarded material ends up in the environment, where it can cause physical and ecotoxicological damage. The accumulation of plastic waste includes debris in a wide range of sizes, with a significant part consisting of microplastics, which has led to an exponential increase in research on this topic, particularly in the last two decades. Considering these aspects, this speech aims to present and discuss issues related to the origins of microplastics, their behavior, fate, and effects, especially in aquatic environments of developing countries, with a particular emphasis on existing gaps in environmental context as well as the analytical challenges for advancing this important field of knowledge.

ETHICAL APPROVAL

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Pairing red wine and stopper: an old issue with new achievements based on multimodal data

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ABSTRACT

The sensory characteristics of wine are a topic studied by several researchers over time, but it continues to be a current and challenging subject. These characteristics are fundamental for the consumer acceptability, which has increasingly aroused their interest to modulate them in line with current market trends and innovation demands. The wine physical-chemical and sensory properties depend on a wide set of factors: they begin to be designed in the vineyard and are later constructed during the various stages of winemaking. Afterwards, the wine is placed in bottles and stored or commercialized. During post-bottling, the wine may suffer several physical-chemical changes, modulated by the position of the bottle, type of stopper, temperature, and storage time, among others, which impact on the oxygen entrance ratio. In the present study, red table wines, stored in a horizontal position for ca. 0.5 and 3 years, using natural cork stoppers, different types of microagglomerated cork stoppers and a screw cap, were characterized. To achieve a holistic view of the changes that may have occurred during bottling, a set of analysis were implemented, namely, determination of volatile components by comprehensive gas chromatography- mass spectrometry with time of flight analyser (GC×GC-ToFMS), determination of phenolic profile by ultra-high-performance liquid chromatography, coupled with tandem mass spectrometry (UHPLC-DAD-MSn), sensorial analysis performed by a trained panel, and also determination of chromatic parameters, SO2 (free and total), acidity (total and volatile) and pH. Chemometric tools were used to explore the data sets, select relevant features, and investigate the networks between features. The fusion data strategy used in this study, that also combines data with high dimensionality, provides new chemical data that allow evaluating the effect of the stopper on red table wines. Physical-chemical and sensory analysis unveiled that the type of stopper modulates the characteristics of the wine, which was more apparent for longer storage time, and its selection may be used as an oenological tool in the construction of the wine identity.

ETHICAL APPROVAL

All the authors agree with the content of this abstract.

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Analytical strategies for the determination of pesticide residues in foods and biological samples

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ABSTRACT

The use of pesticides of different classes in agriculture can generate economic benefits, since they control and combat pests and diseases, protecting the quality of production; however, consumers can be exposed to these compounds through food. They are widely used in agriculture, but after application they are distributed in plants, soil, water or air and can also affect non-target organisms. Considering the risk to human health and the environment associated with excess pesticides often used during food production and storage, monitoring programs for these compounds are necessary. The complexity of most matrices makes it challenging to develop multi-residue methods for the determination of pesticides from different classes in food and biological samples. Most of the methods developed are based on the QuEChERS procedure for sample preparation, with a clean-up step by dispersive solid phase extraction (d-SPE) using new sorbents, including biosorbents, and determination by ultra-high performance liquid chromatography with tandem mass spectrometry (UHPLC-MS/MS) or gas chromatography with tandem mass spectrometry (GC-MS/MS). Other sample preparation strategies may also be suitable for this analysis. We will present an overview of recent developments in this area.

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THE THIN FILM AND ITS CHALLENGING APPLICATIONS ON THE SUSTAINABLE DEVELOPMENT GOALS WAY. A FINE ANALYTICAL APPROACH

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ABSTRACT

The powder photocatalysis (heterogeneous), although it has shown good performance, has the drawback of catalyst recovery, the limitation of its extension of its action in the electromagnetic spectrum, the difficulty of its scaling and the cost associated with its preparation and recovery[1-4]. On the other hand, the thin film allows the fixation of the catalyst in larger areas, increases its efficiency with the rapid action and its scaling is potentially possible without cost for losses and recovery of the catalyst. In addition, and trying to promote the catalytic activation (difference less than 3.0 eV between the valence band VB and the conduction band CB, that is, a GB band gap of those orders) of some catalysts from regions such as the ultraviolet UV and especially in the visible VIS, the thin film allows growth in multilayers so that a combination of photocatalyst compounds with strategies such as multilayer growth or doping of activating elements is an urgent and demanding need. Among the forms of thin film growth is physical vapor deposition PVD, which consists of bombarding in a high vacuum chamber with argon ions in a space of electrical radio frequencies on a target (cathode) of the element to be deposited for adhesion on a substrate. operable (anode) (n-type silicon slides). Here in this film growth process, it becomes important to find the best conditions of power, catalyst feed, growth time and film thickness. First-hand, the application to use this nanotechnology is in the removal of nowadays health risk emergent pollutants such as hormones from wastewater, because no traditional system is capable of achieving the complete mineralization of the contaminants to CO_2 and H_2O, and today only work is done on the transfer of the contamination from the liquid medium to the solid medium, and the other advanced oxidation processes that have this purpose, have not yet been able to be massively demanded and their scaling is compromised, in this way this project seeks to make solid progress in obtaining high quality water in to the SDGs attention in an efficient and scalable way using nanotechnology developed in Romania and Colombia

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ENHANCING THE SUSTAINABILITY OF A MICROEXTRACTION TECHNOLOGY BY USING A NATURAL SORPTIVE PHASE

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ABSTRACT

The key to microextraction technologies lies in the nature of the sorbent phase. Solid sorbents can be classified as either synthetic or natural materials based on their origin. While commercial polymers are commonly used in various microextraction techniques, there is a growing interest in designing solid sorbents using new synthetic materials. In this regard, micro- and nanomaterials have been explored. Alongside these advancements, the innovation of recyclable, natural-origin materials represents a parallel trend in analytical chemistry—a focus that is central to our current research. As previously mentioned, a major challenge in analytical chemistry today is to prioritize eco-efficient or green processes, giving them equal importance to sensitivity and selectivity. Microextraction technology is inherently green, as it minimizes the use of organic solvents during sample preparation. However, the level of analytical "greenness" can be further enhanced by using sorbent phases derived from natural sources.

In this presentation, we highlight several applications of Rotating Disk Sorptive Extraction implemented in our laboratory, utilizing various sorbents derived from natural sources such as peanut shells, cork, avocado seeds, chitosan, and more. In several cases, these materials or their derivatives have demonstrated comparable sorptive behavior to commercial sorbents like Oasis™ HLB. Using these natural sorbents, we have quantified emerging contaminants in wastewater and river water samples from the metropolitan region of Chile [1-3].

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AE-O01

POTENCIAL BIOFUNGICIDA DE ACEITES ESENCIALES FRENTE A FITOPATÓGENOS DE IMPORTANCIA AGRÍCOLA PARA COLOMBIA

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RESUMEN

Los fitopatógenos *Fusarium, Botrytis, Colletotrichum* y *Aspergillus* representan una amenaza para una amplia gama de cultivos de frutas (banano, fresas, mango, nueces, etc.), verduras y hortalizas (Tomate, pimiento, lechuga, etc.), cereales (trigo, maíz, cebada, etc.), flores ornamentales (Rosas, laureles, girasoles, etc.), entre otros, que ocasionan pérdidas económicas a nivel mundial que superan los $100 mil millones de dólares y en Colombia que superan los $300 millones de dólares [1]. Los fungicidas químicos se emplean para el control de estos fitopatógenos. Sin embargo, estos se bioacumulan en el ambiente y ocasionan daños para la salud humana, animal y vegetal, así como la resistencia de los fitopatógenos a estos agentes [1]. En este contexto, surge la necesidad de explorar alternativas más sostenibles y ecológicas, como el uso de aceites esenciales (AE) como una alternativa natural para tratar estos fitopatógenos, debido a sus propiedades antimicrobianas [2]. El objetivo de este trabajo fue evaluar el efecto antifúngico de los AE obtenidos de plantas recolectadas en salidas botánicas o cultivadas en el jardín del Complejo Agroindustrial Piloto CENIVAM sobre el crecimiento de *Fusarium, Botrytis, Colletotrichum* y *Aspergillus*. La actividad antifúngica de los AE se evaluó mediante la determinación del crecimiento fúngico por el método de dilución en placa y exposición de volátiles [2]. Se observó un efecto fungicida de los AE Bio-Reto008, Bio-Reto018, Bio-Reto0045, Bio-Reto0046 y Bio-Reto0103 sobre los cuatro hongos evaluados y un efecto fungistático de los AE Bio-Reto0015, Bio-Reto0080, Bio-Reto0084, Bio-Reto0095, Bio-Reto0098 y Bio-Reto0105 sobre los cuatro hongos evaluados. En conclusión, los AE pueden ser empleados como una estrategia para reducir las enfermedades causadas por *Fusarium, Botrytis, Colletotrichum* y *Aspergillus* en cultivos de frutas, verduras, hortalizas, entre otros.

APROBACIÓN ETICA

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AE-O02

ANÁLISIS DE LA COMPOSICIÓN QUÍMICA DEL AE DE *Cúrcuma longa* OBTENIDO MEDIANTE HIDRODESTILACIÓN ASISTIDA POR MICROONDAS *E HIDRODESTILACIÓN: OPTIMIZACIÓN Y* CONSUMO ENERGÉTICO

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ABSTRACT

Cúrcuma longa L., (Zingiberaceae), es una especie de alto interés biológico. Sus rizomas son utilizados como colorante y aromatizante. Esta especie se cultiva especialmente en India y China. [1] Se ha utilizado en cosmética y en la medicina tradicional, y es reconocida por sus propiedades antiinflamatorias, antioxidantes, antimicrobianas, anticancerígenas y antivirales. [2] Los Aceites esenciales (AE) extraídos de los rizomas de *C. longa*, son ricos en sesquiterpenos, como el zingibereno, ar-turmerona (**1**), α-turmerona (**2**) y β-turmerona (**3**). [3] En esta investigación, el AE del rizoma de esta especie, se obtuvo mediante hidrodestilación asistida por microondas (HDAM) e Hidrodestilación (HD). Se implemento un diseño de Box Behnken con 3 factores: tiempo de irradiación, potencia y volumen de disolvente. Mediante el análisis de superficie de respuesta, se obtuvo para HDAM, un volumen de 132,19 mL., un tiempo de 59 min. y una potencia de 720 W. El porcentaje de rendimiento fue de 4.6 %. Los componentes del AE se analizaron por cromatografía de gases-espectrometría de masas. Se identificaron un total de 50 componentes, estos representaron el 97,77 % para HD y 99,67 % para HDAM. Se reporta a los sesquiterpenos oxigenados como la familia estructural más abundante para ambas metodologías, con porcentajes que oscilaron entre el 89 y 78 %, respectivamente. (**1**) se obtuvo en un 18.920 y 21.50%, (**2**) en 22.677 y 29.60% y (**3**) 14.78 y 16.68%, por HD y HDAM, respectivamente. Los AE extraídos por HDAM mostraron un aumento en los componentes mayoritarios con respecto a la HD, correspondiente al 11 % para (**1**), 32 % para (**2**) y 13.5 % para (**3**). [3] El consumo eléctrico y emisión de CO_2, también fueron evaluados. Los valores de consumo de energía fueron 0.720 kWh para HDAM y 2.2 kWh en la HD. Se generó un ahorro energético por HDAM equivalente a 2 veces menos que lo requerido en la HD. Las emisiones de CO_2 fueron 576 g para HDAM y 1760 g para HD, lo que implicó una notable reducción por HDAM. Los resultados obtenidos en este trabajo muestran como la asistencia por radiación de microondas favorece la extracción de AE de *Cúrcuma longa* desde múltiples aspectos, con un aumento del rendimiento del 32 % del compuesto mayoritario (**2**).

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AE-O03

IDENTIFICATION OF VOLATILE COMPOUNDS IN LEAVES AND FLOWERS OF *Pentacalia vaccinioides* (Kunth) Cuatrec. SPECIES AND THEIR ANTIOXIDANT AND ANTIMICROBIAL STUDIES

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ABSTRACT

Essential oils (EO’s) possess unique properties such as antibacterial, antioxidant, and antiviral activities, which are beneficial across various industries including cosmetics, food, and pharmaceuticals [1]. This study evaluated the antioxidant and antimicrobial activities of EO’s from *Pentacalia vaccinioides* (Kunth) Cuatrec., obtained from fresh and dry leaves and flowers using simultaneous extraction and distillation (SED), hydrodistillation (HD), steam distillation (SD), and solid-phase microextraction (SPME) [2]. The identification and quantification of compounds in the EO’s were performed using gas chromatography coupled with mass spectrometry (GC-MS). The primary secondary metabolites identified in most samples obtained through different extraction techniques were: 1S-α-pinene (~11%), β-phellandrene (~8%), β-pinene (~8%), phenol (~8%), 4-terpineol (~4%), γ-terpinene (~4%), α-nerolidol (~4%), β-thujene (~4%), and limonene (~3%). The EO’s obtained by SD and SED exhibited antioxidant activity with IC_{50} values of 37.1 and 39.4 g/L, respectively. Additionally, the EO’s extracted by SD, SED, and HD demonstrated antimicrobial activity against *Bacillus subtilis* and *Staphylococcus aureus*. This study highlights the variability of results depending on the extraction technique used, the type of plant material employed, and the biological activity evaluated.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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AL-O01

PEPTIDES DERIVED FROM CASEINOMACROPEPTIDE: A POTENTIAL TOOL FOR QUALI-QUANTITATIVE DETERMINATION OF MILK ADULTERATION

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ABSTRACT

Milk serves as food with high nutritional value, whose consumption has increased over the last few years and its production has been affected by adulteration. Cheese whey has become a popular adulterant in the milk industry in Latin America and Europe because of the capability of whey to keep milk taste. Caseinomacropeptide (CMP) has been employed as an adulteration biomarker due to its presence exclusively in whey. However, CMP poses challenges such as high production cost, the glycosylation leading to produce glycomacropeptide (GMP), and the genetic variants which result in low reproducibility analysis and complexity of sample treatment [1]. Therefore, the use of peptides derived from CMP for whey adulteration analysis and determination has been proposed [2]. This study focused on the chromatographic analysis of peptides derived from CMP, specifically the sequence MAIPPKKNQDKTEIPTINT and the peptides produced through the enzymatic hydrolysis of native CMP. Peptide synthesis was carried out by SPPS-Fmoc/*t*Bu strategy and purified via RP-SPE. Analytical methods were developed using a HPLC-DAD and a Bruker Impact II ESI-Q-TOF LC-MS system. It was found that peptides derived from CMP exhibit temperature-dependent conformers, which increase with peptide size and the number of proline residues. A peptide with non-significant isomerism, chromatographic purity over 90%, and production costs around ten times cheaper than commercial standards was selected as the best candidate as an *in-house* standard for the determination and quantification of CMP in adulterated milk.

ETHICAL APPROVAL

The present work does not require ethical approval

AL-O02

CHROMATOGRAPHIC TECHNIQUES FOR THE CHEMICAL PROFILE ANALYSIS OF COCOA FROM SANTANDER

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ABSTRACT

Cocoa beans are characterized by a complex sensory profile, which depends on their post-harvest processes. These define the sensory characteristics, in terms of flavor and aroma, not only of cocoa beans but also of their corresponding liquors. This is why in-depth characterization procedures are required, both for cocoa beans and liquors, in order to recognize the quality of the samples and thus be able to access differentiated markets.

Prior is even more relevant in Colombian cocoa-growing populations, where cocoa crops have become their primary economic source. Therefore, this work aims to characterize cocoa beans and liquors produced in Carmen de Chucuri (Santander) using chromatographic techniques. For this purpose, gas chromatography coupled to mass spectrometry (GC-MS) was used in two complementary analyses. On the one hand, volatile compounds that contribute to the sensory characteristics of cocoa liquors were identified using headspace solid-phase microextraction (HS-SPME). On the other hand, the analysis of fatty acids from cocoa beans was done by liquid-solid extraction, followed by derivatization by transesterification to obtain the volatile methyl esters. In addition, high-performance liquid chromatography (HPLC) was used to quantify theobromine and caffeine in cocoa beans.

Results obtained allowed the characterization of ten samples of cocoa liquors and beans in terms of volatile composition, fatty acid content, caffeine, and theobromine. Compounds such as esters, acids, alcohols, aldehydes, and ketones were identified as responsible for the liqueurs' aroma notes. In addition, statistical analysis (i.e., ANOVA, PCA) allowed for the determination of differences and grouping of the analyzed samples according to the content of chemical species. Further work is needed to develop chemometric tools to facilitate the characterization of cocoa samples in Colombia.

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AL-O04

VALORIZATION OF TANGERINE LEAVES (*Citrus reticulata*): SUPERCRITICAL CO_2 EXTRACTION TO OBTAIN ANTIOXIDANT AND NEUROPROTECTIVE COMPOUNDS

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ABSTRACT

An important approach to enhance the valorization of food waste involves extracting compounds known for their beneficial health properties, such as neuroprotective and antioxidant [1]. More than 600 neurological disorders have been recognized so far, with Alzheimer's disease being the most prevalent [2]. It is estimated that each year in the world citrus processing generates around 14 million tons of residues, including leaves [3]. In this sense, agro-industrial waste valorization represents an economic and environmental alternative for obtaining bioactive compounds. Therefore, this study aimed to identify, using chromatographic techniques, the compounds with potential antioxidant and neuroprotective activity in tangerine leaf (TL) (*Citrus reticulata*) var. Arrayana extracts. First, the extracts were evaluated by a set of in vitro bioactivity assays including enzymatic (acetylcholinesterase and butyrylcholinesterase) and, as well as antioxidants (ABTS, DPPH and ORAC). Considering the ecological character of supercritical CO_2, extraction conditions were optimized considering pressure (100, 200, and 300 bar) and temperature (40, 50, and 60°C). Soybean oil was enriched with optimal extract to evaluate oxidative stability by including it as an ingredient in a food. The extract obtained at 288 bar and 36 ºC, presented a lower degree of lipid oxidation. Gas chromatography-mass spectrometry GC-MS allowed the identification of terpenoids, such as linalool, ho-trienol, thymol, β-caryophyllene, spathulenol, phytol, and squalene in CO_2 extracts. The TL extract obtained with CO_2 showed the greatest potential in terms of biological activity. Therefore, the developed CO_2 extraction method can be benefit from the use of chromatographic techniques to identify bioactive compounds and correlate them with their specific activities and functions, thus offering a sustainable alternative for valorizing mandarin waste.

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AL-O05

LIPID REMODELING IN RESPONSE TO DROUGHT STRESS IN WHEAT PLANTS INOCULATED WITH A TRIPARTITE MICROBIAL CONSORTIUM

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ABSTRACT

The drastic changes resulting from climate change have made drought a major limiting factor in crop production, with wheat being one of the most affected cereals due to its global and national importance. Consequently, there is a pressing need to explore tools to mitigate the effects of water stress, mainly the drought. One promising alternative is the use of bioinoculants in consortia composed of different groups of microorganisms. In this study, we evaluated the lipid profile that mediates the increase in drought tolerance in wheat plants inoculated with a microbial consortium consisting of *Claroideoglomus lamellosum*, *Naganishia albida*, and *Burkholderia caledonica*. Two treatments (control and microbial consortium) with five replicates each were conducted (n = 10). An untargeted metabolomic analysis was performed to identify a broad spectrum of lipids present in the leaves of wheat plants inoculated with the most effective consortium under water stress conditions. The untargeted lipidomic analysis was carried out using a UHPLC-DAD Bruker Elute LC system coupled with a Q-TOF spectrometer Compact (Bruker, Bremen, Germany). Lipid annotation was conducted using the MS-DIAL software version 4.9.221218. The processed data (CSV format) was exported to MetaboAnalyst 6.0 (https://www.metaboanalyst.ca/) for univariate and multivariate analysis. Tolerance under drought conditions was improved by inoculation with the microbial consortium, and this improvement was mediated by an increase in glycerolipids (TG 52:6, TG 53:3, TG 58:6, TG 56:6, EtherDG (DG O-42:4)), sphingolipids (Cer_NS (Cer 44:2;O2)), and sterol lipids (SISE (SE 29:1)). Additionally, significantly expressed lipids were identified, with two sphingolipids—ceramide phosphoinositol (PI_Cer) and ceramide non-hydroxy fatty acid-sphingosine (Cer_NS)— and EtherDG (DG O-42:4) being the most positively and negatively regulated, respectively. This study provides valuable insights into the lipidomic profiling of wheat plants inoculated with different types of microorganisms under water stress conditions.

AMB-O01

BIOCHAR FROM A 'WASTE TO TREASURE' PERSPECTIVE: CONVERSION OF CORN STOVER INTO A CATALYST FOR HYDROGEN PRODUCTION FROM NABH$_4$.

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ABSTRACT

Agricultural production generates 23.7 million tons of food daily [1], resulting in 0.14 trillion tons of waste, expected to increase by 60% by 2050 [2], thereby contributing to global warming. In this context, the utilization of agro-industrial waste for biocomposites, biofuels, and bioenergy production emerges, highlighting its potential to transform 'waste' into valuable products or 'treasure' [1-3]. The aim of this study was to produce biochars derived from corn husk (BCS) impregnated with cobalt and reduced with NaBH$_4$ (BCS-CoB) to obtain catalysts for hydrogen production through sodium borohydride hydrolysis. The catalysts were characterized using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and X-ray diffraction (XRD). The biochars exhibited an increase in yield with cobalt impregnation, rising from 30.9% for BCS to 58.4% for BCS-CoB. SEM analysis of BCS-CoB revealed the formation of highly dispersed amorphous aggregates on the biochar surface, characterized by a rough appearance. EDS indicated an expressive concentration of cobalt and oxygen, indicating successful metal incorporation. XRD results confirmed highly amorphous structures associated to Co-B deposition on the biochar. In catalytic tests, a hydrogen generation rate of 1764.06 mL.min^{-1}.g^{-1} was achieved, under optimized conditions. The catalyst demonstrated potential for reuse in 4 cycles, retaining approximately 50% of its initial activity. Also, the catalyst exhibited magnetic properties, enhancing its practicality and suitability for continuous use, demonstrating the potential of agricultural waste for catalysts development underscores its environmentally friendly nature, utilizing waste that would mitigates its negative environmental impact.

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AMB-O02

ANALYSIS OF POLYCYCLIC AROMATIC HYDROCARBONS EMISSIONS AND THEIR IMPACT IN AIR QUALITY OF THE MANIZALES CITY USING A NOVEL HELIUM GAS BALLOON-SPME AS EXTRACTION DEVICE AND ITS ANALYSIS BY GC-MS

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ABSTRACT

Air pollution is the world's leading cause of environmentally related deaths, and results in tremendous environmental, social and economic costs [1]. World Health Organization (WHO) estimates air pollution is responsible for almost 7 million premature deaths in 2012 [1]. There is a class of pollutants called polycyclic aromatic hydrocarbons, generated by incomplete combustion [2]. They are formed by fused rings of benzene [2]. Its production sources are of anthropic and natural origin [3]. The United States Environmental Protection Agency issued a classification list with 16 compounds of this nature [3]. Different samplings are currently being carried out in the atmosphere of Manizales through the Helium Gas Ballon -SPME-GC-MS. The novel extraction device developed has been usefulness and with a simply assemble for air monitoring. Different types of compounds related to benzene rings have been found. Naphthalene has been found in the Milan Zone (Touristic site) and in the Government Building (city center). Finally, diagnostic relationships will be established on the possible emission sources.

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AMB-O03

IMPACT ON THE EXTRACTION OF DEPSDIDES AND DEPSIDONES FROM *Sticta caulescens* USING GREEN SOLVENTS: TOWARDS A SUSTAINABLE CHEMISTRY OF NATURAL PRODUCTS

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ABSTRACT

Chile is a country with a wide biodiversity of lichens due to both its geographic and climatic conditions. However, knowledge about secondary metabolites of some species is limited, such as *Sticta caulescens* lichen. Therefore, it is important to study extraction and identification methods for secondary metabolites in this species. To address this objective, green chemistry techniques were employed [1], specifically green solvents and unconventional extraction methods, to minimize environmental and health impacts associated with the extraction of secondary metabolites. In particular, microwave-assisted extraction (MAE) was used with ethyl lactate as a green solvent to improve extraction efficiency and minimize environmental impact [2]. Analytical techniques, such as UHPLC-Q/TOF/ESI/MS/MS, were employed for the characterization and tentative identification of secondary metabolites present in *Sticta caulescens* lichen. Conventional extraction techniques, using methanol as solvent, were compared with the unconventional extraction method of MAE using ethyl lactate as green solvent. A total of 21 metabolites were identified and characterized in the lichen *Sticta caulescens* using conventional extraction through maceration with methanol. Additionally, 22 metabolites were identified and characterized using the unconventional MAE with ethyl lactate. These results indicate that MAE, employing ethyl lactate as a solvent, is a viable alternative method for the extraction of secondary metabolites in *Sticta caulescens* lichen.

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AMB-O04

STUDY OF THE UP-TAKE OF NON-STEROID ANTI-INFLAMMATORY DRUGS BY AQUATIC PLANTS

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ABSTRACT

The most frequently consumed medicines in the world are non-steroidal anti-inflammatory (NSAID) [1]. Some of these compounds can enter to the environment through wastewater treatment effluents, which transport them to supply sources, used for consumption or for irrigation of agricultural crops [2]. In this work, the transformation of NSAIDs compounds (ibuprofen, diclofenac, naproxen and piroxicam) was evaluated in the aqueous medium during their interaction with the *Salvinia adnata* (salvinaceae) plant for 25 days, divided into two periods: 1) up-take (15 days), and 2) excretion (10 days), and for 25 days, the interaction of NSAIDs in solution with and without exposure to natural sunlight was evaluated. The extraction of the NSAIDs and their metabolites from the water was carried out using the solid-phase extraction (SPE) with Strata-X® cartridge (100 mg). Extraction efficiencies of 94-99% were obtained, with sample adjustment at pH 6, elution with methanol (12 mL) and without cartridge saturation at three concentration levels (2, 10 and 100 µg L^{-1}). In leaves and roots of the collected plant material, solid-phase matrix dispersion extraction (MSPD) was carried out with a ratio of vegetable material: silica gel modified with C_{18} (1:10), as elution solvent (10 mL) a solution of 3% (v/v) formic acid in ethyl acetate: methanol (60:40 v/v). With the MSPD technique, acceptable extraction efficiencies of NSAID were obtained in the *Salvinia adnata* plant (87-105%). The analysis of the MSPD and SPE extracts was carried out by UHPLC-ESI-Q-*Orbitrap*-HRMS. The hydroxylated metabolites and photochemical degradation product of the NSAID were the main compounds detected and semi-quantified in the aqueous and vegetable samples analyzed. This study could be useful to monitor the process of up-take and excretion of NSAID and their biotransformation products in contaminated with NSAID.

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AMB-O05

Analysis of organochlorine compounds present in leachate fraction from avocado crop soil using the RSDE-SPME technique and gas chromatography with electron capture detector GC-ECD

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ABSTRACT

The intensive agriculture pressures to soil for high performance and low times to recover, in this sense a lot of substances are required for keeping the health of soils such as humus, fertilizers, pesticides, among others, the last one pose significant challenges due to their varied and complex impact on ecosystems [1]. Some pesticides, such as organochlorines (OCs), have the ability to accumulate progressively along the food chain, concentrating on the species' adipose tissues and showing increasing biomagnification as they advance in the food chain. This bioaccumulation poses a significant risk to organisms at higher trophic levels, including humans [2].

The novel method developed is on the green chemistry ideology. For the analysis of OCs in the leachate fraction from avocado crop soils have been required the coupled of the two microextraction well wide known techniques: the RDSE and SPME. The release and extraction of target compounds in one step. The first one holds the solid waste sample and the second one does the extraction in the immersion mode. The lixiviation time and the extraction temperature and time were evaluated using a doehlrt design with 15 experiments. For the validation method was necessary to clean the crop soil sample from the analytes and their interferences and used as blank, and over them was spiked the target analytes to demonstrate the matrix effect, signal/noise ratio, enrichment factor, calibration curve, recovery and precision.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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AMB-O08

ANALYSIS OF CHLORINE DESINFECTION BY-PRODUCTS (HALOACETIC ACIDS AND TRIHALOMETHANES) BY HS-SPME-GC-ECD IN DRINKING WATER FROM CAUCA REGION

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ABSTRACT

The disinfection of water is conducted to remove and deactivate pathogens to ensure drinking water quality safety and protection of public health. Chlorine and its derivatives are still the conventional and highly preferred agents due to their multiple advantages. However, they may react with organic matter present in the raw water, which are not efficiently removed prior to the chlorination process in drinking water treatment plants-DWTP. Therefore, this oxidative reaction promotes the formation of other substances classified as disinfection byproducts - DBP´s, in which the two main groups are Haloacetic acids (HAAs) and Trihalomethanes (THMs) [1]. These compounds represent a risk to human health due to its mutagenic and carcinogenic nature and are currently regulated by Environmental Protection Agency (EPA) [2] and World Health Organization (WHO) [3]. In this research we analyze drinking water samples from DWTP in Popayan city, specifically from the Las Piedras River basin. In this opportunity we use a method based on Head Space-Solid Phase Micro Extraction (CAR/DVB). The trihalomethanes were directly extracted by sample at 60 °C and desorbed in injection port of gas chromatograph-electron capture detector with detection limits of 0.03 µg/L. The HAAs were extracted at first with metil terbutil eter, then were derivatized with methanol and finally the esters derived from acids were extracted by HS-SPME [4] and analyzed as well. The levels were within the permitted limits. Concentrations less than 20 µg/L of chloroform were found and less than 2,0 □g/L of dichloromethane, chlorodibromomethane and bromoform were detected, the WHO guide value was 0.09. While □HAA5 levels were bellow to 60 µg/L, the most abundant was the trichloroacetic acid with less than 41 µg/L.

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AMB-O10

DETERMINATION OF ORGANOCHLORINE-ORGANOPHOSPHORUS PESTICIDES AND SUGARS IN HONEY OF COLOMBIAN APIARIES BY HPLC AND GC

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ABSTRACT

Colombia is one of the countries with the greatest diversity of bee species in the world, with over 600 species. These are fundamental in sustaining ecosystems and crops, in addition, their products have commercial value. Which is why beekeeping has developed and become more technical in recent years in different regions of Colombia [1]. Since 2013, interest in quantifying pesticides in bee products has increased, using high-performance liquid chromatography (HPLC) for the analysis and quantification of these in such matrices, using different sample preparation methods [2]. Liquid-Liquid extraction (ELL) was used in the preparation of honey samples and were analyzed by HPLC - Mass Spectrometry (MS) [3]. The development of the QuEChERS methodology, which consists of the extraction of the sample with solvent followed by cleanup, based on dispersive solid-phase extraction; this method showed adequate recovery percentages and a minimum of interfering substances in fruits and vegetables [4]. In the present work, 3 analytical methodologies are developed for the determination of pesticides and sugars in honey by HPLC and Gas Chromatography (GC) using QuEChERS; the preparation of samples for the determination of organochlorine and organophosphorus pesticides by GC with electron capture detector was established. Also, it in this same preparation, the aqueous phase is taken for the determination of neonicotinoid pesticides by HPLC. Finally, a HPLC methodology is established for glucose, lactose, and fructose determination in honey. In conclusion, these methods allowed to quantify the pesticides and sugars present in the honey from 100 apiaries in Colombia.

Acknowledgments to Colciencias and Universidad del Quindio.

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AMB-O11

DETECTION OF SPECIALIZED METABOLITES BY GC-MS AND LC-MS PRESENT IN SEAWEEDS THE MANGROVES *Rhizophora mangle* AND *Avecennia germinans* FROM BUENAVENTURA – COLOMBIA

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ABSTRACT

Seaweeds are of great interest due to their abundance of bioactive compounds with biotechnological applications in different industries, including pharmaceutical, cosmetic, food and agronomic. The objective of this study was to characterize the phytochemical and nutritional composition of different species of algae associated with mangroves. Samples of *B. calliptera*, *R. riparium* and *C. impudica* were collected in Buenaventura (Valle del Cauca).

The nutritional composition was determined by analyzing the content of ash, protein, crude fiber and minerals. The extracts were obtained with ethanol. The nutritional composition analysis showed variability among species: ash content (16.9 to 31.5%), protein (14.6 to 25.0%) and crude fiber (2.52 to 30.2%). Macro minerals, including nitrogen (2.38 to 4.01%), potassium (3.01 to 3.50%) and sulfur (2.94 to 7.06%) showed little variable ranges, except for sodium (7330-46700 mg/kg). Micronutrients such as iron (1880-9180 mg/kg), manganese (204-4730 mg/kg) and copper (20.7-73.1 mg/kg), showed greater variability. In the preliminary phytochemical characterization, alkaloids, sterols, triterpenes, cardiotonic glycosides and saponins were detected in all species.

These compounds are known for their antioxidant, antibacterial, anti-inflammatory and anticancer properties. Metabolites were analyzed by gas chromatography coupled with mass spectrometry (GC-MS) using a Shimadzu GCMS-QP2010 Ultra, and long-chain methylated molecules and ester derivatives were found. Additionally, the extracts were analyzed with a Q_TOF 6545 electrospray ionization (ESI) mass spectrometer. The analysis was performed in positive ESI mode, with a scanning range of 50 to 1100 m/z (Full scan). Comparison of the compounds was performed using principal component analysis (PCA) and a focus was placed on the detection of phytohormones. These findings are expected to contribute to the knowledge for the sustainable use of mangrove ecosystem resources in the Colombian Pacific region.

CF-O01

COMPARISON OF GC-MS AND UHPLC-ORBITRAP-HRMS FOR THE ANALYSIS OF NOVEL PSYCHOACTIVE SUBSTANCES AND ITS METABOLITES IN FORENSIC SAMPLES

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ABSTRACT

The increase in the abuse of novel psychoactive substances, especially anesthetics and synthetic opioids, has generated a public health and police emergency. In several countries, the rates of deaths and adverse events related to drug use have risen, as well as phenomena related to criminality, gun violence, and mental health problems remarkably in school age teenagers and young adults.

It is an imperative need for the forensic toxicology system determine the best methodologies for the reliable identification of these type of drugs and its metabolites, to contribute to the efficiency of the administration justice, and effective intoxication treatment at emergency services.

In this work, 19 urine forensic samples were analyzed by gas chromatography-mass spectrometry (GC-MS) and UHPLC-Orbitrap-HRMS to examine the advantages and limitations of these commonly used instrumental methods in forensic analysis. The comparison between the two methods indicated that there is significant difference in the performance and analytical results. Both low and high resolution, allow the detection of ketamine as a main component of Colombian NPS cocktail “tusibi”, however, a higher mass accuracy and resolution instrument allowed high-confidence identification of parent drugs and the tentative annotation of several metabolites, in the other hand proposed metabolic pathways, drug-drug interactions mechanism, and intoxication status associated with the cause and manner of death has been possible also.

Keywords: novel psychoactive substances, mass spectrometry, urine, metabolites, drug-drug interaction.

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CF-O02

FORENSIC METABOLOMICS: TRACING CYANIDE-INDUCED METABOLIC CHANGES IN FATALITIES

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ABSTRACT

Accurate detection of cyanide exposure is crucial, particularly in forensic science. However, cyanide's high volatility and potential biochemical conversions in biological samples pose challenges for direct detection, complicating the determination of cause of death. Identifying alternative cyanide metabolites as markers may mitigate false negatives and positives, extending the detection window in poisoning cases. This study aimed to evaluate metabolic changes induced by cyanide exposure in forensic cases using a multi-platform approach, including metabolomics and lipidomics analyses via liquid and gas chromatography coupled with high-resolution mass spectrometry. Results demonstrated clear discrimination between cyanide-exposed and control groups through OPLS-DA models. A total of 92 altered metabolites were identified in cyanide-exposed individuals compared to controls. Significant changes in metabolites primarily included glycerophospholipids (30.7%), glycerolipids (14%), fatty acyls (12.9%), sphingolipids (8.0%), amino acids and analogs (8.0%), among others. Cyanide intoxication disrupted multiple metabolic pathways, including mitochondrial β-oxidation, acylcarnitine accumulation, a shift towards gluconeogenesis in amino acid metabolism, and ammonia homeostasis disturbance, affecting both ammonia recycling and the urea cycle. These pathways are essential for cellular energy production. The altered metabolic profiles provide insight into cyanide poisoning pathways, potentially aiding the development of new forensic diagnostic strategies. The area under the receiver operating characteristic curve was used to assess each model's predictive value. Findings suggest that metabolites such as phosphate and 3-hydroxybutyric acid could serve as diagnostic biomarkers in lethal cyanide poisoning cases. Future studies must evaluate these potential biomarkers' effectiveness in different fatal victim cohorts and validate the suggested panel through a targeted approach.

ETHICAL APPROVAL

Approval was obtained following the Declaration of Helsinki and Colombian laws, including Decree 786 of 1990 on autopsies and viscerotomies.

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Project "Development of new analytical techniques for detecting volatile toxics, carbon monoxide, and cyanide in forensic cases," registered as I-2021-09 at the INMLCF, in collaboration with UTP.

CF-O03

CHEMICAL CHARACTERIZATION BY HS-SPME-GC/MS OF THE VOLATILE FRACTION OF DECOMPOSING MICE

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ABSTRACT

The decomposition process of mammals has been the subject of extensive research, and its study is critical in forensic chemistry [1]. This research aims to determine the chemical composition of the volatile fraction of mice during a decomposition period of three months. Two dead *Mus musculus* mice were buried in a pot with organic substrate and two were placed in aluminum trays. Volatile compounds of decomposing mice were monitored at 1-5,10,15,19,24,30,36,40,43, 50,53,59,72,88 and 110 days by headspace solid-phase microextraction coupled to gas chromatography with mass spectrometry detection (HS-SPME-GC/MS), using a carboxen-poly(dimethylsiloxane) (CAR/PDMS, 85 µm) fibre for HS-SPME monitoring. A total of 42 compounds were tentatively identified by GC/MS in the volatile fraction of decaying mice. On day forty three, the highest emission of compounds was recorded, among which were butanoic acid (37,2%), 4-methylpentanoic acid (20,7%), acetic acid (20,5%), 4-methylbutanoic acid (10,4%), and propanoic acid (2.7%). After analyzing the emitted volatile organic compounds, a decomposition pattern has been established to accurately determine the postmortem interval, allowing for the identification of an approximate time range.

ETHICAL APPROVAL

The project was approved by the ethics committee of the Universidad Industrial de Santander (CEINCI - UIS), Act N° 13 of May 3, 2024.

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EDU-O01

Estudio comparativo de los compuestos volátiles en sudor de mujeres y hombres por HS-SPME-GC-MS

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ABSTRACT

La extracción de compuestos orgánicos volátiles presentes en camisetas de hombres y mujeres jóvenes (entre 20 y 25 años), se realizó mediante microextracción de fase sólida en modo espacio de cabeza y posterior análisis por cromatografía de gases acoplada a espectrometría de masas (HS-SPME-GC-MS) empleando una fibra de Divinilbenceno/Carboxeno/Polidimetilsiloxano.

