LACE & BrMet 2024

29th Latin American Symposium

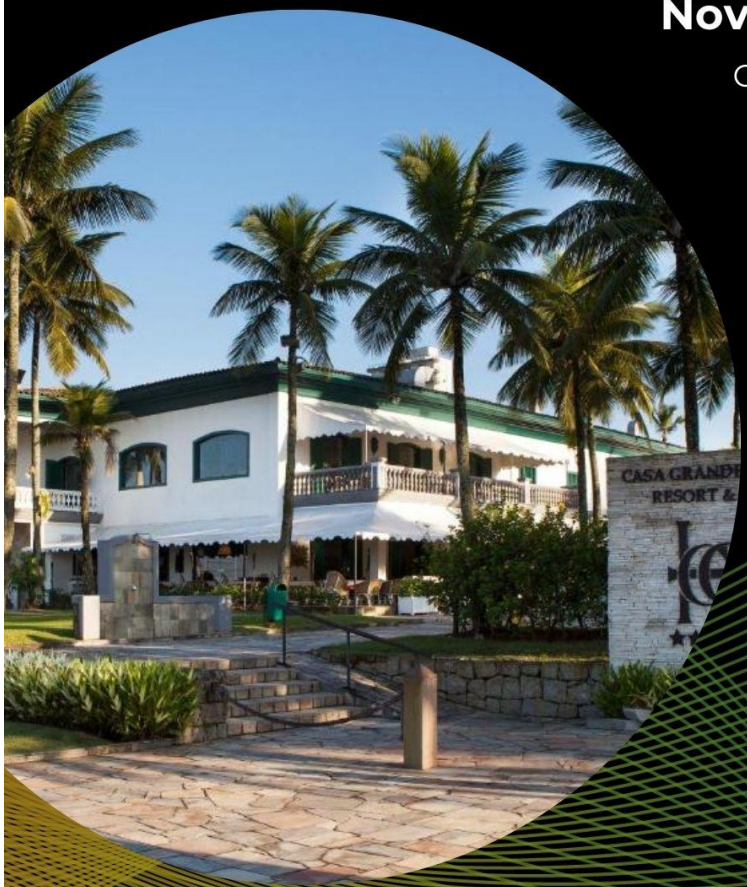
ON CAPILLARY ELECTROPHORESIS,
MICROFABRICATION AND RELATED TECHNIQUES

&

Brazilian Symposium on Metabolomics

November 9 - 12, 2024

Casa Grande Hotel Guaruja
Guaruja - SP - Brazil



BOOK OF ABSTRACTS

LACE 2024 & BrMet

29th Latin-American Capillary Electrophoresis, Microfabrication and Related Techniques Symposium – LACE

&

Brazilian Symposium on Metabolomics – BrMet

November 9th to 12th, 2024
Casa Grande Hotel Guarujá,
Guarujá – São Paulo - Brazil

Book of Abstracts

Book coordinator: Ana Valéria Colnaghi Simionato

Design and layout: Ana Valéria Colnaghi Simionato and Gisele Andre Baptista Canuto

www.lace2024.iqm.unicamp.br

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Symposium Welcoming Remarks

First, we must express our appreciation to all members of the Scientific and Organizing Committee and to the institutions and companies whose generous contributions will help to make this meeting a successful and scientifically rewarding event.

LACE symposium series was created in 1995 in a small meeting in Santiago, Chile with the purpose of keeping Latin American scientists abreast of the latest advances in technology for microseparations, such as capillary electrophoresis and microchip technology, and related techniques.

BrMet intends to join Brazilian metabolomics community to foster scientific discussions, strengthen networking, and disclose the most recent topics performed worldwide on this omics science.

The symposium is structured in four days with initial workshop and short-course, followed by plenary lectures and contributed communications, as well as poster sessions, vendor seminars and exposition. Sessions will include proteomics, glycomics, foodomics, metabolomics, genetic analysis, DNA sequencing and separation, miniaturization and microfluidics, bioanalysis, biotechnology, (bio)pharmaceutical analysis, applications, multidimensional separation approaches, hyphenated techniques, mass spectrometry, novel instrumentation, sample treatment, and more.

The Scientific and Organizing Committees sincerely hope that all aspects of the conference, the scientific sessions, the discussions, the pre-symposium course, and instrumentation exhibition, will serve their intended purposes to advance the science of electroseparations and to foster scientific contacts.

It is our sincere wish that your experience this year in Guarujá be both enjoyable and professionally rewarding.

Our Kindest Regards,

Norberto A. Guzman
Ana Valéria Colnaghi Simionato
Gisele Andre Baptista Canuto
Marcone Augusto Leal de Oliveira
María Segunda Aurora Prado

Chairs of LACE 2024 & BrMet

General Information

Guarujá City

Guarujá is a coastal city located in the state of São Paulo, Brazil. It is situated on the southeastern coast, facing the Atlantic Ocean and is part of the metropolitan area of Santos. Known for its beautiful beaches, Guarujá is a popular tourist destination, especially during the summer months.

The history of Guarujá, dates back to the indigenous peoples who inhabited the region before the arrival of European explorers. The name "Guarujá" is derived from the Tupi language, meaning "sandy beaches" or "seagulls."

Historically, the area began to be explored by Portuguese colonizers in the 16th century. The first European settlements were established along the coast, mainly for trade and agriculture. The construction of the Fortress of Santo Amaro da Barra Grande in the late 1600s and early 1700s marked a significant development in Guarujá's history. This fort was built to protect the coastal area from pirates and invasions and played a role in the defense of the nearby port city of Santos.

Guarujá started to emerge as a resort destination in the late 19th century, attracting wealthy people from São Paulo and other regions. The introduction of the railway system enhanced accessibility, contributing to its growth as a vacation spot. The city continued to develop throughout the 20th century, with a significant increase in population due to urbanization and industrialization.

In recent decades, Guarujá has become a prominent tourist destination, thanks to its beautiful beaches, natural attractions, and growing infrastructure. Today, Guarujá balances its historical roots with modern tourism and urban development. The city's rich history is reflected in its architecture, cultural practices, and ongoing efforts to preserve its historical landmarks.

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Previous Meetings

Chairperson(s)	Location	Year
Norberto A. Guzman	Santiago, Chile	1995
Norberto A. Guzman, Carlos Calvo, and Ethel Guerrero	Santiago, Chile	1996
Norberto A. Guzman, Clyde Carducci, and Juan M. Castagnino	Buenos Aires, Argentina	1997
Norberto A. Guzman, Marina Tavares, and Emanuel Carrilho	São Paulo, Brazil	1998
Norberto A. Guzman, Belinda Vallejo, and Aaron Gonzalez	Acapulco, Mexico	1999
Norberto A. Guzman	Punta del Este, Uruguay	2000
Norberto A. Guzman, and Maria Antonieta Valenzuela	Santiago, Chile	2001
Norberto A. Guzman, and Nora M. Vizioli	Mar del Plata, Argentina	2002
Norberto A. Guzman, Alma Revilla, and Gabriela Vargas	Mexico City, Mexico	2003
Norberto A. Guzman, and Angel Rios	Toledo, Spain	2004
Norberto A. Guzman, Marina F.M. Tavares, and Emanuel Carrilho	Guaruja, Brazil	2005
Norberto A. Guzman, Belinda Vallejo, and Aaron Gonzalez	Queretaro, Mexico	2006
Norberto A. Guzman, and Maria Antonieta Valenzuela	Santiago, Chile	2007
Norberto A. Guzman, and Aaron F. Gonzalez	Puerto Vallarta, Mexico	2008
Coral Barbas, and Marina F.M. Tavares	Sevilla, Spain	2009
Emanuel Carrilho, Marina F.M. Tavares	Florianopolis, Brazil	2010
Bruce McCord, Carlos Garcia, and Marina F.M. Tavares	Miami, USA	2011
Nora M. Vizioli, and Marina F.M. Tavares	Buenos Aires, Argentina	2012
Marina F.M. Tavares	Lima, Peru	2013
Marina F.M. Tavares, and Emanuel Carrilho	Natal, Brazil	2014
Nora M. Vizioli, Marina F.M. Tavares, and Emanuel Carrilho	Cartagena, Colombia	2015
Nora Vizioli, M. Tavares, E. Carrilho, and M. Antonieta Valenzuela	Santiago, Chile	2016

Virginia A. Robinson-Fuentes, and Victor Hugo Abrego-Reyes	Mexico City, Mexico	2017
Maria Fernanda Silva, and Nora M. Vizioli	Mendoza, Argentina	2018
Alberto Escarpa, and Agustin G. Crevillen	Alcala de Henares-Madrid, Spain	2019
-	Cancelled	2020*
Ana Valeria Simionato, Dosil Pereira, and Alberto Fracassi	Brazil (Virtual)	2021
Norberto A. Guzman, and Herbert H. Lindner	Panama City, Panama	2022
Norberto A. Guzman, Virginia A. Robinson, M. Gabriela Vargas, Alma Revilla, and Herbert H. Lindner	Mexico City, Mexico	2023

*In 2020 the LACE Symposium was cancelled due to the COVID-19 pandemic.

Organizers, Collaborators, Scientific Organizations and Sponsors

The Organizing Committee gratefully acknowledge the support and patronage of the following companies, collaborating societies, academic, scientific and technological organizations:

Platinum

Gold

Bronze

No denomination

Choir Performance

The Unicamp Zíper na Boca Choir was established in September 1985 to revive the actvities of the former Unicamp Choir. Its members include students, staff, and professors from various areas of the State University of Campinas (Unicamp) and neighboring community members. Since 1990, it has been associated with NIDIC, now known as CIDDIC (Unicamp's Documentation and Cultural Diffusion Integration Center).

Under the direction and instruction of Vívian Nogueira Dias, the choir maintains a diverse repertoire and extensive performance schedule, including regular concerts with the Unicamp Symphony Orchestra. It actively participates in choir gatherings and festivals, having performed in 11 Brazilian states. The choir has received awards in three editions of the Mapa Cultural Paulista and represented Brazil at the 26th International Choir Festival of Galvez in Argentina.

In 2011, the choir received the "Carlos Gomes Medal" from the Campinas City Hall for its outstanding contributions to the city's artistic and musical scene. In 2015, the choir performed the closing concert of the 46th Campos do Jordão Winter Festival at the Cláudio Santoro Auditorium, in partnership with the Campos do Jordão Young Philharmonic Orchestra.

Among the projects of the group are the choir-scenic productions: The Saltimbancos (2005), ABBA Forever: The Mamma Mia Songs (2010), Queen Rhapsody (2011), Canta Brasil (2012), Love is All You Need: A Tribute to the Beatles (2013), Swingin' with the Saints (2014), Zíper Retrospective: 30 Years (2015), Tomorrow Will Be Another Day (2016), Light, Music, Action (2017), Light, Music, Zíper in Action (2018), 100% Brazil (2019), Zíper 37 Years Old: Back on Stage! (2022), A Watercolor in Samba (2023), and Sambas and Serenades (2024), as well as 19 annual editions of the Unicamp Choirs Festival.

The Virtual International Edition of the festival, held in 2021, brought together 36 guest choirs from 14 Brazilian states and 9 Latin American countries, with online performances broadcast on the Unicamp Zíper na Boca Choir's YouTube channel.

Notable performances include participation in three editions of the International Choir Festival of Chapecó, Santa Catarina, Brazil (2016, 2017, and 2024). A highlight of 2023 was the artistic and cultural exchange with the Choir of the National University of Río Negro in Argentina, culminating in the "Encuentro Binacional de Coros Universitarios", a joint concert held at the Municipal Culture Center of Viedma, the capital of Río Negro, Argentina.

Conductor Vivian Nogueira holds a Ph.D. in Music, a Master's in Arts, and a Bachelor's in Conducting from Unicamp, as well as a Piano degree from the Campinas Musical Conservatory. She has conducted several choirs in the city and has been a faculty member at Unicamp's Department of Music. Among her honors is the "Carlos Gomes Medal," awarded by the Campinas City Hall. Since its inception, she has served as the artistic director and conductor of the Unicamp Zíper na Boca Choir.

CORAL UNICAMP ZÍPER NA BOCA

presents

"Sambas e Serenatas: das ruas do Flamengo aos tempos da brilhantina"

Choros Clássicos

Corta jaca - Machado Careca/ Chiquinha Gonzaga

Flamengo - Bonfiglio de Oliveira

Carinhoso - Pixinguinha

Brejeiro - Catulo da Paixão Cearence/Ernesto Nazareth

Arr: Damiano Cozzella

Adaptação do texto ao arranjo: Vivian Nogueira

Love me Tender - Elvis Presley/Vera Matson

Arr: Roger Emerson

Can't help falling in love - George David Weiss/Hugo Peretti/Luigi Creatore

Arr: Roger Emerson

Suspicious Minds - Mark James

Arr: Weverton Silva

The King of Rock:

Jailhouse Rock - Jerry Leiber / Mike Stoller

Don't Be Cruel - Elvis Presley /Otis Blackwell

Burning Love - Dennis Linde

Arr: Weverton Silva

Sambas da Vila

Canta, canta minha gente

O pequeno burguês

Madalena do Jucu

Devagar, devagarinho

Batuque na cozinha

Casa de bamba

Quem é do mar não enjoa

Ex-Amor

Martinho da Vila/João da Baiana/Heraldo Devagar

Arr: Eduardo D. Carvalho

Ficha Técnica

Regência/Direção Geral e Musical| Vivian Nogueira

Direção Cênica| Lucas Metropolo e Camilla Puertas

Preparação Vocal| Weverton Silva

Solista| Cesar Augusto Barbosa (voz) e Breno Martins (cena)

Instrumentistas | Hively Ferreira (piano); Wenisley Garcia Lima (violino); Osvaldo Baltazar, Vania Monteiro, Silvia Gomes (percussão).

Realização: Unicamp/ ProEEC/Cocen/ Ciddic/Coral Unicamp Zíper na Boca.

Pre-Symposium Courses – Main Topics

The Impact of Capillary Electrophoresis in Clinical Chemistry - Bioanalysis

Lecturers:

[a]**Dr. Norberto A. Guzman**, Princeton Biochemicals Inc, Princeton, New Jersey, USA (www.orcid.org/0000-0001-5504-376X)

[b]**Dr. Herbert H. Lindner**, Medical University of Innsbruck, Innsbruck, Austria (www.orcid.org/0000-0003-1262-9976)

[c]**Dr. Fernando Benavente**, University of Barcelona, Barcelona, Spain (www.orcid.org/0000-0002-1688-1477)

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[c]Bioanalysis group, Department of Chemical Engineering and Analytical Chemistry, Institute of Research and Nutrition and Food Safety, University of Barcelona, Barcelona, Spain.
Correspondence: fbenavente@ub.edu

Topics

1-Norberto Guzman: “Clinical Capillary Electrophoresis: Strategies to get the highest accuracy in clinical diagnosis - Advances in affinity-capture separation technologies.”

2-Herbert Lindner: “Capillary surface chemistry, buffer composition, and pH as important tools to optimize Capillary Zone Electrophoresis of proteins and peptides, protein subtypes, and post-translational modifications.”

3-Fernando Benavente: “Determination of peptide, protein, and microRNA biomarkers using capillary electrophoresis coupled to mass spectrometry.

Abstract

A diagnostic test is any kind of medical test performed to help with the diagnosis or detection of a disease. A systematic review of a particular diagnostic test for a disease aims to bring together and assess all the available research evidence. When a diagnosis is accurate and made in a timely manner, a patient has the best opportunity for a positive health outcome because clinical decision making will be tailored to a correct understanding of the patient's health

problem.

The working diagnosis may be either a list of potential diagnoses (a differential diagnosis) or a single potential diagnosis. Typically, clinicians will consider more than one diagnostic hypothesis or possibility as an explanation of the patient's symptoms and will refine this list as further information is obtained in the diagnostic process. Nonetheless, absolute certainty in diagnosis is unattainable, no matter how much information we gather, how many observations we make, or how many tests we perform. A diagnosis is a hypothesis about the nature of a patient's illness, one that is derived from observations by the use of inference.

The U.S. National Academy of Medicine (formerly the Institute of Medicine) released a report in 2015 describing diagnostic error as a blind spot in the safety field. Still, thousands of patients die every year due to diagnostic errors. Diagnostic error can be defined as diagnosis that was unintentionally delayed (sufficient information was available earlier), wrong (wrong diagnosis made before the correct one), or missed (no diagnosis ever made), as judged from the eventual appreciation of more definitive information. Diagnostic error as an area of patient safety has had insufficient research despite the costs in terms of negative health outcomes, loss of life, income and productivity, health system mistrust and dissatisfaction from both patients and health professionals.

Improving diagnosis in health care is a moral, professional and public health imperative. However, little is known about the full scope of harms related to medical diagnosis and the current estimate range widely. An estimate 795,000 American die or are permanently disabled by diagnostic error each year, confirming the pressing nature of the public health problem.

In the past decade there has been an explosion of new chemical and biochemical approaches and technologies to explore the human immune system with unprecedented precision. Insights into the human immune response to vaccination, cancers, and viral infections such as COVID-19 have come from high-throughput “omics” technologies that measure the behavior of genes, mRNA (single-cell transcriptomics), proteins (proteomics), metabolites (metabolomics), cells (mass cytometry), and epigenetic modifications, coupled with computational approaches.

All of modern medicine is dependent on advances in chemistry, biochemistry, and cell and molecular biology. To ensure the development of healthcare keeps pace with the increasing health challenges our society faces, advancements in chemical science research and modern laboratory tools is absolutely vital. Advancements in science and technology are changing the way we define disease, develop drugs, and prescribe treatments in infectious diseases, chronic diseases, cancer, and rare diseases.

One of the technologies that has contributed to the analysis of a wide range of chemical, biochemical, and cellular entities has been capillary electrophoresis. The advent of capillary electrophoresis as a high-resolution separation and sensitive technology has been a great step toward improved analytical quality for liquid biopsy analysis for diagnostic purposes.

Our laboratories (Guzman, Lindner, and Benavente) have developed, independently and in collaboration, improved capillary electrophoresis methods for disease diagnosis, including revolutionary point-of-care diagnostic technologies. In this course, we will present three different topics on applications of relevance to diagnosis of diseases using the technology of capillary electrophoresis coupled to various detectors and the determination of a panel of biomarkers. A panel of biomarkers is considered better than a single biomarker because it provides a more comprehensive picture of a biological state, leading to improved diagnostic

accuracy, prognostic information, and a better understanding of disease complexity.

Bibliographic References:

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Guzman, N.A.; Guzman, A. Human sputum proteomics: Advancing non-invasive diagnosis of respiratory diseases with enhanced biomarker analysis methods. International Journal of Translational Medicine 2024, 4(2), 309-333, https://doi.org/10.3390/ijtm4020020.

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Pero-Gascon, R.; Sanz-Nebot, V.; Berezovski, M. V.; Benavente, F. Analysis of circulating microRNAs and their post-transcriptional modifications in cancer serum by on-line solid-phase extraction-capillary electrophoresis-mass spectrometry, Analytical Chemistry, 2018, 90(11), 6618-6625, https://10.1021/acs.analchem.8b00405.

Salim, H.; Pero-Gascon, R.; Giménez, E.; Benavente, F. On-line coupling of aptamer affinity solid-phase extraction and immobilized enzyme microreactor capillary electrophoresis-mass spectrometry for the sensitive targeted bottom-up analysis of protein biomarkers, Analytical Chemistry, 2022, 94(19), 6948-6956, https://doi.org/10.1021/acs.analchem.1c03800.