Los compuestos volátiles identificados en la camiseta del hombre, fueron asociados a notas frutales, florales y cítricas, mientras que en la camiseta de la mujer predominaron las notas verdes, florales y cítricas. Se observó que en el sudor de la mujer, la abundancia de compuestos con aroma característico varió entre 0,65% y 21,17%, en comparación, en la muestra de sudor de hombre, la abundancia de estos compuestos estuvo entre 0,27% y 3,29%. Los principales compuestos identificados en el sudor de hombre fueron Limoneno, acetato de isoamilo, n-Decanal y p-Metoxibenzaldehido, y en el sudor de mujer γ-Terpineno, Limoneno, n-Nonanal, n-Decanal, y (E)-2-Hexenal

También se evaluaron los umbrales de olor hombres y mujeres. Se logró evidenciar que las mujeres presentan valores de umbrales más bajos para notas cítrica, frutal y verde, asociadas a citral, acetato de isoamilo y Z-3-Hexenol respectivamente.

Agradecimientos:

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EDU-O02

ANÁLISIS DE COMPUESTOS VOLÁTILES OLFATIVAMENTE ACTIVOS EN ACEITE ESENCIAL DE CANELA Y EUCALIPTO Y SU RELACIÓN MULTIMODAL CON EXPERIENCIAS AUDITIVAS

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RESUMEN

Se realizó la identificación de compuestos en aceites esenciales de eucalipto y canela utilizando cromatografía de gases acoplada a olfatometría y espectrometría de masas (GC-O-MS), mediante la comparación de sus espectros de masas e índices de retención lineal (IRL), calculados y verificados con la base de datos del NIST, además de la evaluación sensorial del perfil cromatográfico por olfatometría.

Se encontró que el eucaliptol constituye el 72,5% del contenido en el aceite de eucalipto, mientras que en el de canela, el eugenol representa el 84,4%, junto con un 1,8% de acetato de cinamilo, responsable de las subnotas características de canela. Además, se exploró la relación entre las propiedades olfativas de estos compuestos y la percepción auditiva, sugiriendo una posible correlación entre las notas olfativas y patrones musicales, integrando un enfoque multimodal que conecta la experiencia sensorial del olfato con la experiencia auditiva.

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PN-O01

CARACTERIZACIÓN QUIMICA DE ALGUNOS COMPONENTES PRODUCIDOS POR *Klebsiella pneumoniae* MEDIANTE CG-EM FRENTE A TRATAMIENTOS CON EXTRACTO ETANÓLICO DE *Hypericum goyanesii*

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ABSTRACT

Klebsiella pneumoniae es una bacteria de la familia Enterobacteriaceae con gran interés científico por su notable resistencia a los antibióticos y su capacidad para causar múltiples infecciones nosocomiales [1]. Uno de los tratamientos de control de la resistencia bacteriana es la inhibición del Quorum Sensing (QS) asociado a la producción de distintos compuestos que son clave en la formación de biopelículas, factores de virulencia y mecanismo de defensa [2]. *Hypericum goyanesii* (HG), es tradicionalmente utilizada para tratar diversas afecciones, por lo anterior, el objetivo de la presente investigación es determinar cómo extractos de HG son capaces de modular la producción de algunos de los componentes generados por *K. pneumoniae* [3].

De esta manera se realizó el montaje con tratamientos a 250 y 125 ppm del extracto etanólico de HG, y en presencia de inoculo de *K. pneumoniae* con densidad óptica de 0.9 (24h – 37°C, 180 rpm) y usando como medio cultivo caldo Luria Bertani (LB), además de los controles positivos y de medio, pasadas 24 horas se realizó la extracción. El residuo se redisolvió para su análisis usando un cromatógrafo de gases acoplado a un espectrómetro de masas (CG-EM) Shimadzu QP 2010 plus, con inyector de tipo Splitless, con gas portador Helio grado 5.0, Flujo de 0.86 mL/min, columna capilar HP-5 MS (30 m x 0,25 x 0,25), con rampas de temperatura iniciando en 70ºC, para el EM se usó una fuente de ionización por impacto electrónico (IE) a 70 eV, y un cuadrupolo en modo full Scan.

De esta manera se logró observar la presencia tentativa de Anfetamina N-Metoxicarbonil (C1) y del 1-triptófano N-formil (C2), entre otros, evidenciando que los compuestos C1 y C2 disminuían en su porcentaje de área en presencia de los tratamientos a las concentraciones evaluadas, dicha disminución más marcada con el compuesto C1, el cual fue comparado con el control de gentamicina que logro una disminución de C1 apenas significativa. En este contexto es importante resaltar que el extracto de HG cumple una función moduladora frente a estos dos compuestos y que posiblemente la disminución de dichos componentes pueda estar relacionado con la comunicación bacteriana.

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PN-O02

UNTANGLING ANCESTRAL WISDOM: BIOACTIVE COMPOUNDS IN AMAZONIAN STEM BARKS USING LC-MS/MS AND GC-MS

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ABSTRACT

This research merges traditional Amazonian knowledge with modern analytical techniques to identify antimicrobial compounds. Aqueous stem barks from *Aspidosperma rigidum* Rusby, *Couroupita guianensis* Aubl, *Monteverdia laevis* (Reissek), and *Protium sagotianum* (Marchand) have been employed as traditional remedies in the Amazon region, mainly against diseases caused by Sars-COV-2 infection [1,2]. We analyzed the metabolic profiles using liquid and gas chromatography coupled with mass spectrometry (UHPLC-MS/MS and GC-MS). The chemical composition of the plants was compared by principal component analysis (PCA). The antimicrobial and toxicity results of their extracts were correlated with their phytochemical profiles by Pearson's correlation. Analysis revealed 20 compounds. *C. guianensis*, inhibited all tested microorganisms, including antibiotic-resistant strains. Molecular networking, i*n silico tools*, and Pearson's correlation suggest that antifungal compounds could belong to the terpene glycoside ($r = 0.918$) and/or phenolic ($r = 0.882$) metabolite classes. This study demonstrates the value of established techniques in uncovering the metabolic profiles of these plants, a key step in identifying potential antimicrobial drugs.

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PN-O03

PRELIMINARY ANALYSIS OF *Tibouchina grossa* BY LC-MS, HPLC-DAD AND ANTIFUNGAL POTENTIAL AGAINST *Fusarium oxysporum*

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RESUMEN

Tibouchina grossa (Melastomataceae) is an endemic species of the Colombian territory traditionally known as seven red leathers. Within its chemical composition, the presence of flavonoids and terpenes stands out, which have shown antifungal activity against phytopathogens that attack crops of commercial interest and are responsible for losses ranging between 20 and 40% of global agricultural productivity [1]. In the control of these phytopathogens, the use of chemical substances that turn out to be of low selectivity, harmful to the environment and humans is common; for this reason, the development of effective and safe phytosanitary agents is of great interest [2]. Due to the above, the purpose of this work was to carry out a preliminary phytochemical characterization of the leaves of *Tibouchina grossa*, where it was possible to preliminarily establish the presence of metabolites such as terpenes, quinones, alkaloids and flavonoids in the ethanolic extract, which is in agreement with other studies carried out on species of the genus such as *T. multiflora*, *T. grandifolia* and *T. urvilleana* [3]. Using HPLC-DAD and comparison with reference standards, the presence of gallic acid, quercetin and rutin was identified in the ethyl acetate fraction, which exhibited a percentage of mycelial growth inhibition of 27.87% at a concentration of 1000 µg/mL against *Fusarium oxysporum*. Finally, LC-MS (ESI, QTof) was used to tentatively identify glycosylated flavonoids such as isorhamnetin-3,4'-diglucoside, isoquercitrin and 3,5-O-di-β-glucoside peonidin, which are authentic markers of the *Tibouchina* genus. This study shows the moderate antifungal potential of *T. grossa* against *F. oxysporum* but suggests this species as an important source of secondary metabolites with another type of biological potential.

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PN-O04

HPLC AND LC/MS ANALYSIS OF PHENOLIC COMPOUNDS EXTRACTED FROM *Alstroemeria* var. Nadya FLOWERS

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ABSTRACT

The genus *Alstroemeria* belongs to the family Alstroemeriaceae, comprising approximately 120 species primarily found in Chile and Brazil. The flowers are known as the Peruvian lily, Inca lily, or lily of the Incas, renowned for their diverse colors. They are of significant commercial interest, with some used as ornamental plants or cut flowers for export [1]. Colombia ranks first in terms of *Alstroemeria* cultivation area [2]. In this study, biomass from *Alstroemeria* var. Nadya flowers were used. Extracts were obtained by ultrasound-assisted solvent extraction (EtOH: H2O, 1% CH_3COOH), and the chemical characterization of the hydroethanolic extracts was carried out by HPLC/DAD and UHPLC-ESI$^{+/-}$/*Orbitrap*-HRMS. The extraction yield was 9.56% and eight compounds were identified: *trans*-cinnamic acid; cyanidin-3-*O*-arabinoside, cyanidin-3-*O*-glucoside, and cyanidin-3-*O*-rutinoside; kaempferol-3-*O*-arabinoside, kaempferol-3-*O*-rutinoside, kaempferol-3-*O*-glucoside, kaempferol-3-*O*-glucoside-7-*O*-glucoside, and kaempferol-3-*O*-sophoroside. LC analysis showed that the extract was rich in phenolic compounds with high biological activity.

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PN-O05

MONOTERPENOID-BASED INSECTICIDES: EXPLORING AROMATIC SPECIES FOR THE CONTROL OF STORED PRODUCT PESTS *Sitophilus zeamais* AND *Tribolium castaneum*

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ABSTRACT

In the search for effective and safe insecticides to control stored grain pests, essential oils (EOs) are emerging as a promising alternative [1]. This study describes the fumigation and contact toxicity of four EOs (*Tagetes zypaquirensis*, *Anethum graveolens*, *Satureja viminea*, and *Minthostachys mollis*) and some of their major constituents against *Tribolium castaneum* and *Sitophilus zeamais*. The study was carried out in the following stages **a)** evaluation of the extraction yield of the EOs using three methods (steam distillation (AV), hydrodistillation (HD) and microwave-assisted hydrodistillation (HDMW)); **b)** chemical characterization of the EOs by GC-MS; **c)** isolation of the main monoterpenoids and preparation of derivatives; **d)** evaluation of insecticidal activity using fumigation and contact toxicity methods of EOs and isolated and synthesized compounds; and **e)** encapsulation of the most active oils in β-cyclodextrin by co-precipitation, characterization of the encapsulated product and evaluation of its fumigant activity against both insects [2,3]. Extraction yields were above 0.49% for *S. viminea*, *M. mollis* and *T. zypaquirensis* with dry material and for *A. graveolens* with fresh material. The best extraction method was HD for *S. viminea* and *M. mollis*, HDMW for *A. graveolens* and AV for *T. zypaquirensis*. The main components of the EOs were α-phellandrene and dill ether in *A. graveolens*, piperitone oxide and R-pulegone in *M. mollis*, R-pulegone and p-menth-3-en-8-ol in *S. viminea*, and dihydrotagetone and myrcene epoxide in *T. zypaquirensis*. *M. mollis* oil showed the highest fumigant activity and contact toxicity against both insects. R-carvone, piperitone oxide and R-pulegone were remarkable for their insecticidal potential. It was observed that the carbonyl group with conjugated double bonds in cyclic monoterpenes is important for the insecticidal activity. The encapsulated EOs showed higher activity against *S. zeamais* compared to *T. castaneum*, achieving the highest efficacy between 96 and 120 hours, with the encapsulated *S. viminea* being the most effective.

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PN-O06

CHEMICAL DIVERSITY OF THREE LICHENS OF GENUS *Graphis* (Graphidaceae) OF THE TROPICAL DRY FOREST FROM THE NORTHERN REGION OF COLOMBIA

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ABSTRACT

Lichens are specialized complex ecosystems formed by algae/fungi living in interspecific symbiosis, which produce secondary metabolites (lichen substances or extrolites) that function as a defense against pathogens/competitors and/or external abiotic factors acting as antibiotics, antifeedants, UV protectants, etc., but also as a tool for taxonomy of lichen-forming fungi [1-3]. In this work, the chemical compositions were determined by TLC/HPLC-DAD/MS (ESI) of total extracts from three lichens belonging to the genus *Graphis* of the tropical dry forest from the northern region of Colombia, and from one of them, two depsidones were isolated/structurally characterized (LC-HRMS, ^{1}H-^{13}C (DEPT135)-NMR). Consequently, the main results were: (i) stictic, norstictic and protocetraric acids were the representative depsidones for *G. dendrogramma* (Tubará), *G. dendrogramma* (Piojó) and *G. supracola*, respectively; (ii) the isolated depsidones were (–)-stictic and (+)-constictic acids from *G. dendrogramma* (Tubará). Therefore, it could be concluded that: (i) for the first time, extrolites other than protocetraric acid have been reported in *G. supracola*, as well as norstictic acid as major lichen-substance for *G. dendrogramma*; (ii) there was a chemical variability between *G. dendrogramma* collected in different places, although they contained stictic acid-derived depsidones, (iii) the main biomarker (stictic acid) reported in the scientific literature for one of *G. dendrogramma* (Tubará) was confirmed, and (iv) for the first time, the specific optical rotation for the isolated depsidones [(–)-stictic acid, (+)-constictic acid] was determined.

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PRE-O01

USE OF A NOVEL LUFFA-BASED BIOSORBENT FOR DETECTION OF PAHs IN WATER SAMPLES

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ABSTRACT

Luffa (*Luffa aegyptiaca*) is a natural fiber from a plant in the Cucurbitaceae family. It is composed of cellulose, hemicellulose and lignin. This material has high porosity, a large contact surface, is economical and biodegradable, which gives it properties that make it a good candidate for sorbent in analyte extraction processes [1]. In this study, the feasibility of applying Luffa as a biosorbent for the extraction of Polycyclic Aromatic Hydrocarbons (PAHs) in aqueous matrices and their subsequent quantification using HPLC-FLD was investigated. The preparation of the material was carried out in two stages; 1) disinfection with ethanol and ultrasound assistance and 2) functionalization with stearic acid, to change the polarity of the sorbent, with SEM and IR studies. For the extraction of PAHs, a portion of luffa is immersed in a standard solution of analytes and shaken for 2 hours to facilitate the transfer of the analytes to the solid support. Subsequently, the sorbent is introduced into an SPE glass cartridge. Using a manifold collector, two washes with ACN are carried out for the desorption of the analytes. The sample is preconcentrated with nitrogen at low flow until dry, and reconstituted with 1 ml of ACN for subsequent quantification by HPLC-FLD. Optimization tests were carried out on sample volume, extraction time, and Luffa mass, obtaining an optimum of 100 ml of sample, 120 minutes of extraction, and 40 g of Luffa mass respectively. The method was validated obtaining precision, accuracy, limit of detection and quantification. The proposed method was applied to real samples obtained from five different points in the city of Viña del Mar, Chile. The results show the great potential of the Luffa plant as a biosorbent, improving analytical parameters such as limit of detection and quantification and increasing the sustainability of the analytical procedure in the detection of PAHs. Furthermore, its functionalization is relatively simple and low cost.

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PRE-O02

CHEMICAL CHARACTERIZATION BY GC/MS AND LC/MS OF *Lippia origanoides*, *Lippia alba* and *Lantana canescens* EXTRACTS

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ABSTRACT

The Verbenaceae family stands out with species such as *Lippa alba*, known for treating diseases of the respiratory and gastrointestinal systems, among others [1]; *Lippia origanoides* has antifungal, anti-mycotoxigenic [2] and antioxidant properties [3]; *Lantana canescens* has anti-inflammatory and anti-hyperalgesic effects [4]. In this study leaves of two species of *Lippia*, a specie of *Lantana*, and their hybridizations were collected at the CENIVAM Agricultural Pilot Center (Bucaramanga, Colombia). The extracts were obtained by solid-phase matrix dispersion (MSPD). The chemical characterization was performed by GC/MS and GC/FID. Thymol (67,80 ± 0,03 %), geranial (51,34 ± 0,03 %), and *trans*-β-caryophyllene (13,90 ± 0,05 %) were the main compounds in *L. origanoides*, *L. alba* and *L. canescens*, respectively. In *L. alba* × *L. origanoides* was piperitenone oxide (36,40 ± 0,07 %), and in seven hybrids between *L. canescens* × *L. origanoides* was *trans*-β-caryophyllene (6,0 ± 0,2 %), (18,2 ± 0,1 %), (19,16 ± 0,04 %), (9,10 ± 0,01%), (15,0 ± 0,02%), (5,390 ± 0,006 %) and (24,22 ± 0,03 %). 43compounds were identified by UHPLC-ESI$^{+/-}$/*Orbitra*p-HRMS in *L. origanoides* (16), *L. alba* (15), and *L. canescens* (12) extracts. Erodyctiol ([M-H]$^{+}$, *m/z* 289.07037), tuberonic acid glucoside ([M-H]$^{+}$, *m/z* 389.18039) and luteolin-glucoside ([M-H]$^{-}$, *m/z* 447,09149) were the main compounds, respectively. In the chemical compositions of the hybrids *L. alba* × *L. origanoides* and *L. canescens* × *L. origanoides*, the compounds detected in the mother were mainly recorded. *trans*-β-Caryophyllene was the major compound in *L. canescens* and *L. canescens* × *L. origanoides* hybrids.

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PRE-O04

SINERGIC COMBINATION OF BIOCHAR AND CHITOSAN FOR THE ADSORPTION OF CARBAMAZEPINE AND ITS METABOLITES BY HPLC-UV DETECTION

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Recently, sample preparation has been linked to the design new sorbents from environmental friendly materials. Based on this, in our work group, sorbent phases from cork, peanut shell, avocado seed, banana peel and chitosan have been studied. Chitosan (CS) is a polymer biodegradable derived from crustacean shells. The -OH and -NH2 functional groups in their structure facilitate a high sorption performance and allow the engineering of structured materials. Despite their versatility, it has inherent drawbacks such as low porosity, high pH sensitivity, high swelling power and low chemical stability [1]. That is why their combination with other materials as carbon-derived is proposed in this work. Biochar (BC) is a porous solid material produced from the thermal decomposition of biomass in an oxygen-limited environment. BC has a specific structure and properties with a high porosity and large specific surface area [2]. Based on these advantages, the reinforcement of CS with wood BC is proposed for the design of a biocomposite material with multifunctional properties.

As a measure to increase the greenness of the methodology we propose the use of biocompatible cross-linking agents as citric acid, oxalic acid and polyethylene glycol methacrylate. To determine the sorbent capacity of carbamazepine and its metabolites, rotating disk sorptive extraction (RDSE) and HPLC-UV detection were used. The best cross linking agent was citric acid, which was selected based on the extractive capacity and mechanical stability of the material. The preparation of the biocomposite is summarized: 500 µL of CS (1%), 50 mg of BC and 30 mg of citric acid were thoroughly shaken by vortex and ultrasound for 30 min. Then, the material was placed in a silicone mold and formed by solvent evaporation. The RDSE was carried out for 60 min at 2000 rpm and the analytes were determined by a previously optimized HPLC-UV method at 220 nm. The results showed an extraction efficiency of the biocomposite close to 42%, synergistically improving the individual materials (BC 13% and CS 5%).

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PRE-O06

SIMPLE AND SENSITIVE HIGH-THROUGHPUT METHOD BASED ON 96-BLADES SPME AND HPLC-FLD FOR DETERMINATION OF OCHRATOXIN A IN WINES AND BEERS

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ABSTRACT

Ochratoxin A (OTA) is a mycotoxin occurring in a variety of commodities, such as grapes and cereals. OTA has been associated with severe pathological outcomes in animals, thus leading to the establishment of regulatory limits of OTA content in food and beverage samples. This work presents a high throughput method for the determination of OTA in wines (white and red) and beer using a 96-blades TFME (thin film microextraction) system and high-performance liquid chromatography coupled to a fluorescence detector (HPLC-FLD). Central Composite Design (CCD) was employed to optimize extraction and desorption times. Under the optimized conditions, within 150 min, 96 samples could be extracted, yielding extraction times of less than 1.6 min per sample. Validation of the method demonstrated proper sensitivity, with quantification limits of 0.01, 0.02 and 0.27 µg/L for red wine, white wine, and beer, respectively. Linearity, within 0.15-30 µg/L, exhibited coefficient of correlation (R^2) better than 0.999 in all matrices. Measured at three levels (0.3, 3.0, and 30 µg/L), precision, expressed as % RSD, and accuracy, expressed as relative recovery, met acceptance criteria established by Brazilian and European Union regulations. The validated method was applied to the analysis of commercial samples. The 96-blade SPME HPLC-FLD method herein presented is simple, features minimal sample handling, low solvent consumption, high sample throughput, low analysis cost and provides selective, accurate, and precise results.

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PRE-O07

MAGNETIC IONIC LIQUIDS FOR THE MONITORING OF BIOMARKERS IN BIOFLUIDS

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ABSTRACT

Magnetic ionic liquids (MILs) are materials derived from ionic liquids that present impressive solvation properties and inherit magnetism. Due to these properties, MILs are excellent candidates as extraction solvents in magnetic-assisted microextraction strategies, this way being applied in areas like bioanalysis, where rapid and highly sensitive analysis are required.

This study focuses on the development of miniaturized analytical methods involving MILs for the monitoring of urinary biomarkers, including hydroxylated polycyclic aromatic hydrocarbons (as cancer biomarkers) and benzophenones (as biomarkers of human exposure to personal care products). Two novel approaches are introduced: 1) dispersive liquid-liquid microextraction (DLLME) using novel bimagnetic MILs [1], and 2) an *in situ* DLLME method with solid effervescent tables prepared with MILs formed by paramagnetic cations [2]. Both applications permit the easy coupling with high-performance liquid chromatography and were successfully applied to the analysis of real samples for voluntary subjects.

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PRE-O08

COMPARATIVE STUDY OF COMPRESSED FLUIDS FOR THE EXTRACTION OF STAPHYLOXANTHIN FROM *Staphylococcus aureus:* CHEMICAL PROFILING, ANTIOXIDANT ACTIVITIES, AND MULTIVARIATE ANALYSIS

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ABSTRACT

Staphyloxanthin (STX) is a virulence factor in *Staphylococcus aureus*, a lipid-based carotenoid found in the bacterial membrane that contributes to resistance against antimicrobial peptides and oxidative stress. Despite being over four decades old, the same STX extraction method is still widely used. In this study, various compressed fluid technologies were employed to extract carotenoids and fatty acids from *S. aureus* cells. These included supercritical fluid extraction (SFE) using CO_2 and ethanol (15%), gas-expanded liquid extraction (GXL) with CO_2 and ethanol (50% and 80%), and pressurized liquid extraction (PLE) with ethanol and ethyl acetate. Five *S. aureus* strains were analyzed, one of which had the CrtM gene, responsible for STX biosynthesis, inhibited. PLE with ethanol, under conditions of 100 bar, 125°C, and 20 minutes, yielded good carotenoid extraction efficiency and selectivity. Carotenoid identification and quantification of 18 carotenoids were carried out using liquid chromatography coupled with diode array detection and tandem mass spectrometry (LC-DAD-MS/MS), revealing significant statistical differences in carotenoid production between the four strains that synthesize bacterial carotenoids, comparing PLE results with conventional extraction methods. Significant differences were also noted in fatty acid profiles across the five strains when analyzed using gas chromatography-quadrupole time-of-flight mass spectrometry (GC-QTOF-MS). Additionally, the antioxidant activities of carotenoid-producing and non-carotenoid-producing *S. aureus* strains were compared. The antioxidant activity results, determined by DPPH and lipophilic ORAC assays, were correlated with carotenoid concentrations in the strains. Principal component analysis (PCA) accounted for 82.13% of the variance in cross-validation, based on the chemical composition and bioactivity of the different extracts. The model predicted a positive effect of ester-4,4´-DNPA, STX, certain STX homologs, and dehydro-STXs, while showing a negative effect of 4,4´-DNPA and other STX homologs in bacterial carotenoids related to oxidative stress tolerance.

PRE-O09

PURIFICATION OF CASEINOMACROPEPTIDE FROM MILK WHEY THROUGH SOLID PHASE EXTRACTION.

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ABSTRACT

The identification of milk adulterated by whey is a recurrent problem in Latin American and European countries due to the difficulties involved in its analysis in terms of sample pretreatment and the high cost of standards. Caseinomacropeptide (CMP) is a biomarker employed in determination of adulterated milk with cheese whey. CMP is normally found in cow's milk at very low concentrations; although, it can be produced by enzymatic hydrolysis of milk with chymotripsin, which specifically cleaves *k*-casein, the main protein present in cow’s milk, yielding two peptides, one which is CMP that remains dissolved in the whey [1]. CMP can also exist as a glycosylated peptide denoted glycomacropeptide (GMP) and it can present two genetic variants denominated CMP-A and CMP-B, which differ on few residues of the sequence. These differences present a significant challenge in standardization of analysis techniques involving these compounds. The present work focuses on CMP obtention from milk whey through RP-SPE purification from different samples containing it. Milk whey extract obtained by RP-SPE was analysed using a Bruker Impact II ESI-Q-TOF LC-MS system, which was found that this strategy allows to separate CMP-A and CMP-B from cow’s milk involving close to none sample pre-treatment, allowing the obtention of a low cost *in-house* standard with potential use as an important biomarker in the milk industry.

ETHICAL APPROVAL

The present work does not require ethical approval

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PRE-O10

FUNCIONALIZACIÓN DE CALIX [4]RESORCINARENOS CON GRUPOS MALEIMIDA POR REACCIÓN DE MANNICH: SEGUIMIENTO DE LA REACCIÓN POR RP-HPLC Y PURIFICACIÓN POR RP-SPE

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ABSTRACT

Los calix[4]resorcinarenos, macrociclos polihidroxilados compuestos por cuatro unidades de resorcinol, son compuestos altamente versátiles y permiten la posterior incorporación de grupos funcionales como maleimidas, que facilitan reacciones modulares. La separación y la purificación de estas macromoléculas, y sus derivados funcionalizados, representan un desafío importante. La reacción de Mannich es empleada para funcionalizar estas macromoléculas, porque permite la adición de grupos en las posiciones 2 de las unidades aromáticas mediante una sustitución electrofílica aromática (SEAr) con aminas primarias o secundarias [1]. En este estudio, se sintetizó C-tetrapropilcalix[4]resorcinareno, y luego fue funcionalizado con 1-(2-Aminoetil)maleimida, en presencia de formaldehído, a pH 7.5. Para el análisis de los productos mono, di, tri y tetrasustituidos se empleó inicialmente una columna Kinetex C18 (2.6 µm, 100 Å) y un gradiente del 5-100 % de acetonitrilo en agua (ambos con TFA 0.05%), durante 10 minutos. Los análisis mostraron baja resolución entre los productos. Posteriormente, se empleó una columna con una mayor porosidad, Chromolith High Resolution RP-18e, con el mismo programa de elución. Esta columna permitió una mejor resolución en los productos de la reacción gracias a sus diferencias en los tipos de poros [2]. Finalmente, el método fue transferido a una columna de RP-SPE, y se logró separar los productos [3], que fueron caracterizados por RP-HPLC y LCMS. En conclusión, fue posible hacer la separación de los productos funcionalizados gracias a la tecnología y metodología empleada con columna monolítica gracias a su mayor tamaño, tipo de poro y estructura continua que facilitó la difusión y separación de estas grandes macromoléculas. En contraste, la columna Kinetex, de tipo core-shell, al presentar poros mas pequeños y limitados a la capa externa de las partículas, restringió la capacidad de separar eficientemente estas macromoléculas de mayor tamaño. Este método de análisis puede ser fácilmente aplicable para otras macromoléculas derivadas de calix[4]resorcinarenos.

ETHYCAL APPROVAL

The present work does not require ethical approval.

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SA-O01

DEVELOPMENT OF A NOVEL, INEXPENSIVE AND RAPID METHOD TO QUANTIFY KREBS CYCLE INTERMEDIATES BY HPLC-UV

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ABSTRACT

The Krebs cycle, or tricarboxylic acid (TCA) cycle, is a vital biological process linked to glycolysis, lipid, and amino acid metabolism. Intermediates of this cycle serve as biomarkers offering valuable insights into pathological conditions related to the absence or overexpression of these compounds. Given the low molecular weight, limited retention in reverse phase, and absence of chromophores in TCA, analytical methods such as liquid chromatography coupled with mass spectrometry (LC-MS) are commonly used due to their sensitivity, precision, and accuracy, though they come at a high cost and require complex instrumentation, trained personnel, and deuterated standards [1]. Alternatively, liquid chromatography coupled with fluorescence, while efficient for TCA analysis, involves complex derivatization pretreatments, adding time and complexity [2]. In this study, a quantitative method using HPLC-UV was developed to analyze nine Krebs cycle intermediates, achieving a resolution greater than 2 in under 9 minutes. Optimization of chromatographic parameters as mobile phase, pH, column selection, workflow, injection volume, and temperature enhanced method performance. This approach demonstrates a satisfactory linear range, low detection limits, and applicability to biological matrices. The simplicity and cost-effectiveness of HPLC-UV make it an accessible alternative to LC-MS and fluorescence-based methods. This study's findings are significant, considering the limited prior research on HPLC-UV for TCA analysis, which has reported issues with resolution and peak shapes [3].

ETHICAL APPROVAL

The present work doesn’t require ethical approval

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SA-O02

COUNTERION EXCHANGE IN BOVINE LACTOFERRICIN PEPTIDES BY SOLID-PHASE EXTRACTION CHROMATOGRAPHY

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ABSTRACT

The most widely used methodology to obtain peptides is solid-phase peptide synthesis (SPPS), in which separation of the peptide from the solid support involves treating the resin-peptide with 92.5% v/v trifluoroacetic acid (TFA). In addition, purification is performed by reverse phase solid phase extraction (RP-SPE) using solvents containing TFA. Therefore, peptides are obtained as trifluoroacetate salt, however, this counterion can affect solubility, secondary structure, toxicity and has great impact on molecular weight causing underestimation of peptide concentration/quantity in activity assays [1,2]. For promising anticancer/antibacterial peptides it is essential to exchange the counterion from trifluoroacetate to hydrochloride or acetate. In this research, RP-SPE-based methodologies were designed, developed, and implemented to simultaneously exchange the counterion and purify the peptide. Critical process steps were identified and parameters such as mobile phase composition (Cl^- or CH_3COO^-), washes and elution program were optimized. Quali-quantified of the counterion exchange reaction and characterization of the final products was performed by RP-HPLC, FT-IR, NMR and LC-MS. The counterion exchange can be performed efficiently, independent of the physicochemical properties of the peptides such as length, polarity, polyvalency, presence of non-natural amino acids or non-protein molecules. The methods developed by RP-SPE are fast, efficient, low-cost and do not require robust instrumentation and can be routinely implemented in SPPS.

ETHICAL APPROVAL

The present work does not require ethical approval

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SA-O04

LIPID METABOLISM DISTURBANCES IN PROSTATE HYPERPLASIA, PROSTATE CANCER, AND METASTATIC PATIENTS: COMPARATIVE INSIGHTS FROM A COLOMBIAN CASE-CONTROL STUDY

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ABSTRACT

Prostate cancer is a significant global health concern, and its prevalence is increasing worldwide. Despite extensive research efforts, the complexity of the disease remains challenging with respect to fully understanding it and enabling early diagnosis, due to population-specific factors such as race, genetics, dietary patterns and lifestyle, which influence the likelihood of developing the disease or its progression, as well as recurrence and mortality rates [1]. Thus, metabolomics has emerged as a powerful approach to understanding prostate cancer by assessing comprehensive metabolite profiles in biological samples [2, 3]. In this study, metabolic profiles of Colombian patients with Benign Prostatic Hyperplasia (BPH), Prostate Cancer (PCa), and Metastatic prostate cancer (Met) were characterized using an untargeted approach that included metabolomics and lipidomics via liquid chromatography and gas chromatography coupled with quadrupole-time-of-flight high-resolution mass spectrometry. Comparative analyses were performed to identify the metabolites responsible for the observed changes. Supervised orthogonal partial least squares discriminant analysis models and univariate analysis *p*-Values among these groups revealed distinct metabolic profiles, mainly associated with lipid biosynthetic pathways, such as unsaturated fatty acid biosynthesis, fatty acid degradation and elongation, and sphingolipid and linoleic acid metabolism. PCa patients showed lower levels of amino acids, glycerolipids, glycerophospholipids, sphingolipids, and carnitines compared to BPH patients. PCa patients had reduced metabolites in the glycerolipid, glycerophospholipid, and sphingolipid groups compared to Met patients. They also had an increase in amino acids and carbohydrates. In addition, we also address how the lipid imbalance in patients with BPH, PCa, and Met changes according to each of the diseases. Thus, our research shows how, in addition to their role as components of cell membranes, lipids play multiple functions in cancer cells, such as tumor growth and metastasis, and play an important role in malignant tumors. These metabolic profiles observed provide insights into the underlying pathways of prostate cancer's progression, potentially aiding the development of new diagnostic and therapeutic strategies.

SA-O05

ALTERATIONS IN K562 LEUKEMIA CELL METABOLISM INDUCED BY THE AQUEOUS EXTRACT OF PETIVERIA ALLIACEA

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ABSTRACT

Despite significant advances in chemotherapy and targeted therapy for the treatment of acute leukemia, high mortality rates and many patients experiencing refractoriness or relapse persist [1]. Alterations in cellular metabolism are related to protection against chemotherapy-induced stress, proliferative capacity, and tumor survival [2]. This metabolic characteristic may be a therapeutic target for natural products, as they can present a wide range of compounds that may act individually or synergistically [3, 4]. *Petiveria alliacea* has traditionally been used to treat breast cancer and leukemia [5, 6]. Previous studies have highlighted that its cytotoxic activity is associated with apoptosis, cell cycle arrest, and alterations in proteins involved in energy metabolism and cell proliferation [7-9]. Since indigenous and rural communities traditionally use aqueous infusions of *P. alliacea* for cancer treatment, this research aimed to thoroughly evaluate the metabolic alterations induced by the aqueous extract named "Esperanza" in K562 tumor cells, as well as the identification of chemical compounds present in the extract. Initially, a non-targeted multiplatform using liquid chromatography and gas chromatography coupled to mass spectroscopy was employed to analyze the endometabolome in K562 cells treated with Esperanza and characterize the extract's chemical composition. Subsequently, various *in vitro* biological activities were conducted to investigate potential mechanisms of action associated with its antitumor activity. *In vitro* tests showed that *P. alliacea* reduced the growth of K562 cells, reduced their glucose consumption, decreased intracellular ATP levels, and decreased oxygen consumption rates. Analysis of the endometabolome revealed glycolytic, phosphorylative, lipid, and amino acid metabolism changes. Especially, a decrease in tyrosine, glutamine, and glutamate, key precursors in the tricarboxylic acid cycle (TCA), was observed, which could contribute to mitochondrial dysfunction. Among the most abundant compounds identified in the extract were amino acids, fatty acids, and cinnamic acids, which may be responsible for biological activity. These results suggest that the antitumor activity of Esperanza in the K562 cell line is attributed to the reduction of metabolites associated with cell cycle arrest, leading to decreased cell proliferation and growth.

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SA-O06

Análisis *in vitro* e *in silico* sugieren una posible correlación entre la clase de flavonoides y la actividad anti-dengue de extractos de *Scutellaria sp*. y *Lippia sp*

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RESUMEN

Antecedentes: La medicina tradicional ha reportado el uso de diversos extractos vegetales para tratar el dengue. Sin embargo, no se ha explorado en profundidad la relación entre la composición química de los extractos y la inhibición del virus del dengue (DENV). Este estudio analizó la influencia del contenido de flavonoides sobre el efecto antiviral in vitro de los extractos de *Scutellaria spp*. *y Lippia spp.* frente al DENV. **Métodos:** Se incluyeron 14 extractos obtenidos por extracción con solvente asistida por ultrasonidos (SE) y extracción por fluidos supercríticos (SFE). Se evaluó la actividad anti-DENV durante la adsorción del virus en células Vero mediante ensayo de reducción del efecto citopático (CPE); la composición química de los extractos se determinó por UHPLC/ESI-Q-Orbitrap-MS. Para explorar la correlación entre el contenido de flavonoides y la reducción del CPE, se aplicaron análisis de agrupamiento y ANOVA. Se utilizó acoplamiento molecular (AutoDock Vina) para predecir la interacción de los flavonoides con el DENV y las proteínas celulares. **Resultados**: Extractos SE de *S. coccinea*, *S. incarnata* y *L. alba* mostraron actividad anti-DENV (IC50 entre 1±1,1 - 81±1,1 µg/mL; SI entre 0.8 - 213), mientras que los extractos SE y SFE de *L. origanoides* fueron inactivos. El análisis de agrupamiento sugiere que un mayor contenido de glucósidos de flavona, en comparación con agliconas de flavona u otro tipo de flavonoides, se asocia con mayor actividad anti-DENV. En general, los glucósidos mostraron mejores afinidades de unión que las agliconas tanto para la proteína E del DENV como para las proteínas de las células Vero (Cl, DY y Axl) que participan en la entrada del virus a la célula. **Conclusión:** El contenido de glucósidos de flavona parece desempeñar un papel clave en la actividad anti-DENV de los extractos vegetales, lo que sugiere su potencial como base para el desarrollo de fitoterapéuticos para el tratamiento del dengue.

ASPECTOS ÉTICOS

La planta se cultivó en parcelas experimentales del Complejo Piloto Agroindustrial del Centro Nacional de Agroindustrialización de Vegetales Tropicales, Aromáticos y Medicinales (CENIVAM), ubicado en la Universidad Industrial de Santander, Bucaramanga, Colombia.

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SA-O07

Computational Structural Analysis and LC-MS/MS Spectra of the 2,3-dimercaptopropanol (BAL, British Anti-Lewisite): A combined theoretical and Experimental Study

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ABSTRACT

This study presents a detailed structural analysis of 2,3-dimercaptopropanol also known as British Anti-Lewisite (BAL) from computational approaches susch as the density functional theory (DFT). Experimentally, electrospray ionization mass spectrometry coupled to a tandem mass analyzer (LC-MS/MS) at collision energies of 10V, 20V and 40V were used to determine the spectra of BAL and the fragmentation pathways for the major ions detected. Comparison of experimental spectra with predicted data in the DrugBank database revealed significant differences because of missing information from LC-MS/MS spectra for dimercaprol. Using the theoretical levels M06-2X/6-311++G(3df,2dp) and G4MP2 the structures and relative energies of the major fragments were determined, obtaining a reliable fragmentation pathway for BAL that aids in the understanding of its fragmentation mechanisms.

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SA-O08

METABOLOMICS STRATEGY BASED ON UHPLC-QTOF/MS EVIDENCE CHANGES IN THE METABOLOME OF HEART AND LIVER MICE ASSOCIATED TO CALAFATE INTAKE AND REDUCTION OF CARDIOVASCULAR RISK.