A Hands-on-Course on Metabolomics: History, Fundaments, and Challenges

Lecturers:

[a,b]**Dr. Marina F. M. Tavares**, University of São Paulo, São Paulo, Brazil

(www.orcid.org/0000-0002-7395-3502)

Co-Coordinator:

[a,b]Daniel R. Oliveira

Duration: 2h theoretical class and 2h (Hands-on/Laptop required)

[a]CEMM (Center for Multiplatform Metabolomics Studies), Sao Paulo, Brazil
[b]Institute of Chemistry, University of Sao Paulo, Sao Paulo, Brazil
**Correspondence: mfmtavar@iq.usp.br*

Objective:

To introduce fundamental and practical aspects of metabolomics, in both targeted and untargeted formats, describing in detail the metabolomics workflow, from the design of experiments to the biological interpretation of the problem under examination, with emphasis on modern analytical techniques commonly used for data acquisition, the statistical concepts involved in the processing of omics data, as well as on a general revision of human metabolism and major metabolic routes.

Justification:

Among the omics sciences and in the context of systems biology, metabolomics has occupied an important niche, because it offers the revolutionary possibility of characterizing the phenotype of an individual to the molecular level, so necessary to aid the understanding of cellular biology towards personalized medicine. Interests in metabolomics have grown considerably in many areas, not only the discovery of biomarkers for early diagnosis of diseases, but include applications in biotechnology and agriculture, development of new pharmaceuticals, nutrition, food quality and safety, environmental chemistry, toxicology, among others.

Syllabus:

This course intends to review the terminology and to discuss the denominations in use in the field of metabolomics, as well to describe systematically its workflow for both untargeted and targeted metabolomics, from the metabolite selection (targeted metabolomics), biological sample collection and preparation, introducing general principles of multiplatform instrumental

analysis in current use for data acquisition, the statistical concepts involved in data processing (using R platform), and finally, to provide an overview of human metabolism and principal biological routes to support biological interpretation of results. Among the analytical instrumentation, GC-MS, LC-MS in both reversed-phase and hydrophilic interaction modes, and CE-MS will be reviewed. The processing of omics data, the methods used for group discrimination, discriminant metabolite selection and structural identification of putative metabolites by assessing metabolomics databases (FiehnLib, KEGG, Metlin, HMDB, MassBank, etc.) as well as MS/MS fragmentation strategies will all be addressed by theoretical and practical lectures using the institution multimedia facility, where the students will have access to real metabolomics datasets and pertinent softwares (XCMS and SIMCA-P). Finally, examples of representative applications of metabolomics will be presented in supervised group discussions.

Bibliographic references:

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Scientific Program

Agenda of Sessions

November 9th to 12th, 2024

At Tereza Cristina Room, Casa Grande Hotel

Saturday, November 9th

Registration: 8:30 – 17:00 h

Pre-symposium course

9:00 – 12:00	**Norberto A. Guzman**, USA **Herbert H. Lindner**, Austria **Fernando Benavente**, Spain	The Impact of Capillary Electrophoresis in Clinical Chemistry - Bioanalysis
13:00 – 17:00	**Marina Franco Maggi Tavares**, Brazil	A Hands-on-Course on Metabolomics: History, Fundaments, and Challenges

Opening Session

Chairperson, ***Dr. Norberto A. Guzman***

18:00 – 18:20	Welcoming Remarks **Norberto A. Guzman**, USA **Ana Valéria C. Simionato**, Brazil **Gisele A. B. Canuto**, Brazil **Marcone A.L. de Oliveira**, Brazil **Maria S. Aurora Prado**, Brazil
18:20 – 19:20 Plenary lecture (**PL-01**)	Metabolic Profiling for Exploring Host-Microbiome Interactions in Human Health: A Chemical Dialogue **Elaine Holmes**, England / Australia
19:30 – 20:30	Choir Performance **Coral Unicamp Zíper na Boca**, Brazil
20:30 – 22:00	Welcome Cocktail

Sunday, November 10th

Registration: 8:30 – 17:00 h

Session 1

Chairperson, ***Dr. Marina Franco Maggi Tavares***

8:30 – 9:10 Plenary lecture (**PL-02**)	The Human Sputum Proteomics: Assessing the Need for Improving Non-Invasive Diagnosis of Infectious Respiratory and Chronic Pulmonary Diseases. A Reevaluation of Protein Biomarkers in the Context of Advanced Analytical Technologies **Norberto A. Guzman**, USA
9:10 – 9:40 (**KN-01**)	Sodium Dodecyl Sulfate Capillary Gel Electrophoresis in the Presence of Propidium Iodide Fluorescent Dye **Andras Guttman**, Hungary
9:40 – 10:00 (**OP-01**)	Fate of One Equation. Application to Capillary Electrophoresis **Bohuslav Gas**, Czech Republic
10:00 – 10:30	Coffee break

Session 2

Chairperson, ***Dr. Andras Guttman***

10:30 – 11:00 (**KN-02**)	Novel Monolithic Capillary Columns for Multimodal Capillary Electrochromatography **Ziad El Rassi**, USA
11:00 – 11:20 (**OP-02**)	Capillary electrophoresis and isotachophoresis applied for analysis and characterization of biologically active (lipo)peptides **Václav Kašička**, Czech Republic
11:20 – 11:40 (**OP-03**)	Building a Drug Delivery Benchtop Microcontrolled Breast-on-a-Chip Microfluidic Platform **Lucas Blanes**, Brazil
11:40 – 12:00 (**OP-04**)	Exploring the versatility of Capacitively Coupled Contactless Conductivity Detection (C^4D) in Conventional and Microchip Capillary Electrophoresis **Dosil Pereira de Jesus**, Brazil
12:00 – 14:00	Lunch recess

Session 3

Chairperson, ***Dr. Maria Segunda Aurora Prado***

14:00 – 14:30 (**KN-03**)	Design of theranostic agents: a major contribution of electrokinetic characterizations **Anne Varenne**, France
14:30 – 14:50 (**OP-05**)	Capillary electrophoresis in the quality control of therapeutic proteins **Nora Vizioli**, Argentina
14:50 – 15:10 (**OP-06**)	Interaction between passion fruit (Passiflora edulis) seed extracts and jambu (*Spilanthes acmella*) aerial parts in topical photoprotective formulations: stability and skin permeation **Carla B. G. Bottoli**, Brazil
15:10 – 15:30 (**OP-07**)	CZE vs. RP-HPLC with inductively coupled plasma mass spectrometry in the investigation of various anticancer drug delivery nanosystems **Magdalena Matczuk**, Poland
15:30 – 16:00	Coffee break

Session 4

Chairperson, ***Dr. Ana Valéria Colnaghi Simionato***

16:00 – 16:30 (**KN-04**)	Unravelling differential antibody proteoform binding with affinity CE-MS **Elena D. Vegas**, The Netherlands
16:30 – 16:50 (**OP-08**)	Tying Cooling Capillaries Around Analytical Capillaries and Provision of a Free Service to the Entire Analytical Chemistry Community **Tarso B. L. Kist**, Brazil
16:50 – 17:10 (**OP-09**)	A New Online Electrokinetic Sample Cleanup Method and the Related Novel Evaluation Approach for APTS Labeled N-Glycan Profiling by Capillary Electrophoresis **Gabor Jarvas**, Hungary
17:10 – 18:00	Poster session, instrument exhibition and book launching
18:00	Poster tear down

Monday, November 11th

Registration: 8:30 – 17:00 h

Session 5 - Brazilian Symposium on Metabolomics (BrMet)

Chairperson, ***Dr. Fernando Benavente***

8:30 – 9:10 Plenary lecture (**PL-03**)	New Advances in High Throughput Metabolomics by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: Doing More with Less! **Philip B. McKibbin**, Canada
9:10 – 9:40 (**KN-05**)	Decoding the Complexity of Cacao Fermentation: Harnessing Metabolomics, Deep Learning, and Big Data **Ian Castro Gamboa**, Brazil
9:40 – 10:00 (**OP-10**)	Metabolomics analysis under NMR point of view **Antônio Gilberto Ferreira**, Brazil
10:00 – 10:30	Coffee break

Session 6 - Brazilian Symposium on Metabolomics (BrMet)

Chairperson, ***Dr. Marcone A. L. Oliveira***

10:30 – 11:00 (**KN-06**)	A multi-omics approach relating disease severity prognosis: A case study for SARS-CoV-2 **Emanuel Carrilho**, Brazil
11:00 – 11:20 (**OP-11**)	Why should one worry about enantioselectivity effects in clinical metabolomics? **Quezia B. Cass**, Brazil
11:20 – 11:40 (**OP-12**)	Understanding Exercise Response Variability: A Metabolomics Perspective. **Alex Castro**, Brazil
11:40 – 12:00 (**OP-13**)	Targeted analysis of gut microbiota-derived metabolites in colonic fermentation models: Investigating the impact of food ingredients **Maricruz Mamani Huanca**, Spain
12:00 – 14:00	Lunch recess

Session 7 - Brazilian Symposium on Metabolomics (BrMet)

Chairperson, ***Dr. Gisele A. B. Canuto***

14:00 – 14:30 (**KN-07**)	Multiomics Approach to Define the Biomolecular Changes Associated with Traumatic Brain Injury
	Yehia Mechref, USA
14:30 – 14:50 (**OP-14**)	Metabolomics for neuropsychiatric diseases differentiation and potential novel treatments study
	Alessandra Sussulini, Brazil
14:50 – 15:10 (**OP-15**)	Geographical Indication Area Expansion for Aroeira Honey Supported by Untargeted Metabolomics
	Adriana Nori de Macedo, Brazil
15:10 – 15:30 (**OP-16**)	Plasma metabolome signatures to predict responsiveness to neoadjuvant chemotherapy in breast cancer
	Andreia de Melo Porcari, Brazil
15:30 – 15:50 (**OP-17**)	Zika Virus in Extracellular Vesicles: Insights from Integrated Proteomic and Metabolomic Dependent Regulation of B Cell and PI3K/AKT/mTOR
	Letícia Gomes de Pontes, Brazil
15:50 – 16:20	Coffee break

Session 8 - Brazilian Symposium on Metabolomics (BrMet)

Chairperson, ***Dr. Elena D. Vegas***

16:20 – 16:50 (**KN-08**)	Applications of microchip electrochemical detection to bioanalysis
	Susan Lunte, USA
16:50 – 17:10 (**OP-18**)	Metabolomics with Q-Orbitrap and Q-Linear Ion Trap – New Solutions for Targeted and Untargeted Analysis
	Caroline Jaegger – Nova Analítica, Brazil
17:10 – 17:30 (**OP-19**)	Separation technique hyphenated with mass spectrometry for improved metabolome coverage, from conventional to miniaturized approaches.
	Serge Rudaz, Switzerland
17:30 – 17:50 (**OP-20**)	Metabolomics in practice: The IonMedicine experience
	Bruna Catussi – Ion Medicine, Brazil

17:50 – 18:00 Photography Session

20:00 Gala Dinner

Tuesday, November 12th

Registration: 8:30 – 13:00 h

Session 9

Chairperson, ***Dr. Quezia B. Cass***

8:30 – 9:10 Plenary lecture (**PL-04**)	Searching alternative drugs to treat infectious and parasitic diseases: the metabolomics approach. **Marina F. M. Tavares**, Brazil
9:10 – 9:40 (**KN-09**)	Characterization of Glycosylated (N-terminal) Pro-B-Type Natriuretic Peptide Forms in Blood Samples of Patients with Severe Heart Failure and its Biological and Medical Implications **Herbert H. Lindner**, Austria
9:40 – 10:00 (**OP-21**)	Exposomics and Emerging Contaminants: A Brief Contribution to Understanding the Pharmaceutical Exposome and Antimicrobial Resistance **Maria de Lourdes Moraes**, Brazil
10:00 – 10:20 (**OP-22**)	Determination of allergenic proteins in food by on-line aptamer affinity solid-phase extraction capillary electrophoresis-mass spectrometry **Fernando Benavente**, Spain
10:20 – 10:50	Coffee break

Session 10

Chairperson, ***Dr. Susan Lunte***

10:50 – 11:20 (**KN-10**)	3D Printed Microfluidic Devices for Separation Science and Chemical Analysis **Adam T. Woolley**, USA
11:20 – 11:40 (**OP-23**)	Advances on the integration of electrochemical and optical detectors to 3D-printed microfluidic devices **José Alberto Fracassi da Silva**, Brazil
11:40 – 12:00 (**OP-24**)	3D Printing with Conductive Polymers in Capillary Electrophoresis and Microchip: Characteristics, Possibilities, and Limitations **Claudimir L. Lago**, Brazil

12:00 – 12:20 (**OP-25**)	How low can we go? – A novel preconcentration strategy for the characterization of intact glycoproteins **Christoph Gstottner**, The Netherlands
12:20 – 13:00	Closing Remarks and Poster Awards Announcement

Poster Session

PP-01
N-glycan biomarkers for early screening of type 2 diabetes:
Sugars against sugar
Rebeka Török, Gábor Járvás, László Korányi, and András Guttman

PP-02
Determination of Glycerol in Biodiesel by Micellar Electrokinetic Chromatography
Carlos Eduardo Lozano-Olvera, M. Elena Paez-Hernandez, Carlos A. Galan-Vidal, Israel S. Ibarra, Jose A. Rodriguez

PP-03
Determination of corticoids in cosmetic cream samples by micellar electrokinetic chromatography
Karen A. Escamilla-Lara, Israel S. Ibarra, Jose A. Rodriguez*

PP-04
Application of Fe_3O_4@SiO-LDH/DS- as an efficient adsorbent for the removal of tetracyclines from milk samples by capillary electrophoresis
Hernán Hernandez, Gabriela Islas, José Antonio Rodriguez, Maria Elena Paez, Juan Manuel Miranda, Irma Pérez, and Israel Ibarra*

PP-05
Simple and low-cost platform for fluorescence measurements integrated with microcontrollers.
Mathias Stahl Kavai, José Alberto Fracassi da Silva

PP-06
Determination of cocaine residues and metabolites in breast milk:
a special approach for milk banks
Bruno Bernacchi, Maria Paranhos, Rafaella Aredes, Eliani Spinelli, Flávia Marques

PP-07
Determining major Capsaicinoids in pepper by capillary electrophoresis with UV detection using dual-surfactant in BGE: method development and validation
João Pedro R. Mansano and Lucas M. Duarte*

PP-08
Multivariate data analysis for carbohydrate profiling in isothermal wort
Rafaella S. Aredes, Fernando C. Peixoto, Leandro A. Sphaier, Vinicius N. H. Silva, Lucas M. Duarte, Flávia F. C. Marques

PP-09
CE-ICP-MS on the hunt for liposomal rejuvenation potion
Joanna Zajda, Karolina Ogórek, Kinga Nowak, Oliwia Gutowska, and Magdalena Matczuk

PP-10
Capillary electrophoresis for the determination of carbohydrates in lignocellulosic biomass through acid hydrolysis
Rafaella S. Aredes, Daniel G. S. Quattrociocchi, Vinicius G. C. Madriaga, Giovanni Offrede, Maria C. S. Paranhos, Thiago M. Lima, Lucas M. Duarte, Flávia F. de C. Marques

PP-11
Simultaneous separation of artesunate and mefloquine in fixed-dose combination tablets by CZE-UV
Jéssica Cordeiro Queiroz de Souza, Paula Rocha Chellini, Alessandra Lifsitch Viçosa, Marcus Vinícius Nora de Souza, and Marcone Augusto Leal de Oliveira

PP-12
Primaquine analysis in pharmaceutical formulation using multiple and short end injections by capillary zone electrophoresis with UV detection
Jéssica Cordeiro Queiroz de Souza, Paula Rocha Chellini, Marcus Vinícius Nora de Souza, and Marcone Augusto Leal de Oliveira

PP-13
UHPLC-MS/MS Analysis on Brachyotum naudinii Triana Composition and its Toxic and Antimicrobial Activities
Marco Rolando Aronés Jara, Kirianova Godoy Bautista, Edgar Cárdenas Landeo, Edith Eveling Conislla Cáceres, Eylen Almendra Ortiz Pérez, María Segunda Aurora Prado

PP-14
Fast Stability-Indicating RP-HPLC Method for Determination of Antiarrhythmic Drug Amiodarone in Pharmaceutical Formulation
Marcos Joseph Benites Neyra, Anas Rashid, María Segunda Aurora Prado

PP-15
Lifelong Exercise and Metabolic Health: Differential Serum Metabolite Responses in Young and Master Athletes
Luciele Guerra Minuzzi, Alex Castro, Karsten Krüger, José Cesar Rosa-Neto, Antônio G. Ferreira, Ana Valéria Colnaghi Simionato, Fabio Santos Lira

PP-16
Determination of Sucralose Using Capillary Electrophoresis with Capacitively Coupled Contactless Conductivity Detection
Gabriela Ribeiro, Dosil de Jesus

PP-17
The Evaluation of Galectin-1 – Glycopeptide Interactions by Affinity Monolith Chromatography
Maria Butnariu and Dušan Koval

PP-18
Determination of amino acids in retina of the chicken embryo through capillary electrophoresis
Marcos M. Gouvêa, Rafaella S. Aredes, Marcelo C. P. Almeida, Flávia F. C. Marques

PP-19
Chemical profiling of Amazonian Propolis using a metabolomics approach
Brícia Marques Parreiras, André Rodrigo Rech, and Adriana Nori de Macedo

PP-20
Determination of multiclass antibiotics by capillary electrophoresis using the AQbD approach
Natália Salles, Felipe Santos, Alan Jacoud, Mirelle Silva, Heron Torres Silva, and Maria Lourdes Moraes

PP-21
Low-Resolution CZE-MS screening data of urine samples associated with deep learning modeling for discriminative classification of COVID-19
Marcone Augusto Leal de Oliveira, Claudimir do Lago Neto, Fernando Silva Lopes, Luiz Henrique Cantarino Adriano, Lúcio Marco de Lemos, Olívia Brito de Oliveira Moreira, Raphaela Cristina Cancela Marquesa

PP-22
3D-Printed Porous Microstructures and their Role in Electromambrane extraction
Mayra Venturini Paschoarelli, Juan Matias Santos, Reverson Fernandes Quero, Dosil Pereira de Jesus

PP-23
Synergic effect evaluation of antiplatelets and statins on infarcted patients: a targeted metabolomics approach
Novais, K., Cieslarova, Z., Magaldi, M., Barros, L.A., Lago C.L., Oliveira, D.R., Fonseca, F.A.H., Izar, M.C., Tavares, M.F.M., Lopes, A.S.; Klassen A.