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ABSTRACT

Polyphenols are bioactive substances involved in the prevention of chronic diseases, such as cardiovascular disease. Calafate, endemic to the Chilean-Argentine Patagonia, has a high polyphenol content [1]. In the present study, the aim was to demonstrate the effect of calafate on cardiac and hepatic metabolism and its relationship with cardiovascular protection (CVD). To this end, a previously characterized Calafate extract was administered to C57BL/67 mice fed a high-fat diet. A metabolomics strategy based on UHPLC-QTOF/MS assessed post-consumption changes in the tissue metabolome. Samples were treated and analysed by UHPLC-DAD-QTOF using 3 chromatographic methods. Data processing was carried out in MetaboScape and MetaboAnalyst software. Databases (KEEG, HMDB, etc.) were used for annotation. Exploratory PCA analysis showed a separation of groups indicating an effect of calafate on the cardiac and hepatic metabolome. A total of 46 significant (ANOVA $p<0.05$) features (metabolites) have been identified. An increase in inositol metabolites, and a decrease in carnitines, aminoadipic acid, inosine and hypoxanthine were found. Calafate reduces oxidative stress and increases energy metabolism favoring cardiovascular protection.

ETHICAL APPROVAL

Ethics Committee of Universidad de Concepción (CEBB E425-2019)

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PRESENTACIONES POSTER

AE-P02

EVALUACIÓN DE LA ACTIVIDAD REPELENTE E INSECTICIDA DE LOS ACEITES ESENCIALES DE *Piper ceanothifolium* Kunth, *Piper marginatum* Jacq., *Piper divortans* Trel. & Yunck y *Piper reticulatum* L. SOBRE *Sitophilus zeamais* Motschulsky (COLEOPTERA: CURCULIONIDAE).

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ABSTRACT

El gorgojo de maíz, *sitophilus zeamais* es uno de los insectos más importantes de los cereales almacenados, los cuales pueden causar pérdidas sustanciales que oscilan entre el 20% y el 30% del producto en las zonas tropicales y subtropicales del mundo [1][2]. Sin embargo, los pesticidas químicos con un amplio espectro de actividad, es la columna vertebral para el tratamiento de este tipo de plagas, pero debido a los problemas asociados al uso de estos insecticidas convencionales como la presencia de residuos peligrosos y desarrollo de resistencias, se ha hecho necesaria la búsqueda de alternativas ecológicas como los bioplaguicidas [1].

El objetivo de la presente investigación fue evaluar la actividad repelente e insecticida de manera individual y su vez potenciar la actividad insecticida a través de combinaciones de los aceites esenciales de *p. ceanothifolium*, *P. marginatum*, *P. divortans*, y *P. reticulatum* en proporciones 1:1, 1:3, 3:1 sobre adultos de *S. zeamais*. Estas plantas pertenecientes a la familia de las Piperáceas fueron recolectadas en Lázaro, zona rural del municipio El Carmen de Bolívar. Los aceites esenciales fueron obtenidos por hidrodestilación convencional, con un rendimiento de 0,08% para *P. ceanothifolium*, *P. marginatum* obtuvo la mayor cantidad de AE con un 0,62%, seguida por *P. reticulatum* con un 0,17%, y *P. divortans* con un 0,13% por cada 500 g de material vegetal. Las actividades repelentes e insecticidas se evaluaron por los métodos de área de preferencia y dispersión de gas [3]. Todos los aceites evaluados mostraron actividad repelente a una concentración de 1 $\mu L/cm^2$ destacando principalmente el aceite de *P. reticulatum con un 93%*, seguidamente de *P. ceanothifolium* con un 87%, *P. marginatum* con un 80%, y *P. divortanas* con un 73%. Los porcentajes de mortalidad en la acción insecticida de los aceites evaluados demuestran mortalidad del 100% de los insectos durante las primeras 24 horas de exposición a diferentes concentraciones, permitiendo calcular las concentraciones letales (CL_{50} y CL_{95}) para cada uno de ellos. *P. reticulatum* (CL_{50} =0,084 uL/cm^3 y CL_{95}= 0,305 uL/cm^3), *P. ceanothifolium* (CL_{50} =0,097uL/cm^3 y CL_{95}= 0,213 uL/cm^3), *P. marginatum* (CL_{50} =0,230 uL/cm^3 y CL_{95}= 0,697 uL/cm^3), y *P. divortanas* (CL_{50} =0,210 uL/cm^3 y CL_{95}= 0,396 uL/cm^3).

AE-P03

Determinación de los compuestos volátiles del aceite esencial de *Piper peltatum* L., y su capacidad insecticida y repelente sobre el *Sitophilus zeamais* y *Canthocelides obtectus*

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ABSTRACT

En este estudio, se evaluó el potencial insecticida y repelente del aceite esencial (AE) de *Piper peltatum* L. contra dos plagas agrícolas, *Sitophilus zeamais* y *Acanthocelides obtectus*. Estas plagas, conocidas comúnmente como gorgojo del maíz y gorgojo del frijol, respectivamente, representan una amenaza para el almacenamiento de granos a nivel mundial [1]. Estas plagas reducen el valor comercial y las características organolépticas de los cereales y las legumbres. El maíz es uno de los principales alimentos en la dieta de millones de personas en el mundo, y el frijol es una gran fuente de proteínas [2] [3]. Por estas razones, se utilizan insecticidas sintéticos para controlar estas plagas, los cuales son tóxicos y se bioacumulan en los seres humanos [4], por ello los biocidas naturales derivados de plantas, ofrecen una solución prometedora debido a su menor impacto ambiental, menor toxicidad para los humanos y otros organismos no objetivo, y su potencial para reducir la resistencia de las plagas[5]. Para la extracción del AE de *P. peltatum* se utilizó la técnica de hidrodestilación y se separaron e identificaron los compuestos volátiles presentes en el aceite mediante cromatografía de gases acoplada a espectrometría de masas (GC-MS). La actividad insecticida del aceite esencial de *P. peltatum* L., se evaluó mediante bioensayos de fumigación y la repelencia por área de preferencia [6].

Los resultados de la identificación mostraron que los compuestos mayoritarios del AE de *P. peltatum* son el cariofileno (17,3 %), el germacreno D (12,1 %), el *cis*-calameneno (10,6 %) y el curcumeno (8,632 %). En los ensayos de fumigación, el AE fue efectivo, y se determinaron las concentraciones letales (CL) mediante un análisis probit. Para *A. obtectus* se obtuvieron CL_{50} (0,0071 µL/cm^3) y CL_{95} (0,0195 µL/cm^3), y para *S. zeamais* se obtuvieron CL_{50} (0,00351 µL/cm^3) y CL_{95} (0,00695 µL/cm^3). La actividad repelente, evaluada mediante el método de área de preferencia, mostró que el AE seguía una relación dosis-respuesta y tenía una bioactividad similar a la de compuestos comerciales. El aceite esencial de *Piper peltatum L*. posee un alto potencial como agente insecticida y repelente natural contra *Sitophilus zeamais* y *Acanthocelides obtectus*. Estos hallazgos sugieren que este aceite esencial podría ser una alternativa efectiva y ecológicamente viable para el manejo integrado de plagas en sistemas de almacenamiento de granos, reduciendo la dependencia de insecticidas sintéticos.

AE-P05

COMPOSICIÓN QUÍMICA VOLÁTIL Y EVALUACIÓN DE LA ACTIVIDAD REPELENTE E INSECTICIDA DEL ACEITE ESENCIAL DE *Hyptis suaveolens (L.) Poit.* SOBRE *Sitophilus zeamais* Motschulsky (COLEOPTERA: CURCULIONIDAE).

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ABSTRACT

La producción de cereales como el maíz desempeña un papel fundamental en la seguridad alimentaria, constituyendo entre el 50% y el 60% de la dieta humana[1]. Sin embargo, las etapas de poscosecha y almacenamiento presentan desafíos significativos debido a la proliferación de plagas, que pueden causar pérdidas del 20% al 30%. Entre las plagas responsables del daño primario en el maíz se encuentra el gorgojo del maíz, *Sitophilus zeamais*[2]. Para combatir estas plagas, es común el uso de pesticidas químicos de amplio espectro, pero presentan preocupaciones por sus efectos tóxicos en el medio ambiente. En busca de alternativas ecológicas, los bioplaguicidas obtenidos a partir de metabolitos secundarios de plantas, entre ellos los aceites esenciales (AE), han demostrado eficacia por la toxicidad de sus componentes activos[3]. Este estudio evalúa la actividad repelente e insecticida del AE de *Hyptis suaveolens* contra *Sitophilus zeamais* y determinar su composición química volátil. El AE se obtuvo mediante hidrodestilación asistida por un brazo Clevenger, y su composición química se identificó usando cromatografía de gases acoplada a espectrometría de masas (GC/MS). La actividad repelente se evaluó con el método del área de preferencia, y la insecticida mediante fumigancia, calculando las concentraciones letales (CL50 y CL95), ambas actividades fueron evaluadas para el AE y algunos de sus componentes[4]. El rendimiento del AE de *Hyptis suaveolens* fue del 1.2%, y el análisis por GC/MS identificó 36 compuestos, siendo los mayoritarios α-Fenchol (39,27%), Eucaliptol (24,14%), β-Cariofileno (4,76%), Isoborneol (4,23%) y Spathulenol (4,07%). La actividad repelente del AE mostró una relación dosis-respuesta similar al compuesto comercial (Stay off ®), y componentes como el eugenol, α-pineno y β-pineno también presentaron actividad repelente. En cuanto a la actividad insecticida, se calcularon las siguientes concentraciones letales: AE de *Hyptis suaveolens* (CL_{50} = 0,094 $\mu L/cm^3$ y CL_{95} = 0,205 $\mu L/cm^3$), Eugenol (CL_{50} = 0,094 $\mu L/cm^3$ y CL_{95} = 0,197 $\mu L/cm^3$), α-Pineno (CL_{50} = 0,336 $\mu L/cm^3$ y CL_{95} = 0,661 $\mu L/cm^3$) y β-Pineno (CL_{50} = 0,079 $\mu L/cm^3$ y CL_{95} = 0,360 $\mu L/cm^3$). Este estudio evidencia el potencial del AE de *Hyptis suaveolens* y algunos de sus componentes como agentes repelentes e insecticidas contra *Sitophilus zeamais*, ofreciendo una alternativa ecológica a los pesticidas químicos.

AE-P06

COMPOSICIÓN QUÍMICA VOLÁTIL Y EVALUACIÓN DE LA ACTIVIDAD REPELENTE E INSECTICIDA DEL ACEITE ESENCIAL DE *BURSERA GRAVEOLENS* SOBRE *SITOPHILUS ZEAMAIS* MOTSCHULSKY

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ABSTRACT

El uso excesivo de pesticidas químicos en el control de plagas agrícolas causa problemas ambientales, resistencia en plagas y riesgos para la salud. Por ello, se busca alternativas sostenibles como los aceites esenciales (AE) por sus propiedades insecticidas, entre otras[1]. La producción de maíz es esencial para la seguridad alimentaria, aportando entre el 50% y el 60% de la dieta humana. Aunque puede almacenarse sin perder valor nutricional, las plagas como el *Sitophilus zeamais* causan grandes pérdidas en su etapa de cosecha, poscosecha y almacenamiento[4], especialmente en regiones tropicales y subtropicales, con daños de hasta el 18.3% en 48 días[6]. Para el control de *S. zeamais* se han propuesto plaguicidas botánicos, los cuales actúan mediante varios mecanismos. Entre estos métodos de acción se incluyen la repelencia, la inhibición y la desnaturalización de proteínas, lo cual depende del tipo de compuesto botánico[2][5]. Este estudio tiene como objetivo evaluar la actividad repelente e insecticida del AE de *Bursera graveolens* contra el *Sitophilus zeamais* y determinar la composición química volátil del aceite esencial.Para la hidrodestilación de AE se utilizó un aparato tipo Clevenger, y se analizó por cromatografía de Gases acoplada a Espectrometría de Masas(GC-MS)[3]. Para el AE de *B. graveolens* se obtuvo un rendimiento del 0.25%. El análisis de GC-MS evidenció la presencia de 45 compuestos, siendo los mayoritarios limoneno (52.2%), germacreno D (13.0%) y α-cadinol (3.2%). La actividad repelente se evaluó mediante el método de área de preferencia [3]. El aceite esencial de *B. graveolens* muestra una eficacia notable a corto plazo a comparación del Stay off que muestra una mayor consistencia y eficacia a largo plazo. Con la actividad insecticida evaluada por el método de fumigación[3], se lograron calcular las concentraciones letales (CL$_{50}$ y CL$_{95}$) tanto para el AE como para los patrones. El AE de *Bursera graveolens* (CL$_{50}$ = 0.166 uL/cm3 y CL$_{95}$ = 0.336 uL/cm3), limoneno (CL$_{50}$ = 0.289 uL/cm3 y CL$_{95}$ = 0.439 uL/cm3), α-pineno (CL$_{50}$ = 0.366 uL/cm3 y CL$_{95}$ = 0.661 uL/cm3). Con esta investigación se logró demostrar la potencial actividad repelente e insecticida del AE de *B. graveolens* y algunos de sus componentes sobre *S. zeamais*.

APROBACIÓN ÉTICA

De acuerdo con la metodología empleada en esta investigación no se requieren consideraciones éticas para la realización de este proyecto llamado "COMPOSICIÓN QUÍMICA VOLÁTIL Y EVALUACIÓN DE LA ACTIVIDAD REPELENTE E INSECTISIDA DEL ACEITE ESENCIAL DE Hyptis suaveolens (L.) Poit. SOBRE Sitophilus zeamais Motschulsky (COLEOPTERA: CURCULIONIDAE)". No se realizó muestreos en los que se requieran muestras provenientes de seres humanos, por lo que no se hizo uso de consentimientos informados, ni de algún otro formato en las que se necesitó el permiso de una persona natural.

AE-P07

OPTIMIZACIÓN DEL PROCESO DE EXTRACCIÓN DEL ACEITE ESENCIAL DE RIZOMAS DE *Curcuma zedoaria* (Zingiberaceae) MEDIANTE HIDRODESTILACIÓN ASISTIDA POR MICROONDAS

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ABSTRACT

La cúrcuma blanca (*Curcuma zedoaria*), de la familia Zingiberaceae, es una planta medicinal originaria de la India, cultivada también en Brasil y Asia. Se utiliza como condimento y tónico para tratar trastornos menstruales, vómitos, dolor de muelas, cáncer cervical, hepatitis e inflamación. [1] Su aceite esencial (AE) es rico en compuestos como la curzerenona, 1,8-cineol, p-cimeno, α-felandreno y β-turmerona, los cuales tienen actividades antimicrobianas, anticancerígenas, analgésicas, antioxidantes, cicatrizantes, antiinflamatorias, insecticidas y cardioprotectoras. [2] El AE del rizoma de *Curcuma zedoaria* se aisló mediante hidrodestilación asistida por microondas (HDAM). El procedimiento de extracción se optimizó utilizando una metodología de superficie de respuesta con un diseño de Box-Behnken, empleando tres factores: tiempo de extracción, potencia de irradiación y relación sólido-líquido. Las condiciones óptimas para la extracción del AE con HDAM fueron un tiempo de 45 minutos, una potencia de irradiación de 900 W y una relación líquido-sólido de 8:1, logrando un rendimiento máximo de 1,94 ± 0,01%, bajo estas condiciones. Además, se evaluó un pretratamiento de ultrasonido (US+HDAM) que mostró un aumento en el rendimiento del 9,9%, debido al efecto mecánico de cavitación que facilita la liberación del AE. La composición química de los AE se analizó mediante cromatografía de gases-espectrometría de masas, revelando que los sesquiterpenos oxigenados (83,6%) son sus principales componentes, de los cuales la curzerenona (41,14%) y el ácido vetivénico (26,29%) son los constituyentes mayoritarios. La curzerenona se destaca por tener un gran potencial antioxidante, antibacteriano, antifúngico y cardioprotector, por lo que el AE de Curcuma *zedoaria* podría emplearse en aplicaciones médicas y alimentarias. [3], [4] Tanto la HDAM como la US+HDAM se proponen como métodos alternativos eficientes y ecoamigables, ya que ofrecen un mayor rendimiento, menor consumo de electricidad y reducidas emisiones de CO_2 en comparación con métodos convencionales.

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AE-P08

EXTRACCIÓN DE ACEITE ESENCIAL DE RIZOMAS DE *Hedychium coronarium* (Zingiberaceae) MEDIANTE HIDRODESTILACIÓN ASISTIDA POR MICROONDAS: OPTIMIZACIÓN Y COMPOSICIÓN QUÍMICA

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ABSTRACT

Hedychium coronarium, comúnmente conocido como jengibre mariposa, es una planta originaria de Asia, que se ha clasificado como invasora en América del Sur. Los rizomas de esta planta son ricos en aceites esenciales (AE) con un alto contenido de monoterpenos, entre los cuales predominan el eucaliptol, β-pineno, α-pineno y α-terpineol.[1] Los componentes principales del AE exhiben propiedades biológicas significativas, incluyendo actividades antimicrobianas, larvicidas, antiinflamatorias, antihelmínticas, antioxidantes, antiofídico y fitotóxicas.[2] El AE de los rizomas de *Hedychium coronarium* se extrajo mediante hidrodestilación asistida por microondas (HDAM). Para optimizar la extracción, se utilizó un modelo de superficie de respuesta con un diseño Box-Behnken (DBB), considerando tres factores: tiempo de extracción, potencia de irradiación y volumen de H_2O. Posteriormente, se evaluó un pretratamiento de ultrasonido (US+HDAM) y se compararon ambos métodos en términos de rendimiento y composición química. El contenido metabólico de los AE se analizó mediante cromatografía de gases acoplada a espectrometría de masas (CG-EM). Los componentes del AE se identificaron por similitud de tiempos de retención, espectros de masas proporcionados por la biblioteca NIST 2013 e índices de Kovats con una serie de alcanos C_8-C_{25}. Los rendimientos de los AE obtenidos en el DDB variaron entre 0.053% y 0.2155%, demostrando que el tiempo y la potencia de irradiación del microondas tienen un efecto significativo sobre el rendimiento de extracción. Las condiciones óptimas en la HDAM fueron un volumen de H_2O de 360 mL, una potencia de irradiación de 300 W y un tiempo de extracción de 60 min, logrando un rendimiento del 0.242%. El US+HDAM mejoró el rendimiento en un 18% y no modificó significativamente la composición de los AE. El análisis por CG-EM reveló un total de 25 compuestos en los AE, siendo los mayoritarios el Nezukol (67.91%) y el Óxido de cariofileno (7.99%). Este estudio identificó las condiciones óptimas para la extracción de AE por HDAM, destacando la importancia del tiempo y la potencia de irradiación. Además, se confirmó que la combinación de ultrasonido y microondas mejora los rendimientos sin alterar significativamente la composición química.

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AE-P09

ESSENTIAL OILS OF THE PIPER GENUS; PROMISING ANTIMICROBIAL RESOURCE

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ABSTRACT

The *Piper* genus, which belongs to the Piperaceae family, is considered one of the oldest families in Asia and tropical America where multiple species are found and used in traditional medicine. Its essential oils are rich in monoterpeton, diterpenes and sesquiterpenes that have diverse biological activities [1]. In the present study, the essential oils of *Piper glabratum*, *P. friedrichsthalii*, *P. cumanense* and *P. ibaguense* were identified and characterized by gas chromatography with mass selective detector (GC-MS). As a result, about 90 compounds were identified in this species. These oils were tested against the fungus *Moniliophthora roreri* and the Oomicota *Phytophthora palmivora*, species of microorganisms associated with losses of up to 80% of fruit production in the cocoa crop, resulting in many economic losses. [2]. Showing promising bioactivity for agricultural product development.

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AE-P10

Cymbopogon martinii (POACEAE) STEAM DISTILLATION STUDY

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ABSTRACT

Cymbopogon martinii is an aromatic plant of the Poaceae family that is distilled to obtain an essential oil (EO) that is widely used in the production of perfumes, cosmetics, pharmaceuticals, hygiene products and insecticides [1]. The EO of *C. martinii* is characterized by its fragrant rose aroma and its biological activities as an antibacterial [2] and insect repellent for disease transmission vectors, such as dengue, zika, chikungunya, yellow fever, among others (e.g. *Aedes aegypti*) [3]. The objective of this study was to determine the steam distillation variables that allow obtaining high EO yields from *C. martinii* plants grown in Barbosa, Santander. The EO of fresh *C. martinii* plant material was obtained by steam distillation in a 1 m^3 stainless steel still. The effect of the variables charge density, vapor flow and distillation time on the EO yield were evaluated by applying an experimental design 2^3. The EO was characterized by gas chromatography coupled to mass spectrometry (GC/MS) and gas chromatography with flame ionization detector (GC/FID). The highest yield of EO was 0.43% and the individual steam flow and combined factors charge density-time had a significant effect on the response. The major EO compounds of *C. martinii* were geraniol (85 ± 2%) and linalool (3.1 ± 0.7%).

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AE-P11

EVALUATION OF THE XAVIER *et al.* MODEL FOR STEAM DISTILLATION OF COMMERCIAL AROMATIC PLANTS

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ABSTRACT

Steam distillation is an ancient technique used to obtain essential oils (EO) [1]. Xavier *et al.* [2] described the obtaining of EO as a process that occurs in stages, distillation of the free oil from the broken cells and diffusion from inside the intact cells, with good results for obtaining EO from *Baccharis* spp. The objective of this research was to evaluate the model proposed by Xavier *et al*. [2] for the distillation of fresh plant material of citronella (*Cymbopogon winterianus*) and palmarosa (*C. martinii*), and dried plant material of geranium (*Pelargonium graveolens*) and patchouli (*Pogostemon cablin*). The plant material was steam distilled in 1 and 2 m^3 stills, with a charge density between 63 and 339 kg/m^3, steam flow between 620-1500 mL/min and distillation time of 1.5-5.2 h, depending on the aromatic species and the capacity of the equipment used. The EO was collected every 10, 15 or 20 min, depending on the plant, and the cumulative essential oil yield curve was plotted as a function of time. The model of Xavier *et al*. [2] was simulated for each distillation and the kinetic parameters were fitted by minimization of the sum of squared errors between experimental and predicted data, the concentration and transition time were calculated and the level of fit was determined with the goodness criterion mean square error (MSE). The model of Xavier *et al*. [2] described the steam distillation of geranium, patchouli, citronella and palmarosa species in 1 and 2 m^3 stills with a good fit between experimental and predicted data, MSE values less than 3.17×10^{-3}.

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AE-P12

CHEMICAL CHARACTERIZATION BY GC/MS OF *Ocimum minuta* ESSENTIAL OIL

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ABSTRACT

The genus *Ocimum* includes approximately 35-150 species considered annual and perennial herbaceous plants and shrubs. In Colombia, native and cultivated species such as *Ocimum americanum* L., *Ocimum basilicum* L., *Ocimum campechianum* L., and *Ocimum gratissimum* L. have been recorded [1,2]. The genus *Ocimum* has been the subject of several studies to explore its biological properties such as insecticidal, antifungal, antimicrobial, and antioxidant. These properties are attributed to the diverse presence of terpenes, phenylpropanoids, and some flavonoids in the extracts and EOs of *Ocimum* plants [2,3]. This study was focused on basil plants cultivated and harvested at the Centro Nacional de Investigaciones para la Agroindustrialización de Especies Vegetales Aromáticas y Medicinales Tropicales (CENIVAM). Plant material (leaves, stems, and flowers) was distilled by microwave-assisted hydrodistillation (MWHD). The yield of obtaining the essential oil was 0.36%. The identification of the EO compounds was performed by GC/MS. In the *O. minuta* EO, eugenol (60.1%), (*E*)-β-caryophyllene (26.4%), β-elemene (7.6%), humulene (1.6%) and caryophyllene oxide (1.5%), were the principal components. The essential oils (EOs) contain compounds that have demonstrated biological activities including anticancer, antimicrobial, and cytotoxic properties [4]. This study adds to the research on the chemical components of *Ocimum* plants in Colombia. The findings suggest potential applications in traditional medicine and other industrial sectors.

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AE-P13

PROTECTIVE AND MATURATION DELAY EFFECT OF AN ESSENTIAL OIL FORMULATION ON THE RIPENING OF AVOCADOS CULTIVATED IN SANTANDER, COLOMBIA

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ABSTRACT

The avocado, *Persea americana* Mill (Lauraceae), is a tree native to Mesoamerica that produces an edible berry. It is a climacteric fruit, which means that it continues to ripen after it has been harvested [1]. Currently, the development of edible coatings based on essential oil (EO) formulations with antioxidant, antimicrobial, or antifungal activities allows the development of new methodologies for the preservation of the organoleptic properties of fruits [2,3]. The upcoming research will assess the impact of a formulation of essential oils on preserving the physical, chemical, and sensory properties of *P. americana* fruits. Avocados were grown in the municipality of San Vicente de Chucurí, Santander, Colombia. The fruits were disinfected with a sodium hypochlorite solution at a concentration of 200 ppm and allowed to dry. An EO formulation was applied to the avocados and changes in weight, firmness, color, pH, total soluble solids content, antioxidant activity, and total phenols were monitored for a period of 15 days, every five days. Preliminary tests showed significant variations in pH, with higher values in untreated fruit. Regarding color change, a more accelerated variation was observed in untreated fruit. The application of an EO formulation on fruits allowed determining the possible protective and ripening retardant effects. Variation in color intensity was also observed in fruits with EO formulation. Therefore, tests will be conducted in which the concentration will be varied. Further measurements related to avocado quality, specifically changes occurring during ripening, are required to evaluate the effectiveness and mode of action of the AE formulation.

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AE-P14

MONITORING THE MAJOR COMPONENTS OF *Turnera diffusa* ESSENTIAL OIL INCORPORATED INTO A NANOEMULSION FOR THE TREATMENT OF CUTANEOUS LEISHMANIASIS

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ABSTRACT

The encapsulation of essential oils (EOs) in nanoemulsions provides an effective solution for their integration into cosmetic and pharmaceutical formulas, addressing the volatility and low solubility of EOs in specific solvents [1]. The European Union (EU) mandates that medicines for human use must comply with Directive 2001/83/EC. This directive stipulates that each product must contain information about the qualitative and quantitative composition of the medicine [2]. This study aimed to use extraction techniques to determine the chemical composition of the volatile fraction of a nanoemulsion containing *T. diffusa* essential oil as an adjuvant for treating cutaneous leishmaniasis. Volatile organic compounds in a nanoemulsion were sampled *in vitro* with HS-SPME. CAR/DVB/PDMS (50/30 µm, Supelco S.A., USA) fiber was exposed to the compounds emitted by the sample (50 mg) for 20 min at 60 °C. The analysis was performed on a GC/MS. The major components of the nanoemulsion volatile fraction were 4,5-di-*epi*-aristolochene (34%), $C_{15}H_{24}$ [*m/z* 204 (37%), 161 (72%), 133 (63%), 107 (100%) and 93 (94%)] (11%), *p*-cymene (8%), and co-elution of valencene and β-selinene (8%). The volatile compounds of *T. diffusa* essential oil are still present in the nanoemulsion studied after seven months of storage.

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AE-P15

CHEMICAL CHARACTERIZATION BY GC/MS OF *Minthostachys mollis* (LAMIACEAE) ESSENTIAL OILS DISTILLED IN SANTANDER

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ABSTRACT

The genus *Minthostachys* has around 17 species, among which is *Mintostachis mollis*. *M. mollis* is a woody shrub and endemic species from the South American Andes [1] that has been widely used in traditional medicine to treat different respiratory and digestive diseases [2], it also has insecticidal properties [3]. In this study, two species of *M. mollis* were collected in Santa Barbara, Santander (Colombia). The first species was collected at 6°56'16.4" N 72°57'44.5" W and the second was collected at 6°56'27.3" N 72°57'32.0" W. The EOs were obtained by microwave-assisted hydrodistillation (MWHD) using a Clevenger-type equipment. The EO chemical composition was determined by GC/MS on both polar and non-polar columns, using linear retention indices, mass spectra, fragmentation patterns and standard compounds for identification. The main components in the EO distilled from plants collected in different harvest varied. *trans*-Piperitone oxide (49.6 %), menthone (8.9 %) and piperitenone oxide (4.8 %) were the main components present in the first EO of *M. mollis*, the extraction yield from plant material was 0.26 % (w/w). For the second EO the main components were menthone (46.1 %), pulegone (13.3 %), piperitone (12.1 %), *trans*-β-caryophyllene (7.0 %) and the extraction yield was 0.37 % (w/w). Two different EO compositions were identified for the same plant species. Oxygenated monoterpenes were predominant in the composition of both *M. mollis* EO. The chemical composition of the EO distilled from plants of the same species but grown in different spots, may vary substantially, as we showed in this study. This suggest that it is possible to obtain substantial quantities of different bioactive ingredients of the same plant species for use as potential pharmacological agents.

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AE-P16

EFFECT OF CULTIVATION TYPE ON YIELD AND QUALITY OF ESSENTIAL OILS OF COMMERCIAL PLANT SPECIES

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ABSTRACT

The biosynthesis and accumulation of secondary metabolites in plants is related to several aspects, among which are: genetic factors, environmental conditions of the crop, agronomic management, harvest time and postharvest treatments [1]. The objective of this study was to determine the effect of the type of crop, monoculture or polyculture, on the yield and quality of essential oils (EO) of citronella (*Cymbopogon winterianus*), palmarosa (*C. martinii*), rosemary (*Salvia rosmarinus*), thyme (*Thymus vulgaris*), geranium (*Pelargonium graveolens*) and patchouli (*Pogostemon cablin*). Fifteen experimental units were established in the municipality of Barbosa (Santander, Colombia). For each unit, two monocultures and a polyculture consisting of the two interspersed species were evaluated. The EO were obtained by microwave radiation-assisted hydrodistillation (MWHD) and the analysis of their chemical composition was performed by gas chromatography coupled to mass spectrometry (GC/MS) and gas chromatography with flame ionization detector (GC/FID). The relative amounts (%) of the majority compounds in the EO of the commercial species were: citronella [citronellal (32-33%)], palmarosa [geraniol (85%)], rosemary [α-pinene (21%), 1,8-cineole (19-20%), camphor (16-17%)], thyme [*p*-cymene (25-40%), γ-terpinene (11-15%), thymol (25-36%)], geranium [citronellol (11-14%), geraniol (33-39%)] and patchouli [patchoulol (47%), α-guaienol (9-10%), α-bulnesene (9%)]. The chemical compositions of EO obtained from plants grown in monocultures did not show significant differences compared to EO from plants in polycultures.

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AE-P17

ESSENTIAL OILS FROM NATIVE PIPER SPECIES IN THE CONTROL OF STRAWBERRY PHYTOPATHOGENS

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ABSTRACT

Strawberries are globally significant due to their popularity, but they are highly perishable and susceptible to fungal infections, leading to rot and substantial economic losses. Essential oils (EOs) are promising for controlling pests and phytopathogens in agriculture, with the *Piper* genus being particularly notable for its fungicidal properties and high EO content. This study aims to: (i) identify the main chemical constituents in the EOs of seven native *Piper* species (*P. aduncum, P. crassinervium, P. fuligineum, P. gaudichaudianum, P. lhotzkyanum, P. malacophyllum, P. tuberculatum*), and (ii) evaluate their Minimum Inhibitory Concentration (MIC) against the phytopathogen *Botrytis cinerea* Pers. Dry leaves of the seven species were subjected to hydrodistillation for four hours, in triplicate. The EOs were analyzed using GC-MS and GC-FID on Shimadzu GC-2010 Plus and Agilent 7890A gas chromatographs, respectively, with a fused silica capillary column HP-5MS (30 m × 0.25 mm × 0.25 µm). Identification of the main constituents was achieved by comparing mass spectra and retention indices with reference data and literature [1,2]. The MIC was determined using the broth microdilution method. The predominant classes of compounds in the EO studied were as follows: arylpropanoids for *P. aduncum* (84.3%) and *P. gaudichaudianum* (71.3%); sesquiterpenes for *P. crassinervium* (64.5%), *P. lhotzkyanum* (60.0%), and *P. tuberculatum* (68.4%); mono and sesquiterpenes for *P. malacophyllum* (35.9% and 42.2%); and sesquiterpenes and oxygenated sesquiterpenes for *P. fuligineum* (30.5% and 34.4%). In in vitro tests, among the essential oils studied, those from *P. gaudichaudianum* (MIC of 20 $\mu L\ mL^{-1}$) and *P. aduncum* (MIC of 60 $\mu L\ mL^{-1}$) demonstrated the most effective inhibition of *Botrytis cinerea* spores. In comparison, the commercial fungicide iprodione has a MIC of 10 $\mu g\ mL^{-1}$. These promising results highlight the potential o these essential oils as viable alternatives to commercial fungicides, positioning them as effective biofungicides for controlling *B. cinerea*.

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AE-P18

EFFECT OF FERTILIZATION LEVEL ON ESSENTIAL OIL YIELD OF *Pelargonium graveolens, Salvia rosmarinus* y *Thymus vulgaris*

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ABSTRACT

The yield and essential oil (EO) composition of aromatic plants can vary by genetic factors and agroecological conditions of the cultivation site, postharvest management, and method of production [1]. The objective of this work was to evaluate the effect of fertilization level on the essential oil (EO) yield of geranium (*Pelargonium graveolens*), rosemary (*Salvia rosmarinus*) and thyme (*Thymus vulgaris*). At the headquarters of the Universidad Industrial de Santander, municipality of Barbosa, the experimental culture of the three species studied was planted and their EO was obtained by microwave radiation-assisted distillation (MWHD). The crop of each species was divided into two areas to evaluate the two levels of fertilization, the first level consisted of a mixture of chemical synthesis fertilizer (triple-15) and a mineral soil conditioner (ABOB), and the second level was a mixture of distillation residue compost and ABOB. The yield of geranium EO (0.39%) was higher than that reported by other authors [2], while that of rosemary (0.9%) [3] and patchouli (1.2%) [4] was lower. The yield of geranium and thyme showed significant differences between the fertilization levels evaluated, being favored by chemical-organic fertilization (triple 15-ABOB). The yield of rosemary EO did not show significant differences; however, the use of organic-compost fertilization (ABOB-compost) was determined because it meets the nutritional requirements of the aromatic species and reduces crop maintenance costs.

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AE-P19

USO DE ACEITES ESENCIALES PARA EL CONTROL DE *ASPERGILLUS FUMIGATUS* Y *ASPERGILLUS FLAVUS*

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RESUMEN

Aspergillus fumigatus y *Aspergillus flavus* son hongos patógenos que representan una amenaza para la salud humana y la seguridad alimentaria, *A. fumigatus* es un agente etiológico de infecciones respiratorias graves, especialmente en individuos inmunocomprometidos, mientras que *A. flavus* es conocido por producir aflatoxinas, compuestos altamente tóxicos y carcinogénicos que contaminan cultivos como el maíz y el maní [1]. El control de estos hongos ha sido mediante fungicidas sintéticos, los cuales presentan inconvenientes como la generación de resistencia y efectos adversos sobre el medio ambiente [1]. En este contexto, los aceites esenciales (AE) surgen como una alternativa prometedora por sus propiedades antimicrobianas [2]. El objetivo de este proyecto fue evaluar el efecto de los aceites esenciales obtenidos de plantas recolectadas en salidas botánicas o cultivadas en el jardín del Complejo Agroindustrial Piloto CENIVAM, sobre el crecimiento de *A. fumigatus*-SIBYG3 y *A. flavus*-SIBYG4. La actividad antifúngica de los AE se evaluó mediante la determinación del crecimiento fúngico por el método de dilución en placa y exposición de volátiles [3]. Los AE Bio-Reto0018 y Bio-Reto0008, presentaron un porcentaje de inhibición superior al 80% sobre el crecimiento de *A. flavus*-SIBYG4 y *A. fumigatus*-SIBYG3. En conclusion, los AE pueden ser empleados como una alternativa para tartar las enfermedades producidas por *A. fumigatus y A. flavus.*

APROBACIÓN ETICA

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AE-P20

ESTUDIO *IN VITRO* DE LA EFICACIA DE ACEITES ESENCIALES EN LA INHIBICIÓN DEL CRECIMIENTO DE *FUSARIUM OXYSPORUM*-SIBYG1

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RESUMEN

Fusarium oxysporum es un hongo filamentoso presente en suelos, climas cálidos y suelos húmedos, de rápido crecimiento en el laboratorio, temperatura óptima 28 °C, sus colonias varían de blanco a rosado [1]. La marchitez por *Fusarium* es considerada entre las diez enfermedades más importantes en la historia de la agricultura [2]. La forma convencional de abordar esta problemática es mediante el uso de pesticidas, pero estos tienen consecuencias negativas para el medio ambiente (contaminación, la degradación e infertilidad del suelo), y la salud humana (anemia, esterilidad, cáncer y diversos trastornos) [2]. Una alternativa es el uso de aceites esenciales (AE), que han demostrado tener actividad antioxidante y antimicrobiana contra hongos [1]. El objetivo de este proyecto fue evaluar el efecto de los aceites esenciales obtenidos de plantas recolectadas en salidas botánicas o cultivadas en el jardín del Complejo Agroindustrial Piloto CENIVAM, sobre el crecimiento de *Fusarium oxysporum*-SIBYG1. La actividad antifúngica de los AE se evaluó mediante la determinación del crecimiento fúngico por el método de dilución en placa y exposición de volátiles [3]. Los AE Bio-Reto0018, Bio-Reto0015, Bio-Reto0046, Bio-Reto0045, Bio-Reto0008, Bio-Reto0080, y Bio-Reto0103, presentaron un porcentaje de inhibición superior al 80% sobre el crecimiento de *F. oxysporum*-SIBYG1. En conclusion, los AE pueden ser empleados como una alternativa para tartar las enfermedades producidas por *F. oxysporum.*

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AE-P21

EVALUACIÓN DE LA ACTIVIDAD ANTIFÚNGICA IN VITRO DE ACEITES ESENCIALES SOBRE EL CRECIMIENTO DE FUSARIUM GRAMINEARUM-SIBYG2

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RESUMEN

Fusarium graminearum es el principal agente causal de fusariosis en cereales debido a la producción de micotoxinas y la liberación de enzimas extracelulares [1]. Este daño genera pérdidas de rendimiento de hasta el 50% en los cereales debido a la reducción de la calidad del grano, para contrarrestar esta problemática, se recurre al uso de plaguicidas, los cuales presentan efectos negativos en la salud humana y el medio ambiente [1]. Una alternativa prometedora es el uso de aceites esenciales (AE), que contienen compuestos químicos como carvacrol, timol, citral, flavonoides, ácidos fenólicos, terpenoides y lignanos, que han demostrado tener actividad antioxidante y antimicrobiana [2]. El objetivo de este proyecto fue evaluar el efecto de los aceites esenciales obtenidos de plantas recolectadas en salidas botánicas o cultivadas en el jardín del Complejo Agroindustrial Piloto CENIVAM, sobre el crecimiento de *Fusarium graminearum*-SIBYG2. La actividad antifúngica de los AE se evaluó mediante la determinación del crecimiento fúngico por el método de dilución en placa y exposición de volátiles [3]. Los AE Bio-Reto0018, Bio-Reto0046, Bio-Reto0008, y Bio-Reto0103, presentaron un porcentaje de inhibición superior al 70% sobre el crecimiento de *F. graminearum*-SIBYG2. En conclusion, los AE pueden ser empleados como una alternativa para tartar la fusariosis en trigo causada por *Fusarium graminearum*.

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AE-P22

GC/MS ANALYSIS OF ESSENTIAL OILS FROM LEAVES AND FLOWERS OF *Varronia curassavica* (BORAGINACEAE) COLLECTED IN SANTANDER, COLOMBIA

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ABSTRACT

Varronia curassavica (Boraginaceae) is an aromatic plant native to South America [1]. Traditionally, it has been used as an antipyretic and anti-inflammatory. The main compounds in the essential oil of *V. curassavica* are α-pinene, β-caryophyllene, and germacrene D, which have demonstrated anticancer activity *in vitro* in prostate, breast, and lung cancer cells [2]. In this work, the essential oils from the leaves and flowers of *V. curassavica* were obtained by microwave-assisted hydrodistillation (MWHD). The distillation flask was placed inside a household microwave oven (Samsung, 2.45 GHz, 1600W) with a side hole through which an external glass condenser was connected to the distillation flask containing the plant material (200 g) and water (400 g). The microwave oven was operated in 4 cycles of 15 minutes at 60% maximum power. The essential oil was decanted using a Dean-Stark condenser and dried with anhydrous sodium sulfate. *V. curassavica* essential oils were characterized using GC/MS and quantified by GC/FID. *trans*-β Caryophyllene (15.7%), α-pinene (13.4%), and germacrene D (13.3%) were the major compounds in the essential oil from *V. curassavica* leaves. Higher levels of α-pinene (20.4%) and germacrene D (14.2%) were found in the essential oil of *V. curassavica* flowers. Flowers play a crucial role in attracting pollinators. Volatile terpenes, such as α-pinene, play an important role in the production of aromas that attract pollinating insects, this could be the reason why the presence of α-pinene is more abundant in flowers than in leaves, where α-pinenosole fulfills the function of keeping predators away from the plant.

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AE-P23

CARACTERIZACIÓN PRELIMINAR DE DIFERENTES EXTRACTOS DE *Spathodea Campanulata*: UN ESTUDIO SOBRE SU COMPOSICIÓN QUÍMICA

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ABSTRACT

El presente estudio se enfoca en la extracción y caracterización de compuestos volátiles y no volátiles de tulipán africano (*Spathodea campanulata)* especie arbórea introducida a Colombia en la década de 1930 y ampliamente distribuida en la región del Cauca. Esta especie vegetal se caracteriza por un notable efecto insecticida de la planta sobre especies animales, incluyendo chinches, coccinélidos, véspidos y dípteros [1].

La metodología empleada para la caracterización incluye el estudio de flores frescas (almacenadas máximo 24 horas) mediante tres técnicas para el análisis de compuestos volátiles y semivolátiles con el objetivo de determinar la composición de la siguiente manera: un análisis de compuestos volátiles mediante la técnica de HS/GC-MS (de sus siglas en inglés) en cuyo método se empleó una columna TG-5MS 30 m x 0.25mm x 0.25 µm (5% fenilo) con flujo de He de 1.0 mL/min. La temperatura del horno y jeringa fueron 40°C con incubación de 30 min. La temperatura del puerto de inyección fue de 80°C y en el horno se realizó una rampa de temperatura entre 40°C a 200°C cuyo. La temperatura del detector fue de 230°C y se realizó un *full scan* entre 35 a 300 umas. Los resultados permitieron la identificación preliminar del *flavour* en flores. En el siguiente paso se realizó la técnica de hidrodestilación (realizada durante 4 horas), mediante el empleo de un Clevenger para la obtención de aceite esencial e hidrolato [2]. Las muestras obtenidas fueron analizadas por HPLC-DAD (de sus siglas en inglés). Luego, mediante la técnica de extracción asistida por microondas se empleó como solvente una solución 1:1 etanol-agua. Las condiciones usadas para la extracción fueron una potencia de 600W durante 25 minutos procurando que la temperatura no superará los 80 °C. Posteriormente el extracto se rotaevaporó hasta sequedad para eliminar el solvente en exceso y se efectuó un tamizaje fitoquímico cualitativo del extracto obtenido por microondas [3]. Este estudio multitécnico aporta información valiosa sobre la composición química de *S. Campanulata* y establece una metodología para la caracterización integral de compuestos bioactivos en especies vegetales.

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AE-P24

GC/MS ANALYSIS OF THE VOLATILE FRACTIONS OF *Varronia curassavica* (BORAGINACEAE) COLLECTED IN SANTANDER, COLOMBIA

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ABSTRACT

Varronia curassavica Jacq. (Boraginaceae) is an aromatic subshrub that grows wild in Colombia [1]. Few studies with essential oil compounds from *V. curassavica* confirmed anti-inflammatory activity [2]. The volatile fractions of *V. curassavica* EO obtained at different times during steam distillation were compared in this research work. In total, 83 kg of fresh plant material from aerial parts were collected and chopped. Fractions were collected every 20 min for two hours. The volatile fractions of the EO of *V. curassavica* were obtained by steam distillation and characterized by gas chromatography using two columns, polar (DB-WAX) and apolar (DB-5MS), coupled with a mass selective detector (MSD) with electron ionization (EI, 70 eV). The major compounds of the fractions collected in the first 20 min were (*E*)-β-caryophyllene (26.4%), α-pinene (21.4%), germacrene D (14.8%), β-pinene (9.6%) and for the last 20 min were α-bisabolol (18.3%), (*E*)-β-caryophyllene (16.8%), and germacrene D (8.5%). The fractions enriched in terpenes such as (*E*)-β-caryophyllene and α-pinene, which have anti-inflammatory, analgesic and anxiolytic potential, may have applications in medicines to treat ailments and calm anxiety. Those enriched in compounds such as α-bisabolol and germacrene D, which have anti-inflammatory, anti-irritant and antibacterial activity, possibly have applications in cosmetics.

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AE-P25

CHEMICAL COMPOSITION BY GC/MS AND LC/MS OF ESSENCIAL OILS AND EXTRACTS ISOLATED FROM GERANIUM (*Pelargonium graveolens*), AND THEIR ANTIOXIDANT ACTIVITY

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ABSTRACT

Pelargonium graveolens (Geraniaceae) is an aromatic and medicinal plant native to South Africa, and its essential oil (EO) is widely used in cosmetic products, aromatherapy, and as a food flavoring [1]; it has been shown to have antibacterial, immunostimulant, antioxidant, hypoglycemic and antiinflammatory properties [2]. In this study, the chemical composition of the essential oil and extract of *P. graveolens* was analyzed. *P. graveolens* plants were collected in the experimental plots of CENIVAM (Barbosa, Colombia) and were distilled by microwave radiation-assisted hydrodistillation (MWHD) using Clevenger apparatus, with a Dean-Stark trap and microwave radiation heating set at 60% capacity (1350 W) for 60 min (15 min x 4). GC/MS and GC/FID were used for the chemical characterization of the EO; the major compounds identified were geraniol (45 ± 1%), citronellol (8 ± 1%), decanoic acid (7 ± 3%), linalool (5.4 ± 0.7%), 10-*epi*-γ-eudesmol (5 ± 1%), and *iso*-menthone (4.4 ± 0.3%). The extracts were analyzed by LC/MS, in positive and negative ion acquisition modes; were identified rutin, catechin, epigallocatechin, gallic acid, kaempferol-3-*O*-arabinoside, quercetin-*O*-hexoside-pentoside and luteolin-7-*O*-glucoside. The antioxidant activity of extracts was evaluated by ORAC and ABTS$^{+\bullet}$ methods; the µmol Trolox$^{®}$/g extract values of the *P. graveolens* extract were 2100 ± 344 167 µmol Trolox$^{®}$/g extract by the ORAC method, and 900 ± 167 µmol Trolox$^{®}$/g extract by the ABTS$^{+\bullet}$ method. The geranium EO distilled from plant material cultivated in Santander, Colombia, fulfills the specifications established in the ISO 4731:2012. The extracts obtained from the post-distillation material were rich in antioxidant compounds, such as flavones, flavanols and coumarins.

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AE-P26

GC/MS AND GC/FID ANALYSIS OF THE MAJOR COMPOUNDS OF THE ESSENTIAL OILS OF LEMONGRASS DISTILLED IN SANTADER, COLOMBIA.

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ABSTRACT

Cymbopogon flexuosus (Poaceae family) is a perennial aromatic plant commonly known as lemongrass. It’s distributed around the world, specifically in the tropical and subtropical regions of Asia and Africa. [1,2]. Its preparations or infusions are used in traditional medicine for their anxiolytic, analgesic, and diuretic effects [3]. The plant material was cultivated and collected in Bucaramanga and Barbosa, Santander, Colombia, and its essential oil was obtained by microwave-assisted hydrodistillation (MWHD). The identification of compounds was performed by GC/MS, on a GC 6890 Plus gas chromatography (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS column [5%-phenyl-poly(methylsiloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d_f)] and a DB-WAX [poly(ethylene glicol), 60 m x 0.25 mm (i.d.) x 0.25 (d_f)], and the quantification of these compounds was carried out by the GC/FID, using *n*-tetradecane as internal standard. Identification was based on mass spectra study (MS; electron ionization, 70 eV, coincidence > 95%), and the linear retention indices measured on the polar and non-polar columns. In the *C. flexuosus* EO, the geranial (38.0-50.8%) and neral (27.2-34.1%) were the principal compounds, and flash point [84-86 °C], optical rotation [(-)1.58-(+)1.03], refractive index [1.485-1.493] and relative density [0.8847-0.9037] were determined. The neral amount (27-34%) in the EO distilled from lemongrass, cultivated in Santander (Colombia) fulfills (25-35%) of the ISO 4718:2004 recommendation. The *C. flexuosus* EO distilled from plants grown in Santander (Colombia) contain vital bioactive compounds with medicinal and edible resources, therefore, they have a wide field of application in industry.

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AE-P27

CHEMICAL CHARACTERIZATION BY GC/MS OF *Piper aduncum* ESSENTIAL OILS

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ABSTRACT

The *Piper* genus is composed of about 1500 species grown in tropical and subtropical regions, its wide diversity makes of the Piperaceae family one of the major contributor to the Colombian biodiversity. In folk medicine, the *Piper* plants are used to treat inflammations, cuts, gastrointestinal problems, and also as an analgesic [1]. In this study, leaves, inflorescences and roots of *Piper aduncum* species (200 g) were collected from plants cultivated at the CENIVAM Agricultural Pilot Center (Bucaramanga, Colombia). Essential oil (EO) distillation, which was carried out by microwave-assisted hydrodistillation (MWHD), using a Clevenger-type equipment. The GC/MS and GC/FID was performed on both polar and non-polar columns, mass spectra, linear retention indices and standard compounds were used for EO constituent identification. The EO yields (*w/w*) obtained for leaves, inflorescences, aerial parts, and roots were 0.16%, 0.27%, 0.24%, 0.49%, respectively. The abundant components in *P. aduncum* EO were hydrocarbon monoterpenes (39%) and oxygenated monoterpenes (59%). Piperitone and 1,8-cineol were compounds present in the EO, distilled from different plant. Phenylpropanoid such as dillapiole were also found in all *Piper* EOs.

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AE-P28

GC/MS ANALYSIS OF *Salvia Rosmarinus* ESSENTIAL OIL OBTAINED BY MICROWAVE-ASSISTED HYDRODISTILLATION AND STEAM DISTILLATION

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ABSTRACT

Salvia rosmarinus Spenn (rosemary) is an aromatic plant of the Lamiaceae family. The essential oil (EO) of *S. rosmarinus* has antioxidant, anti-inflammatory and antimicrobial properties [1]. The rosemary plants were obtained from experimental plots of the CENIVAM research center. EOs were obtained by microwave-assisted hydrodistillation (MWHD) and steam distillation (SD). MWHD was performed in a microwave oven coupled to a Clevenger apparatus with a Dean-Stark trap [2]. SD was performed using a 0.1 m^3 stainless steel still. Each EO was analyzed by gas chromatography coupled to mass spectrometry (GC/MS) in *split* mode (1:30). EO compounds were identified by comparing their retention times and indices, mass spectra and fragmentation patterns with those of spectral databases, and certified reference substances. The main compounds were camphor (17-18%), α-pinene (12-14%) and 1,8-cineole (14-16%). The EO yield obtained by MWHD (0.84% w/w) was 2.6 times higher than that obtained by SD (0.32% w/w). The composition of EO obtained by MWHD corresponds better to the composition recommended by the International Organization for Standardization ISO 1342:2012, compared to the composition of the EOs distilled by SD.

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AE-P29

GC/MS STUDY OF *Steiractinia aspera* ESSENTIAL OILS OBTAINED FROM DIFFERENT CROPS IN SANTANDER (COLOMBIA) BY STEAM DISTILLATION

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ABSTRACT

Steiractinia aspera is a plant from the Asteraceae family, native to Colombia [1]; although its hydroethanolic extracts have shown good antioxidant properties *in vitro* [2], there has been little research conducted on the properties and composition of its essential oil. Chemical characterization of *S. aspera* essential oil was performed by GC/MS using both polar (DB-WAX) and non-polar (DB-5MS) chromatographic columns (60 m). *Split* injection (1:30, 1 μL) and MSD (EI, 70 eV) were used. The experimental mass spectra and linear retention indexes and those from spectral databases and standard compounds were used as confirmatory identification criteria. The essential oil was obtained by steam distillation of *S. aspera* aerial parts. The plants were collected in Bucaramanga (2019) and Barbosa (2021), Santander (Colombia). A total of 36 compounds were identified in the essential oil from Bucaramanga (2019), with the major constituents being α-pinene (24.9%), β-pinene (14.8%), β-phellandrene (10.1%), and germacrene D (13.1%). In the essential oil from Barbosa (2021), 56 compounds were identified, with α-pinene (27.3%), germacrene D (19.1%), limonene (8.2%), and *trans*-β-caryophyllene (8.2%) being the most abundant. For both plant harvests (2019, 2021) the major constituents were α-pinene and germacrene D. However, the overall chemical composition of the essential oils showed significant variation between the two different years and places of harvesting.

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AE-P30

CHEMICAL CHARACTERIZATION BY GC/MS AND GC/FID OF ESSENTIAL OIL FROM *Thymus vulgaris* L. PLANTS CULTIVATED IN COLOMBIA

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ABSTRACT

Thymus vulgaris L. (Lamiaceae), is a perennial, medicinal and aromatic shrub of the Mediterranean region and has an increasing economic importance for North America, Europe, North Africa and Asia [1]. The major constituents of *T. vulgaris* are thymol, carvacrol and flavonoids known to have insecticidal, antibacterial, anti-flatulent and acaricidal properties [2]. Vegetal material was collected and then distilled by microwave radiation assisted hydrodistillation (MWHD) in the small villages of Barbosa, Chipatá, Puente Nacional and Vélez (Santander, Colombia). The identification of the different compounds found in the essential oil (EO) was performed by GC/MS, using GC 6890 Plus (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS column [5%-phenyl-poly-(methylsiloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] and a DB-WAX [poly-(ethylene glicol), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] and quantification by the GC/FID. In *T. vulgaris* EO were found as major components: thymol (24.7-41.1%), *p*-cimene (15.1-42.2%), γ-terpinene (4.4-21.3%) y linalool (2.0-3.5%), that reached 80% of the total chromatographical area. The values of the relative amounts of linalool obtained in this study act in accordance with the values reported in ISO 19817:2017 [3]. The essential oil of *T. vulgaris* distilled from plants grown in Barbosa, Chipatá, Puente Nacional and Vélez (Santander, Colombia) has shown to have high quality standard attributes that may be of considerable interest for areas like pharmacology, agriculture, biochemistry, medicine and chemistry in which many of the compounds that were identified in the EO may be used for multiple applications.

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AE-P31

EVALUACIÓN DE DIFERENTES MÉTODOS PARA LA EXTRACCIÓN DE ACEITE ESENCIAL DE RIZOMAS DE *Hedychium coccineum* (Zingiberaceae): RENDIMIENTO Y COMPOSICIÓN QUÍMICA

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ABSTRACT

Hedychium coccineum (Zingiberaceae) es comúnmente conocido como lirio jengibre escarlata, que se utilizaba como planta ornamental originaria de Asia y se conoce localmente como Aichhia y Mansila. [1] Sus rizomas contienen aceites esenciales (AE) ricos en monoterpenos y sesquiterpenos como el E-nerolidol, acetato de borneol, espatulenol, linalool, elemol y borneol. [2] Se ha informado que el AE de H. coccineum tiene propiedades antimicrobianas, insecticidas, nematicidas, antiinflamatorias, herbicidas y antiproliferativas. [3] Para optimizar la extracción de estos AE, se utilizó un diseño experimental Box-Behnken (DBB) que evaluó el tiempo de extracción, la potencia de irradiación y el volumen de agua. Además, se probó un pretratamiento con ultrasonido (US+HDAM) y se compararon los resultados. La composición química de los AE se analizó mediante cromatografía de gases acoplada a espectrometría de masas (CG-EM). Se identificaron componentes usando la biblioteca NIST 2013 y los índices de retención de Kovats usando alcanos de C_8 a C_{25} como referencia. Los rendimientos de AE variaron entre 0.0996% y 0.2134%, mostrando que el tiempo de extracción y la potencia de irradiación influyen significativamente en los resultados. Las condiciones óptimas para HDAM fueron 480 mL de agua, 700 W de potencia y 50 minutos de extracción, con un rendimiento del 0.2248%. El pretratamiento con ultrasonido mejoró el rendimiento en un 10% sin alterar notablemente la composición de los AE. En total, se identificaron 40 compuestos, destacando nerolidol (17.42%), linalool (15.29%), espatulenol (10.66%) y acetato de bornilo (9.73%). Este estudio identificó las condiciones óptimas para la extracción de AE mediante HDAM y mostró que la combinación de ultrasonido y microondas mejora los rendimientos sin afectar de forma notable la composición química de los aceites.

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AE-P32

GC/MS AND GC/FID ANALYSIS OF *Eucalyptus globulus* (MYRTACEAE) ESSENTIAL OIL DISTILLED IN SANTADER, COLOMBIA.

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ABSTRACT

Eucaliptus globulus is a genus of the Myrtaceae family native to Australia and Tasmania. Four varieties are known and has two types of leaves. *E. globulus* has up to 100 meters in height [1] and its leaves contain bioactive components that make it important in human nutrition, pharmaceutical, sanitary, agricultural and cosmetic industry [2]. For this study, the *E. globulus* leaves were collected in Bucaramanga Santander (Colombia) and the essential oil was obtained by microwave-assisted hydrodistillation (MWHD). The EO chemical composition was performed by GC/MS, on a GC 6890 gas chromatography (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS column [5%-phenyl-poly(methylsiloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d_f)] and a DB-WAX [poly(ethylene glicol), 60 m x 0.25 mm (i.d.) x 0.25 (d_f)], and the quantification of these compounds was carried out by the GC/FID, using *n*-tetradecane as internal standard. The identification was based on mass spectra study (MS; electron ionization, 70 eV, coincidence > 95%), and the linear retention indices were measured on the polar and non-polar columns. The main components identified in the *E. globulus* EO were eucalyptol (57,4%), α-pinene (15%) and limonene (6,3%). These components contribute significantly to the biological activity of *E. globulus* EO due to its anti-inflammatory, analgesic and antimicrobial properties, making the EO an important component in many medicines for treatment nasal congestion, colds and respiratory diseases.

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AE-P33

GC/MS AND GC/FID CHEMICAL CHARACTERIZATION OF *Pogostemon cablin* ESSENTIAL OIL DISTILLED IN SANTANDER, COLOMBIA

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ABSTRACT

P. cablin, commonly known as patchouli, is an aromatic plant belonging to the Lamiaceae family. This plant is native to the southern and southeastern regions of Asia. Patchouli reaches a height of 1.0 to 1.2 meters and is characterized by its lush green leaves [1,2]. The essential oil (EO) of *P. cablin* is used in the cosmetics industry, especially in the production of body lotions and perfumes [3]. For this study, the plant material was cultivated in the towns of Barbosa, Chipatá and Puente Nacional, Santander, Colombia. The EO was obtained by microwave radiation assisted hydrodistillation (MWHD). The compounds in the EO were identified using gas chromatography coupled with mass spectrometry (GC/MS), on GC 6890 Plus (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS [5%-phenyl-poly-(methylsiloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] and DB-WAX [poly-(ethylene glicol), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] columns and quantification by the GC/FID. In the analysis of *P. cablin* EO, pachulol (33.7-48.7%), α-bulnesene (6.4-12.9%), α-guaiene (8.4-12.0%), seychellene (5.9-8.7%) and α-pachulene (3.8-5.1%), were identified as major components. The *P. cablin* EO distilled from plants grown in Santander, Colombia, have high quality standard characteristics for their commercialization as raw material in the pharmaceutical, food and cosmetic industries.

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AE-P34

CHEMICAL COMPOSITION BY GC/MS AND GC/FID OF *Lippia origanoides* ESSENTIAL OIL CULTIVATED IN SANTANDER COLOMBIA

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ABSTRACT

Orégano de monte (*L. origanoides*) is an aromatic plant with large, lance-shaped leaves, white flowers and round, highly branched stems [1]. The essential oil (EO) of *L. origanoides* is mainly made up of thymol, carvacrol and phellandrene (major compounds) [2,3]. In folk medicine, orégano de monte has been used as an antiseptic and antimicrobial [4]. Plant material was collected in the small village of Barbosa, Santander, Colombia. The EO was obtained by microwave radiation assisted hydrodistillation (MWHD). The identification of the compounds present in the EO was performed by GC/MS, on GC 6890 Plus (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS columna [5%-phenyl-poly-(methylsiloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] and a DB-WAX [poly-(ethylene glicol), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)] and quantification by the GC/FID. In *L. origanoides* OE, carvacrol (35.1-50.8%), thymol (12.3-18.7), γ-terpinene (9.812.3%), *p*-cymene (9.3-10.1%), α-humulene (1.2-2.6%) and β-myrcene (1.8-2.4%) were identified as major components. *L. origanoides* OE distilled from plants grown in Barbosa, Santander, Colombia, have high quality standard characteristics that are of great interest to the pharmacology, agriculture, biochemistry, medicine and chemistry sectors.

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AE-P35

EXTRACTO DE *Scutellaria coccinea* Kunth DE COLOMBIA INHIBE LA REPLICACION IN VITRO DEL VIRUS DENGUE SEROTIPO 2

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RESUMEN

El dengue es la arbovirosis más frecuente en Colombia, el número de casos ha incrementado más del 200% en 2024 comparado con 2023 [1]. Dado que aún no se ha descubierto un antiviral para el tratamiento del dengue y la medicina tradicional continúa siendo la alternativa, se requiere investigar el potencial farmacológico de plantas medicinales de Colombia. *Scutellaria coccinea* (Alegría) tiene diversos usos medicinales [2], se desconoce su utilidad para el tratamiento del dengue. **Objetivo:** Determinar el efecto del extracto de *S. coccinea* sobre la replicación del virus del dengue (DENV-2) en células hepáticas humanas (HepG-2). **Metodología:** El extracto fue obtenido mediante extracción hidroalcohólica asistida por ultrasonido. La citotoxicidad se determinó con el ensayo de MTT y el efecto antiviral se investigó tratando las células con seis concentraciones y cuantificando la proteína viral NS1 usando un estuche comercial de ELISA. **Resultados:** El tratamiento con el extracto de las células hepáticas infectadas con DENV-2 redujo el nivel extracelular de NS1 en 93% (CI_{50} de 41 ± 1.2 µg/mL). La concentración citotóxica 50 fue 663 ± 1.1 µg/mL y el índice de selectividad 15.9. Los resultados indican que el extracto de *S. coccinea* posee efecto inhibitorio *in vitro* relevante sobre el virus DENV-2. **Conclusión:** *S. coccinea* podría ser seleccionada para investigaciones dirigidas al descubrimiento de un fitoterapeútico para el dengue.

ASPECTOS ÉTICOS

La planta se cultivó en el Jardín Botánico del Centro Nacional de Investigaciones para la Agroindustrialización de especies vegetales aromáticas y medicinales tropicales (CENIVAM), UIS, Bucaramanga, Colombia.

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AL-P01

UNVEILING THE HIDDEN CHEMISTRY OF *Ilex guayusa* THROUGH GC-MS: THE IMPACT OF LIGHT AND AGE ON ITS VOLATILOME AND ANTIOXIDANT CAPACITY

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ABSTRACT

Ilex guayusa, a native tree of the Amazon Region, has aroused interest due to its use in the industry as an energizing drink and for the presence of secondary metabolites with antioxidant properties. However, the optimization of harvest conditions to maximize these products is still under development [1]. The main objective of this work was to determine the volatilome and antioxidant capacity under the influence of different light intensity conditions and maturation state of *I. guayusa* leaf extracts in three different chakras. Gas chromatography coupled to mass spectrometry was used to analyze the volatile compound profile in the extracts, and the antioxidant capacity was evaluated using the ABTS and DPPH methods. The component profile showed differentiation according to samples harvested in age ranges of 4 to 6 years and 6 to 10 years, as well as between those harvested in light and shade conditions, while the collection site did not have an impact on the metabolite composition. 23 metabolites were identified, of which acetophenone, 4-viniloguaiacol, 4-methoxyphenol, chalcone increased in shade condition in an age range of 6 to 10 years, while theobromine and ethyl 1-methylpipecolinate were more abundant in plants of 4 to 6 years. On the other hand, antioxidant capacity was affected by both light, age and collection site. Samples harvested in the absence of light and with ages in a range of 6 to 10 years increased the antioxidant power, in addition to those harvested in Alto Pano, which suggests that, although the volatile compound profile is not affected by the location of the chakra, the profile of higher molecular mass compounds probably varies significantly according to the location. These results emphasize the importance of optimizing cultivation practices and environmental conditions to improve the quality and antioxidant benefits of *Ilex guayusa*

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AL-P02

PRESSURIZED LIQUID EXTRACTION FOR THE RECOVERY OF BIOACTIVE METABOLITES FROM DEFATTED SEJE (*Oenocarpus bataua Mart.*): A CONTRIBUTION TO THE FOOD UTILIZATION OF AMAZONIAN PALMS

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ABSTRACT

Seje is the seventh most abundant palm in the Amazon and its oleaginous fruits have been traditionally used as foods. The fruits also contain bioactive compounds, which have not been comprehensively explored[1]. Several techniques have been applied to recover bioactive compounds with antioxidant capacity of phenolic nature from a wide range of fruits and vegetables. Pressurized liquid extraction (PLE) is an effective method to recover polar compounds by applying green solvents, such as EtOH and water[2]. This study developed a PLE process for extracting a Seje polar fraction rich in anthocyanins with antioxidant activity. Soxhlet (cyclohexane, 12 h, 50 °C, and 150 mbar) was used as a pretreatment for exhaustive defatting Seje pulp. The polar fraction from defatted pulp was obtained under PLE conditions after an optimization process employing a central composite design and multiple desirability function. Two factors at three levels were considered: solvent composition (%EtOH in the mixture EtOH/H_2O: 40, 60 and 80% *v/v* at pH 2.0 adjusted whit formic acid) and temperature (50, 75 and 100 °C). Response factors were extraction yield, total phenolic content (TPC), total flavonoid content (TFC), cyanidin-3-glucoside content (C3G), cyanidin-3-rutinoside content (C3R), and antioxidant activity (EC_{50} and TEAC). TPC, TFC, EC_{50}, and TEAC were performed by colorimetric methods[2], while C3G and C3R were determined via UHPLC-MS/MS dynamic-MRM triple quadrupole equipped with an electrospray source operating in positive ionization mode. The optimized MRM transitions for C3G and C3R were 449.1→287.1 *m/z* and 595.2→287.1 *m/z*, respectively. All results were maximized at the conditions of 70 °C and with 45% EtOH. Bioactive rich extracts from defatted Colombian Amazon Seje were characterized for the first time applying this approach, showing a broad concentration of anthocyanins (C3G and C3R). This application can be considered a successful demonstration of the great potential of the proposed methodology to effectively obtain natural extracts with potential bioactivity.

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AL-P03

UHPLC-ESI-Q-*Orbitrap*-MS STUDY OF BIOGENIC AMINES ISOLATED FROM FISH

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ABSTRACT

Biogenic amines (BAs) are produced by the decarboxylation of free amino acids (FAA) in food by microorganisms (e.g., bacteria) [1]. High BA content is associated with health issues (migraines, intoxication, and hypertension) and poor food quality [2]. Their high reactivity with nitrites to generate nitrosamines, potentially carcinogenic compounds, poses a public health risk [3]. In Colombia, fish consumption is part of the daily diet [4], however, an inadequate storage and transport process can lead to BA formation. In this study, we identified and quantified biogenic amines in tuna fish during a ten-day storage period using UHPLC-ESI-Q-*Orbitrap*-MS. The extracts were obtained using matrix solid-phase dispersion technique (MSPD), with modified C_{18} silica gel as adsorbent and methanol as elution solvent. BAs chemical identification in the extracts was carried by UHPLC-ESI-Q-*Orbitrap*-MS. Various biogenic amines were identified in tuna, *i.e.*, histamine $C_5H_{10}N_3$ $[(M+H)^+$, *m/z* 112.0869] and its typical ion-product at *m/z* 95.06037 $C_5H_7N_2$ $[(M+H)-NH_3]^+$, tyramine $C_8H_{12}NO$ $[(M+H)^+$, *m/z* 138.0913] and its ion-product at *m/z* 121.0647 C_8H_9O $[(M+H)-NH_3]^+$, putrescine $C_4H_{13}N_2$ $[(M+H)^+$, *m/z* 89.10732] and its ion-product at *m/z* 72.0807 $C_4H_{10}N$ $[(M+H)-NH_3]^+$ and cadaverine $C_5H_{15}N_2$ $[(M+H)^+$, *m/z* 103.1229] and its ion-product at *m/z* 86.0964 $C_5H_{12}N$ $[(M+H)-NH_3]^+$. The results showed the presence of biogenic amines in tuna fish. Histamine was the most abundant BA present in tuna extracts.

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AL-P04

MYCOTOXIN CONTENT IN PROTEIN SUPPLEMENTS

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Mycotoxins are secondary metabolites of fungi that pose a significant threat to global food security due to their adverse effects on human health. These compounds are characterized by high chemical stability and ubiquity. Simultaneous exposure to several mycotoxins produced by the same or different fungal species increases the risk of food toxicity [1].

This study aimed to determine the mycotoxin content of three protein supplements. The research material consisted of two plant-based proteins (rice and pea) and whey protein concentrate (WPC). Mycotoxin levels were estimated by separation techniques with the use of immunoaffinity columns (DON-Test ™ DON Testing System, VICAM, Watertown, USA; Zearala-Test ™ Zearalenone Testing System, G1012, VICAM, Watertown, USA) and an Agilent chromatography system (Santa Clara, CA, USA) coupled with the 6470 double quadrupole LC/TQ mass spectrometer.

Eight mycotoxins were detected in the analyzed proteins, including deoxynivalenol, aflatoxin B1 (AFB1), fumonisin B1 (Fum B1), fumonisin B2 (Fum B2), zearalenone (ZEN), ochratoxin, T-2, and HT-2 toxins. WPC was characterized by the highest sum of mycotoxins (172.76 µg/kg). However, plant-based proteins characterized similar levels of analyzed substances, 111.79 and 111.60 µg/kg for rice (RPI) and pea proteins (PPI), respectively. The most abundant mycotoxin in WPC and RPI samples was HT-2 toxin, while the dominant compound in RPI was ZEN.

Contamination of protein supplements with mycotoxins may be a significant problem in the dietary supplement sector, and it may have serious health consequences, including carcinogenic, cytotoxic, and inflammatory effects. Therefore, it seems appropriate to continue research on determining the standards of acceptable levels of toxins of fungal origin for a wider group of food products.

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AL-P05

NUTRITIONAL COMPOUNDS AND TOXIC ELEMENTS IN DIETARY SUPPLEMENTS FROM YOUNG BARLEY (*Hordeum vulgare L.*)

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ABSTRACT

Cereal grasses are perceived as superfoods, and as a result, their popularity is constantly increasing. In light of these facts, the content of bioactive ingredients (polyphenols, micro and macro elements, antioxidants activity) in dietary supplements containing green barley was examined. Furthermore, in order to assess the safety of consuming supplements containing young barley, the presence of environmental contaminants (pesticides, PAHs, heavy metals) was also investigated and compared with existing legislation, with a risk assessment also performed. The research material consisted of dietary supplements containing young barley, which were present on the Polish market between 2021 and 2023. The material comprised 14 samples in the form of tablets or capsules, 13 powdered barley grass and 4 juices. The supplements were purchased from pharmacies or online stores. Samples in the form of powder and juices did not require preliminary preparation for analysis, while tablets and capsules were ground to obtain a homogeneous powder. The total polyphenols content (TPC) and the antioxidant activity (AO) were determined by standard spectrophotometric methods. Phenolic acids concentration were analyzed by high-performance liquid chromatography–diode array detection (HPLC-DAD) as well as neonicotinoid pesticides. The other pesticides and PAHs was conducted by gas chromatography–mass spectrometry (GC-MS). Toxic elements were analyzed using inductively coupled plasma mass spectrometry (ICP-MS) and mineral content via atomic absorption spectrometry (AAS). Overall, the research findings indicated that although young barley powders exhibited a substantial amount of macro and microelements, in particular iron, potassium and calcium, they were also most contaminated with cadmium, lead and pesticides that makes them dangerous to the human organism. In turn, dietary supplements in the form of tablets or capsules frequently contain additional bioactive ingredients that may enhance their beneficial health properties. However, the results of this study indicate that they may also be a significant source of some harmful substances. Consequently, it is difficult to recommend which form of young barley supplement can be consumed without the risk to human health. Furthermore, our finding demonstrated that even products with the organic farming label also can contain the contaminants such as heavy metals and pesticide residues.

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AL-P06

CHEMICAL CHARACTERIZATION BY LC/MS OF XANTHOPHYLLS IN YELLOW CORN EXTRACTS

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ABSTRACT

Chicken meat and skin pigmentation are of great interest due to consumer preferences, particularly toward yellow hues in certain regions. Besides being a nutritional component in poultry feed, yellow corn is a natural pigment to enhance the color of chicken skin and egg yolk [1]. Xanthophylls, pigments found in corn, are crucial in this process, and their quantification is essential to meet quality and food safety standards [1]. This research aimed to determine by LC/MS the xanthophylls extracted from *Zea mays*. Yellow corn extracts were obtained by solvent extraction and solid-phase matrix dispersion (MSPD) techniques. The extraction yield by solvent extraction (13 ± 2%) was higher than that obtained for MSPD (5.00 ± 0.01%) Xanthophylls chemical identification in the extracts was carried by UHPLC-ESI-Q-*Orbitrap*-HRMS Three xanthophylls were detected in *Z. mays* extracts, i.e., lutein $C_{40}H_{56}O_2$ (*m/z* 568.42748, Δppm = 0.3), zeaxanthin $C_{40}H_{56}O_2$ (*m/z* 568.42748, Δppm = 1.9), and cryptoxanthin $C_{40}H_{56}O$ (*m/z* 552.43256, Δppm = 0.4). The information on the chemical composition of xanthophylls in yellow corn extracts could be useful for the poultry industry of the department of Santander.

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AL-P07

COMPARATIVE ANALYSIS OF AROMA EXTRACTION FROM COLD BREW COFFEE OF DIFFERENT VARIETIES (*Castillo*, *Colombia*, and *Caturra*)

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ABSTRACT

Coffee is one of the most widely consumed beverages worldwide, largely because of its inherent hedonic character. This characteristic has driven the continuous reinvention of the beverage aimed at creating new sensory profiles that appeal to the public. In this context, Cold Brew coffee has emerged as a beverage made through prolonged cold extraction, which imparts distinctive flavors and aromas to coffee, different from the traditional ones, contributing to its notable increase in popularity. However, limited information is available on the aroma of beverages and how it is affected by different variables. Therefore, this study aimed to characterize the sensory-active compounds in the aroma of Cold Brew coffee using gas chromatography coupled with olfactometry and mass spectrometry (GC-O-MS). To achieve this, volatile composition extraction was optimized and validated using headspace solid-phase microextraction (HS-SPME). Sample analyses using olfactometry were conducted with a trained sensory panel, identifying 15 compounds that exhibited sensory activity with descriptors such as floral, caramel, sweet, and almond. Initially, a single coffee variety was used, which led to the question of how these sensory-active compounds might be affected by the variety used in the beverage preparation. Therefore, the *Castillo*, *Colombia*, and *Caturra* varieties, which are common in Colombia, were selected to investigate how the sensory profile is influenced, and to determine the aroma descriptors associated with each variety. This revealed that various coffee types possess unique combinations of compounds in varying amounts.

ETHICAL APPROVAL

According to the University EIA Ethics Committee in its case CEI-202485-6, the project was approved under technical, scientific, and ethical conditions.

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AL-P06

IMPACT OF COFFEE QUALITY (HIGH, MEDIUM, LOW) ON THE EXTRACTION OF SENSORY-ACTIVE VOLATILE COMPOUNDS IN COLD BREW

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ABSTRACT

Coffee is one of the most consumed beverages worldwide; therefore, it is important to thoroughly investigate its properties. The flavor of a coffee beverage is influenced by factors such as coffee variety, roasting level, and extraction method (e.g., cold brew or hot extraction). These variables affect the chemical compounds produced, which in turn affect the sensory experience and quality of the coffee, particularly in methods such as cold brew, which produces a smooth and refreshing beverage with more fruity and floral notes, and less acidity. However, research on this method is very limited, so there are many aspects of coffee prepared using this method, which are still unknown. This study aimed to determine whether the sensory-active volatile compounds responsible for the aroma in Cold Brew vary according to the quality (high, medium, or low) of the coffee used for extraction. This will be done using the sample preparation technique of solid-phase microextraction (SPME), the HeadSpace method, and gas chromatography coupled with olfactometry (GC-O). The HS-SPME method has been validated in previous studies, making it effective for the analysis of volatile compounds [1]. This allows the identification of different types of aroma descriptors in beverages, including the presence of pleasant or unpleasant smelling compounds, which are perceived with varying intensities.The most characteristic descriptors for low-quality coffee were burnt, smoke, and earthy; for medium quality, there were caramel, woody, roasted, and chocolate notes; and for high quality, fruity, floral, and fresh aromas stood out.In this way, the objectives of using an optimized extraction method for volatile compounds and understanding the relationship between different coffee qualities and these compounds were achieved.