PP-24
Untarget analysis of human skin derived fibroblast cells exposed to phthalates by GCxGC-Q-TOFMS/MS
Nayara Silva Fraga, Josimar Marques Batista, Thais Fernandes Bassani, María José Gonzáles, Michele Angela Rodrigues, Dawidson Assis Gomes, Zenilda de Lourdes Cardeal, and Helvécio Costa Menezes

PP-25
Metabolomic fingerprint of cytotoxic extract from Gram-positive bacteria recovered from Itaguaré Beach (SP, Brazil)
Daniela C. Russo, Dhiego B. Rigato, Renan S. Oliveira, Anelize Bauermeister, Paula C. Jimenez

PP-26
Untargeted metabolomic evaluation of the mefloquine for Leishmania amazonensis treatment
Heiter V. M. Boness, Hanna C. de Sá, Vinicius P. C. Rocha, Milena B. P. Soares, and Gisele A. B. Canuto

PP-27
Understanding feline mammary carcinoma by untargeted metabolomics
Hanna C. de Sá, Alessandra Estrela-Lima, Gisele A. B. Canuto

PP-28
Experimental design applied to the optimization of sample plasma preparation for untargeted metabolomic analysis
Erika T. de J. C. Cruz, Giulia B. B. Afonso, Mirtes F. S. de Freitas, Gisele A. B. Canuto

PP-29
Clinical metabolomics in the study of acute kidney injury (AKI)
Daniel R. Oliveira, Joao P. S. Farah, Lúcia C. Andrade, Marina F. M. Tavares

PP-30
Molecular Signatures of Wilms Tumor issued by Metabolomic and Transcriptomic Integrative Analysis
Pedro H. Godoy Sanches, Bruna M. S. Pereira, Alex A. R. Silva, Danilo C. Oliveira, Natália A. S. Miyaguti, Paulo A. Faria, Beatriz de Camargo, Mariana Maschietto, and Andréia M. Porcari

PP-31
Comparative metabolomic evaluation of cisplatin and synthetic tellurium compounds in search of drug candidates for lung cancer treatment
Jessica Oliveira Fernandes Mantoanelli, Tharcisio Citrangulo Tortelli Junior, Roger Chammas, Alcindo Aparecido dos Santos, and Marina Franco Maggi Tavares

PP-32
Clinical metabolomics in the study of patients with COVID-19 and acute kidney injury (AKI)
Lucas H. F. D. Silva, Joao P. S. Farah, Natalia C. P. dos Santos, Lúcia C. Andrade, Daniel C. Pimenta, Marina F. M. Tavares

PP-33
LC-HRMS for prospecting secondary metabolites of aqueous extract of *Strychnos peckii* B.L.Rob.
Fernando Cassas, Carla L.G. Santos, Felipe M. A. da Silva, Quezia Cass

PP-34
Cationic Dyes with High Molar Absorption Coefficients to be Used as Labels or Co-ions in Capillary Electrophoresis
Carlos Eduardo Rodrigues, and Tarso B. Ledur Kist

PP-35
Hypolipemiants and antiplatelets treatments in patients with ST-segment elevation myocardial infarction: Semi-targeted lipidomics of the BATTLE-AMI study
Carolina R. C. Picossi, Joao P. S. Farah, Marina F. M. Tavares, Coral Barbas, Francisco Javier Rupérez

PP-36
Untargeted metabolomics to reveal the mechanism of action of potential drugs against Chikungunya
Danielle dos R. Lucas, Giselle F. Ribeiro, Carolina B. Moraes, Lúcio Freitas-Junior, Alcindo A. Santos, Joao Pedro S. Farah, and Marina F. M. Tavares

PP-37
Rationalizing solvent effects on the MEKC separation of natural and synthetic steroids using QSRR
Claudinei A. Silva, Carolina R.C. Picossi, Vanessa M. Carpentieri, Cristina Sumie Nizuma Matsumoto Sorio (*in memoriam*), João P.S. Farah, and Marina F.M. Tavares

PP-38
Comparison of different Acquisition Modes - untargeted urinary metabolome analysis of COVID-19 patients
Danilo Oliveira, Alex Ap. Rosini Silva, Pedro Henrique Godoy Sanches, Raquel M. Rodrigues-Peres, Andreia M. Porcari

PP-39
Noncovalent Labeling of Proteins in Sodium Dodecyl Sulfate Capillary Gel Electrophoresis
Felicia Auer, Andras Guttman

PP-40
Metabolomics evaluation of the kynurenine pathway in COVID-19 associated to acute kidney injury by LC-MS
Felipe Monferdine Aggio, Mariana Feitosa Custódio, Marina Franco Maggi Tavares, Lúcia da Conceição Andrade, Carla Beatriz Grespan Bottoli, Ana Valéria Colnaghi Simionato

PP-41
Study of metabolic alterations linked to the SARS-CoV-2 virus and the use of low-level laser as anti-inflammatory therapy in zebrafish (Danio rerio).
Leonardo Santos Alexandre, Vinicius Guimarães Ferreira, Ives Charlie Silva, and Emanuel Carrilho

PP-42
Refining Extraction Techniques for Alpha and Beta Acids in *Humulus lupulus*: Chemical Analysis via CD-MEKC-UV and HPLC-DAD
Eiriz, D. N., Pavon, V. E. Z., Mansano, J. P. R., Silva, D. S., Carvalho, A. S., Rocha, L. M., Fernandes, C. P. B., Duarte, L. M.

PP-43
Evaluating the mechanism of action of novel Te-based drugs for the treatment of Schistosomiasis with an untargeted metabolomics approach
Vinicius B. Fernandez, Rafaela Freitas, Eliana Nakano, Alcindo A. Dos Santos, João P. S.Farah, Marina F. M. Tavares

PP-44
Study of polysaccharide hydrolysis by capillary electrophoresis with direct UV detection
Giovanni Offrede, Thallis M. Souza, Lucas M. Duarte

Abstracts – Plenary Communications

PL-01

Metabolic Profiling for Exploring Host-Microbiome Interactions in Human Health: A Chemical Dialogue

Elaine Holmes

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Metabolic profiling of biofluids such as urine, plasma or fecal water in combination with multivariate statistical modeling tools, can provide a window for investigating the impact of disease on human health. High-resolution spectroscopic methods (NMR spectroscopy, CE-MS, LC-MS, GC-MS etc) are used to generate information-dense metabolic profiles that carry information relating both to genetic and environmental influences, including contributions from the diet, xenobiotics and gut microbiome.

The contribution of the gut microbiota to human health and disease is undisputed, yet the mechanisms by which the microbiome exerts its effects remain poorly understood. Co-evolution of host and microbiome has influenced the functionality of both the microbiome and host such that metabolic complementarity exists within the microbiota and that critical biosynthetic pathways are provided for the host that significantly extend host metabolic capacity. Of all the 'omics' technologies, metabolomics provides one of the most accessible windows on investigating the impact of the microbiome on human health since metabolic profiles of easily obtainable biofluids such as blood plasma and urine carry information relating both to genetic and environmental influences, including microbiome-diet and microbiome-xenobiotic interactions.

High resolution spectroscopy together with multivariate mathematical modelling has been used to model the metabolic consequences of perturbing the microbiota and to profile the effects of nutritional interventions on both the metabolism and the microbiome. Basic studies in germ free and antibiotic-treated animals have shown dramatic changes in the urinary and faecal metabolomes, which are largely restored to 'normal' following recolonization. Recent research indicates that the microbial metabolites can be predictive of response to drug treatment and to diet. This presentation describes the use of metabolic profiling to evaluate the impact of the gut microbiome on human health and focuses on the chemical dialogue between the host and its microbial partners.

PL-02

Human Sputum Proteomics: Advancing Non-Invasive Diagnosis of Respiratory Diseases with Enhanced Biomarker Analysis Methods.

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Many ailments can be diagnosed while they are asymptomatic, meaning that the patient has no signs or symptoms of a progressing disease. If caught in their initial stage of formation, these maladies can be effectively treated, leading to successful outcomes; curative therapies can halt diseases from advancing to improve the quality of life, and long-term survival of the patient. Still, cutting-edge upgrades in precision technologies are not only necessary for early, reliable, affordable, and rapid disease detection, but vital for the well-being of people and the future of global public health.

The emerging role of non-invasive approaches for medical diagnostics has been liquid biopsies based on genomic biomarkers. As such, biological fluids permit any measurable molecular indicator or signature to provide valuable information on individual's wellness and/or disease. Among the bodily secretions used for non-invasive diagnostics is sputum, a complex viscous hydrogel meshwork, that has gained growing recognition as a rich source of biomarkers to unveil infectious respiratory and chronic pulmonary diseases, and serve as a determinant to reveal other illnesses.

As per the World Health Organization, the burden of respiratory conditions is exacerbated by factors, ranging from considerable subjection to air pollution and occupational contaminants, to tobacco smoking and second-hand smoke, in addition to poor socio-economic status. Due to the likely increase of these determinants, respiratory tract ailments are on the rise, putting stress on healthcare facilities and services worldwide. I therefore highlight the need to use expectorated or induced sputum specimens as a routine source for testing valuable protein biomarkers to diagnosis these chronic maladies, to predict inflammation and disease progression, as well as to monitor the effectiveness of treatments. Further, I will discuss the urgency for fast and reliable point-of-care methods employing miniaturized analytical instruments to detect and quantify crucial protein biomarkers in sputum specimens, and limitations faced when dealing with their complex matrices.

PL-03

New Advances in High Throughput Metabolomics by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: Doing More with Less!

Meera Shanmuganathan, Zachary Kroezen, Erick Helmeczi, Biban Gill, Ritchie Ly, and Philip Britz-McKibbin

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Keywords: Metabolomics, Lipidomics, CE-MS, Biomarker discovery, Multiplexed separations

High throughput methods are needed in mass spectrometry (MS)-based metabolomics to tackle large-scale epidemiological studies for biomarker discovery in support of preventative health. This includes more objective assessment of lifestyle and dietary exposures as potential modifiable factors in chronic disease risk. However, conventional methods using chromatographic separations coupled to high resolution MS are slow, resource-intensive, and require complicated data processing steps prone to error. Herein, multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) is introduced as a robust, low-cost and multiplexed separation platform for untargeted analysis of ionic metabolites and lipids under aqueous or non-aqueous buffer conditions, respectively. I will outline the ten-year evolution of MSI-CE-MS technology that takes advantage of a serial injection format of up to 13 samples within a single analytical run. Recent advances in developing a customized software tool for automated processing of serum metabolome data sets in MSI-CE-MS via migration time indices will be discussed given challenges related to long-term migration time drifts. We validated this approach to identify serum biomarkers associated with cognitive development in a national nutritional survey of children across Brazil. I will also outline recent applications of MSI-CE-MS technology used in the discovery of urinary biomarkers associated with recent exposures, including tobacco smoke, coffee intake and red meat consumption from participants in 14 countries globally. Lastly, the potential to perform rapid lipidomic analyses after chemical derivatization will also be presented as a strategy to greatly expand CE-MS metabolome coverage beyond polar/hydrophilic metabolites.

Bibliographic references:

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PL-04

Searching alternative drugs to treat infectious and parasitic diseases: the metabolomics approach.