ETHICAL APPROVAL

According to the University EIA Ethics Committee in its case CEI-202485-6, the project is approved under technical, scientific, and ethical conditions.

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AL-P10

ANALYSIS BY GC/MS AND LC/MS OF RESIDUAL PESTICIDES IN BLUEBERRIES OBTAINED COMMERCIALLY IN BUCARAMANGA, SANTANDER

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ABSTRACT

Blueberries are an emerging crop in Colombia. Given its success in other neighboring countries, such as Chile and Peru, it is expected that blueberry farming will become more prominent soon [1]. Considering its potential for exportation, it is important to explore methods for determining contaminants, such as pesticides, in this fruit. The objective of this study is to analyze commercial blueberry samples using GC-MS/MS and LC/HRMS for the determination of a multi-residue pesticides. Blueberry extracts were obtained using two extraction techniques, i.e. ultrasound-assisted extraction (UAE) and QuEChERS procedure. Analysis of the extracts was carried out by GC-QqQ-MS and LC-ESI-Q-*Orbitrap*-HRMS. Out of 38 pesticides analyzed, 10 pesticides were detected in the samples. Three of them, imidacloprid (71,3 µg/kg), carbendazim (34,84 µg/kg) and thiamethoxam (3,67 µg/kg), were detected above the maximum residue level established in Colombia for this crop.

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AL-P11

A COMPREHENSIVE APPROACH TO OLIVE OIL ANALYSIS: LIPIDS SEPARATION AND CLASSIFICATION USING HPTLC AND RPLC-QTOF

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ABSTRACT

Olive oil (OO) is a staple in the Mediterranean diet [1], and only its extra virgin olive oil (EVOO) offers health benefits due to its lipid composition [2,3]. Lipids can be beneficial for health, making it essential to study their composition in OO. Reverse-phase liquid chromatography coupled to mass spectrometry (RP-LC-MS) is the most widely used technique for the qualitative and quantitative determination of the metabolic profile of OO [3]. However, this technique may encounter ion suppression issues due to overlapping lipids from different families, making the use of deuterated standards by lipid family insufficient. A solution to this problem is high-performance thin layer chromatography (HPTLC) which can preliminary separate lipids by family due to its simplicity and speed. For this purpose, a direct analysis of the oil dissolved in MTBE/MeOH (2.3:0.7) was performed using HPTLC to separate lipids by family. The fractions were then extracted from the plate and analyzed by RPLC-QTOF using a Phenomenex Kinetex C18 100 x 4.6 mm 2.6 µm column, with a mobile phase gradient of acetonitrile/water (60:40 v/v) and isopropanol/acetonitrile (90:10 v/v) at a flow rate of 0.6 mL/min. Our results demonstrate successful separation of lipid families on HPTLC plates, visualizing mono-, di- and triglycerides, cholesteryl esters, etc. Subsequently, we investigated whether the lipids in the olive oil could differentiate between extra virgin (VE) and non-extra virgin (NO-VE) categories. For this purpose, a total of 24 samples (17 VE and 7 NO-VE) were analyzed, with 18 samples used for the calibration model and 6 for validation. After autoscaling and mean-centering pretreatment, a calibration and global classification rate of 100% was achieved, with a Q2 of 0.764. This method successfully identifies specific lipids in Chilean olive oil and classifies oils according to their quality.

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AL-P12

A VOLATILOMICS APPROACH FOR COMPARING THE VOLATILE PROFILES OF RUMS FROM DIFFERENT PARTS OF THE WORLD USING HS-SPME-GC-MS

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ABSTRACT

Although rum is a widely consumed alcoholic beverage worldwide [1], there is no universally accepted standard for its classification or labeling [2]. Various classification systems exist, including terms such as “Golden,” “Premium,” “Añejo,” and “Reserva,” which are often dictated by the regulations of each country [2]. In this study, the volatile profiles of rums from multiple countries were analyzed using Headspace Solid-Phase Microextraction coupled with Gas Chromatography-Mass Spectrometry (HS-SPME-GC-MS) to identify characteristic compounds that could potentially categorize or classify rums based on their country of origin. The Global Natural Products Social Molecular Networking (GNPS) and MetaboAnalyst platforms were employed for multivariate and chemometric statistical analysis of the features identified in the rum samples [3]. Additionally, some characteristic compounds were tentatively identified using GNPS platform databases, standard mixtures, and retention indices. The volatile profiles obtained through HS-SPME-GC-MS, combined with statistical analyses using extensively recognized omics platforms, revealed significant differences between rums from different countries.

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AL-P13

EVALUATION OF THE ANTIOXIDANT CAPACITY OF TOTAL EXTRACT AND FRACTIONS OF THE PLANT SPECIES *Achyrocline bogotensis*

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ABSTRACT

Worldwide, deterioration caused by oxidation processes affects the quality, safety and shelf life of products manufactured by the pharmaceutical, food and cosmetic industries [1]. Therefore, there has been a growing interest in the search for substances of natural origin with antioxidant potential to delay or prevent oxidation processes [2]. In this work, antioxidant capacity was evaluated using the $ABTS^{+\cdot}$ and $DPPH^{\cdot}$ methods, and preliminary phytochemical analysis (PPA) and quantification of phenols and flavonoids in extracts and fractions of the plant species *Achyrocline bogotensis* was carried out. A hydroethanolic extract (HEE) was made by maceration and subsequent liquid-liquid fractionation with solvents of lower to higher polarity using hexane (HFr), dichloromethane (DFr) and water (AFr). The PPA assays allowed the identification of flavonoids, glycosides, tannins, sesquiterpenic lactones, carotenoids, coumarins and steroids. The concentration of phenols and flavonoids for the HEE was 256.3 ± 25.5 mg GAE/g and 36.2 ± 1.2 mg QE/g, respectively. Contents of 46.8 ± 2.8 mg GAE /g and 48.2 ± 0.5 mg QE/g were found in HFr, 178.1 ± 16.4 mg GAE/g and 114.4 ± 3.5 mg QE/g in DFr, and 260.5 ± 22.9 mg GAE/g and 26.0 ± 0.50 mg QE/g in AFr for phenols and flavonoids, respectively. The determination of the antioxidant capacity of the total extract and the fractions using $ABTS^{+\cdot}$ and $DPPH^{\cdot}$ allowed the calculation of the 50% inhibitory concentration (CI_{50}), finding values of 12.3 ± 0.6 ppm and 30.9 ± 0.1 ppm for HEE, 56.4 ± 0.3 ppm and 300.9 ± 2.3 ppm for HFr, 12.1 ± 0.1 ppm and 20.2 ± 0.5 ppm for DFr and 9.9 ± 0.3 ppm and 15.7 ± 0.01 ppm for AFr, respectively. In conclusion, the total extract and the fractions of *Achyrocline bogotensis* show antioxidant capacity with AFr having the highest activity, and this may be related to the content of phenolic compounds. * GAE: gallic acid equivalent. QE: quercetin equivalent.

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AL-P14

VOLATILOME AND FATTY ACID PROFILES OF THE "SUERO COSTEÑO"/MILK FROM CÓRDOBA (COLOMBIA): CHEMICAL CRITERIA AS SUPPORT FOR THE DESIGNATION OF AUTOCHTHONOUS-REGIONAL PRODUCT IDENTITY

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ABSTRACT

Suero costeño (SC) is an autochthonous food from the northern region of Colombia, produced mainly in an artisanal way and by spontaneous fermentation of raw cow´s milk (RM). It has a smooth texture and a characteristic flavor (sour/salty taste and acrid/ rancid odor) which is well accepted by consumers [1,2]. As an artisanal dairy product, this research focused on establishing of the product identity from the chemical compositions (by GC-FID/MSD) of the volatile fractions (by HS-SPME and SDE) and fatty acids (as FAME) present in SC and RM samples, from eight localities in the department of Córdoba (Colombia) and five different manufacturing methods. Thus, the most important findings were: (i) both RM and SC were mainly constituted by $C_{16:0}$ (21-29%), $C_{18:1}$ (13-23%), $C_{18:0}$ (12-17%) and $C_{14:0}$ (7-12%) acids, as well as SFA (59-69%), MUFA (26-36%), PUFA (2-5%), ω-3 (0.2-1.2%), ω-6 (0.5-1.6%) and ω-9 (19-30%) acids, with no significant differences between them ($p>0.05$); (ii) compositional differences ($p<0.05$) were observed in the volatile fractions between RM and SC samples, as well as between SC samples due to the manufacturing processes used; nevertheless, it was possible to establish a volatilome profile for the type of food; (iii) the main constituents that contributed to the chemical identity of this dairy product were ethyl esters (C_2-C_{12}, $C_{10:1}$(cis-D^9)-$C_{18:1}$(cis-D^9)), aliphatic alcohols [(2E)-tridecen-1-ol, C_2, isoamyl alcohol]/aldehydes (C_{16}, C_{14}), methyl alkyl ketones (2-pentadecanone, 2-tridecanone, 2-undecanone), sesquiterpenes (β-caryophyllene, a-humulene), monoterpenes (limonene), benzoic acid, benzenethanol along with SCFA and acetoin.

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AL-P15

Influence of the addition of coffee bean extract on the physicochemical properties of chitosan-alginate films

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ABSTRACT

The demands of consumers for the high quality foods have contributed to an increased interest in the development of edible packaging. The biodegradable films and coatings can be produced from the natural polymers, such as, proteins, polysaccharides or their combination, which are perfectly biodegradable and safe to environment. Among the films based on polysaccharides, chitosan and alginate films have attracted particular interest for maintaining quality and extending shelf-life of fruits, vegetables, meat, poultry, seafoods, and cheeses by reducing dehydration, controlling respiration, enhancing product appearance and improving mechanical properties. The aim of this study was to develop the novel chitosanalginate (1:0.3 m/m) based films (CHALG) incorporated with the extracts of coffee beans of different degree of roasting (2.5%, m/m), as well as to estimate their structural, mechanical (DMA), thermal (DSC) and mechanical properties. The water-ethanolic extracts (40:60, v/v) obtained from the green coffee beans, and those of different degree of roasting were tested in terms of the content of phenolic compounds (TPC), chlorogenic acids (CQAs), free phenolic acids (TPA), and antioxidant activity estimated in the reaction with DPPH radical. Among the studied samples, the extract of green coffee was characterized by the highest content of phenolic compounds determined by means of high performance liquid chromatography (HPLC); whereas, the extract of light roasted coffee exhibited the highest antioxidant activity. The dark roasted coffee extract was characterized by the lowest values of the mentioned parameters. The five various films enriched with the coffee extracts were obtained. ATR-FTIR analysis verified the interactions between chitosan and alginate being components of the studied films as well as between CHALG composite and the components of the coffee extracts. Coffee extracts improve the thermal and mechanical properties of the films tested. All the films with coffee extracts have a higher elongation at break and higher strength compared to the base film. DMA analysis allowed significant differences to be observed in the films studied. The storage modulus is responsible for the elastic behaviour of the 1st order bonds in the material. Extracts significantly increase the storage modulus and the loss modulus in the films tested.
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AMB-P01

Effects of climate change on the mobility of organophosphates pesticides in soils of the Arroyo Grande coastal aquifer, Bolivar, Colombia

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ABSTRACT

The modelling of the effects of climate change on the transport of organophosphate pesticides in soils and the risk to the groundwater of the coastal aquifer of Arroyo Grande in the Northern of the Colombian Caribbean it is a necessity in the present. This aquifer is a source of fresh water used for agricultural activities and for the supply of drinking water, located at the north of the department of Bolívar and is an area of great projection for the development of tourism in which there are no policies for the sustainable use of this valuable resource[1]. Three points in this area were choose, where organophosphate pesticides are used to combat crop pests are characterized for their hydro-geochemical parameters. The modeling was adjusted from tests of undisturbed soil columns where the concentration of the organophosphate pesticides Chlorpyrifos© and Parathion© are monitored between two months. The pesticides were extracted by Soxhlet using a mixture of 1:1 n-hexane and acetone for 4 hours and quantified by Gas Chromatography coupled with Mass Chromatography[2]. Then, the transport of pesticides in the soil columns is modeled with the MACRO 5.2, because this software has shown good results to model and simulate the transport of pesticides in countries like Norway and the Netherlands[3]. This model will use to simulate the direct effects generated by climate change like as the increase in the temperature and the decrease in the rainfall in the future scenarios throw 25 years between 2025 - 2050. This simulation is proposed according to RCP 8.5 model[4], given that model anticipate among the indirect effects going to generate by climate change are the increase in the use of pesticides and the use of new wells to supply the water demand in the region, for these reasons is important evaluate the probability of risk of the Arroyo Grande aquifer groundwater. This project tries to contribute to the planning of policies that serve for the sustainable development of the land use as well as the water resource of great socioeconomic potential for the department of Bolívar in Colombia.

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AMB-P02

CUANTIFICACION DE PESTICIDAS ORGANOCLORADOS EN SEDIMENTOS MARINOS SUPERFICIALES DEL ARCHIPIELAGO DE NUESTRA SEÑORA DEL ROSARIO (ISLAS DEL ROSARIO, CARTAGENA, COLOMBIA)

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ABSTRACT

Los pesticidas organoclorados (OCPs) se caracterizan por ser altamente liposolubles y tóxicos [1]. Por tal motivo la presencia de estos compuestos en sedimentos marinos representa una amenaza para los organismos acuáticos, afectando el medio ambiente y la salud humana a través de la cadena trófica [2]. La literatura reporta que puede ocasionar enfermedades como cáncer hepático, malformaciones urogenitales, efectos en la espermatogénesis, aborto espontáneo, síntomas neuropsicológicos y psiquiátricos [3], y a nivel ambiental afecta la reproducción, crecimiento, y procesos fisiológicos de los organismos acuáticos [4]. El objetivo principal de esta investigación fue determinar las concentraciones de OCPs presentes en doce zonas de muestreo del archipiélago de nuestra señora del rosario. La extracción de los OCPs en los sedimentos se realizó mediante un método de extracción solido – líquido (soxhlet), para la separación e identificación de los analitos se empleó un cromatógrafo de gases acoplado a un detector de micro-captura de electrones (GC-μECD). El estudio evidenció la presencia de 6 pesticidas de los 7 estudiados, siendo el lindado y metalocloro los pesticidas con más incidencias en las zonas de muestreo. Las islas donde se encontró mayor contenido residual de OCPs en sedimentos fueron: Isla Grande, Isla Múcura, Isla Maravilla e Islote, con concentraciones que oscilan entre $1.40x10^{-5}$-$1.48x10^{-3}$g/kg, $2.60x10^{-6}$-$1.17x10^{-4}$μg/kg, $1.10x10^{-6}$-$1.14x10^{-4}$μg/kg, $4.24x10^{-8}$-$3.58x10^{-4}$μg/kg, respectivamente. Aunque los valores no sobrepasan los límites establecidos en la NOAA, si son inquietantes ya que los OCPs fueron prohibidos en el territorio colombiano por el decreto 305 de 1988, y se hallan trazas de estos pesticidas en algunas islas consideradas áreas protegidas.

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AMB-P04

PSYCHO-VOLATILOMICS OF ACOUSTIC STIMULI IN SEEDS OF (Phaseolus vulgaris): AN EXPLORATION USING SPME GC-MS

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Plants react to stimuli present in the environment in order to adapt and survive to changing environmental conditions, they emit volatile organic compounds in response to changes such as: water stress, herbivory, infection by phytopathogens (bacteria, fungi) [1-5]. The importance of these secondary metabolites during germination, growth, reproduction, fruit production is a very important topic to implement alternative methods and beneficial stimuli in plants and thus avoid the use and elimination of agrochemicals and exogenous fertilizers generating soil degradation, contamination of aquatic and terrestrial ecosystems, causing a decrease in the quality of the ecosystem in general. For this reason this study develops a method based on the application of acoustic stimuli to improve the conditions of growth, germination and behavioral change, showing positive effects during development, facilitating physiological processes with nutrient absorption, protein synthesis, photosynthesis and general development of the plant [2-4] in the germination stage of a species of agricultural interest (Phaseolus vulgaris). The best seeds were chosen taking into account morphological characteristics such as: uniform color, absence of spots showing disease, the seeds were put into germination using 100 mL beakers and were placed in a place guaranteeing equal conditions of light, temperature and humidity. For the analysis of volatiles, a closed 6.5 cm3 glass chamber was used where the plant was exposed to acoustic stimuli and adsorption process for 45 min, using two types of acoustic stimuli (major and minor tonality) and a control treatment where there was no acoustic exposure. SPME solid phase microextraction was performed, using gray fiber (CAR/DVB/PDMS), then a gas chromatography equipment coupled to GC-MS mass spectrometry (QP2010 Plus) with 45 min extraction method was used, left in thermal desorption for 10 min, to finally obtain the chromatogram of the mapped VOCs volatile organic compounds, in parallel length of hypocotyl and root were taken from day 6. The research presented here is linked to precision agriculture, crop breeding and behavioral psychology studies.

Key words: VOCs, SPME, germination, environment, agriculture, behavior.

AMB-P10

ELECTROCHEMICAL AND PHOTOELECTROCHEMICAL DEGRADATION OF OXYTETRACYCLINE AND OXOLINIC ACID ON Ti/TiO$_2$ MODIFIED ELECTRODES

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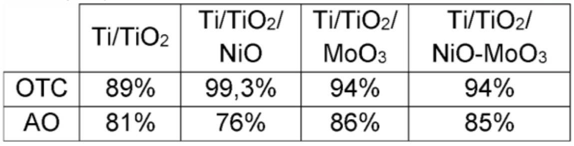
ABSTRACT

The use of antibiotics has increased in recent years in the livestock industry. This is mainly due to its low cost, ease of handling and its broad spectrum of activity against bacteria. Among the most used are the tetracycline, quinolone and sulfone families that are used for the prevention and treatment of diseases [1]. The contamination of surface and wastewater with these compounds has been recognized as an issue of environmental interest in many countries. Therefore, the development of methodologies capable of decomposing, transforming or reducing these contaminating compounds is essential.

Currently, the use of electrochemical methods has received considerable attention, with TiO$_2$ being one of the most studied compounds for those reactions that can produce chemical modifications in this type of contaminants [2].

In this work, the degradation of oxytetracycline and oxolinic acid was evaluated by electrochemical (EC) and photoelectrochemical (PEC) methods using Ti/TiO$_2$ and modified Ti/TiO$_2$ electrodes. Ti/TiO$_2$ electrode was prepared by anodizing in an acid medium using 0.5 M H_2SO_4 + 0.13 M NH_4F. Ti/TiO$_2$ modified electrodes were then modified with Ni oxide (NiO) and Mo oxide (MoO$_3$) by drop-coating. The degradation reaction was carried out using these electrodes by electrolysis at controlled potential and the concentration of the antibiotics was controlled by HPLC-DAD measuring at a specific wavelength for each antibiotic. The results indicate that there is a dependence of the degradation percentage on the electrode used, showing that the modification of the TiO$_2$ film influences the degradation process of the antibiotics (**Table 1**).

Table 1: % Degradation of oxytetracycline (OTC) and oxolinic acid (AO) with Ti/TiO$_2$ and Ti/TiO$_2$ modified electrodes.



	Ti/TiO$_2$	Ti/TiO$_2$/ NiO	Ti/TiO$_2$/ MoO$_3$	Ti/TiO$_2$/ NiO-MoO$_3$
OTC	89%	99,3%	94%	94%
AO	81%	76%	86%	85%

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AMB-P11

REMOVAL OF ARSENIC FROM AQUEOUS SOURCES USING A BIOADSORBENT PRODUCED FROM LYCHEE SEEDS (LITCHI CHINENSIS).

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ABSTRACT

Arsenic is one of the contaminants that has received the most attention due to its classification as a group-A carcinogen through water consumption, with the World Health Organization establishing a limit concentration of 10-100 ppb for drinking/irrigation water [1]. For these reasons, new methods are emerging as a necessity for the removal of arsenic. The aim of the following study was to develop bioadsorbents using lychee seeds. Two bioadsorbents were prepared from dried lychee seed (DLS) and another modified with iron (DSL-F) and used for the removal of arsenic III, V and organic. Firstly, it was observed that the surface characteristics were altered by the iron modification, with a significant increase in the surface area, which rose from 0.0170 m^2/g (DLS) to 21.9690 m^2/g (DLS-F). In addition, the zero charge point (PCZ) of DLS was found to be 5.44 and of DLS-F 3.56 respectively. Finally, the arsenic removal capacity of both materials at different pH was studied. The highest removal results were 6,90% for DLS at pH 9 for As III and 9.05 % for As V at pH 3, while DLS-F had its removal efficiency at pH 11 for As III (77.05 %), pH 5 (As V 100.38 %) and pH 11 (organic As 40.97 %). This is probably due to the distribution of arsenic species, for example, arsenious acid (V) has pKa = 2.3 and arsenious acid (III) has pKa = 9.3; This means that for both species at the best adsorption pH, they will be mainly in their basic form, in the same sense the PCZ of the material shows that its surface at both pHs will be negatively charged, which would explain the low adsorption values for DLS, however, DLS-F showed high removal rates due to Fe-As interaction or through the interaction of Fe with the non-bonding electron pairs of the oxygen that are bound to arsenic. These results show that lychee/seed modified with iron is an adsorbent with excellent results for removing arsenic from aqueous matrices allowing the use of waste with low added value that could minimize the cost of water treatment processes.

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AMB-P12

COMPARATIVE ANALYSIS OF THE ACTIVITY OF HETEROPOLYACID CATALYSTS IN HOMOGENEOUS PHASE TO OBTAIN BIODIESEL FROM THE OIL EXTRACTED FROM *Persea Americana Mill*. LORENA VARIETY WASTE

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ABSTRACT

One of the main attractions of biodiesel is that it can be obtained from any raw material rich in triglycerides, mainly from vegetable oils, which makes the resource practically inexhaustible. The avocado *Persea amercana Mill.* Lorena variety is produced in tropical and subtropical countries of the five continents. In Colombia, several types of avocado are grown, of which the Lorena variety is the only native one. In the last decade this fruit has presented an increase in its production volumes due to its importance in the human diet; however, a significant volume of production is lost for overripening, pests and defects in fruit quality causing a environmental impact associated with the generation of agricultural waste, which translates into economic losses and low productive efficiency in the sector. The objective of this study was to carry out a comparative analysis of the catalytic activity of heteropolyacid catalysts to obtain biodiesel from the oil extracted from the Lorena variety avocado and thus generate a use of the agroindustrial waste of this fruit. Two catalysts were used: phosphotungstic acid $H_3PW_{12}O_{40}$ (HPW) and Silicotungstic acid $H_4SiW_{12}O_{40}$ (HSiW) to obtain biodiesel. Different catalytic conditions such as catalyst concentration, reaction time and reaction temperature were evaluated. The progress of the reaction was continuously monitored by taking aliquots at one-hour intervals and analyzing them by GC/MS and catalytic parameters such as conversion and selectivity were calculated. The best catalytic conditions for HPW were: 1 mol %, 3 hours and 60 °C for 99% conversion of oleic acid, while with HSiW the best conditions were: 1 mol %, 4 hours and 60 °C, for 99% conversion of oleic acid. With the above, it was established that the HPW catalyst presented the best catalytic conditions. This work is a contribution to the sustainable development of the Colombian agroindustrial sector since it allows the generation of added value and utilization of *Persea americana Mill.* Lorena variety residues.

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AMB-P13

DECARBOXYLATION OF DICLOFENAC AND FORMATION OF ARTEFACTS IN THE HOT GC INJECTION PORT

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ABSTRACT

Diclofenac is a commonly used anti-inflammatory drug and it is synthesized using an indolinone derivative. Due to the thermal unstability of diclofenac, an intramolecular cyclization product (impurity A) may be formed, or the oxidation of the decarboxylated diclofenac products to an alcohol (-CH_2OH, impurity C), an aldehyde (-CHO, impurity B), and other derivatives can be observed [1,2]. A hot GC injection port was coupled to a temperature controller; the effect of carrier gas type (air or helium), temperature (100, 150, 200, 250, and 300 °C), and preparation solvent (ethyl acetate, methanol or dichloromethane) were studied. The splitless injection mode was used, a flow rate was set at 1 mL min^{-1}, and an injection volume was 2 µL. A DB-5MS short column (0.12 m x 0.25 mm x 0.25 µm) was connected to the injection port, and the column outlet was introduced into ethyl acetate (0.5 mL); the injection lasted 1 min. Each eluate recovered in ethyl acetate was concentrated to dryness, reconstituted in water: methanol (1:1) and analyzed by UHPLC-ESI$^+$-*Orbitrap*-HRMS. The best analytical response obtained by LC/MS for diclofenac and its impurities A, B, C was obtained using water and methanol as mobile phase, with 0.2% (v/v) formic acid, and with the capillary voltage set at 3.5 kV. The variation coefficients were in the range of 0.04-0.2% and 0.6-4% for retention times and chromatographic areas, respectively. Minimum detection and quantification levels values were found to be between 0.2-0.9 µg L^{-1} and 0.6-3 µg L^{-1}, respectively. It was shown that in helium gas the formation of impurity A (γ-lactam) was predominant, while in the presence of air, impurities B and C were mainly formed, through a possible intermediate 2,6-dichloro-*N*-(*o*-tolyl)aniline. This study contributes to the understanding of the diclofenac thermal decomposition and the elucidation of different reaction mechanisms, which some thermolabile compounds could experiment in the hot GC injection port.

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AMB-P14

MICROBIOLOGICAL AND CHEMICAL METHODS IN SCREENING FOR BACTERIAL RESISTANCE TO ANTIBIOTICS IN WASTEWATER TREATMENT PLANTS (WWTPS) AND THEIR CONTRIBUTION TO THE CONCEPT OF ONE-HEALTH.

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ABSTRACT

The contamination of water sources by water from industrial, agricultural and hospital sectors has recently gained great relevance, finding in these waters a high load of contaminants such as antibiotics, disinfectants, remains of medicines, hormones, among others, (1-2) as well as detecting high concentrations of pathogenic microorganisms, harmful to human health and the ecosystem, including enterobacteria, fecal coliforms and Gram-negative bacilli fermenters and non-fermenters of lactose, and others, such problems suggest a challenge for their elimination, mitigation and establishment of effective solutions for their control (3-5). This research relates the presence of emerging antibiotic-type contaminants in a hospital wastewater treatment plant (WWTP) in the department of Caldas, with resistance to AMR antimicrobials and how this multisectoral problem affects humans, the environment and the entire ecosystem, based on the concept of a single health to obtain a comprehensive approach to this situation. In this study, persistent resistance to ciprofloxacin and ceftriaxone was found to be greater than 80% in total heterotrophic bacteria. In the coliform group, the following was observed: Ceftriaxone 48% resistant at MIC and greater than 90% in the three lower concentrations. For ciprofloxacin, resistance was found at MIC with values higher than 90 %. In Gram-negative bacilli and Enterobacteriaceae (lactose fermenters and non-fermenters), a tendency to acquire resistance to ampicillin was observed, showing percentages of resistance higher than 90 % at the lowest concentration (1 μg L-1). In parallel to these, analysis was performed by HPLC high performance liquid chromatography identifying two drugs (amoxicillin and cephalexin) in the influent waters of the WWTP, in 5 samples, and quantifying cephalexin in a concentration of 2 mg L-1, thus finding that emerging antibiotic type contaminants are intensifying the phenomenon of AMR.

Key words: Contaminants, Water, Ecosystem, AMR, WWTP, Selective Pressure

Antibiotic consumption in secondary and tertiary hospitals in Colombia: national surveillance from 2018-2020. Rev Panam Salud Publica/Pan Am J Public Heal. 2023;47:1–8.

AMB-P015

ESTANDARIZACIÓN DE UNA METODOLOGÍA POR MEDIO CG-EM PARA IDENTIFICACIÓN Y CUANTIFICACIÓN DE DICLOFENACO Y LORATADINA COMO CONTAMINANTES EMERGENTES

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ABSTRACT

El agua es el bien más valioso del mundo, buscar herramientas para reducir y hacer seguimiento a su contaminación genera continuidad a los procesos de protección de los recursos hídricos. En este trabajo se presenta la estandarización de una metodología por CG-EM que tiene por objetivo, realizar el seguimiento del proceso de biodegradación llevado a cabo por la especie de microalga de agua dulce *Chlorella vulgaris* sobre los fármacos diclofenaco y loratadina. Los dos hacen parte del grupo de contaminantes emergentes, los cuales se detectan a bajas concentraciones en los cuerpos de agua, con efectos tóxicos sobre el entorno acuático y en la salud. Para la estandarización se establecieron las mejores condiciones para identificar los dos analitos mediante el mismo método. Los análisis se realizaron en un cromatógrafo de gases Trace 1300 (Thermo Scientific). Se utilizó una columna TG-5MS 30 m x 0.25mm x 0.25 µm (5% fenilo) y se empleó He como gas portador a 1.0 mL/min. La temperatura del puerto de inyección fue de 250°C en modo splitless. En el horno se estableció una rampa de temperatura que inició en 150°C, después 20°C/min hasta 220°C durante 1,0 min y finalmente 10° C/min hasta 300°C durante 1,0 min. Se estableció un tiempo de corrida de 17 min. Los espectros de masas se obtuvieron en el modo full scan (m/z: 35 a 400 umas) con el modo de ionización de impacto electrónico a 70 eV. Las temperaturas de la línea de transferencia y fuente de ionización fueron 280°C y 260°c respectivamente. Los tiempos de retención fueron 7.30 y 15.9 min para el diclofenaco y loratadina, respectivamente. Se realizaron curvas de calibración con seis niveles de concentración con los dos analitos en una misma solución. Se obtuvo un comportamiento lineal entre 15,0 mg/L a 40,0 mg/L ± 0,1 para la loratadina y 10,0 mg/L a 45,0 mg/L ± 0,1 para el diclofenaco. Se evaluó la precisión y robustez. La metodología descrita permite el seguimiento de los posibles procesos de biodegradación de los dos contaminantes que permitirá establecer el tipo de metabolitos generados al exponerlos antes a la microalga *Chlorella vulgaris*.

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AMB-P08

ESTUDIO DE INHIBICIÓN DEL CRECIMIENTO DE ESPECIES DE HONGOS DE LA PODREDUMBRE BLANCA EN PRESENCIA DEL ANTIBIOTICO DOXICICLINA

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ABSTRACT

Los recursos hídricos están cada vez más limitados y su calidad está comprometida por diversos contaminantes, incluidos los contaminantes emergentes (CE), como la doxiciclina, un antibiótico que al ser utilizado extensamente para prevenir y tratar enfermedades infecciosas en humanos y animales es motivo de preocupación ya que su presencia constante en el agua puede alterar los ecosistemas acuáticos, afectar el sistema endocrino humano y promover resistencia bacteriana a los antibióticos [1]. Por lo anterior, este trabajo pretende estudiar el efecto de la doxiciclina en el crecimiento de 3 especies de hongos de pudrición blanca (*Irpex Lacteus*, *Phanerochaete Sordida y Bjerkandera sp.*) como paso inicial para el posterior empleo de estos microorganismos en la degradación del CE en medio acuoso. Para ello se cortaron discos de 5 mm de diámetro del borde exterior de cepas de dos semanas de antigüedad cultivadas en un medio sólido que contenía en gL^{-1}: glucosa (20), extracto de levadura (2), peptona (1.5), KH_2PO_4 (1), $MgSO_4$ (0.5) y agar (15) incubados a 30 °C. Los discos se colocaron asépticamente en el centro de placas de Petri de 90 mm de diámetro con 25 ml de medio sólido suplementado con doxiciclina en concentraciones de 10, 50, 100, 200, 300, 400 y 500 ppm. Cada especie se inoculó en tres placas, además de placas de control sin antibiótico, incubadas entre 25 y 30 °C. Se midió el diámetro del halo de crecimiento en días distintos para calcular el porcentaje de inhibición [2]. Los resultados mostraron que la doxiciclina inhibe el crecimiento de las tres especies de hongos comparado con el cultivo control, siendo el hongo *Phanerochaete Sordida* la especie que presento mayor inhibición a una concentración de 300 ppm con un porcentaje de inhibición de 93,05%, a comparación de la especie *Bjerkandera sp.* e *Irpex Lacteus* las cuales presentaron porcentajes de inhibición a esa misma concentración del 39,99% y 20,44% respectivamente. Considerando que la dosis administrada en humanos es 200 mg/día, las concentraciones máximas establecidas para la exposición del contaminante con los hongos son adecuadas para el posterior estudio de la biodegradación de doxiciclina en agua.

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AMB-P019

OPTIMIZACIÓN DEL METODO DE ENCAPSULACIÓN DE LA MICROALGA *Chlorella vulgaris* PARA POSTERIOR EMPLEO EN LA BIOREMOCIÓN DE CONTAMINANTES EMERGENTES EN AGUA

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ABSTRACT

La contaminación de cuerpos de agua con contaminantes emergentes representa un desafío ambiental considerable. Algunos fármacos como la loratadina y el diclofenaco hacen parte de este grupo, los cuales se encuentran en cantidades de trazas. Este estudio se enfoca en la encapsulación de la microalga *Chlorella vulgaris* utilizando alginato de sodio y cloruro de calcio realizando el seguimiento de su estabilidad en el tiempo en el medio acuoso. Para optimización de las esferas se llevó a cabo un diseño experimental 3^k, k=3. Los factores fueron el tamaño de la esfera, $CaCl_2$ y alginato. El tamaño de la gota fue medido con 3 tipos de goteros, se estableció midiendo la cantidad de esferas que llenaban un volumen de 1 mL encontrando valores de 26, 15 y 10 gotas por mL para los goteros 1, 2 y 3 respectivamente. Las relaciones de $CaCl_2$ con alginato de sodio en un volumen constante de 200 mL de agua fueron 0,2510, 0,3760 y 0,5051 g. El diagrama de pareto indicó la influencia significativa del tamaño de la esfera y la concentración del $CaCl_2$. Se procedió con un diseño de superficie de respuesta con puntos extremos a un intervalo de confianza del 95%, evaluando valores de 0,625 y 0,125 g de $CaCl_2$. La ecuación del diseño de superficie fue E = 6975 + 1748 A+ 1757 C - 2916 B -722 A*A- 722 C*C - 722 B*B+ 491 A*"C + 388 A "B + 1266 C*B; donde A: alginato, B: tamaño de gota y C: cloruro de calcio. El resultado de la superficie indicó que la mejor relación para las esferas es una relación 1:1 de $CaCl_2$ con alginato y con el tamaño de esferas realizado con el gotero 2. Se alcanzó una estabilidad de 6 días de las esferas en medio acuoso (sin rompimiento). Estos resultados sugieren que la metodología empleada es adecuada para el desarrollo de las cápsulas destinadas a la biodegradación de los contaminantes propuestos, por lo anterior, se plantea el empleo de las esferas para encapsular la microalga *Chlorella vulgaris* para estar inmersas en medio acuoso contaminado con loratadina y diclofenaco.

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AMB-P021

MÉTODO MULTI-RESIDUO PARA LA IDENTIFICACIÓN Y CUANTIFICACIÓN DE PESTICIDAS EN AGUA SUPERFICIAL POR UHPLC/ESI-Q-ORBITRAP-MS

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RESUMEN

Introducción: El aumento en la demanda de productos agroquímicos tipo pesticida ha conllevado a una creciente contaminación de las cuencas hidrográficas [1]. En Colombia, se tiene un marco normativo que incluye el monitoreo de pesticidas, es por ello que en el presente trabajo se optimizó y validó una metodología para la determinación multi-residuo de pesticidas en agua utilizando cromatografìa líquida de alto eficiencia acoplada a espectrometría de masas Q-*Orbitrap*. **Metodología:** Para la identificación y cuantificación de pesticidas se usó un sistema de Cromatografía líquida UHPLC *Ultimate* 3000 (*Thermo Scientific*), acoplado a un espectrómetro de masas Q-Exactive (*Thermo Scientifi*c), con una interfaz de electro-nebulización (ESI). La separación de los analitos se realizó en una columna Raptor C18, 150 mm, L x 2,1 mm, I.D. x 2,7 µm. La obtención de los analitos se realizó por extracción en fase sólida (SPE) con cartuchos Oasis HLB [2]. El flujo de la fase móvil fue de 0,3 mL/min y la aguja ESI se operó a 250 °C, el voltaje del capilar se fijó en 3,5 Kv. **Resultados:** Se optimizó y validó un método analítico para la extracción, identificación y cuantificación inequívoca de más de 100 pesticidas en matrices de agua que tienen amplio uso en la industria colombiana. Los criterios de confirmación fueron la comparación de los tiempos de retención, el espectro de masas y el patrón isotópico del analito y el estándar certificado adquiridos mediante el modo *Data Independent Acquisition* (DIA). El método validado mostró buen desempeño para las pruebas de linealidad, repetibilidad, precisión, exactitud, recuperación y robustez. **Discusión:** Los resultados muestran que el modo de adquisición DIA es idóneo para realizar el *screening* y la adquisición simultánea en modo *full scan* se presentó como la mejor opción para realizar la cuantificación de más 100 pesticidas. **Conclusiones:** El cumplimiento de criterios de aceptación que normalmente la US EPA considera en sus métodos de referencia, demuestra que el presente método. El método validado fue usado para determinación de pesticidas de acuerdo con el programa de monitoreo del recurso hídrico de la jurisdicción de la CAR Cundinamarca.

APROBACIÓN ÉTICA

Durante el desarrollo del presente trabajo no se realizaron estudios en animales o humanos.

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AMB-P022

ESTANDARIZACIÓN DE UNA METODOLOGÍA PARA LA DETERMINACIÓN DE NITRATOS, NITRITOS Y SULFATOS EN AGUA LLUVIA POR ESPECTROFOTOMETRÍA UV-VIS USANDO INTERCAMBIADORES IÓNICOS

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ABSTRACT

El propósito de este trabajo es estudiar la capacidad de absorción, selectividad, regeneración y robustez de diferentes resinas (SAC, WAC, SBA, AMB y mixtas) en el análisis de contaminantes ambientales presentes en agua de lluvia, empleando espectrofotometría UV-Vis para la cuantificación de NO_3^- (270 nm), NO_2^- (540 nm) y SO_4^{2-} (540 nm). El estudio se inició con el diseño de captadores pasivos de agua lluvia, apoyados por aerosoles espaciales proporcionados por la UNAM. Según el protocolo utilizado para la determinación de estos analitos, se emplearon 30 g de cada resina. Se determinó el volumen muerto de las resinas y posteriormente se adicionaron soluciones con concentraciones conocidas de NOx (250 ppm) y SOx (500 ppm), respetando las concentraciones permitidas. El intercambio de un anión por su contraión está controlado por la relación equivalente del anión dado al contraión univalente (es decir, $[R_n^{+} B^{n-}]/[R^{+} A^{-}]$) en la fase de resina a aquella (es decir, $[B^{n-}]/[A^{-}]$) en el agua de alimentación durante el agotamiento (o salmuera durante la regeneración).[1] Los resultados indicaron que, para la retención de sulfatos, la resina SBA mostró un intercambio iónico eficiente, en cuanto a la retención de NO_3^-, el intercambiador Amberlyst 15 demostró la mayor eficiencia, mientras que para NO_2^-, el intercambiador mixto superó a las otras resinas, siendo el más selectivo para este ion. En términos de regeneración, todas las resinas superaron un 95% de recuperación, excepto el lecho mixto, cuya regeneración no fue posible. En cuanto a la capacidad de trabajo a diferentes pH, todas las resinas fueron eficientes en el rango de 0 a 14, con excepción del intercambiador fuertemente alcalino, cuyo rango efectivo fue de 0 a 7. En conclusión, cada resina presenta ventajas y selectividad específica hacia ciertos analitos, lo que sugiere la importancia de considerar las características de la muestra y los objetivos del análisis al seleccionar la resina más adecuada. Estos hallazgos permitieron un monitoreo y cuantificación efectivos de contaminantes en agua de lluvia, constituyendo un método alternativo para el análisis de la contaminación atmosférica.