Ana Paula G. Fernandes,[a,b] Robert Ivan Schumacher,[b] Maria Júlia M. Alves,[b] Alcindo A. Santos,[b] João P.S. Farah,[a,b], and Marina F.M. Tavares[a,b,*]

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Keywords: metabolomics, neglected diseases, infectious diseases, parasite, drugs

The Center for Multiplatform Metabolomics Studies (CEMM) at IQ-USP, implemented during the COVID-19 pandemics (August 2020), inaugurated a novel research front, that intends to explore the potential of targeted and untargeted multiplatform metabolomics to reveal the mechanism of action at molecular level of candidate drugs to the treatment of infectious and parasitic diseases. Among the diseases of interest there are included infectious diseases: chikungunya and yellow fever (arboviruses), both neglected in Brazil, and COVID-19, considered an emergent disease; in addition there are included several neglected parasitic diseases: leishmaniasis (visceral form is re-emergent) and Chagas disease, both caused by protozoa, and schistosomiasis, caused by helminths. There are hundreds of compounds being screened at the moment using high-throughput and/or high-content screening techniques; such compounds result from the efforts of CEMM collaborators, locally and abroad, working on the synthesis, extraction, purification, as well as theoretical calculations, and they are originated from computer simulations, natural products, synthetic chemicals libraries, and drug repositioning. Preliminary results for Leishmaniasis will be presented demonstrating the impact of the listed drug classes into the parasite metabolism. The results generated so far may contribute in a concerted manner to elucidate the broad action of several candidate drugs against infectious and parasitic diseases, paving the way into the searching of novel alternative therapies.

Acknowlegements:

Fapesp 2019/24107-5; CNPq 304983/2022-5

Abstracts – Keynote Communications

KN-01

Sodium Dodecyl Sulfate Capillary Gel Electrophoresis in the Presence of Propidium Iodide Fluorescent Dye

Andras Guttman[a,b*], Felicia Auer[b]

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Keywords: sodium dodecyl sulfate, capillary gel electrophoresis, proteins, propidium iodide, temperature, gel concentration, electric field

Sodium dodecyl sulfate capillary gel electrophoresis is one of the frequently used methods for size-based protein separation in molecular biology laboratories and the biopharmaceutical industry. To increase throughput, quite a few multicapillary electrophoresis systems have been recently developed, but most of them only support fluorescence detection, requiring fluorophore labeling of the sample proteins. To avoid the time-consuming derivatization reaction, we developed an on-column labeling approach utilizing propidium iodide in SDS-CGE of proteins, a dye only used before for nucleic acid analysis. As a key ingredient of the gel−buffer system, the oppositely migrating positively charged propidium ligand in migratio complexes with the SDS-proteins, therefore, supports in situ labeling during the electrophoretic separation process, not requiring any extra pre- or postcolumn derivatization step. A theoretical treatment is given to shed light on the basic principles of this novel online labeling process, also addressing the influence of propidium iodide on the electroosmotic flow, resulting in reduced retardation. The effects of the three most important user-adjustable separation parameters (temperature, gel concentration, and electric field strength) were also investigated on the electrophoretic mobility and resolution of SDS-protein complexes in the presence of propidium iodide in the gel-buffer system.

Bibliographic references:

F. Auer, A. Guttman, In Migratio Noncovalent Fluorophore Labeling of Proteins by Propidium Iodide in Sodium Dodecyl Sulfate Capillary Gel Electrophoresis, *Analytical Chemistry*, 2024, 96, 10969−10977

KN-02

Novel Monolithic Capillary Columns for Multimodal Capillary Electrochromatography

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Keywords: Capillary electrochromatography, Chiral separation, Achiral Separation, Reversed phase, Hydrophilic interaction

The previously developed poly(carboxyethyl acrylate-coethylene glycol dimethacrylate) precursor monolith (carboxy monolith) was exploited in preparing columns for CEC having nonpolar n-alkyl and anthracenyl, polar and chiral ligands that led to RPC, π interactions, hydrophilic interactions, and enantioseparations, respectively. The chiral carboxy monolith, was obtained by reacting the monolith with (S)-(-)-1-(2-naphthyl) ethylamine (NEA). The NEA column allowed not only enantioseparations in RPC via its chiral site but also the separation of nonpolar species via its achiral site offering both hydrophobic and π-π interactions for aromatic compounds. The octadecyl carboxy monolith was obtained by reacting the monolith with octadecylamine yielding a monolith with typical RPC behaviors. The anthracenyl carboxy monolith was obtained by reacting the precursor monolith with 2-aminoanthracene, which showed π and hydrophobic interactions, and separated aromatic compounds with superior selectivity than observed with octadecyl carboxy monolith. Finally, the polar carboxy monolith was prepared by reacting the carboxy monolith with TRIS, which separated polar and slightly polar species.

KN-03

Design of theranostic agents: a major contribution of electrokinetic characterizations

Laura Trapiella-Alfonso[a], Bich-Thuy Doan[a], G. Ramirez-Garcia[b], Fanny d'Orlyé[a], Anne Varenne[a]*

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[b]*Biofunctional Nanomaterials Laboratory, Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, Querétaro, 76230, México*
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Keywords: nanotheranostics, auto-assemblies, electrokinetic methodologies, physico-chemical characterization, protein corona, drug delivery

The use of nanomaterials as theranostic tools presents great potential to improve the efficiency and overcome many drawbacks of current theranostic objects, such as lack of targeting, biocompatibility or biodistribution, short lifetime or toxicity. In this context, the formation of complex and smart supramolecular nanostructures from synthetic material or natural building blocks is a key strategy to exploit in nanomedicine. So as to generate efficient nanostructures, it is crucial to control their formation in terms of size and surface charge density, their functionalization if necessary, to determine their behaviour/ auto-assembly and colloidal stability in different pH and ionic strength media, to characterize the protein-corona formation, to study targeted drug delivery strategies and imaging properties. Electrokinetic methods represent an interesting tool for these physico-chemical characterizations to limit animal testing, as will be highlighted with some nanostructurations developed in our group.

Bibliographic references:

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KN-04

Unravelling differential antibody proteoform binding with affinity CE-MS

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Keywords: affinity CE, mass spectrometry, antibodies, binding, Fc receptors

Antibodies recruit immune responses via interaction with different Fcγ receptors (FcRs). These interactions are strongly influenced by structural features of the antibody, including glycosylation. Unfortunately, common approaches, such as SPR provide an overall affinity response for all different glycoforms present in the sample.
We have exploited the capabilities of affinity CE-MS to study the binding of antibodies and FcRs in a proteoform-resolved fashion. To this end, the FcR receptors were added to the BGE whereas the mixture of antibody glycoforms were injected in the CE. Due to the low amounts of receptor required, the developed platform was ideal for testing a variety of FcRs, namely FcγRIIa, FcγRIIb, FcRn and FcγRIIIa and including different allotypic variants. As anticipated, Fc glycosylation was key for the binding. Hemiglycosylated antibodies showed strong decrease in the binding affinity towards the FcγRs while non-Fc glycosylated forms showed near no binding. Fc-glycoforms behaved differently between receptors with clear differences for afucosylated and high mannose variants. Interestingly, different receptor allotypes also revealed glycan-sensitive differences.

KN-05

Decoding the Complexity of Cacao Fermentation: Harnessing Metabolomics, Deep Learning, and Big Data

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Keywords: metabolomics, Theobroma cacao, transference of knowledge, deep learning.

Brazil's vast biodiversity is a crucial asset for global conservation and sustainability. The Nucleus of Bioassays, Biosynthesis, and Ecophysiology in Natural Products (NuBBE) plays a vital role in preserving and sustainably utilizing this biodiversity. Through metabolomics, molecular biology, metabolic engineering, and bioinformatics, NuBBE has developed tools like the NuBBE-DB to map the chemical and biological properties of plants and microorganisms. In recent studies, we applied these technologies to the fermentation of cacao (*Theobroma cacao*), an economically important resource for Amazonian communities. By employing metabolomics and chemoinformatics, combined with deep learning and big data, we analyzed cacao seed fermentation to predict the metabolic variability of exudates, using chemical fingerprints. These insights provide a better understanding of microbial interactions, crucial for improving chocolate quality. Our overreaching goal is to transfer this knowledge to local cacao producers, promoting sustainability and enhancing their livelihoods. This research promises to boost cacao production quality and support Amazonian communities.

KN-06

A Multi-Omics Approach Relating Disease Severity Prognosis: A Case Study for SARS-CoV-2

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Keywords: metabolomics, disease severity, mass spectrometry, covid, chemometrics

This presentation explores how multi-omics, particularly metabolomics, provides critical insights into metabolic disruptions caused by SARS-CoV-2, aiding in the prognosis of disease severity. By analyzing plasma metabolomes from 110 individuals, including SARS-CoV-2 patients and controls, several metabolites—such as glycerol, 3-aminoisobutyrate, and formate—were found to be dysregulated. These alterations impacted key metabolic pathways, including phenylalanine and lipid metabolism, which are tied to energy production and immune responses. The study also revealed polar metabolites, like glycerol and acetate, as potential prognostic biomarkers, showing strong predictive power for disease severity. Dysregulated glycerophospholipid and sphingolipid pathways were linked to immune evasion and increasing severity, while phenylalanine metabolism disturbances correlated with cardiac and neurological risks. This lecture will highlight how metabolomics can help clinicians anticipate disease progression and tailor interventions to improve patient outcomes in COVID-19 cases.

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KN-07

Multiomics Approach to Define the Biomolecular Changes Associated with Traumatic Brain Injury

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Keywords: TBI, LC-MS/MS, Metabolomics, Proteomics/Glycoproteomics, Glycomics

Traumatic Brain Injury (TBI) results from an external force on the head, causing temporary or permanent brain function impairment. Investigating TBI involves understanding its complex pathophysiology. Multiomics analysis of serum and cerebrospinal fluid (CSF) samples—encompassing proteomics, glycomics, glycoproteomics, and metabolomics— facilitate comprehensive understanding of TBI. We analyzed here blood serum and CSF samples from-free controls (n=19) and patients with mild TBI (mTBI) (n=19) at days 1, 3, and 5 post-injury using LC-MS/MS. Our findings revealed distinct molecular signatures in TBI patients compared to controls, highlighting pathways related to inflammation, oxidative stress, and neuroprotection. Proteomics identified key proteins in the acute inflammatory response and neuronal repair. Metabolomics indicated alterations in energy metabolism and neurotransmitter levels. Glycomics revealed changes in brain-specific glycans, while glycoproteomics showed changes in glycoproteins functioning as immune system receptors. This study underscores the value of multi-omics approaches in unraveling TBI's complex biological landscape.

KN-08

Application of Capillary and Microchip Electrophoresis to Investigate Oxidative Modifications of Proteins and Oxidative Stress

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Oxidative stress is involved in many diseases including Alzheimer's Disease, autoimmune disease and cancer. Reactive nitrogen and oxygen species (RNOS) are generated during oxidative stress and can react with proteins and other macromolecules *in vivo* and cause cell damage. In this presentation, the use of capillary (CE) and microchip electrophoresis (ME) for the determination of RNOS and their reaction products with amino acids and proteins is presented. Using this separations-based approach, it is possible to monitor multiple species simultaneously and resolve both endogenous and exogenous interferences. Both these techniques require small volumes, exhibit fast analysis times and yield high separation efficiencies. This makes it possible to monitor transient RNOS directly, as well as investigate the production of RNOS in single cells. A variety of detection methods can be employed with CE and ME including UV, fluorescence and electrochemical detection. ME with LIF detection has been evaluated for the indirect determination of RNOS in microglia lysates following reactions with RNOS specific dyes (1). The electrophoretic separation makes it possible to monitor several RNOS in a single run, as well as to isolate the reaction product from potential interferences.

CE and ME with electrochemical detection (EC) is particularly well suited to studies of oxidative stress since redox reactions are involved in their production. Both peroxynitrite and nitric oxide have been detected directly using ME-EC (2-3). In these studies, the use of ME-EC for the separation and selective detection of RNOS modified amino acids and peptides was evaluated. Oxidative ME-EC was employed for the separation and selective detection of the products of tyrosine and phenylalanine with the hydroxy radical using ligand exchange MEKC (5). Since there are very few reducible analytes in biological samples, reductive ME-EC was also investigated for the selective detection of nitrotyrosine containing species in the presence

of a large amount of tyrosine and potential interferences. Lastly, a method combining ME with bipolar electrochemistry and chemiluminescence detection was developed as an approach to improve the limits of detection for reductive ME-EC.

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KN-09

Characterization of Glycosylated (N-terminal) Pro-B-Type Natriuretic Peptide Forms in Blood Samples of Patients with Severe Heart Failure and its Biological and Medical Implications

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Keywords: natriuretic peptides, glycosylation, NT-proBNP, heart failure, nano-LC-MS

B-type natriuretic peptide (BNP) is a hormone secreted from cardiac myocytes as a response to myocardial stretch and stress. The biologically active C-terminal cleavage product of the pro-hormone proBNP and its inactive N-terminal counterpart (NT-proBNP) have been proven to be useful for ruling out heart failure (HF) and to correlate with HF disease severity and prognosis. However, several factors, such as biological and individual variability as well as the structural microheterogeneity of these polypeptides are far from being completely understood, which is important, as both peptides are the most powerful predictors of morbidity and mortality related to certain heart diseases at present. An overview is given, how our lab contributed significantly to unravel the molecular complexity of NT-proBNP by identifying its molecular diversity. Moreover, the unambiguous identification of all glycosylation sites of NT-proBNP and the determination of the detailed structure of the glycan chains based on the application of specific enzymes and MS fragmentation techniques is discussed. These results open new avenues for the development of more advanced quantitative assays in the future.

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KN-10

3D Printed Microfluidic Devices for Separation Science and Chemical Analysis

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Keywords: 3D printing, microfluidics, monoliths, integrated analysis

3D printing offers promising capabilities in the creation of innovative microfluidic systems for analytical applications. We use 3D printing to form integrated devices that can carry out separations of biomolecules. Our custom-built 3D printer utilizes digital light processing–stereolithography to make microfluidic devices that include valves, pumps and separation channels. We form monolithic columns in these 3D prints for the enrichment and purification of analytes related to diseases. We have performed solid-phase extraction of proteins and peptides related to preterm birth risk and sequence-selective retention and detection of mosquito-borne virus RNA. We also have carried out high-performance microchip electrophoresis in these 3D printed microfluidic systems. We are leveraging valves and pumps that can be made in 3D printed devices to combine upstream sample preparation steps with downstream analysis in an automated fashion. Integrated 3D printed microfluidic systems offer significant advantages in lowering detection limits, reducing reagent and sample needs, and automating analyses.

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Abstracts – Oral Communications

OP-01

Fate of One Equation. Application to Capillary Electrophoresis.

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Keywords: continuity equation, electromigration, numerical simulation software, PeakMaster, Simul

Electrophoresis utilizes a difference in movement of charged species in a separation channel or space for their spatial separation. A mathematical consequence of the mass conservation law is the continuity equation which is acting whenever there is a movement of mass and which can be formulated as a partial differential equation. The continuity equation is a beautiful law, concise in formulation and boundlessly rich in solution, which even nowadays can reveal very unexpected consequences and phenomena, such as oscillations[1]. Attempts at the analytical solution of the continuity equation in electrophoresis go back to the Kohlrausch's days. However, in spite of effort of mathematicians, the full analytical solution has not been presented until now. Therefore the scientist try to obtain useful results by another ways: extracting conservation functions, by means of moving boundary approximation, by linearization, and of course by numerical solution.

The presentation reviews (i) derivation of conservation functions from the conservation law as appeared chronologically, (ii) deals with theory of moving boundary equations, (iii) presents the linear theory of electromigration, (iv) shows the abilities of the last generation of numerical simulation software – PeakMaster and Simul.

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OP-02

Capillary electrophoresis and isotachophoresis applied for analysis and characterization of biologically active (lipo)peptides

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Keywords: capillary zone electrophoresis, capillary isotachophoresis, neuropeptides, acidity constant, effective charge

Capillary zone electrophoresis (CZE) and isotachophoresis (CITP) were employed for analysis and physicochemical characterization of neuropeptides regulating food intake (ghrelin, prolactin-releasing peptide, and cocaine- and amphetamine-regulated transcript peptide) and their lipidized analogs containing covalently attached octanoic, myristic or palmitic acids. Purity degree of synthetic (lipo)peptides (LPs) was quantified by CZE in acidic background electrolytes (BGEs) at pH 2.0 using various coatings of fused silica capillary suppressing sorption of LPs to inner capillary wall.
Acidity constants, pKa, of ionogenic groups of LPs and actual mobilities of their ionic forms were determined by a nonlinear regression analysis of pH dependence of their effective mobilities measured by CZE in BGEs within a wide pH range (2.00-10.50) at 25 mM ionic strength and 25°C. Effective charge of LPs was estimated by CITP in cationic electrolyte system at pH 4.0 using the dependence of the CITP zone length of LPs on their effective charge and injected amount [1, 2]. The effective charge of polycationic LPs was found to be significantly lower than the number of basic amino acids in their molecules.

Acknowledgement

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OP-03

Building a Drug Delivery Benchtop Microcontrolled Breast-on-a-Chip Microfluidic Platform

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Keywords: Organs-on-a-Chip, Instrumentation, Breast-on-a-chip, Palbociclib

Organ-on-a-chip devices are essential tools for replicating human physiology in controlled environments. This presentation focuses on a breast-on-a-chip platform designed to mimic breast tissue and tumor microenvironments in luminal A breast cancer models. Two platforms were built: one with a single syringe pump and another with two microcontrolled syringe pumps, both integrated with temperature control systems. These platforms allow for precise control of the cell culture environment and enable experiments on a conventional lab bench without incubators, offering greater flexibility. MCF-7 and T47D cells were seeded in different chip models, connected to the temperature controlled platform that delivered a constant flow of cell medium and Palbociclib at various concentrations (33 µM, 20 µM, 16.5 µM, and 10 µM) for 48 hours. Cell proliferation was assessed using microscopy and Ki67 assays. Higher Palbociclib concentrations (33 µM and 20 µM) significantly reduced proliferation and altered cell morphology compared to lower concentrations. These results indicate the model's effectiveness in drug testing for breast cancer.

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OP-04

Exploring the versatility of Capacitively Coupled Contactless Conductivity Detection (C^4D) in Conventional and Microchip Capillary Electrophoresis

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Keywords: conductivity detection, environmental, food, instrumentation, microfluidic

The first applications of Capacitively Coupled Contactless Conductivity Detection (C^4D) capillary electrophoresis (CE) emerged in 1998. Since then, several applications of the CE-C^4D to determine various analytes have been reported. One of the advantages of the C^4D is its ability to detect compounds with low UV-visible absorption without the need for derivatization steps. Moreover, C^4D requires simple and low-cost instrumentation, making it easy to adapt to microfluidic devices (microchips) used for CE separations. This presentation will show some novel applications of the CE-C^4D in developing analytical methods for determining compounds of environmental and food interest. Additionally, it will discuss innovative integrations of this detection method into a thread-based and 3D-printed microfluidic device for CE, highlighting the versatility of the C^4D.