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AMB-P023

ESTUDIO DE INHIBICIÓN DEL CRECIMIENTO DE ESPECIES DE HONGOS DE LA PODREDUMBRE BLANCA EN PRESENCIA DEL ANTIBIOTICO DOXICICLINA

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ABSTRACT

Los recursos hídricos están cada vez más limitados y su calidad está comprometida por diversos contaminantes, incluidos los contaminantes emergentes (CE), como la doxiciclina, un antibiótico que al ser utilizado extensamente para prevenir y tratar enfermedades infecciosas en humanos y animales es motivo de preocupación ya que su presencia constante en el agua puede alterar los ecosistemas acuáticos, afectar el sistema endocrino humano y promover resistencia bacteriana a los antibióticos [1]. Por lo anterior, este trabajo pretende estudiar el efecto de la doxiciclina en el crecimiento de 3 especies de hongos de pudrición blanca (*Irpex Lacteus, Phanerochaete Sordida y Bjerkandera sp.*) como paso inicial para el posterior empleo de estos microorganismos en la degradación del CE en medio acuoso. Para ello se cortaron discos de 5 mm de diámetro del borde exterior de cepas de dos semanas de antigüedad cultivadas en un medio sólido que contenía en gL^{-1}: glucosa (20), extracto de levadura (2), peptona (1.5), KH_2PO_4 (1), $MgSO_4$ (0.5) y agar (15) incubados a 30 °C. Los discos se colocaron asépticamente en el centro de placas de Petri de 90 mm de diámetro con 25 ml de medio sólido suplementado con doxiciclina en concentraciones de 10, 50, 100, 200, 300, 400 y 500 ppm. Cada especie se inoculó en tres placas, además de placas de control sin antibiótico, incubadas entre 25 y 30 °C. Se midió el diámetro del halo de crecimiento en días distintos para calcular el porcentaje de inhibición [2]. Los resultados mostraron que la doxiciclina inhibe el crecimiento de las tres especies de hongos comparado con el cultivo control, siendo el hongo *Phanerochaete Sordida* la especie que presento mayor inhibición a una concentración de 300 ppm con un porcentaje de inhibición de 93,05%, a comparación de la especie *Bjerkandera sp.* e *Irpex Lacteus* las cuales presentaron porcentajes de inhibición a esa misma concentración del 39,99% y 20,44% respectivamente. Considerando que la dosis administrada en humanos es 200 mg/día, las concentraciones máximas establecidas para la exposición del contaminante con los hongos son adecuadas para el posterior estudio de la biodegradación de doxiciclina en agua.

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AMB-P024

METAL-FREE BIOMASS AND BIOCHAR FROM AGRICULTURAL WASTE AS CATALYST TO GENERATE HYDROGEN

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ABSTRACT

The environmental challenges posed by the growing accumulation of agricultural waste have underscored the need for sustainable practices that enhance water resource efficiency and enable the production of valuable products from waste [1]. The objective of this work was to evaluate the use of agricultural biomass and biochars derived from it as catalysts for hydrogen generation through the methanolysis of $NaBH_4$. Biomasses were selected based on their high consumption rates and the generation of untreated waste, specifically coffee husks (C), corn husk (CH), banana leaves (BL), and chicken litter (CF). The raw biomasses were subjected to slow pyrolysis at varying temperatures, resulting in biochars denoted as C400, C500, C750, C900, CH400, BL400, BL500, CL400, CL500, and CL600, where the letter represents the biomass type and the number indicates the pyrolysis temperature, in degrees Celsius. The use of these materials as catalysts in $NaBH_4$ methanolysis allowed the evaluation of different variables influencing hydrogen generation, including pyrolysis temperature, biomass type, and catalyst type. In general, the biomasses exhibited higher activity than the biochars, with CH demonstrating the highest hydrogen generation rate (HGR) at 93.6 mL/min·g. Additionally, for the biochars, there was a consistent decrease in HGR with increasing pyrolysis temperature, despite the biomass type used in the biochar production. These results can be attributed to the reduced availability of oxygenated and nitrogenated functional groups, which likely act as catalytic sites during the reaction. To compare this performance with metal-impregnated catalysts, CH was impregnated with cobalt and pyrolyzed at 400 °C, resulting in a cobalt-impregnated biochar. This material exhibited a lower HGR (78.8 mL/min·g) compared to the untreated biomass. These findings demonstrate that agricultural residues hold significant potential as catalysts for hydrogen production, given their high availability, low cost, and practicality, without the need for metal incorporation, which could introduce risks of leaching and loss of activity.

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AMB-P025

IDENTIFICATION OF FATTY ACIDS IN ARCHAEOLOGICAL SAMPLES BY L-L EXTRACTION AND GAS CHROMATOGRAFY-MASS SPECTROMETRY: AN ARQUEOMETRICAL APPROACH

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ABSTRACT

Archaeological studies have shown that there are chemical indicators that provide information related of past human activities. The fatty acids are one of them, that have been found in archaeological remains [1]. In this work, soil samples from the Aguazuque archaeological site located in the Sabana de Bogotá, Colombia, which has an occupation during the initial middle and late Holocene (8000-2500 B.P.) associated with hearth areas and human burials, were processed to associate the type of resources, both animal and plant, that are being used by these human groups of the past. On the arqeometrical approach, the samples were extracted with dichlorometane: methanol 1:1, then, refluxed with adittion of boron trifluoride in 14% methanol as derivatizing agent and heptane as extracting solvent. Finally, the extract was analyzed by gas chromatograph-mass spectrometry detection [2]. Long-chain saturated fatty acids such as hexadecanoic acid, palmitic acid, lignoceric acid, tridecanoic acid, stearic acid, and others were identify.

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CF-P01

EFFICIENCY EVALUATION OF AN ECO-FRIENDLY ADSORBENT BASED ON MONTMORILLONITE, HYDROXYAPATITE AND GELATIN ON THE REMOVAL OF STEROID HORMONES AS EMERGING CONTAMINANTS FROM WATER SAMPLES

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ABSTRACT

A focal point that attracts the attention of researchers is the search for alternatives that eliminate part of the pollution caused by domestic, industrial and hospital waste present in the wastewater that reaches the wastewater treatment plants (PTAR). Among the emerging pollutants are steroid hormones, which are classified as endocrine disruptors (EDCs) because they affect the endocrine system of exposed organisms. In the present investigation, it is proposed to employ a novel eco-friendly adsorbent phase composed of montmorillonite (MMT), hydroxyapatite (HAP) and gelatin (Gel) named (MMT/HAP/Gel) as adsorbent component packed in a rotating disk, which is an interesting alternative to extract emerging pollutants by evaluating the adsorption efficiency of steroid hormones: 17α-ethinylestradiol (EE2), 17β-estradiol (E2), estrone (E1) and estriol (E3) from both domestic and hospital wastewater [1]. The fully characterization of the novel hybrid material respect to the molecular weight distribution of the gelatin and then the structural, thermal and morphological issues have been done. In addition the chromatographic methodology optimization for the identification of the hormones achieving their optimal separation and identification was necessary, for evaluating the real adsorption capacity of the material through the implementation of rotating disk sorptive extraction RDSE as a modern sample preparation technique[2,3].

ETHICAL APPROVAL

not applicable

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CF-P02

CHEMICAL CHARACTERIZATION OF THE VOLATILE FRACTION OF DECOMPOSING CHICKEN USING HS-SPME-GC/MS

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ABSTRACT

During the decomposition of a cadaver, various chemical and biological processes produce volatile organic compounds (VOCs) that are crucial for locating and recovering victims, as well as determining the post-mortem interval (PMI) [1]. This research aimed to determine the best extraction variables using HC-SPME (fiber type and exposure time) for GC-MS analysis of the volatiles emitted during chicken decomposition. Four chicken thighs (202 g) were placed in glass containers with an opening to introduce the SPME fiber. Four SPME fiber coatings were tested: PDMS (100 μm), PDMS/DVB (65 μm), CAR/PDMS (85 μm), DVB/CAR/PDMS (50/30 μm), and three extraction times were tested: 30 min, one and two hours during a decomposition period of five days. Volatile compounds were analyzed by gas chromatography coupled to mass spectrometry (GC/MS). With the CAR/PDMS fiber, more compounds were extracted (six) than those obtained with the DVB/CAR/PDMS (three), PDMS/DVB (one), and PDMS (none). A total of 24 compounds were tentatively identified by GC/MS in the volatile fraction of chicken tissue for the three extraction times. The total chromatographic area obtained during a one-hour SPME fiber exposure did not exhibit significant differences, based on the Student's t-test, when compared to the areas obtained with a two-hour SPME fiber exposure. The major VOCs identified by GC/MS were dimethyl disulfide (40,1%), phenol (23,7%), indole (11,4%), ethyl 3-methylbutanoate (4,6%), and dimethyl trisulfide (4,1%). Sulfur compounds, phenols, and indoles are reported as volatiles in mammalian decomposition, which are the products of amino acid degradation by bacteria.

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EDU-P01

FROM THE BLACKBOARD TO THE LABORATORY: LEARNING CHROMATOGRAPHY THROUGH THE VAN DEEMTER EQUATION

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ABSTRACT

The van Deemter equation is a valuable tool for understanding the chromatographic process and meeting the challenges of chromatographic separation in HPLC and GC. With the educational objective of introducing the van Deemter equation to students and HPLC/GC users, experimental activities were designed and implemented to facilitate the understanding and usefulness of the equation. In the first stage the relationship between the retention factor *k* and the percentage of organic eluent (B) was determined for three analytes and S was calculated. From these the students selected the optimum %B to determine the Van Deemter equation in a packed column and a monolithic column. By performing isocratic runs at different mobile phase flow rates, the relationship between flow rate and pressure, retention factor, resolution, peak asymmetry and number of theoretical plates was established. The relationship between the theoretical plate height and the linear velocity of the mobile phase was determined and the data were fitted to the van Deemter and Knox curves. The optimum flow rate for each analyte was determined and the efficiency and differences of monolithic and packed columns in chromatographic separation were established.

ETHICAL APPROVAL

The present work does not require ethical approval

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EDU-P02

UNDERGRADUATE TRAINING IN CHROMATOGRAPHY: THE CRUCIAL ROLE OF SOLID-PHASE EXTRACTION AS A TOOL FOR COMPLEX SAMPLES PRETREATMENT.

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ABSTRACT

Sample pretreatment is an essential step for RP-HPLC separation of complex mixtures to ensure accuracy, reliability, and quality of results. While techniques such as filtration, crystallization, and decantation are commonly employed in sample pretreatment, the significance of Solid Phase Extraction (SPE) is often undervalued in experimental procedures. SPE is widely used for sample pretreatment and enrichment, utilizing a solid adsorbent that selectively retains analytes, effectively removing impurities and isolating target analytes. This work provides a practical guide applied to undergraduate academic training, emphasizing the importance of SPE in the separation and enrichment of complex samples. The experimental process included column activation and conditioning. Subsequently, to elute the sample through the column, using previously prepared fractions with varying concentrations of acetonitrile. Finally, the fractions were collected and analyzed by RP-HPLC to identify which ones contain the analytes. In conclusion, it was possible to enrich and eliminate interferences present in the complex sample in a cost-effective and reliable manner, facilitating the identification of each analyte. This method is easily applicable in undergraduate academic environments.

ETHICAL APPROVAL

The present work does not require ethical approval

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EDU-P03

LEARNING THROUGH RP-HPLC METHOD DEVELOPMENT: ISOCRATIC AND GRADIENT ELUTION AS TOOLS FOR ANALYSIS OF COMPLEX SAMPLES

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ABSTRACT

The development and optimization of chromatographic methods are fundamental for the precise quantification of analytes on complex samples in various analytical applications. This work emphasizes the importance of developing both gradient and isocratic methods as an educational strategy for students of analytical chemistry courses. The pedagogical approach to comparing these two methods allows students to improve their understanding of the main principles and variables that impact chromatographic separation. Initially, students analyze a complex mixture carrying out a gradient method with the following conditions: Solvent A (Water-TFA 0.05%) and Solvent B (Acetonitrile), using a gradient from 5 to 100% acetonitrile over 10 minutes. The employed column was a C18 type B (100 × 4.6 mm, 3 µm) at room temperature and a flow rate of 1.0 mL/min. Subsequent adjustments are made to optimize the retention factors (k^*) [1] and (α^*), accomplished by modifying the gradient time, flow rate, gradient interval, solvent strength and nature, temperature, column pH, and ionic pair concentration [2]. The objectives include achieving a baseline resolution ($Rs \geq 2.0$) and minimizing the run time. Following the results obtained from the gradient method, an isocratic method is developed for the quantification of the target analyte, once again optimizing the retention factor (k) [3]. Students compared the advantages and limitations of each method, observing that the gradient method offered improved control over peak resolution and greater flexibility in separating complex analytes. However, the isocratic method proved to be faster and more efficient for the quantification of individual analytes once parameters were optimized. This practice allowed students to apply theoretical concepts in a practical setting, deepening their apprehension of the theory applied to chromatographic separation.

ETHICAL APPROVAL

The present work does not require ethical approval.

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EDU-P04

EXPLORING HPLC SYSTEM DIAGNOSTIC IN EDUCATION: BRIDGING THEORY WITH PRACTICE

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ABSTRACT

Reverse Phase High Performance Chromatography (RP-HPLC) is considered one of the most important analytical techniques in different research fields such as the pharmaceutical industry and forensic sciences. In order for this technique to work appropriately, HPLC systems must follow certain regulations and align to determined parameters that assure its well-functioning, which can be verified through HPLC diagnostic protocol. Exploring these experiments in an educational context serves students of different academic levels to identify the importance of certain elements in an HPLC system such as the well-functioning of gradient systems and proportionality valves, as well as linearity of the detector's response [1]. Taking a do-it-yourself pedagogical approach, students are encouraged to pilot the device and learn different aspects of software functionalities and particularities of different HPLC systems. Students start by performing a no-column system diagnosis, where they evaluate the performance of proportionality valves, flow and gradients prepared by the pump system. From this first diagnostic step, they are encouraged to compare the results with acceptance criteria and state conclusions around the performance of the system, as well as to determine parameters of importance for the development of chromatographic methods such as dwell time (t_D) and mixing time (t_{mix}) [2]. Following this, students perform an on-column diagnosis procedure, where they evaluate the linearity of the detector response by analyzing different injection volumes of a determined analyte and the suitability of the detector's response by observing the variance on retention times (t_R) and detector signal generated by multiple injections of the same analyte. It was observed that these diagnostic procedures help students understand to a better degree the functioning of HPLC systems and the importance of the different parameters being evaluated and help for a better understanding of topics overlooked on theoretical courses by connecting them to a practical environment. Students get a tighter grip on aspects required for a good performance of HPLC systems.

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EDU-P05

SYNTHESIS AND ANALYSIS OF COMPOUNDS WITH ORGANOLEPTIC PROPERTIES FOR THE FORMULATION OF A FLAVORING

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ABSTRACT

The organoleptic properties of each compound are given by the interaction between these and the senses of living beings. In the case of smells, specifically the interaction with the olfactory receptors, smells have great relevance in various industries such as food, which is related to the quality of the product, intensity of flavors and consequently how it is perceived by consumers. Some smells that can be easily recognized are the result of the mixture of other scents. In this case, a couple of compounds with odoriferous properties were synthesized through Fischer-Speier esterification to use them in a mixture that gave as a final product a flavoring with a tutti-frutti smell. The compounds chosen for the synthesis were isoamyl acetate (banana odor) [1], ethyl butyrate (pineapple odor), cinnamic acid (cinnamon odor) [2] and methyl anthranilate (grape odor).

To carry out the Fisher reactions, different carboxylic acids were mixed with alcohols, depending on the desired product, in the presence of a catalyst (sulfuric acid). Something that was noticed was that the reagents had very different odors from the products which helped to determine whether the reaction had been carried out or not. The products obtained were analyzed by infrared spectroscopy (IR), Nuclear Magnetic Resonance (NMR), gas chromatography coupled to mass spectrometry (GC-MS) and olfactometry (GC-O) in order to analyze the purity and yield of the reactions. Three out of four desired compounds were successfully synthesized, yet the yield percentage was lower than expected. Finally, some compounds that were product of reactions that could not be carried out either due to extended reaction times or uncommercial inputs were added; however, it was decided to add them to the project because they provide the properties that are being sought in a tutti-frutti scented flavoring. Among these added compounds are: aldehydes, essential oils, alcohols and lactones.

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MET-P01

UNRAVELING METABOLITE DIVERSITY IN AMAZON PLANTS WITH ANTIMICROBIAL PROPERTIES: UNTARGETED METABOLOMICS PROFILING OF *Piper aduncum* AND *Grias neuberthii*

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ABSTRACT

Leaves from *Piper aduncum* and *Grias neuberthii* are used in Ecuador amazon communities as traditional medicine for their antiseptics and antihemorrhagic agents [1,2]. The present study aims to elucidate the chemical composition of methanolic extracts of *Piper aduncum*, and *Grias neuberthii* leaves from Tena, Ecuador, due to their potential as a source of antimicrobial compounds. The leaves from both plants were macerated using methanol. The resulting extracts were lyophilized, screened for phytochemical constituents, and their antimicrobial activity was evaluated against six different microorganisms. UHPLC-QTOF-ESI-MS/MS was carried for metabolic profile elucidation, where compounds such as ellagic acid and corosolic acid were identified in *G. neuberthii* leaf extracts, and likely related to the effective inhibition of all 6 microorganisms, even reaching considerably low concentrations for some strains like *Staphylococcus aureus (MIC: 0,9*mg/mL*)*. While *P. aduncum* leaves also showed active inhibition of all 6 microorganisms, less metabolites could be identified. Initial results indicate the presence of a wide spectrum of secondary metabolites, phenols and flavonoids being more prominent. In summary, this research underscores the significance of *P. aduncum* and *G. neuberthii* as sources of bioactive compounds.

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MET-P02

METABOLÓMICA DE *Kalanchoe pinnata* Y *Witheringia solanacea* MEDIANTE UPLC-MS/MS: EXPLORACIÓN DE COMPUESTOS BIOACTIVOS Y ACTIVIDAD ANTIMICROBIANA DE PLANTAS AMAZÓNICAS

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RESUMEN

Las plantas juegan un papel importante en el ecosistema, no solo por producir oxígeno, sino también por los valiosos metabolitos secundarios que contienen, usados en medicina tradicional [1]. Este estudio se centra en dos especies destacadas, *Kalanchoe pinnata* y *Witheringia solanacea*, reconocidas por sus propiedades únicas y su uso ancestral en Tena, Napo, Ecuador. El objetivo fue identificar el perfil químico de las hojas secas de ambas plantas y determinar la actividad antimicrobiana de estos extractos. Se prepararon extractos liofilizados de ambas plantas con metanol para un análisis fitoquímico inicial y se evaluó su actividad antimicrobiana contra seis microorganismos patógenos. Mediante UHPLC-QTOF-ESI-MS/MS, se caracterizó el perfil metabólico, identificando quercitrina, ácido cafeico y ácido p-cumárico en *K. pinnata*, que inhibió efectivamente *Staphylococcus aureus* (CMI: 62.5 mg/mL). En *W. solanacea*, rutina, ácido clorogénico y ácido salicílico mostraron actividad contra *S. aureus* y *Bacillus subtilis* (CMI: 1.95 mg/mL y 62.5 mg/mL respectivamente). Resaltando flavonoides y ácidos fenólicos como compuestos notables en ambas especies. En síntesis, este estudio enfatiza el valor de estas plantas como ricas fuentes naturales de compuestos bioactivos con potencial terapéutico.

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MET-P03

PERFIL METABOLÓMICO Y ACTIVIDAD ANTIMICROBIANA DE *Ilex guayusa* MEDIANTE UPLC-MS/MS: IDENTIFICACIÓN DE COMPUESTOS BIOACTIVOS

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RESUMEN

Las plantas nativas, silvestres y semicultivadas son fundamentales para las comunidades amazónicas ecuatorianas, proporcionando productos esenciales para su supervivencia y sustento económico. Entre estas plantas destaca *Ilex guayusa*, una planta milenaria distribuida en las provincias orientales del Ecuador, utilizada históricamente en infusiones con diversos fines: enjuague bucal, estimulante para aliviar el cansancio y tratamiento de indigestiones [1]. Con el fin de identificar los compuestos responsables de las propiedades antibacterianas en las infusiones de guayusa, se han analizado hojas jóvenes y adultas en tres chacras de la provincia de Napo, Ecuador. Se recolectaron hojas de las chacras ubicadas en Alto Tena, Alto Pano y Alto Talag en dos estadios: jóvenes (4–6 años) y adultas (8–10 años). Los extractos acuosos se obtuvieron mediante procesos de secado, macerado, filtrado y liofilizado, y luego se usaron en los ensayos antimicrobianos. Mediante UPLC-MS/MS, se caracterizó el perfil metabólico, identificando ácido 5-O-cafeoilquínico, 3,5, ácido dicafeoilquínico y luteína, los cuales se encontraban en mayor proporción en los extractos con efecto antibacteriano sobre *Klebsiella pneumoniae* (CMI: 500mg/mL) y *Candida albicans* (CMI:500mg/mL). En conclusión, se destacan compuestos fenólicos y carotenoides como compuestos principales en esta planta, asociando de esta forma a compuestos responsables de la capacidad antibacteriana en extractos vegetales, de acuerdo a su estado de maduración y ubicación.

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MET-P04

UHPLC-ESI-ORBITRAP-MS/MS A VERSATILE TOOL FOR THE IDENTIFICATION OF LICHENIC SUBSTANCES

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ABSTRACT

Lichens constitute a mutualistic symbiosis between mycobionts and photobionts (fungi with microalgae and/or cyanobacteria). [1] Resulting in an organism morphologically different from each of its components as a totally new entity. Since ancient times they have been used as a source of dyes, cosmetics and as medicine for the treatment of some diseases such as bronchitis, asthma, leprosy, among others. This type of individuals are important because they are a source of phenolic secondary metabolites of different types and their active principles can be applied in food, natural medicine, antibiotic and antitumor applications. [2] Using advanced analytical techniques such as UHPLC-ESI-Orbitrap-MS/MS, we can obtain an efficient profiling of the metabolite complex, which allows us to find substances of industrial, cosmetic and medicinal interest. In addition, it allows us to use them as chemotaxonomic markers that could be helpful for their identification, since lichens are often similar in appearance but the typical chemotaxonomic differentiation is marked.

Financial Support Ministry of Science, Technology and Innovation (Minciencias), the Ministry of Education, the Ministry of Industry, Commerce and Tourism and ICETEX, Program Ecosistema Científico–Colombia Científica, from the Francisco José de Caldas Fund (Grant RC-FP44842-212-2018) and funds from Fondecyt Regular 1230414 (ANID).

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MET-P05

STUDY OF THE BIODIVERSITY OF WILD MACROMYCETE FUNGI FROM THE BOTANICAL GARDEN OF THE UNIVERSITY OF CALDAS USING VOLATILOMIC TOOLS FOR BIOPROSPECTING PURPOSES: A CONTRIBUTION TO INCREASING THE COMPETITIVENESS OF THE BIOTECHNOLOGY SECTOR IN COLOMBIA.

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ABSTRACT

The present research is aimed at generating a process of exploration of the chemical biodiversity of wild macromycete fungi found in the Botanical Garden of the University of Caldas, located in Manizales – Caldas (Colombia), in order to identify the biogenic volatile organic compounds (BVOC's) and the constitution of a volatilome of these species. The central problem identified lies in the scarce knowledge about the fungal biodiversity of native macromycete species in the forests of Caldas and in Colombia in general [1]. The multiple attributes and properties of macromycetes lead to recognize their value, sustainable use and their potential integration into bioeconomic and circular processes that can contribute to the sustainability of fungal biodiversity. Therefore, it is intended to fill a knowledge gap around fungal biodiversity that exists in the department of Caldas and the Botanical Garden of the University of Caldas, in order to analyze in terms of the biotechnological potential expressed in valuable metabolites, not only by the transformation, but also by the documentary collection around the volatilomic footprint and the potentialities related to the studies of biological activities, which allow the orientation towards scientifically supported products. In this sense, a metabolomic approach was carried out for the identification of potential biomarkers or biomolecules of value, coming from the metabolism of macromycetes, applying two microextraction techniques: a) field extraction by dynamic headspace (DHS), b) field and laboratory extraction by solid phase microextraction (SPME) and a separation technique that is gas chromatography coupled to mass spectrometry (GC-MS) for the identification of the BVOC profile with both extraction methods. For this volatilomic study, 32 samples of the different genera and species of macromycetes found in the Botanical Garden of the University of Caldas were analyzed, which allowed to know and confirm the volatile profile, in addition to providing relevant information to understand its ecology. It should be noted that there is a high richness of different volatile 8-carbon secondary metabolites such as: 1-octen-3-ol, 1-octen-3-one, 3-octanone and 3-octanol, among others, which are related to the volatilomic profile of macromycetes [2]. These results can be applied both in the field of conservation and care of ecosystems, as well as in the development of the agri-food and pharmaceutical industries.

MET-P06

UNTARGETED LIPIDOMICS OF STRAWBERRY (*Fragaria x ananassa*) PLANTS INOCULATED WITH MICROBIAL CONSORTIA AND GROWING UNDER DROUGHT CONDITIONS

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ABSTRACT

Strawberry is a plant species highly susceptible to drought. An alternative for helping to tolerate drought stress in plants is the use of bio-inoculants such as bacteria, arbuscular mycorrhizal fungi (AMF), and yeasts. However, to date, no studies have been performed oriented to evaluate the response at the metabolomics level in strawberry plants inoculated with consortia growing under drought conditions. Liquid chromatography-based metabolomics coupled to mass spectrometry have been effective techniques for profiling plant metabolite changes in response to stress [1]. This has contributed to the current understanding of metabolite regulation in many plant species in response to different environmental conditions, including drought [2-4]. The aim of this study was to identify through untargeted metabolomics the lipid profiles that mediate the effects on increased drought tolerance in strawberry plants due to the inoculation with two microbial consortia (*Claroideoglomus claroideum* + *Naganishia albida* + *Burkholderia caledonica* (CS1) and *Funneliformis mosseae* + *Candida guillermondii* + *Bacillus tequilensis* (CS2)). A total of three treatments (control, CS1 and CS2) with five replicates were conducted (n = 15). All treatments were maintained at 85% of water holding capacity (WHC) of soil for 30 days after transplanting. From day 31, irrigation was discontinued until soil moisture reached 30% WHC. CS1 inoculation allowed an improvement in tolerance under stress conditions, and this improvement was mediated by an increase in glycerolipids (DG 27:3, DG 44:7, OxTG 43:2;O and DGTS 42:1), sterol lipids (STSE (SE 29:2/28:3) and AHexCAS. Furthermore, only significantly expressed lipids were found in the control/CS1 comparison, being Hemibismonoacylglycerophosphate (HBMP 55:12|HBMP 18:3_15:4_22:5) and Diacylglycerol (27:3) the most positively and negatively regulated, respectively. This study provides useful information for lipidomic profiling of strawberry plants inoculated with different types of microorganisms growing under water stress conditions.

MET-P07

COMPOSITIONAL VARIATION OF COMPOUNDS WITH POTENTIAL FOR BIOTECHNOLOGICAL USE IN *Piper cumanense* AND *P. aduncum* IN THE CONTEXT OF CLIMATE CHANGE

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ABSTRACT

Piper is an abundant and species-rich tropical genus of wild peppers considered a group of model plants for studies of phytochemical diversity given its great variability and its potential for use in Biotechnology. Altitudinal variation in metabolites may also result from greater herbivore specialization and greater diversity of trophic interactions at lower altitudes, and herbivory is influenced locally by community attributes such as host plant abundance. More concentrated resources and plant stress are expected to increase variation.

To achieve this objective, an altitudinal gradient from 800 to 2200 meters above sea level was established and abiotic factors (altitude, amount of light, soil pH) and biotic factors (herbivory) were characterized in natural distribution sites of the two species. In each *Piper* individual, samples were taken from 10 leaves with and without herbivory. These samples were preserved in paper bags and dried with silica gel until they reached the laboratory. From each sample, 0.3 g of dry material was ground and extracts were prepared with 1.5 ml of methanol. After vortexing, sonicating on ice and reducing in Centrifuge and Centrivap until the extract was completely dry, it was stored at -80°C until analysis. For chromatographic analysis by LCMS, 2 ml of mass grade methanol were added. Metabolic profiling of the extracts was performed using analytical platforms (MzMine and Metabolanalyst). Site-level variables, such as altitude, seasonality and herbivory, explain the variation in the composition of metabolites found in both *P. cumanense* and *P. aduncum*.

Our data demonstrate that seasonality, altitude and herbivory explain variation in wild *Piper* composition within populations and between species. It will be important to understand which variables operate at both regional and local scales that influence herbivory patterns and compositional and structural variation of metabolites. Future research addressing the causes and effects of soil variation in the context of climate change will help determine the ecologically significant factors that produce levels of phytochemical variation.

OT-P01

OPTIMIZATION OF MASS SPECTROMETRY IMAGING (MSI) USING MALDI-TOF IN THE CONTEXT OF ALZHEIMER'S DISEASE

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ABSTRACT

Alzheimer's disease (AD) is a neurodegenerative disease with an insidious onset. This disease ranks among the top 10 causes of death worldwide. The main cerebral characteristics associated with AD consist of the accumulation of misfolded β-amyloid protein outside neurons, and the accumulation of a hyperphosphorylated form of tau protein in the intracellular space, causing changes at the brain level [1]. The present study aimed to optimize the treatment of mouse brain samples for Mass Spectrometry Imaging (MSI). Three frozen methods were proved: $N_2(l)$, isopentane, and box immersion in $N_2(l)$. Coronal sections (10 µm) were made, mounted on MALDI IntelliSlides, and covered with two types of matrix: 2,5-dihydroxybenzoic acid for positive mode and 9-Aminoacridine for negative mode. MALDI-TOF/TOF autoflex® maX analyzed the histological sections. Data processing (.imzML) was carried out in Bruker's SCiLS software, normalizing the data by the total ions. The images obtained by the freezing method with isopentane showed greater sample integrity compared to direct freezing in $N_2(l)$ and in the box. Both matrices allowed the acquisition of molecular images. It was possible to optimize image acquisition for MSI in negative and positive modes.

ETHICAL APPROVAL

This study was approved by Ethics Committee of Universidad de Concepción (CEBB 1617-2024).

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OT-P02

Outer coating of montmorillonite-type clay on a biopolymer based on agro-industrial waste from the Eje Cafetero region (Valencia orange peel) for potential use in food packaging

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Films made from biopolymers are increasingly in popular in food packaging due to their ability to take advantage of materials that are often discarded, their biodegradability and their compatibility with food products. The goal of this study was to increase the barrier to water of pectin films using montmorillonite (MMT) as an additive and a thin clay coating. Films were developed using pectin extracted from the albedo of the Valencia orange varying pH, solvent: raw material ratio (mL:g), and extraction time (min). Half of those films were produced by mixing the pectin biopolymer with MMT and the other half were coated with MMT using Magnetron Sputtering [1]. Controls consisted of neat pectin. Each film was cut into small pieces and placed in an environmental chamber set at 23 °C and 50 % RH for 48 hours. ANOVA was performed to find differences among treatments. Before and after the clay coating process, the films were characterized by Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM-EDS) [2]. The water vapor permeability (WVP) of all the films was measured using permeation cells. The SEM-EDS results show the presence of clay in both types of films (~2 % of Si). The FTIR results corroborated the presence of pectin and clay in the films. The best performing film was the one resulting from the mixture of pectin with MMT, which reduced the WVP of the neat pectin film by approximately one order of magnitude ($p < 0.05$), NIAS tests are also carried out by HS-SPME CG-MS with food simulant. In conclusion, the first attempt of external coating of montmorillonite-type clay on pectin with the magnetron sputtering technique is reported. This study demonstrates that the water barrier of the pectin film can be improved when MMT is used as an additive or as a thin layer obtained by magnetron sputtering and none NIAS from bioplastic has been released.

Keywords: *Bioplastic, clay, Magnetron Sputtering, montmorillonite, pectin.*

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OT-P03

SÍNTESIS VERDE DE NANOPARTÍCULAS DE Cu y/o CuO, CON EXTRACTOS VEGETALES DE PLANTAS DEL BOSQUE SECO TROPICAL, CESAR, CARIBE COLOMBIANO

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ABSTRACT

Las nanopartículas (NPs) son estructuras metálicas con tamaños inferiores o iguales a 100 nm [1], dicho tamaño les confiere propiedades catalíticas, antimicrobianas y anticancerígenas, que, les permite tener aplicación en diversos campos. Las NPs se pueden obtener mediante síntesis verde, económica y ambientalmente sostenible. Los extractos vegetales (EV), con metabolitos encargados de la reducción y estabilización de las sales metálicas, son usados para la obtención de NPs. En este estudio se planteó la obtención de NPs de cobre y/u óxido de cobre (Cu-NPs o CuO-NPs), mediante síntesis verde, haciendo uso de EV acuosos provenientes de *Guazuma ulmifolia* (guásimo), *Caesalpinia coriaria* (dividivi), y *Cleome viscosa* (cola de rata), plantas típicas del Bosque Seco Tropical, Bs-T, del Caribe Colombiano. Inicialmente, se implementó un diseño experimental factorial de 2^3 para evaluar el efecto de las variables (concentración del metal-CM, temperatura y concentración del EV), sobre el rendimiento de NPs, usando el EV de *H. sabdariffa* como agente reductor. Luego, se evaluó la formación de NPs, con los EV de *C. viscosa*, *C. coriaria* y *G. ulmifolia*. Las espectroscopias UV-Vis y FTIR se usaron para determinar las señales características de NPs. Para el EV de *H. sabdariffa*, se alcanzó el mayor rendimiento de NPs a 80°C, 10% p/v de EV, y 2mM para la CM. Entre las especies vegetales del Bs-T, con *C. coriaria* se alcanzó el mayor rendimiento de NPs, seguido por *C. viscosa* y *G. ulmifolia*. Mediante UV-Vis, se observaron máximos de absorción, definidos a 215 nm y 280 nm, para las NPs sintetizadas con *C. coriaria*. En contraste, para las NPs obtenidas con EV de *C. viscosa* y *G. ulmifolia*, con picos menos pronunciados a 317 nm y 315 nm, respectivamente. Las señales FTIR, relacionadas con vibraciones de enlaces metálicos (Cu-O) [2], se observaron con mayor intensidad para las NPs obtenidas a partir de *C. coriaria* (577 cm^{-1}) y *C. viscosa* (598 cm^{-1}). Se concluyó que, la formación de NPs se favoreció a temperaturas y concentración de agente reductor (EV) altas.

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OT-P04

DETERMINATION OF THE OCTANOL-WATER PARTITION COEFFICIENT OF PEPTIDES DERIVED FROM BOVINE LACTOFERRICIN BY RP-HPLC-DAD.

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ABSTRACT

The distribution of a substance between two immiscible solvents can be measured using LogP this physicochemical parameter indicates the degree of lipophilicity or hydrophilicity of a substance. LogP provides valuable information on cell permeability, solubility, toxicity, pharmacokinetics and structure-activity relationship of drug candidates [1]. Through the development and implementation of an RP-HPLC-DAD methodology, the partition coefficient n-octanol-water ($LogP_{o/w}$) of peptides containing the palindromic sequence, RWQWRWQWR [2] and two drugs was determined. It was established that peptide sequence differences generated significant variations in the n-octanol/water partition coefficient, a fundamental physicochemical parameter in the pharmacokinetics of these promising molecules. For the standardization of the analysis method, acetaminophen and tryptophan were used as model analytes; the method allowed determining partition coefficient values significantly close to those reported in the literature. Finally, the experimentally obtained LogP values using two systems octanol-water (1:5 and 1:10 v/v) were compared with the values reported by a prediction tool, showing discrepancies with the experimentally obtained data. Our results indicate that this method can be implemented to determine the partition coefficient of peptides, a crucial parameter in the development of promising drugs.

ETHICAL APPROVAL

The present work doesn't require ethical approval

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OT-P05

GLOBAL METABOLIC ALTERATIONS IN COLORECTAL CANCER CELLS INDUCED BY BAMBOO LEAF EXTRACT OBSERVED BY UHPLC-QTOF-MS AND ^{1}H-NMR

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ABSTRACT: Metabolic alterations are increasingly recognized as an important aspect of cancer, serving as a potentially interesting area for identifying therapeutic targets [1,2]. Previous studies have demonstrated the cytotoxic potential of bamboo leaf extract obtained from *G. incana* (BLEGI) against HCT-116 colon cancer cells [3]. However, its molecular mechanisms on tumor cells have not been studied. This study aimed to apply an untargeted metabolomic approach based on advanced analytical techniques such as ultra-high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (UHPLC-QTOF-MS) and proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy to analyze the endometabolome and exometabolome and reveal the metabolic alterations in HCT-116 cells after BLEGI treatment. Univariate and multivariate statistical analyses were then applied for data analysis. The methodological design included the evaluation of cell viability of the extract by an MTT assay and immunofluorescence analysis using an LPS-stimulated macrophage model. UHPLC-QTOF-MS and ^{1}H-NMR were employed for the analysis of the metabolome of the cells to investigate the intra- and extracellular changes. As a result, BLEGI extract showed potent cytotoxic activity with an IC_{50} value of 1.23 µg/mL. The metabolomic analysis revealed 98 differential metabolites involved in glutathione metabolism, the tricarboxylic acid cycle, and lipoic acid metabolism, among others. Of the differential metabolites, a significant decrease in reduced glutathione (GSH) and an increase in oxidized glutathione (GSSH) were found, related to an imbalance of oxidative stress in the cells, causing different processes related to apoptosis such as chromatin condensation, nuclear fragmentation, cytoplasmic shrinkage, and the formation of apoptotic bodies. The observed changes in glutathione metabolism possibly suggest apoptotic cell death induced by increased oxidative stress in the cells, confirmed by immunofluorescence analysis evidencing the formation of apoptotic bodies. Furthermore, BLEGI demonstrated a significant inhibitory capacity of nitric oxide (NO) in macrophage cells, showing significant inhibitory effects against NO production, with values of 8.44 ± 0.38 µM at a concentration of 2 µg/mL, comparable to the positive control. The metabolomic analysis of colon cancer cells in this study offers an approach to understanding the mechanism of action and gaining new insights into therapeutic targets for the treatment of this disease.

OT-P06

TARGETED ISOLATION OF FLAVONE GLYCOSIDES WITH CYTOTOXIC POTENTIAL BY CENTRIFUGAL PARTITION CHROMATOGRAPHY (CPC)

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ABSTRACT: *Guadua incana* Londoño is a bamboo plant that represents a valuable source of bioactive compounds with promising pharmacological properties [1,2]. A previous metabolomic study determined that the high composition of flavone glucosides present in the ethanolic extract obtained from the leaves of *G. incana* showed a positive correlation with cytotoxic activity [3]. However, to date, there are no reports of the isolation of cytotoxic compounds in this species. This study aimed to perform the fractionation of the leaf extract of *G. incana* for the purification and identification of cytotoxic compounds, guided by a metabolomic and bioactivity approach. For this purpose, the plant material collected in the municipality of Montenegro (Quindío/Colombia) was used to obtain the ethanolic extract. Purification was carried out by successive separations using Centrifugal Partition Chromatography (CPC), employing a solvent system in varying proportions of EtOAc-BuOH-H_2O (EBuWat) from 8:2:10 *v/v/v* to 2:8:10 *v/v/v*, flowed by Sephadex LH-20 column in a 100% methanol system. Finally, the evaluation of the cytotoxic activity of the obtained compound against HCT-116 colon cancer cells was carried out by the MTT assay. The results of the phytochemical study, guided by the metabolomic approach, allowed the isolation of a flavone glucoside, identified as isoschaftoside (**1**). The compound **1** was elucidated by spectroscopic techniques (UV and ^{1}H and ^{13}C-NMR), spectrometric techniques (LC-MS-QTOF), and comparison with experimental data reported in the literature. Compound **1** has been reported in other plant species; however, for *G. incana* this represents the first report. Finally, it was determined that compound **1** exhibits potent cytotoxic activity with an IC_{50} value of 13.26 µM, comparable with the positive control. This study provides experimental validation of the results obtained in previous correlation studies of the chemical profile and biological activity of *G. incana* and corresponds to the first isolation of flavone glucosides from this bamboo and within the genus.

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OT-P07

QUANTITATIVE ANALYSIS OF BOLENONE IN WISTAR RATS BY ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-HIGH RESOLUTION MASS SPECTROMETRY (ORBITRAP)

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ABSTRACT

Boldenone (BL) is an anabolic steroid developed for veterinary growth promoter used in meat production, but also used by amateur and high-performance athletes. Its frequent detection in biological samples has raised concerns about food and environmental safety, as well as potential negative effects in various sports modalities[1]. In this study, a high performance liquid chromatography-quadrupole-Orbitrap mass spectrometry (HPLC-Q-Orbitrap-MS) involved data target acquisition by Parallel Reaction Monitoring (PRM) with QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) extraction, was developed and validated for analysis of alpha and beta BL in plasma samples. Boldenone undecylenate (UBL; 0.5 mg/kg) was administered intramuscularly to males (M) and females (F) Wistar rats, and samples were collected for 60 days. The limit of quantification (LLOQ) was mostly at 0,5 ng/mL, with recoveries within 85–110%, and precision-RSDs <20%. The validation parameters were satisfactory, quantifiable BL concentrations were found in 86% of 1450 plasma samples, the plasma concentrations (C_{max}) for αBL-F and βBL- F were 8.23 and 24.71 ng/mL and for αBL-M and βBL-M were 7.34 and 34.33 ng/ml, respectively. As one of the first reports for this specie, this method was used to evaluate the pharmacokinetics[2] and biodistribution of BL in plasma and tissues of Wistar rats.

ETHICAL APPROVAL

The development of this work was approved by the Ethics Committee of the Faculty of Sciences of the National University of Colombia (Act 08 of 2021).

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PN-P01

CARACTERIZACIÓN QUÍMICA DE ALGUNOS COMPONENTES PRODUCIDOS POR *Klebsiella pneumoniae* MEDIANTE CG-EM FRENTE A TRATAMIENTOS CON EXTRACTO ETANÓLICO DE *Tibouchina grossa*

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RESUMEN

La resistencia a los antimicrobianos (RAM) es una de las principales amenazas contra la salud pública y se asocian 4,95 millones de muertes en 2019 según la Organización mundial de la salud (OMS) [1]. *Klebsiella pneumoniae* fue clasificada recientemente por la OMS como patógeno priorizado en el grupo crítico debido a su alta resistencia a antibióticos de tercera generación [1], esto debido a cambios génicos asociados a la comunicación y defensa bacteriana, mediada por metabolitos de distintos tipos producidos por la bacteria [2,3]. El objetivo de la presente investigación es la caracterización química mediante Cromatografía de gases acoplada a espectrometría de masas (CG-EM) de algunos componentes producidos por *K. pneumoniae* frente a tratamientos de distintas concentraciones de la especie vegetal *Tibouchina grossa* (TG).

Para lo anterior se realizaron diferentes concentraciones del extracto de TG que fueron agregados junto con la bacteria, cultivada previamente en caldo LB a una DO de 0,9 (24h, 37 °C, 180 rpm). Adicionalmente se realizaron controles de crecimiento bacteriano, medio y un control positivo (Gentamicina a 0,79 ppm). Posteriormente se realizó la extracción de los metabolitos, usando para su análisis un CG-EM Shimadzu QP 2010 plus, en modo splitless, con helio como gas portador (0,8 mL/min), con una columna capilar HP-5 MS, (30 m x 0,25 x 0,25), una fuente de ionización por impacto electrónico a 70 eV y un cuadrupolo en modo full-scan.

Así las cosas, se observó la presencia de tres posibles compuestos propios de la bacteria: anfetamina N-metoxicarbonil (K1), 1-triptofano N-formil (K2) y 3-bencilhexahidropirrolo[1,2-a]pirazina-1,4-diona (K3), los cuales fueron modulados en presencia del extracto de TG, evidenciando para el caso de K3 que este presento mayor porcentaje de área comparado con el control de bacteria y frente a gentamicina usada como control positivo, es de resaltar que este compuesto ha sido aislado de bacterias en otros trabajos como antibiótico contra cepas multirresistentes. De esta manera se establece que posiblemente la presencia de los extractos podría cumplir una función moduladora lo que conlleva a incrementos en los metabolitos producidos por la bacteria y que podrían relacionarse con mecanismos de defensa o de comunicación.

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PN-P02

PHYTOCHEMICAL ANALYSIS, ANTIOXIDANT CAPACITY AND PHENOL CONTENT OF *Jatropha gossypiifolia*

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ABSTRACT

The family Euphorbiaceae comprises about 300 genera and 8000 species. Euphorbiaceae spp. are characterized by their milky sap and unisexual flowers [1]. These plants, distributed in tropical regions of the planet, are noted for their diverse biological activities, including cytostatic, cytotoxic and anticancer effects. Species of the genera *Ricinus* and *Jatropha* are characterized by their pharmacological properties and biotechnological applications (nanoparticles, biodiesel). In the present study, a chemical analysis of *Jatropha gossypiifolia*, collected in Valledupar, Cesar, was carried out. Aqueous and methanolic extracts (AE and ME) were obtained from fresh parts of the plant. The plant extracts (PE) were filtered, brought to dryness (40°C) and refrigerated until use (4°C). Carbohydrates and flavonoids were qualitatively detected by phytochemical screening. Total phenol content (TPC) was evaluated by the Folin-Ciocalteau method, as gallic acid equivalents (mg GA/g PE). Ultra-high efficiency liquid chromatography with Orbitrap mass detector, UHPLC-ESI-ORBITRAP-MS, was used for the detection of polyphenols. Antioxidant activity (AA) was determined by colorimetric assay with 2,2-diphenyl-1-picrylhydrazyl radical (DPPH), as the equivalent concentration of PE to decrease the DPPH concentration by 50% (EC_{50}, ppm PE/ppm initial DPPH). PEs from fruits showed higher carbohydrate content, while those from leaves showed a higher proportion of flavonoids. The TPCs found in the PEs were: 112 ± 2, for leaf ME; 69.3 ± 0.9, for leaf AE; 93.8 ± 0.9, for stem ME; 89 ± 4, for fruit ME; 67.8 ± 0.4, for fruit AE. Leaves presented the highest TPC, followed by stems and fruits. Meanwhile, the EC_{50} were: 2.80 ± 0.14, for leaf AE; 1.41 ± 0.06, for leaf ME; 2.31 ± 0.09, for fruit AE; 0.89 ± 0.01, for fruit ME; and 3.79 ± 0.05, for stem ME. Fruits presented higher AA, followed by leaves and stems. In general, the ME presented higher TPC and AA.

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PN-P03

ANTIOXIDANT CAPACITIES AND PHENOLS CONTENT OF *Guazuma ulmifolia, Cleome viscosa* and *Caesalpinia coriaria*

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ABSTRACT

The high biological diversity of Colombian Caribbean region, provides access to diverse genetic resources that constitute a unique opportunity to implement innovative and efficient strategies for their sustainable use. In particular, the Tropical Dry Forest (TdF) is undergoing changes that threaten the conservation of biodiversity and ecological services provided by this ecosystem. In the present study, a chemical analysis of *Guazuma ulmifolia*, *Cleome viscosa* and *Caesalpinia coriaria*, typical plants of the Bs-T of the Colombian Caribbean, was carried out to support the importance of these species in the restoration or conservation of the Bs-T, and for economic activities, where biodiversity is used for the development of bioproducts, which can have applications in traditional medicine, cosmetics or livestock or agricultural activities, among others [1]. Aqueous plant extracts (APE) were obtained from ripe fruits of *G. ulmifolia*, fresh leaves of *C. viscosa*, and green fruits of *C. coriaria*, collected in the municipality of La Paz, Cesar. The APEs were filtered, brought to dryness (40°C), and refrigerated until use (4°C). The total phenol content (TPC) was evaluated by the Folin-Ciocalteau method, as gallic acid equivalents (mg GA/g PE) [2]. Ultra-high efficiency liquid chromatography with Orbitrap mass detector, UHPLC-ESI-Orbitrap-MS, was used for the detection of polyphenols in PEs. The antioxidant activity (AA) was determined by colorimetric assay with 2,2-diphenyl-1-picrylhydrazyl radical (DPPH), as the equivalent concentration of PE to decrease the concentration of DPPH by 50% (EC$_{50}$, ppm PE/ppm initial DPPH). The TPC found in the PEs were: 8.5 ± 0.3, for *G. ulmifolia*; 42.8 ± 0.4, for *C. viscosa*; and 510 ± 028, for *C. coriaria*. The green fruits of *C. coriaria* presented the highest TPC followed by leaves of *C. viscosa*, and fruits of *G. ulmifolia*. While, the EC$_{50}$ were of: 37 ± 2, for *G. ulmifolia*; 7.4 ± 0.3, for *C. viscosa*; and 0.093 ± 0.002, for *C. coriaria*. In general, the PE of the green fruits of *C. coriaria* presented the highest TPC and AA.

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PN-P04

GC-MS AND LC-MS IDENTIFICATION OF SECONDARY METABOLITES ISOLATED FROM *Cestrum nocturnum*

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ABSTRACT

Cestrum nocturnum (Solanaceae) is a native species for ornamental use due to the different volatile organic compounds (VOCs) responsible for the sweet fragrance of the flowers [1]. This species has different alkaloids [2], mainly tropane alkaloids, which are commonly found in plants of the Solanaceae family [3]. *C. nocturnum* flowers were obtained from experimental plots at the CENIVAM research center. Volatile organic compounds in *C. nocturnum* flowers were sampled *in vitro* with HS-SPME. CAR/PDMS (85 µm) fiber was exposed to the compounds emitted by flowers (2 g) for 30 min at 60 °C. The analysis was performed on a GC/MS. Alkaloid extraction was carried out by matrix solid-phase dispersion (MSPD), using C_{18} silica as a dispersant, a 1:4 ratio between plant material and dispersant, and methanol (99.8%) as eluent. The extract analysis was performed by UHPLC-ESI-Q-*Orbitrap*-MS. The major components of the *C. nocturnum* flower volatile fraction were linalool, benzaldehyde and phenylacetaldehyde. Nicotine and scopolamine were identified by UHPLC-ESI-Q-*Orbitrap*-MS in the *C. nocturnum* extract. The information on chemical composition of *C. nocturnum* plant secondary metabolites found could be useful for pharmaceutical, flavor and fragrance industries.

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PN-P05

PERFILES QUÍMICOS OBTENIDOS POR UHPLC-ESI-ORBITRAP-MS/MS DE *Ramalina celastri* DE COLOMBIA Y CHILE

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ABSTRACT

Lichens are symbiotic organisms consisting of a fungus and one or more photobionts such as algae or cyanobacteria. In this association, the fungus provides protection and nutrients while the photobiont produces food through photosynthesis. Likewise, several species of lichens have been characterized by their biological activity and chemical composition. Such is the case of *Ramalina celastri*, a species of epiphytic lichen with cosmopolitan distribution that has become a species of biotechnological interest [1]. In addition, its chemical composition may vary according to local environmental conditions, in this study a chemotypic comparison of the species identified in Colombia and Chile is made. UHPLC-ESI-MS/MS was used and between the two specimens a total of 63 compounds were identified, grouped mainly in depsides, depsidones, lipids, diphenylether derivatives and dibenzofurans. Likewise, a significant difference was found between the identified constituents of each locality, which confirms that there is a relationship between the localities and their components, determining the chemotype of this species.

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PN-P06

ESTUDIO DEL PERFIL LIPÍDICO DE ACEITE DE AGUACATE PROVENIENTE DEL CASANARE - LIPID PROFILE STUDY OF AVOCADO OIL FROM CASANARE

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ABSTRACT

This study analyzed the fatty acid composition of cold-pressed avocado pulp oil obtained by two distinct methods (mechanical extrusion-ME and hydraulic pressing-HP) from ripe fruits harvested in the Department of Casanare. The FAMEs from the oils were obtained by two different methods: the first method involved saponification with KOH in MeOH followed by methylation (BF_3 in MeOH); the second method involved dissolving the oil in heptane and subsequent transesterification with KOH in MeOH. The obtained FAMEs were analyzed by GC-MS. Both methods gave similar results, but the second method was preferred due to its simplicity.

The oil yield obtained by ME was 2.0% on a wet basis (10.3% on a dry basis), and by HP, it was 4.0% (20.6% on a dry basis). GC-MS analysis determined that the major fatty acids were oleic (48.4%-49.4%), palmitic (27.0%-28.8%), and linoleic (14.0%-14.9%), with no significant differences between the two extraction methods. Differences in the fatty acid composition compared to other varieties could be related to factors such as soil type, climate, or agricultural management, which may influence the lipid profile of each avocado variety [1].

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PN-P07

LC-MS AND HPLC-ABTS$^{+\bullet}$ANALYSIS OF PHENOLIC COMPOUNDS FROM *Dianthus caryophyllus* spp. FLOWERS

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ABSTRACT

Dianthus caryophyllus (Caryophyllaceae, family) is distributed in Europe, Asia, North America, and mountainous regions in Africa [1]. The objective of this study was to determine chemical composition and antioxidant activity of *Dianthus flower* extracts, as possible ingredients in cosmetic products. *D. caryophyllus* flowers were obtained from FLORES FUNZA S.A., Bogotá, Colombia. The extract was obtained by solid-liquid extraction with acidified (1% HCl) ethanol-water (3:1, v/v). Flower extract analysis was carried out using an UHPLC Dionex^{TM} UltiMate^{TM} 3000 (Thermo Fisher Scientific, Bremen, Germany), coupled to an Orbitrap^{TM} mass detector (Exactive Plus, TFS, Bremen, Germany). On-line ABTS$^{+\bullet}$ antioxidant activity was determined using an HPLC 1200 Infinity (Agilent Technologies, Palo Alto, CA, USA), coupled to a Pinnacle PCX post-column derivatizer (*Pickering Laboratories*, Mountain View, CA, USA). Kaempferol-(glucosylrutinoside), kaempferol-diglucoside, kaempferol-robinobioside, kaempferol-sophorotrioside-rhamnoside, kaempferol-diglucoside, kaempferol-robinobioside, *p*-coumaric acid, kaempferol-rhamnoside-glucoside, ferulic acid, kaempferol-3-glucoside, isosalipurposide, naringenin, and kaempferol were identified by LC-MS using the exact masses of the protonated target compounds, comparison with MS/MS metabolite data base, and using certified standards. *p*-Coumaric acid, ferulic acid, kaempferol-3-glucoside, naringenin, and kaempferol were identified by HPLC-DAD-ABTS$^{+\bullet}$ using UV-Vis spectra, retention times and certified standards. Kaempferol (3%) and kaempferol-glycosides (50%) showed the highest contribution to the antioxidant activity of the extract.

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PN-P08

CHEMICAL CHARACTERIZATION AND BIOLOGICAL ACTIVITIES OF *Posoqueria latifolia* FLOWER EXTRACT

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ABSTRACT

The jasmine tree (*Posoqueria latifolia* Rudge. Roem. & Schult, Rubiaceae), according to its colloquial (vernacular) name, is native to the neotropical region, growing in Mexico, Bolivia, and southern Brazil [1,2]. Looking for beneficial natural ingredients in cosmetic and pharmaceutical products, in this work fragrances and flower extracts were obtained from *P. latifolia*. Volatile and extract chemical characterization was carried out; antioxidant, cytotoxic, sensitizing, and photoprotective activities were evaluated in this work. The volatile fraction isolated by HS-SPME from *P. latifolia* flower was analyzed by GC-MS. *P. latifolia* flower extract was obtained by solid-liquid extraction with acidified (HCl, 1%) ethanol-water (50:50) and analyzed by LC-MS. The antioxidant activity was determined by ORAC and HPLC-ABTS$^{+\bullet}$ methods. Cytotoxic activity was determined in six human cell lines by the MTT method. The sensitizing effect was evaluated by quantifying ELISA chemokine IL-8 in human monocyte culture. The photoprotective effect was established according to sun protection factor (SPF) and critical wavelength (λ_c) methods. Fifty-three compounds were isolated by HS-SPME from *P. latifolia* flower fragrance. The major components were (*E*)-β-ocimene (12%), (*Z*)-hex-3-en-yl acetate (20%), and methyl salicylate (29%). *P. latifolia* flower extracts contain flavonols, phenolic acids, and stilbenoids. According to HPLC-ABTS$^{+\bullet}$ results, chlorogenic acid (29%) and rosmarinic acid (28%) showed the major contribution to the observed flower extract antioxidant activity. *P. latifolia* flower extract exhibited antioxidant and photoprotective activities and did not show a tendency to cause toxicity. *P. latifolia* flower extract could be used as a natural ingredient in cosmetic and pharmaceutical products.

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PN-P09

PHYTOCHEMICAL COMPOSITION AND BIOLOGICAL ACTIVITY OF CEMPASÚCHIL (*Tagetes erecta*) ROOT EXTRACT FROM MEXICO: IN VITRO EVALUATION IN CELLULAR MODELS RELEVANT FOR POTENTIAL ANTI-OBESOGENIC/ANTI-DIABETIC USE

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ABSTRACT

The cempasúchil plant (*Tagetes erecta*) holds significant cultural importance in Mexico, where it is used as a floral tribute during the Day of the Dead festivities and plays a crucial role in traditional medicine. A preliminary analysis of root and stem extracts from this plant, using untargeted metabolomic methodologies, revealed a diverse array of constituents in the total extract. Gas chromatography-tandem mass spectrometry (GC-MS/MS) identified 31 components, including phenolic compounds and thiophenes, while liquid chromatography-tandem mass spectrometry (LC-MS/MS) detected various flavonoid glycosides. Comprehensive biological evaluation was performed to assess the potential applications of these extracts in treating type 2 diabetes mellitus (T2DM). In vitro studies using relevant cellular models demonstrated the anti-obesogenic and anti-diabetic properties of the extracts. Notably, the DCM and BuOH fractions showed a significant increase in glucose uptake (30%) at 100 μg/mL in C2C12 myotubes and reduced triglyceride content in HepG2 hepatocytes and 3T3-L1 adipocytes. These effects may be attributed to polyphenols such as ρ-hydroxybenzaldehyde (ρ-BN) and its derivatives, known for their anti-diabetic properties. In summary, the activity assays suggest promising potential for these extract fractions as sources for developing novel treatments for T2DM, thereby opening new avenues for treating this prevalent disease.

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PN-P10

ENANTIOSEPARATION OF DIFFERENT RACEMIC MIXTURES BY CAPILLARY ELECTROPHORESIS USING CYCLODEXTRINS AS CHIRAL SELECTORS

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ABSTRACT

Enantioseparation remains a significant challenge in analytical chemistry owing to the structural similarity among analytes. HPLC and GC are common techniques used to address this issue. However, CE was selected for this study due to its efficiency, rapid analysis, cost-effective reagents, minimal residue production, and methodological versatility [1-5]. This work investigates the resolution of tryptophan and duloxetine enantiomers using CE-UV with cyclodextrins (α, β, γ) as chiral selectors. The procedure began with a 0.1M NaH_2PO_4/H_3PO_4 buffer adjusted to pH 2.5, and the optimization involved varying parameters including the applied voltage, temperature, injection method and detection settings. Optimal conditions for tryptophan separation were 9kV running voltage, 30°C, electrokinetic injection (7kV), and detection at 220 nm, achieving a resolution of 3.64 with 4% of α-CD. On the other hand, for duloxetine the procedure required the substitution of electrokinetic injection with hydrodynamic (50 mm bar) and the functionalization of β-CD to HP-β-CD via an etherification reaction with propylene oxide to enhance solubility. Under these optimized conditions and with a 7% of HP-β-CD a maximum resolution of 1.63 was obtained. The optimized methods achieved a sufficient resolution (>1,5) for both mixtures within brief analysis times and highlighted the importance of selecting a chiral selector of comparable size to the analyte to facilitate effective separation through necessary interactions.

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PN-P11

UHPLC-DAD-QTOF-MS CHROMATOGRAPHIC PROFILE OF THE ACTIVE FRACTION OF *Tillandsia usneoides* AND ITS POTENTIAL ACTIVATION OF THE ERK AND PI3K SIGNALING PATHWAYS, IN PRIMARY NEURON CULTURES

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ABSTRACT

Extracts obtained from medicinal plants have been shown to have therapeutic potential against neurological diseases due to their neuroplasticity-modulating capacity[1]. Probably through the activation of some signaling pathways such as the extracellular signal-regulated kinase (Erk) pathway and the phosphoinositol 3-kinase (PI3K-Akt) pathway[2,3]. A species shown to have neuroplasticity-inducing activity *in vitro* is *Tillandsia usneoides*, specifically the ethyl acetate fraction (AcOEt)[4]. Considering the above, the objective of this study was to chemically characterize the AcOEt fraction and evaluate the inducing potential of the activation of the Erk and PI3K pathways in cortical neurons of Wistar rat embryos. The plant material (leaves and stems) was extracted with EtOH and the resulting extract was fractionated by vacuum chromatography, then an analysis was carried out by High-performance Thin-Layer Chromatography (HPTLC) and an analysis by Ultra Performance Liquid Chromatography coupled to Diode Array Detector (UPLC-DAD) and coupled to Mass Spectrometry (UHPLC-MS-QTOF). UV detection was performed at 254nm and 360nm and MS detection was performed between 100 and 1000 m/z. The activating potential of the signaling pathways was evaluated by Western Blot assays of the p-Akt proteins (of the PI3k pathway) and p-Erk. The chromatographic profile of the AcOEt fraction was obtained and the compounds 5,7,4'-trihydroxy-3,6,3',5'-tetramethoxyflavone and 3,5,7,4'-tetrahydroxy- 6,3',5' trimethoxyflavone were tentatively identified. Regarding the activation of the pathways, an increase in the phosphorylation of the Akt and Erk proteins was evident at 5 minutes after treatment. Demonstrating a direct effect of the fraction on the signaling pathways.

ETHICAL APPROVAL

The culture was performed after approval by the Institutional Committee for the Care and Use of Laboratory Animals of the Pontificia Universidad Javeriana (CICUA)(FUA-0057-18).

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PN-P12

EXPLORING THE EFFECTS OF EXTRACTION CONDITIONS ON PHENYLPROPANOID-RICH ESSENTIAL OILS FROM *Piper* SPECIES: INSECTICIDAL ACTIVITY AGAINST STORED GRAIN PESTS AND MECHANISTIC INSIGHTS

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ABSTRACT

Essential oils (EOs) from *Piper* species, rich in phenylpropanoids, have emerged as a promising alternative for pest control, offering topical insecticidal properties by contact, making them an interesting alternative to explore as insecticides against cereal pests such as *Sitophilus zeamais* and *Tribolium castaneum,* which have developed resistance to traditional chemical controls [1]. In this sense, the present work aims to characterize the insecticidal potential of AEs from 4 species of the genus *Piper* and their phenylpropanoids for the control of *S. zeamais* and *T. castaneum*. To this end, the methodology included four phases: **1)** Extraction of AEs from plant material subjected to different growth conditions of *P. auritum*, *P. aduncum*, *P. hontonii* and *P. asperiusculum*, using three extraction methods (steam distillation, hydrodistillation and microwave-assisted hydrodistillation), **2)** chemical characterization of the AEs by GC-MS, **3)** isolation of the main phenylpropanoids and preparation of derivatives and **4)** evaluation of contact insecticidal activity and inhibition of acetylcholinesterase (AChE), catalase (CAT) and glutathione-S-transferase (GST) in EOs, isolated compounds and synthetic derivatives [1-3]. Extraction yields were found to be higher than 0.1%, and in general it was observed that shade favored the production of EO and increased the phenylpropanoid content, which was higher than 30%. The oils of the four *Piper* species showed insecticidal activity against *S. zeamais* with LD_{50} between 124 and 200 µg/insect. The oil of *P. auritum* was the only one active against *T. castaneum* with LD_{50} below 100 µg/insect. Five phenylpropanoids were toxic by contact, safrole being the most active against both insects. Hydrogenations, coniferaldehyde formation, epoxidations, Wacker oxidations and demethylations did not increase insecticidal activity. The EOs, phenylpropanoids and derivatives did not inhibit the catalytic activity of GST, AChE and CAT by more than 50% at the maximum concentration evaluated; however, the enzyme with the greatest inhibition was GST with the AEs and phenylpropanoids.

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PREP-P01

DESARROLLO DE UNA METODOLOGÍA TFME EN BASE A LUFFA FUNCIONALIZADA CON UN SOLVENTE EUTÉCTICO PROFUNDO PARA LA EXTRACCIÓN DE HIDROCARBUROS AROMÁTICOS POLICÍCLICOS EN AGUAS NATURALES.

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Este trabajo se centra en la investigación de un material adsorbente de origen natural para la remoción de contaminantes orgánicos, específicamente utilizando la esponja de Luffa (*Luffa aegyptiaca*) como base sortiva [1]. Este material lignocelulósico, se implementó como soporte base para aplicar una metodología de microextracción en película delgada (TFME) en la extracción de Hidrocarburos Aromáticos Policíclicos (PAHs) desde muestras de aguas de río y mar. La detección instrumental fue realizada utilizando cromatografía líquida de alta presión acoplada a un detector de fluorescencia (HPLC-FLD). La Luffa se destaca por ser un biomaterial económico, reutilizable y efectivo para la adsorción de contaminantes en muestras de agua [2] pero su uso como biosorbente en preparación de muestra ha sido poco explorada. Debido a su carácter natural polar, el biomaterial fue funcionalizado con diferentes mezclas de solventes eutécticos profundos de carácter hidrofóbico (HDES) como: lidocaína-mentol, mentol-timol, timol-lidocaina, lidocaina-Ácido decanoico, en diferentes mezclas molares, obteniéndose los mejores resultados con las mezclas que presentan lidocaína y mentol. Parámetros de extracción como: tiempo de extracción, volumen de HDES y volumen de eluyente fueron optimizados con un diseño experimental multifactorial. El método propuesto fue aplicado a muestras reales obtenidas de cinco puntos diferentes de la ciudad de Valparaíso, Chile. Los resultados muestran el gran potencial del fruto de la Luffa como biosorbente, mejorando parámetros analíticos como límite de detección y cuantificación y aumentando la sustentabilidad del procedimiento analítico en la detección de PAHs. Además, su funcionalización es sencilla y de bajo costo. La técnica de microextracción desarrollada permitió preconcentrar sobre 30-60 veces dependiendo del analito. Esta metodología innovadora combina las ventajas de emplear un material natural potenciado con las propiedades de los HDES, ofreciendo una solución eficiente y sostenible para el análisis y extracción de estos contaminantes en el agua.

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PREP-P02

PRELIMINARY STUDY IN THE EVALUATION OF EMBRIONIC VIABILITY IN BOVINE THROUGH VOCs ANALYSIS BY HS-SPME-GC-MS

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ABSTRACT

The VOCs can be emitted by a multitude of biological samples [1]. Recent studies have shown promising potential for the diagnosis of several diseases [2]. On the other hand, animal reproduction represents a worldwide concern due to fertility decrease. To overcome this drawback, the assisted reproductive technology (ART) has irrupted as the most important alternative for getting pregnant. The most effective form of ART is *in vitro* fertilization (IVF). However, the success rate may be less than 50% in some cases. A very important factor that contributes to IVF success is the selection of the most appropriate and viable embryo from the available cohort [3]. In this study, a preliminary analysis has been carried out in order to evaluate the Volatile Organic Compounds (VOCs) emitted by bovine embryos during their development and before their *in vitro* fertilization. Initially, blank samples such as culture medium, mineral oil and Petri dishes used during embryo maturation were analyzed by Head Space-Solid Phase Micro Extraction (SPME) and Gas Chromatography-Mass Spectrometry (GC-MS), then, embryos were analyzed as well. As preliminary results some compounds were identified in culture medium such as ethyl acetate, ethylbencene and derivatives, beta-myrcene, D-limonene, isopropyl palmitate, beta-pinene, 3-octanone and others, while in the mineral oil were identified some compounds such as ramified hydrocarbons and bencene derivatives. Also, in Petri dishes compound were identified as butylated hydroxytoluene, ethylbenzene and derivatives, d-limonene and camphor.

ETHICAL APPROVAL

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PREP-P03

PURIFICATION OF CASEINOMACROPEPTIDE FROM MILK WHEY THROUGH SOLID PHASE EXTRACTION.

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ABSTRACT

The identification of milk adulterated by whey is a recurrent problem in Latin American and European countries due to the difficulties involved in its analysis in terms of sample pretreatment and the high cost of standards. Caseinomacropeptide (CMP) is a biomarker employed in determination of adulterated milk with cheese whey. CMP is normally found in cow's milk at very low concentrations; although, it can be produced by enzymatic hydrolysis of milk with chymotripsin, which specifically cleaves *k*-casein, the main protein present in cow’s milk, yielding two peptides, one which is CMP that remains dissolved in the whey [1]. CMP can also exist as a glycosylated peptide denoted glycomacropeptide (GMP) and it can present two genetic variants denominated CMP-A and CMP-B, which differ on few residues of the sequence. These differences present a significant challenge in standardization of analysis techniques involving these compounds. The present work focuses on CMP obtention from milk whey through RP-SPE purification from different samples containing it. Milk whey extract obtained by RP-SPE was analysed using a Bruker Impact II ESI-Q-TOF LC-MS system, which was found that this strategy allows to separate CMP-A and CMP-B from cow’s milk involving close to none sample pre-treatment, allowing the obtention of a low cost *in-house* standard with potential use as an important biomarker in the milk industry.

ETHICAL APPROVAL

The present work does not require ethical approval

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PREP-P04

APPLICATION OF SOLID PHASE MICROEXTRACTION COUPLED TO GAS CROMATOGRAPHY IN THE ANALYSIS OF VOLATILE FRACTION FROM HUMAN EMBRYO CULTURE MEDIUM

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ABSTRACT

In the last years, an increase in the infertility rate worldwide has been estimated, which is between 10-15% [1]. This problem is related to genetic, environmental, and nutritional factors, among others [2]. Artificial fertilization programs developed in European Union countries have allowed the study of embryonic development in order to determine its viability. Generally, a morphological characterization of the embryo is performed. However, some information can be lost during the process [3], resulting in an unsuccessful fertilization case [3]. Volatolomic techniques allows us to complement this study and determine key factors of embryonic development in its different states. In this research, an analytical methodology was developed for the sampling and identification of volatile compounds from human embryos. The culture medium (blastocyst) and its volatile fraction were monitored by headspace solid-phase microextraction coupled to gas chromatography- mass spectrometry detection (HS-SPME-GC-MS), with divinylbenzene/carboxene/polydimethylsiloxane (DVB/Carboxen/PDMS, 50/30 μm) fiber. 20 mg of each culture medium was incubated at 38 °C. Volatile compounds were exposed to the fiber for 2 h. The compounds were identified tentatively by comparison between the mass spectrum reported in spectral data base NIST 14. Some compounds identified in the samples 68TUKS5, 69TUKS2 and 72TUK-S1 were decane 3,7-dimethyl and dodecane, 2-methyl. The results shown that volatile organic compounds are produced through embryonic development.

ETHICAL APPROVAL

The human embryo study protocol was approved from the Research Ethics Committee of University of Tartu

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PREP-P05

FRACTIONATION OF EXTRACTS BY RP-SPE: A USEFUL TOOL TO ASSESS PEPTIDE METABOLISM IN CUNNINGHAMELLA ELEGANS

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ABSTRACT

The use microorganisms in vitro to simulate the metabolism of molecules with pharmacological and toxicological importance in mammals is useful in preliminary studies of activity and safety, and has several advantages of cost-efficiency, bioethics, and facility. Fungal models such as the Cunninghamella family that present high level of expression of enzyme systems similar to mammalian ones and therefore are able to metabolize a wide variety of substances such as drugs, pharmaceuticals, pesticides, among other. However, their use in biotransformation studies of peptides of pharmacological interest has not been reported. The objective of this project was to study the metabolism of two anticancer peptides derived from Bovine Lactoferricin RWQWRWQWR and RWQWRWQWOrn, using the in vitro model of *Cunninghamella elegans*. Peptide synthesis was carried out by SPPS-Fmoc/tBu strategy and the peptides were purified by RP-SPE, and characterized by RP-HPLC and LC-MS. The fungal was treated with the peptide and culture supernatants were fractioned by RP-SPE chromatography and analyzed by HPLC-DAD and a Bruker Impact II ESI-Q-TOF LC/MS. Intact peptides and peptide fragments were identified, suggesting that the peptides were partially metabolized and that RP-SPE fractionation is useful for identifying metabolites from *C. elegans* culture supernatant.

ETHICAL APPROVAL

The present work does not require ethical approval

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PREP-P07

CHARACTERIZATION AND FUNCTIONALIZATION OF LUFFA *(LUFFA ACUTANGULA)* AS A BIOSORBENT FOR THE DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS IN AQUEOUS MATRICES.

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In this study, the feasibility of applying the Luffa sponge (*Luffa Acutangula*) as a biosorbent for the determination of Polycyclic Aromatic Hydrocarbons (PAHs) in aqueous samples was investigated. According to the reported literature, this biomaterial stands out for being a natural, economical, reusable and compostable material [1]. In this context, the new biosorbent was used as a more ecological alternative to classical sorbents, in the solid phase extraction technique. For the study, benz[a]anthracene, chrysene, benzo[a]pyrene, benzo[b]fluoranthene, benzo[g,h,i]perylene, benzo[k]fluoranthene, dibenz[a,h]anthracene were used as target analytes.

The preparation of the biomaterial was carried out in two stages; first, the biosorbent was disinfected with a 70% ethanol solution, assisted by ultrasound. Then, it was functionalized, in increasing solutions with stearic acid ($C_{18}H_{36}O_2$) with 0.8, 1.2, 1.6 and 2.0%, to modify the polarity by forming a hydrophobic coating. For the extraction of the analytes, the new $1cm^3$ biosorbent was immersed in the 50 ug/L solution for the 7 analytes under study, and stirred for 120 min. The desorption of the analytes was performed with acetonitrile (ACN) and vacuum, followed by a preconcentration to dryness with nitrogen gas at low flow. Finally, the sample was reconstituted with 1 mL of ACN, for its instrumental detection by high pressure liquid chromatography coupled to a fluorescence detector. The optimization of the extraction variables was carried out by means of a univariate analysis, studying the effects of: stirring time, sample volume, Luffa mass and elution volume, obtaining optimal conditions of 120 minutes of stirring, 100 mL of sample, 0.35-0.4 g of Luffa mass and 10 mL of ACN for elution. The method was validated by obtaining the analytical parameters of precision and accuracy and was applied to real water samples from the Viña del Mar region, an area recently affected by a large wildfire.

Finally, the biomaterial was characterized. The physical analysis was performed using Scanning Electron Microscopy (SEM) which revealed the presence of a hydrophobic coating on the surface of the plant, allowing the adsorption of the analytes on the solid support. The chemical analysis, a study performed using FT-IR, showed the formation of new bonds between stearic acid and Luffa, the signals at 1463 and 1430 cm^{-1} may originate from lignocellulosic residues and the hydrogen bonds of stearic acid, which are those that favor the adsorption of PAHs.

PREP-P08

GC/MS STUDY OF THE TROPANIC ALKALOIDS IN FLOWERS AND LEAVES EXTRACTS FROM *Datura metel* L.

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ABSTRACT

Datura metel L. (Solanaceae) is an annual herb that grows between 0.5-1 m. The plants are slightly furry, and the shoots are usually dark violet. It is widely used by people both as a drug and ornamental plant and it is grown all over the world [1]. The whole plant is considered a narcotic, anodyne, and antispasmodic, while the leaves, bark, and seeds are also separately used in extractions [2]. *D. metel* flowers were collected from CENIVAM research experimental plots (UIS, Bucaramanga, Colombia) and lyophilized for 48 h, extraction was made using MSPD (Matrix Solid-Phase Dispersion) method using dry plant material (0.88 g), silica gel C_{18} (3.53 g), and dichloromethane (10 mL) as elution solvent, extraction was cleaned using HCl solution (5 mL, 1% w/v) and *n*-hexane (5 mL) by triplicate, then alkaloids were extracted from aqueous solution using dichloromethane (5 mL) by triplicate. MSPD extract was analyzed by GC/MS, on GC 6890 Plus (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS column [5%-phenyl-poly-(methyl siloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)]. Atropine and scopolamine were the major compounds identified in D. metel flower extract; the presence of tropane alkaloids confirming the narcotic properties of this plant, the compounds extracted may be of substantial interest for pharmacology, biochemistry, and other chemistry areas.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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PREP-P09

GC/MS STUDY OF THE TROPANIC ALKALOIDS IN FLOWERS AND LEAVES EXTRACTS FROM *Datura metel* L.

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ABSTRACT

Datura metel L. (Solanaceae) is an annual herb that grows between 0.5-1 m. The plants are slightly furry, and the shoots are usually dark violet. It is widely used by people both as a drug and ornamental plant and it is grown all over the world [1]. The whole plant is considered a narcotic, anodyne, and antispasmodic, while the leaves, bark, and seeds are also separately used in extractions [2]. *D. metel* flowers were collected from CENIVAM research experimental plots (UIS, Bucaramanga, Colombia) and lyophilized for 48 h, extraction was made using MSPD (Matrix Solid-Phase Dispersion) method using dry plant material (0.88 g), silica gel C_{18} (3.53 g), and dichloromethane (10 mL) as elution solvent, extraction was cleaned using HCl solution (5 mL, 1% w/v) and *n*-hexane (5 mL) by triplicate, then alkaloids were extracted from aqueous solution using dichloromethane (5 mL) by triplicate. MSPD extract was analyzed by GC/MS, on GC 6890 Plus (Agilent Technologies, AT, Palo Alto, CA, USA), equipped with a mass selective detector MS 5973 Network (AT, Palo Alto, CA, USA), using a DB-5MS column [5%-phenyl-poly-(methyl siloxane), 60 m x 0.25 mm (i.d.) x 0.25 (d.f.)]. Atropine and scopolamine were the major compounds identified in D. metel flower extract; the presence of tropane alkaloids confirming the narcotic properties of this plant, the compounds extracted may be of substantial interest for pharmacology, biochemistry, and other chemistry areas.

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PREP-P10

GRAPHENE-CHITOSAN BIOSORBENT: A NOVEL APPROACH FOR PESTICIDE ASSESSMENT BY MICROEXTRACTION IN FOOD MATRICES

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ABSTRACT

Rising global concerns about pesticide residues in food due to health risks have increased the need for advanced assessment methods. Miniaturized techniques such as microextraction by packed sorbent (MEPS) are effective for concentrating target analytes and removing interferences, enabling accurate trace-level detection [1]. Recent developments in sorbent technology have introduced hybrid sorbents, with graphene-based materials showing significant potential. However, combining these with biopolymers, such as chitosan (CS), in MEPS methods remains largely unexplored, particularly their application in food analysis through microextraction protocols [2]. In this study, silica-graphene oxide@chitosan (SiGO@CS) was synthesized through an in-situ reaction, followed by freeze-drying and packing the sorbent into MEPS syringes for extracting atrazine and thiamethoxam from corn and tomato samples, respectively. Characterization confirmed the successful modification of the graphene-based polymer with CS. Method optimization identified the draw/eject and washing cycles as the most significant parameters. The method demonstrated limits of detection (LOD) and quantification (LOQ) ranging from 0.020 to 0.045 μg L^{-1} and 0.045 to 1.0 μg L^{-1} for atrazine and thiamethoxam, respectively, with accuracy values between 92% and 100%. Compared to traditional sorbents, the biosorbent showed superior extraction efficiency and notable reuse capability (more than 15 times). Local sample analysis revealed atrazine at concentrations below the LOQ reference. The SiGO@CS biosorbent proved effective in MEPS for pesticide assessment in corn and tomato samples, offering a green alternative to traditional and non-eco-friendly microextraction methods. This study demonstrated the SiGO@CS sorbent as a sustainable and efficient solution for pesticide residue analysis in food safety.

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PREP-P11

EXPLORING THE VERSATILITY OF GRAPHENE OXIDE FUNCTIONALIZED WITH IONIC LIQUIDS FOR THE MICROEXTRACTION OF EMERGING CONTAMINANTS IN DIFFERENT MATRICES

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ABSTRACT

Graphene-based materials, particularly graphene oxide (GO), are noted for their high surface area, conjugated structure, and potential for functionalization, enhancing their adsorption capacity and allowing for polarity modification [1]. This study developed sorbents by functionalizing GO with two imidazolium ionic liquids (ILs) containing imidazolium cations: 1-vinyl-3-hexylimidazolium ([VHiM]Br) and 1-vinyl-3-(butyl-4-sulfonate)imidazolium (ViImC4S), using “thiol-ene” click chemistry [2]. These materials were evaluated for their extraction capacity for five triazine herbicides (atrazine, ametryn, propazine, prometryn, and simazine) in environmental waters and four parabens (methyl, ethyl, propyl, and butyl parabens) in cosmetic matrices. ViImC4S@GO demonstrated high recovery values, retaining over 60% of herbicides and 80% of parabens due to multiple adsorption mechanisms. The zwitterionic ViImC4S modified the polarity of GO, resulting in a sorbent with greater affinity for medium- and low-polarity pesticides and parabens compared to commercial C18 or Strata-X particles. The ViImC4S@GO was used in stir bar sorptive extraction (SBSE) for triazines in river and groundwater and dispersive solid-phase microextraction (d-µSPE) for parabens in soap, moisturizer, and facial sunscreen, followed by ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS). Optimized parameters achieved excellent equilibrium conditions for extraction and desorption. Both methods showed good linearity ($r^2 \geq 0.99$), with limits of quantification (LOQ) ranging from 0.0014-0.45 ng mL^{-1} for triazines and 0.9-4.0 ng mL^{-1} for parabens and analyte recoveries of ≥ 50%. Real sample analysis revealed no triazine residues in water samples, while paraben concentrations in “paraben-free” cosmetic samples were below the LOQ of the method. In conclusion, functionalizing GO with ILs enhances the efficiency of microextraction methods, improving the sorption of emerging contaminants with varying polarity in complex matrices.

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PREP-P13

DEVELOPMENT OF A NOVEL METHOD FOR THE DETERMINATION OF HORMONES IN SOLID WASTE BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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ABSTRACT

In this study, A solvent-free simple and efficient method for the quantification of Hormones in solid waste matrices is proposed. The new approach involves the extraction, clean up and pre-concentration of Estrone (E1), Estradiol (E2), and Ethinylestradiol (EE2), in a single step using simultaneously a rotating disk contained the solid sample and solid phase microextraction where the fiber is directly immersed in the water used as solvent for extraction of the target compounds from the rotating disk [1]. The rotation of the disk facilitates the solid/water equilibrium of the congeners contained in the solid waste which are extracted by the SPME fiber [2]. In order to improve extraction efficiency, parameters considered important such as pre-equilibrium, extraction time, temperature, ionic strength and the presence of organic solvent are investigated and optimized. Good linearity is achieved with a correlations coefficient of 0.9952, 0.9912 and 0.996; quantification (LOQ) limits were between 0.61and 2.19µg g^{-1}. The accuracy and precision providing recoveries 78.1 – 89.2% for the Hormones in three levels of fortification and the relative standard deviations between 3.3% and 9.5%. These results showed that the method is a promising alternative for hormones analysis determination in solid wastes.

ETHICAL APPROVAL

The request does not apply.

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PREP-P14

EXTRACTION OF BIOACTIVE COMPOUNDS FROM PROMISING AMAZONIAN FRUITS (*Mauritia flexuosa, Eugenia stipitata, Myrciaria dubia, Theobroma grandiflorum*) USING NON-POLAR NATURAL DEEP EUTECTIC SOLVENTS (NADES) AS ALTERNATIVE SOLVENTS

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ABSTRACT

The extraction of bioactive compounds using environmentally friendly techniques has become essential. Organic solvents (acetone, methanol, propanol, hexane, dichloromethane, or a combination of these) have good extraction capacity for bioactive compounds; however, they present many inherent disadvantages, such as low boiling points, flammability, high toxicity, and poor biodegradability [1,2]. Moreover, using these organic solvents in extraction methods reduces the applicability of the extracts [1,2]. One of the alternatives that have emerged in the last decade is the use of NADES, which offer significant advantages over traditional solvents like methanol, hexane, and dichloromethane, as NADES are biodegradable, easy to prepare, and have low volatility and toxicity [3,4]. By 2030, agricultural productivity and the incomes of small-scale food producers, such as Amazonian fruit growers, are expected to double [5]. As a result, this study aimed to extract non-polar bioactive compounds from promising fruits native to the Amazon region using NADES. The natural products chosen for extraction include Canangucha (*Mauritia flexuosa*), Araza (*Eugenia stipitata*), Camu-camu (*Myrciaria dubia*), and Copoazu (*Theobroma grandiflorum*). The extracts obtained using NADES were compared with those obtained through traditional solvent extraction methods. Subsequently, the extracts were analyzed using HPLC-DAD-MS/MS.

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PREP-P15

SÍNTESIS Y CARACTERIZACIÓN DE SOLVENTES EUTÉCTICOS PROFUNDOS PARA SU EMPLEO COMO EXTRACTANTES DE CONTAMINANTES EMERGENTES EN MUESTRAS ACUOSAS

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RESUMEN

A través de los años, los solventes convencionales han sido empleados en diversos procesos de extracción, sin embargo, se ha presentado interés en el desarrollo de alternativas ecológicas con el fin de generar el menor impacto ambiental, surgiendo así los Solventes Eutécticos Viscosos (DES) como aquella alternativa hacia la química verde. Este tipo de solventes están conformados por dos tipos de componentes: Una molécula donadora de enlaces de hidrógeno (HBD) y una aceptora de enlaces de hidrógeno (HBA) que en la proporción molar adecuada generan un líquido con un punto de fusión mucho menor que el de los dos componentes por separado, siendo así posible su uso como disolvente a temperatura ambiente convirtiéndose en un complemento llamativo para las técnicas de extracción [1]. El mecanismo de síntesis de estos solventes se basa en las interacciones moleculares entre los componentes que forman el solvente pero aún no es claro y por lo cual la caracterización de estos solventes es importante para contribuir al establecimiento de este mecanismo. Por lo anterior, en el presente trabajo se establece fortalecer el conocimiento de estos solventes por medio de la caracterización, con el fin de aportar a la elucidación de sus estructuras y así comprender cómo es su comportamiento con el analito cuando es empleado en aquellos procesos de extracción. Para ello, fueron sintetizados DES basados en Ácido cítrico y Glicina en proporciones molares distintas y posteriormente caracterizados mediante análisis físicos (viscosidad y densidad) y espectroscópicos (NIR, IR, RMN y Raman), donde estos últimos permitieron una comparación con los espectros de los compuestos de partida y obteniendo como resultado un cambio de ciertas señales con las que se determinaron la ocurrencia de estas interacciones. El empleo de estos solventes en técnicas miniaturizadas como la microextacción líquido-líquido dispersiva (DLLME) han revelado eficacia en el análisis de muestras con analitos presentes en cantidades de trazas cómo es el caso de los Contaminantes Emergentes (CE), siendo su capacidad extractora amigable con el medio ambiente la principal motivación a su aplicación.

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PREP-P16

SOIL-BASED ANALYSIS OF TOMATO ROOT VOLATILES BY GAS CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY

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ABSTRACT

The rhizosphere is a complex environment, which houses a wide variety of interactions that occur between plants, microorganisms and even animals [1]. Plants can detect and respond to neighboring plants [2]. These detection and signaling interactions can occur both above ground and below ground, and mostly happen through chemical signaling by volatile organic compounds (VOCs). Above ground signaling interactions have been widely studied and well stablished; they are mediated by VOCs such as ethylene, benzoate and several volatile terpenes among many others [3]. Belowground signaling interactions and the VOCs involved in them remain relatively understudied. Three different varieties of tomato (*Solanum lycopersicum*) were planted, and small, 3D printed hollow chambers made from polylactic acid (PLA) filament were carefully buried in the soil next to the roots. These chambers were made with a meshed, net-like surface to allow volatiles into the hollow space while keeping dirt and other solids out. Solid-phase microextraction (SPME) was used to extract VOCs from the hollow chambers, using a polydimethylsiloxane (PDMS, 85 μm) fiber. VOC analysis was performed by gas chromatography coupled to mass spectrometry (GC-MS) with MSD (EI, 70eV) using a DB-WAX column (60 m). Many compounds were identified, some of them reported by other authors in aerial parts of the plant. The overall volatile composition was observed to change throughout the duration of the experiment, as the tomato grew and matured.

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PREP-P17

CHEMICAL CHARACTERIZATION BY UHPLC/ESI+-*ORBITRAP*-MS OF HYDROETHANOLIC POST-DISTILLATION WASTE EXTRACT OF *PSIDIUM SARTORIANUM*

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ABSTRACT

Psidium sartorianum is a small tree from the Myrtaceae family that can be found throughout central and South America [1]. Its extract has shown antibacterial and antifungal properties [2], however, it has not been chemically characterized by analytical methods yet. The chemical composition of hydroethanolic extract from post-distillation waste of *P. sartorianum* was analyzed. Aerial parts of the plant were employed, and the extract was obtained by ultrasonic assisted extraction of the ground waste, using 70% ethanol. The mass spectra and retention times of certified standards were used as one of the identification criteria for chemical characterization by UHPLC/ESI-*Orbitrap*-MS. A total of 17 compounds were detected, confirmatory data were obtained for five of these compounds, and the remaining 12 were tentatively identified; of the 17 compounds eight were flavonols, 4 were flavanols and 3 were flavanones and the remaining 2 were proanthocyanidins. Flavonols were amongst the most abundant compounds present in the hydroethanolic extract of post-distillation waste of *P. sartorianum*, followed by flavanols and flavanones.

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PREP-P18

COMPARISON OF QUECHERS AND P-QUECHERS EXTRACTION METHODOLOGIES FOR THE DETERMINATION OF MULTI-RESIDUE VETERINARY DRUGS IN FOOD MATRICES OF ANIMAL ORIGIN BY LC/MS

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ABSTRACT

The intensive use of veterinary drugs in the livestock industry has generated a growing concern for food safety, since veterinary drug residues (VDRs) remaining in animal tissues intended for human consumption can have adverse effects, such as carcinogenicity, hypersensitivity, alteration of the intestinal flora and, even, in the most severe cases, antimicrobial resistance [1]. In this study, an effective method for the extraction, detection and quantification of VDRs in samples of animal origin was evaluated. The extraction efficiency of the analytes was evaluated by comparing the QuEChERS techniques and a modified version of p-QuEChERS [1,2]. Subsequently, qualitative and quantitative analysis of VDRs was performed by liquid chromatography coupled to mass spectrometry with an Orbitrap detector. The p-QuEChERS method was superior to QuEChERS in the extraction efficiency of VDRs, particularly for sulfonamides, from 22-32% with QuEChERS to 61-73% with p-QuEChERS. Tetracyclines went from 11-22% to 73-90%, and some macrolides from 17-28% to 40-57%. However, the QuEChERS technique was more effective (49-65%) in the extraction of some fluoroquinolones compared to p-QuEChERS (11-26%). The implemented p-QuEChERS method will allow the monitoring of VDRs in different matrices of animal origin and will ensure food safety for consumers.

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PREP-P19

IMPLEMENTATION OF A METHOD FOR EXTRACTION AND ANALYSIS OF MULTI-RESIDUE VETERINARY DRUGS IN ANIMAL TISSUE BY LC/MS

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ABSTRACT

The inappropriate use of veterinary drugs in the livestock industry can lead to the presence of residues of these drugs in animal foods intended for human consumption, which represents serious risks to public health [1]. This project focuses on the implementation and validation of a modified analytical method: p-QuEChERS [2] By implementing some figures of merit, such as detection limits, recovery, reproducibility, repeatability and robustness, applied to animal tissue matrices obtained locally at five points of sale in Bucaramanga and its surroundings. The extracts were obtained using the p-QuEChERS method, and chromatographic analysis by UHPLC-ESI+-Orbitrap-HRMS, the best analytical responses were obtained using water and methanol as mobile phase, with 0.1% (v/v) formic acid, 0.5 mM ammonium formate, with a capillary voltage of 3 kV.The drugs studied included sulfonamides (7), anthelmintics (5), fluoroquinolones (5), macrolides (4), tetracyclines (3), coccidiostats (3), beta-lactams (3), tranquilizers (2), beta-agonists (2), amphenicol (1) and lincosamide (1). The coefficients of variation were in a range of 0.06-0.66% and 1.60-24.83% for retention times and chromatographic areas, respectively. Recoveries were obtained in the range of 55% to 75%, with detection limits of 0.1 to 2.5 µg/L for most analytes and quantification limits of 2 to 20 µg/L. The correlation coefficients (r^2) reached a value of 0.99. Traces of 2-aminoflubendazole, azaperone, chlortetracycline, danofloxacin, fenbendazole, flumequine, ractopamine and tetracycline were detected in local sampling at concentrations of 1 to 5 µg/kg, mainly in beef and pork muscle samples. These results demonstrate that the analytical parameters of the evaluated method allow the extraction, detection and quantification of even traces of drugs well below the established Maximum Residue Limits (MRLs), ensuring food quality and safety.

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PREP-P20

EXTRACCIÓN E IDENTIFICACIÓN DE COMPUESTOS FENÓLICOS DE CANANGUCHA (*Mauritia flexuosa*) UTILIZANDO DISOLVENTES EUTÉCTICOS PROFUNDOS NATURALES (NADES)

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ABSTRACT

La Canangucha (*Mauritia flexuosa*) de la familia *Arecaceae*, es una palma que se cultiva al sur de la amazonia colombiana [1]. Esta fruta se caracteriza por tener un alto contenido de polifenoles, dentro de los cuales se encuentra quercetina, apigenina, luteolina, ácido cafeico, acido ferúlico y ácido clorogénico como el más abundante (1,15 mg/g peso fresco) [2]. Sin embargo, la extracción de estos compuestos, haciendo uso de disolventes convencionales representa un gran riesgo para el medio ambiente, una de las alternativas que ha surgido para la extracción de compuestos bioactivos es el uso de disolventes de origen natural, como es el caso de los disolventes eutécticos profundos naturales (NADES, Natural Deep Eutectic Solvents por su sigla en inglés) [3, 4]. En este trabajo se llevó a cabo la preparación los NADES, se caracterizaron mediante (IR y TGA), se determinaron sus propiedades fisicoquímicas (densidad y viscosidad), posteriormente se realizó la extracción de compuestos fenólicos de pulpa de canangucha (*Mauritia flexuosa*) utilizando el NADES y un disolvente convencional (Metanol), además de la respectiva identificación de dichos compuestos mediante cromatografía liquida acoplada a espectrometría de masas en tándem (LC-MS/MS), por último, se realizaron ensayos de actividad antioxidante (DPPH y ABTS) y determinación del contenido de fenoles totales (CFT). Se detectaron 11 compuestos, de los cuales se identificaron 6 compuestos fenólicos (ácido clorogénico, apigenina C-hexósido-C-pentósido, apigenina 6,8-di-C-glucósido, luteolina-8-C-(6"-O-p-benzoil)-glucósido, apigenina-6-C-Desoxihexosa-O-hidroximetil ácido glutárico y quercetina-3-O-glucósido) siendo el ácido clorogénico el compuesto mayoritario. Tanto el área relativa de los compuestos extraídos, el contenido de fenoles totales (1569,60 mg EAG/100 g peso seco) y la actividad antioxidante ABTS (10235,50 mg ETx/100 g peso seco) revelaron que el mejor NADES para la extracción de los compuestos fenólicos fue (Cloruro de colina: Glicerol (1:2) 30% H_2O).

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PREP-P21

DEVELOPMENT OF A TWO-LEVEL EXPERIMENT DESIGN FOR THE OPTIMIZATION OF A HS-SPME-GC-MS METHOD FOR THE STUDY OF RUMS FROM COLOMBIA AND BRAZIL

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ABSTRACT

Rum is an alcoholic beverage primarily produced in the Caribbean and Central America, and distributed globally [1]. A key factor influencing a consumer's decision to buy rum is its aroma, largely attributed to the chemical diversity of its volatile organic compounds (VOCs) [2]. Therefore, a two-level experimental design was implemented, incorporating a Plackett-Burman design for screening and a central composite design (CCD) for response surface analysis [3,4]. This aimed to maximize the adsorption of VOCs on the Solid Phase Micro Extraction (SPME) fiber, using the area of esters, a main chemical family in rums, as the response. The study found that sample dilution and salting out are the primary factors affecting the adsorption of these compounds. Consequently, a HS-SPME-GC-MS method was developed for analyzing VOCs in rums using a two-level experimental design which allowed the identification of differentiating compounds between the volatile profiles of rums from Brazil and Colombia.

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PREP-P22

A NEW COATING INK BASED ON A LIGHT-CURING POLYMER AND A METAL-ORGANIC FRAMEWORK TO DEVELOP MIXED MATRIX MEMBRANES FOR THIN-FILM MICROEXTRACTION

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ABSTRACT

The use of polymers in analytical sample preparation is nowadays widely extended due to their capacity to act as an efficient extraction material but also as a blinder connecting other materials to the polymer. Their high agglutinant power ensures adequate incorporation of other materials like magnetic nanoparticles, metal organic frameworks (MOFs), ionic liquids, carbon-based materials, and covalent organic frameworks, among others. MOFs are quite interesting crystalline materials formed by metal ions (or clusters) coordinated with organic ligands, with high versatility and impressive surface area, thus being quite successful extraction materials to be combined with polymers forming microextraction devices, such as mixed matrix membranes (MMMs) for thin-film microextraction. Besides, it is worth mentioning light-curing polymers. They are very interesting materials due to their capacity to solidify when exposed to UV light. This property makes possible to produce an initial liquid coating ink (in combination with another material, like MOFs) and then becoming solid under UV radiation.

In this study, we propose the development of a new MMM using cellulose as support and coated with a light-curing polymer@MOF ink through the bar-coating technique. MMMs based on these materials are deeply characterized, as assessed in a screening studying for the determination of a variety of contaminants of emerging concern.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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PREP-P23

THIN-FILM MICROEXTRACTION DEVICES BASED ON A VARIETY OF MATERIALS, INCLUDING SILVER NANOPARTICLES OR IONIC LIQUIDS AND DERIVATIVES: APPLICATION TO THE REMOVAL OF PHENOLS FROM AQUEOUS SAMPLES

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ABSTRACT

Thin-film solid-phase microextraction (TF-SPME) is an interesting analytical sample preparation technique able to solve limitations of conventional SPME with fibers. This technique is based on using thin layers of the extraction material, thereby using higher amount of sorbent compared to SPME fibers (thus increasing the extraction capacity), without increasing the extraction time. The lack of selectivity of the devices based on polydimethylsiloxane (PDMS), the extraction material mostly used in TF-SPME, is solved in this study by introducing new materials. Among them, solid materials, such as silver nanoparticles and polymeric ionic liquids, and liquid materials, such as neat ionic liquids and their magnetic derivatives, are proposed as alternatives in TF-SPME devices. As a proof of concept, these devices have been used for the removal of phenols from aqueous samples.

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PREP-P24

IDENTIFICATION OF SECONDARY METABOLITES PRODUCED BY *Cannabis sativa L.* DURING DIFFERENT MOMENTS IN THE FLOWERING CYCLE USING GAS CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY (GC-MS)

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ABSTRACT

In order to know and understand the floral biology (biochemistry) of the Cannabis sativa plant. L. The present study aimed to investigate the physiological response of the plant, through the synthesis of chemical compounds with therapeutic potential at different stages of the flowering stage. For this, the chemical extraction technique of ethanolic maceration was used, subsequently the solid phase microextraction (SPME) for the capture of the metabolites present in the oily matrix, the chromatographic, separation and identification analysis was carried out by means of gas chromatography. coupled to mass spectrometry (GC-MS). The results reveal a dynamic physiological response, with variations in the composition and concentration of the different metabolites, identifying several families in the ethanolic extract: cannabinoids (cannabidiol and tetrahydrocannabinol), terpenes, phenols, and other families in minor proportions; Its presence in the flower varies according to the floral development in the field.

ETHICAL APPROVAL

This study did not require ethical endorsement, since it did not relate the study to humans or animals.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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SA-P01

SORPTIVE MICROEXTRACTION WITH A ROTATING DISK OF STEROID HORMONES: USING A HYBRID MATERIAL BASED ON THE FUNGUS AND MONTMORILLONITE AS ADSORBENT PHASE FROM AQUEOUS SAMPLES

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ABSTRACT

One of the current environmental problems is continuous exposure to emerging contaminants (ECs). Among these, steroid hormones are especially critical, as they disrupt the normal functioning of the endocrine system in exposed organisms (EDCs) [1,2]. To address this challenge, an interesting strategy has been proposed: the bioremediation process. In this process, enzymes such as laccase and peroxidase are used to degrade contaminating compounds. An important source of these enzymes is the fungus *Pleurotus ostreatus*. Its biomass and enzymes promise to be useful in the elimination of ECs. However, a limitation in using enzymes is that their stability and activity decrease over time. To overcome this obstacle, immobilization has been used as a strategy. This technique favors the stability of enzymes, preserves their activity, promotes their reuse and reduces their cost. In this context, natural materials with adsorbent characteristics, such as montmorillonite (MMT), are presented as a novel alternative. MMT is an inexpensive and non-toxic material that can serve as a support for the biomass of the fungus or its enzymes [3]. Hybrid materials have been developed from the combination of MMT with *P. ostreatus*. These materials were synthesized using three procedures in an aqueous medium and an open reactor: growth of the fungus in the presence of MMT (MMT/Mixture), combination of MMT with the enzymatic arsenal of the fungus (MMT/Broth) and mixing of the biomass with MMT (MMT/Biomass). To evaluate its potential in the removal of 17α-ethinyl estradiol (EE2), 17β-estradiol (E2), estrone (E1) and estriol (E3) in aqueous matrices, the RDSE (rotating disk under optimized conditions) method was used [4]. The samples were analyzed on a HPLC-UV equipment. The results showed an extraction equivalent to that obtained with the commercial Oasis® HLB adsorbent, without significant differences. This demonstrates the amphipolarity of the materials explored and their potential in terms of cost-benefit ratio, since the precursor materials have a low production value. In conclusion, these hybrid materials constitute an interesting alternative to eliminate emerging steroid hormone-type contaminants in aqueous matrices.

ETHICAL APPROVAL

Does not apply.

FINANCIAL SUPPORT AND ACKNOWLEDGEMENTS

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SA-P02

PHYTOCHEMICAL STUDY AND ANTIMPLASMODIAL ACTIVITY OF *Miconia aeruginosa*

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ABSTRACT

Malaria is a tropical neglected disease produced by protozoa belonging to *Plasmodium* genus and transmitted by *Anopheles sp*. [1]. This illness is the cause of death of at least 2 million people around the world and the sickness of circa 400 million every year [2]. Currently, there are very few drugs to treat it and the parasite is resistant to most of them [3]. Because of this, the search for new antimalarial drugs is urgent. Due to the results of a previous antiplasmodial screening, where *M. auriginosa* showed promising in vitro activity (13,6 mg/mL), this work aims to study the phytochemical composition and their role in the biological activity of this plant. The ethanolic extract of the leaves was prepared by percolation and a phytochemical analysis for 10 secondary metabolites was performed. Additionally, an open column fractionation was made and the obtained fractions were tested in vitro against *P. falcimarum*, strain FCR-3. As a result, in the ethanolic extracts were found flavonoids, such as leucoantocyanidins, triterpens, saponins, and tannins. The most active fractions were identified and their composition was studied by an HPLC-MS analysis. The isolation and purification process are ongoing.

ETHICAL APPROVAL

The Ministry of Environment and Sustainable Development has granted us with the contract 249 to access genetic resources and derivative products to perform this work. As the biological test are performed in vitro no further ethical approval is needed.

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SA-P03

PHYTOCHEMICAL ANALYSIS OF TWO SAMPLES OF *Solanum americanum* Mill.

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ABSTRACT

In the rural northwest area of the Tolima Department, plants of the *Solanum* genus are used by folk population to treat skin diseases. This work aims to perform the phytochemical evaluation of two of them by analyzing and comparing their phytochemical composition and establish a potential correlation between the presence of secondary metabolites and the cicatrizating activity. A total of 16 extracts, 8 whole ethanolic and 8 aquose, were prepared from the leaves, stems, roots, and fruits of two plants (SNA y SNB) classified as *S. americanum.* Each one of the ethanolic extracts was tested for secondary metabolite presence and their chemical profiles were obtained, by TLC and HPLC-MS as well. For the aquose extracts, the presence of alkaloids and flavonoids was examined. Alkaloids and terpenes were found in both plants and in all the organ tested. Flavonoids were in both plants, but only in leaves and stems. As a result of the importance of alkaloids and its relationship with the improvement of skin conditions [1], a comparative semi-quantitative analysis of these secondary metabolites in both plants and their organs was performed. For SNA, the leaves exhibited the highest proportion of alkaloids (39%), in comparison to fruits, steams, and roots, the least showed the least with 14%. In the case of SNB, the fruits had the highest proportion of alkaloids (36%) and stems the least (13%). Additionally, the alkaloid profiles of SNA y SNB were compared and significative cuali-quiantitative differences were observed not only between organs, but also between SNA and SNB. These chemical differences could be related to the morphological differences of both studied plants.

ETHICAL APPROVAL

The Ministry of Environment and Sustainable Development has granted us with the contract 249 to access genetic resources and derivative products to perform this work.

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SA-P04

TENTATIVE IDENTIFICATION OF CHEMICAL CONSTITUENTS OF *Vaccinium floribundum* BY GC-MS AND EVALUATION OF THEIR ANTIOXIDANT ACTIVITY

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RESUMEN

Vaccinium floribundum Kunth (Ericaceae), commonly known in Colombia as mortiño, is a species native to the Colombian moors and widely used due to its antioxidant properties, which is why it has been attributed therapeutic, anticancer, antiaging and antitumor applications [1]. Taking into account the above, the purpose of this research was the tentative identification of the chemical constituents present in the leaves of this species and the evaluation of its antioxidant activity. Successive separations by column chromatography led to the obtaining of a mixture of flavonoids reported in other species of the Ericaceae family [2] and composed of quercetin and hyperoside and the isolation of three compounds, a coumarin, a lactam and a flavonoid (3-(2-(diethylamino)ethyl)-7-hydroxy-4-methylcoumarin, 3-benzylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione and hyperoside), which were tentatively identified using GC-MS and by comparison of their mass spectra with those reported in the literature. The determination of the antioxidant capacity in extracts and fractions from the leaves of the species was carried out by the DPPH free radical capture method, where it was shown that the ethanolic extract and the dichloromethane and ethyl acetate fractions presented an inhibitory effect of 50% at concentrations between 100 and 200 ppm, with IC_{50} values of 98.1387, 146.1595 and 115.5450 ppm respectively, the above allowed to establish that the ethanolic extract and the fractions studied present a promising antioxidant capacity compared to the reference antioxidant substance Trolox, which presented an IC_{50} of 103.0176 ppm.

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SA-P05

TITLE: DEVELOPMENT OF A VANCOMYCIN QUANTIFICATION METHOD ON HUMAN PLASMA BY UHPLC-UV

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ABSTRACT

Vancomycin (VCN) is the preferred antibiotic for treating gram-positive infections, including Methicillin-Resistant *Staphylococcus aureus* (MRSA)[1]. Despite its narrow therapeutic window, variable pharmacokinetics, and dose-dependent nephrotoxicity[1], it is widely used in the clinical field of Colombia. This necessitates the development of protocols for optimal administration and dosing, such as therapeutic drug monitoring (TDM), which measures drug concentration in plasma and its effects[1]. This project aims to develop and validate a method for quantifying VCN in human plasma using UHPLC-UV. The method was developed taking in account other validated methods on the literature [2-4]. It employs a wavelength of 240nm, a Kinetex™ EVO C18 column (100 x 2.1mm, 2.6 µm), and gradient elution with mobile phases of 0.1% formic acid and methanol with 0.1% formic acid. Sample preparation involves protein precipitation with methanol, using caffeine as the internal standard. The method demonstrated positive results, with calibration curves showing an R^2 of 0.9967 and back-calculated accuracies around ±7%. Minimal interference was observed in two different lots of human plasma at the retention time of the VCN over a range of 0.5µg/mL to 100µg/mL. Future validation will follow the ICH M10 guidelines, aiming to establish this method as the basis for a VCN quantification service.

ETHICAL APPROVAL

The present project was approved by the investigation ethics committee of the Universidad del Atlántico on March 21 of 2023

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SA-P08

MECHANISMS AND METABOLIC CHANGES INDUCED BY CRUZIOSEPTIN PEPTIDES AGAINST TRYPANOSOMA CRUZI

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ABSTRACT

Current treatments for Chagas disease face several challenges, underscoring the need for new therapeutic alternatives [1]. In this regard, antimicrobial peptides (AMPs) have shown promise as potential options [2]. There are multiple families of AMPs, including cruzioseptins, which are characterized by having short sequences (<32 amino acids), cationic, hydrophobic, and structured in an α-helix. Cruzioseptins were previously identified in the frog *Cruziohyla calcarifer* and have been shown to exhibit antibacterial and anti-Leishmania activity [3,4]. This study focused on assessing the trypanocidal potential and related mechanisms of action of synthetic peptides from the cruzioseptin family across different stages of *Trypanosoma cruzi*. The trypanocidal and selective effects of four synthetic peptides (CZS-1, CZS-5, CZS-7, and CZS-11) were evaluated on various *T. cruzi* isolates (X-1081, MG, Ds, and Y) and human erythrocytes. The mechanisms of action for the most promising peptide were explored using DNA release assays, electron microscopy, and untargeted metabolomic and lipidomic analyses with liquid and gas chromatography coupled with quadrupole time-of-flight mass spectrometry. All tested peptides were effective against epimastigotes, with CZS-5 being the most selective (Selectivity Index = 42.6). CZS-5 maintained efficacy across various epimastigote strains and showed activity against metacyclic trypomastigotes (IC_{50} = 25.1 μM). In the intracellular stage, CZS-5 reduced the release of trypomastigotes from cells but did not impact the number of intracellular amastigotes. DNA release assays, scanning electron microscopy, and metabolomic and lipidomic analyses suggested that CZS-5 disrupts the parasite's membrane in a time-dependent manner (2 and 4 hours). Notably, there were consistent increases in phosphatidylserines and decreases in phosphatidylinositols and phosphatidic acids, supporting previous findings of membrane alterations after cruzioseptin treatment. Additionally, changes in metabolic pathways associated with energy production were observed, with increases in biosynthetic pathways related to carbohydrates and fatty acids, while amino acid metabolism decreased. These biosynthetic pathways may be meeting the energy requirements for cellular membrane remodeling. CZS-5 shows promising antiparasitic activity against different stages of *T. cruzi*, acting through membrane disruption and critical metabolic alterations.

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SA-P12

DESARROLLO DE UN MÉTODO DE ANÁLISIS QUÍMICO INSTRUMENTAL PARA LA DETERMINACIÓN DE TAMOXIFENO, 5-FLUROURACILO Y ANASTROZOL EN MUESTRAS DE SANGRE POR GC-MSD

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RESUMEN

El Tamoxifeno, el Anastrozol y el 5-Fluorouracilo son medicamentos ampliamente utilizados en el tratamiento del cáncer de mama. La determinación precisa de estos compuestos farmacológicos en muestras biológicas es esencial para evaluar la eficacia y seguridad de los tratamientos médicos, especialmente en sangre. Para la cuantificación de estos compuestos, se utiliza un sistema GC-MSD de Agilent Technologies con la siguiente configuración: Inyector Automático 7683, Puerto de Inyección Split/Splitless, Cromatógrafo de Gases 7890A (GC), Detector de Espectrometría de Masas 5975 (MSD), Software MassHunter Versión 10.0 y Base de Datos NIST Versión 2.3. Se utilizó el modo de inyección Splitless con la Columna Agilent DB-35ms (122-3832) (30 m, 0.25 mm, 0.25 µm). Después de identificar la estructura molecular de los compuestos, se concluyó que el 5-Fluorouracilo es una molécula con muy baja volatilidad, por lo que se derivatizó utilizando N,O-Bis(trimethylsilyl)trifluoroacetamida (BSTFA), un potente donador de trimetilsililo. Esta modificación aumenta la volatilidad del 5-Fluorouracilo y mejora su respuesta en el detector GC/MSD, confirmado que el BSTFA es el agente derivatizante más efectivo para estas muestras, lo que respalda su idoneidad para analizar estos compuestos. Para el Tamoxifeno y el Anastrozol, la derivatización no fue necesaria.

El método analítico para la determinación de Tamoxifeno, Anastrozol y 5-Fluorouracilo en muestras de sangre mostró un comportamiento lineal dentro del rango de concentración requerido, con un R^2 superior a 0.995. La curva de calibración se preparó utilizando el método de adición estándar con sangre como matriz. El coeficiente de variación (CV%) menor al 5% en la repetibilidad indica que el método es consistente y fiable.

APROBACION ÉTICA

N/A

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IMPLEMENTING METHODOLOGIES FOR ELASTIN PURIFICATION AND ANALYSIS TO TRACK THE ELASTASE ACTIVITY CHANGES DURING SKIN AGEING

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ABSTRACT

Elastin is an extracellular matrix protein that provides elasticity and resilience to tissues. It comprises units of tropoelastin, which is cross-linked through desmosine and isodemosine (DES/IDES), unique to elastin, forming an extremely durable and insoluble biopolymer. It is continuously degraded during its lifespan, mainly by enzymes called elastases. Elastin damage is associated with skin ageing and diseases such as aneurysms and atherosclerosis [1]. Studies of elastin degradation request the implementation of purification methods that preserve the integrity of the fibre and methodologies for the quantification of markers. This study used skin samples from donors aged 26 to 31 and 66 to 86 years. Initially, two elastin purification methods were evaluated: the hot alkali method [2], which includes reflux with organic solvents and alkaline hydrolysis, and the Schmelzer method [3], which uses solvents, chaotropic agents, cleavage agents and trypsinization. The integrity of the elastin fibre was determined by scanning electron microscopy and the presence of residual collagen using modified Masson's Trichrome staining. Elastin was digested with Cathepsin V (EC 3.4.22.43) and Metalloproteinase 9 (EC 3.4.24.35) in a ratio of 1 nM enzyme: 50 µg of elastin. Finally, a methodology for quantifying DES/IDES by ion-pair liquid chromatography was implemented [4]. The purification methods evaluated do not allow elastin isolation due to the remnant of the epidermis in the skin samples, so a previous treatment with ammonium hydroxide was carried out before mechanically removing the epidermis. Only the Schmelzer method, with modifications, maintains the integrity of the elastin fibres according to the age group. The elastin content is 12,3 and 20,0 mg elastin/g skin in young and older adults, respectively, with few collagen residues. The methodology for quantifying DES/IDES using HPLC-ion pair and detection at 275 nm is selective, linear (3 to 30 ppm), repeatable and inexpensive. The integrity of the elastin fibre influenced the amount of DES/IDES released by some elastases. The methods implemented allow the elastin fibres to preserve their integrity and quantify markers of their degradation, which can be used to study changes in the activity of other elastases involved in skin ageing.

ETHICAL APPROVAL

The study (Hermes Code 51042) was approved by the ethics committee of the Facultad de Ciencias - Universidad Nacional de Colombia and Hospital Universitario Clínica San Rafael (Bogotá, Colombia) and carried out in compliance with the Declaration of Helsinki.

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