OP-05

Capillary electrophoresis in the quality control of therapeutic proteins

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Keywords: capillary electrophoresis, therapeutic proteins, isoelectric focusing, capillary gel electrophoresis, size heterogenity

In the early 2000s, capillary electrophoresis (CE) was seen as a novelty. Nowadays, it's widely utilized for quality control globally, offering automated, high-resolution techniques with on-line detection. Traditional electrophoretic methods like SDS-PAGE and IEF gels were once common in biopharmaceutical release testing, but they are cumbersome, involve hazardous reagents, and suffer from variability and reproducibility issues due to inconsistency in staining and destaining steps. Consequently, many biotech companies have turned to CE methods such as capillary electrophoresis sodium dodecyl sulfate (CE-SDS), capillary isoelectric focusing (CIEF), and capillary zone electrophoresis (CZE) as more practical alternatives. With user-friendly instruments, regulatory-compliant software, and tailored assay kits for protein and monoclonal antibody analysis, CE has emerged as a viable replacement in quality control labs, establishing release specifications for therapeutic proteins. Each year, new research contributes to the understanding of therapeutic proteins through various CE modes. In this talk we will review the CE methods in use and an update on CE advances that promise to be valuable in the quality control of therapeutic proteins.

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OP-06

Interaction between passion fruit (*Passiflora edulis*) seed extracts and jambu (*Spilanthes acmella*) aerial parts in topical photoprotective formulations: stability and skin permeation

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Keywords: piceatannol, spilanthol, passion fruit, paracres, emulsions, formulation stability.

Among the more than 8,000 currently elucidated plant phenolic compounds, piceatannol, obtained from passion fruit seed (*Passiflora edulis*), is presented as a potential dermocosmetic active ingredient candidate with in vitro demonstrated photoprotective and skin regenerative properties. The delivery of this molecule to the deeper layers of the skin, however, is challenging. In this sense, permeation-promoting molecules can be associated with piceatannol to help it diffuse beyond the stratum corneum, and spilanthol, present in the aerial parts of paracres (*Spilanthes acmella*), in addition to its recognized anti-wrinkle action, exhibits this property. To protect the skin against the deleterious effects of the environment, it is fundamental to block sun radiation through organic and inorganic sunscreens. We will discuss the interaction between passion fruit seed and paracress aerial part extracts in terms of formulation stability and *in vitro* skin permeation on the Strat-MTM (Merck Millipore) synthetic model. First, we will show the obtaining of a passion fruit seed extract by microwave assisted extraction (MAE), which has not been described in the literature so far. Following that, we will present the results of a stability study of passion fruit and paracress extracts in a base emulsion (B_{em}) added with organic (O_{em}) or inorganic (I_{em}) sunscreens, in which it was observed that they did not affect their physical stability, but chemical interactions occurred in all formulations. Piceatannol was only found in B_{em} after 12 days of temperature cycling (5 and 40 °C), and both it and spilanthol were incompatible with the inorganic sunscreens in the proposed emulsion. Finally, we will show the *in vitro* permeation profile of piceatannol through the Strat-MTM membrane, revealing that, in the proposed formulation, it reached the dermis equivalent, reaching deeper layers in the presence of spilanthol and organic sunscreens.

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OP-07

CZE vs. RP-HPLC with inductively coupled plasma mass spectrometry in the investigation of various anticancer drug delivery nanosystems

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Keywords: CZE-ICP-MS, RP-HPLC-ICP-MS, nanomaterials, drug delivery systems, cisplatin

The treatment of cancer often includes chemotherapy with the application of cytotoxic drugs, e.g., cisplatin. The limitations of its use are a lack of selectivity towards cancerous targets, which, along with highly cytotoxic properties, results in numerous severe side effects and fastly observed drug resistance. The way to overcome the mentioned obstacles is to ensure the effective transportation of cisplatin directly to targets using various nanomaterials as nanovehicles. A combination of nanocarrier and anticancer drugs is called anticancer drug delivery system (DDS).

To effectively investigate the formation and changes of DDSs, there is an acute need to monitor the final product and all constituents in the probed mixture. This way of characterizing DDSs is possible by employing hyphenated techniques with analyte-specific inductively coupled plasma mass spectrometer (ICP-MS) detection.

In the frame of the presentation, CZE-ICP-MS and HPLC-ICP-MS will be compared as tools for direct, qualitative, and quantitative monitoring of cisplatin DDS formation profiles during one analysis. Herein, two nanomaterials were used as cisplatin vehicles – gold and liposomes.

The research was financed in the frame of the WUT Research University Excellence Initiative grant (1820/83/Z01/2022).

OP-08

Tying Cooling Capillaries Around Analytical Capillaries and Provision of a Free Service to the Entire Analytical Chemistry Community

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Keywords: Joule effect, temperature control, cooling, thermal band broadening

Capillary Electrophoresis is a separation technique that uses small volumes of environmentally friendly buffer solutions. The instrumentation is of low cost and, in some cases, exhibits separation efficiencies of up to 10 million theoretical plates. In this presentation the author calls the attention to some underexplored advantages of using efficient and radially symmetric temperature control in CE (*Kist*). For this the author developed an automated capillary tying machine and provides this free service to the entire analytical chemistry community. The operation of this machine will be explained using videos and a series of cooling capillaries (n = 4, 5, and 6) tied around analytical capillaries will be shown. To obtain a good match and prefect closing of the n cooling capillaries (with outer diameter ODc) around the analytic capillary (with outer diameter ODa), one must choose the right n and ODc. The ideal ODc for a given n is given by: $ODc = ODa \sin(\pi/n) [1 - \sin(\pi/n)]^{-1}$. This is the master equation for tying cooling capillaries around analytical capillaries.

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OP-09

A New Online Electrokinetic Sample Cleanup Method and the Related Novel Evaluation Approach for APTS Labeled N-Glycan Profiling by Capillary Electrophoresis

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Since glycans in most of the cases lack chromophore or fluorophore groups, their CE analysis usually requires tagging by a charged fluorophore. To speed up the derivatization reaction, a large excess of the labeling reagent is typically used, therefore, a purification step is necessary prior to CE analysis using the industry standard low pH gel-buffer system. In addition to representing an extra sample preparation step with the associated labor and cost, the purification process also holds the risk of losing some of the sample components. In this presentation we demonstrate an online electrokinetic sample cleanup process with electroosmotic flow (EOF) assisted separation in a bare fused silica capillary using alkaline pH background electrolyte and normal polarity of separation voltage [1]. The use of the new 150 mM caproic acid - 253 mM Tris (pH 8.1) running buffer facilitated the entrance of the sample components of interest into the separation capillary, while the excess labeling reagent was excluded, therefore, did not interfere with the detection. Next to the radically new separation method, the required novel data evaluation method will be introduced as well [2].

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OP-10

Metabolomics analysis under NMR point of view

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Keywords: NMR, 2D NMR, Metabolomics, body fluids

The omics research certainly needs to make use of very powerful and precise experimental tools and Nuclear Magnetic Resonance (NMR) is one of them, especially when the study involves body fluids as urine, plasma and serum. However, NMR have some advantages which include: *i)* easy sample preparation – typically a simple pH correction using buffer solution, centrifugation or filtration, addition of stock solution with D_2O plus internal reference (TSPA-d4 or DSS-d4) and using a few well know protocols for it[1,2]; *ii)* reproducibility – the samples could be run in different days, with different operators and different equipment's presenting the same results[3]; *iii)* compounds identification and quantification in the same analyses and samples; *iv)* unnecessary use of analytical standards for identification or quantification of each compounds; *v)* and automated operation after sample thawing. Additionaly, information obtained from NMR measurements have been recently used in data bank and artificial intelligence (AI) to be applied in clinical analysisof body fluids[4].

One of the advantages for NMR is the use data bank and AI, but such information may be checked experimentally to reinforce the findings. 2Ds NMR experiments allow obtaining information about the compounds molecular structure using: COSY – comparing the neighbors hydrogens information (chemical shift and multiplicity); HSQC – to find the chemical shifts of the hydrogen attached to the directly carbon, HMBC – chemical shifts of the neighbors' carbons attached with the same hydrogens and from J-Resolved to get the multiplicity of a non-resolved multiplets. In some cases, it is also possible to use the HSQC-TOCSY experiments, although this mode can be runed only once for the matrix and not for each compound.

Certainly, the two major restrictions to use NMR approach is the natural low sensitivity, compared with other techniques, and the signals overlaps in the hydrogen's spectra.

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OP-11

Why should one worry about enantioselectivity effects in clinical metabolomics?

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Keywords: chiral biomarkers; amino acids; stereoisomers, 2D-LC, metabolites

Stereochemical analytical protocols have been mostly overlooked in target or non-target metabolomic profiling. Most protocols rely in derivatization, since the formed diastereomeric mixture are separated by achiral liquid chromatography. Moreover, the analysis of amino acids by chiral chromatography, for instance, is compromised by the structural isomers and diastereoisomers present in the mixture. Another drawback for measuring enantiomeric ratio is the higher proportion of the L-enantiomer. Nevertheless, the importance of disclosing the enantiomeric signature of the end product of a biochemical process, has been the motif for pursuing enantioselective separations. To this end, it is well recognized that D-amino acids are biomarkers with diagnostic value for a series of diseases. In a recent study, D-Asn (asparagine), D-Ser (serine), D-Ala (alanine), and D-Pro (proline), were found in all patient's plasma samples with chronic kidney disease, and the percentage of D-Asn and D-Ser have shown good correlation with the estimated glomerular filtration ratio of the patients. By another hand, chiral hydroxycarboxylic acids have been related to metabolic diseases. For instance, D- and L-2-hydroxyglutaricacid are normal endogenous metabolites, but they are biomarkers of the three inborn acidurias. In this talk, methods for chiral metabolomics will be overseen considering the importance of disclosing chiral biomarkers and their diagnostic and prognostic clinical value.

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OP-12

Understanding Exercise Response Variability: A Metabolomics Perspective

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Keywords: Metabolomics, NMR, Cardiorespiratory Fitness, Endurance Training, High-intensity interval training

Cardiorespiratory fitness (CRF) levels represent a strong predictor of all-cause mortality. However, there is wide variability in CRF responses (responsiveness) to standardized exercise doses. Identifying the molecular factors affecting CRF responsiveness contributes to biomarker discovery and personalized exercise prescription. This study investigated the baseline serum and intramuscular metabolomic profiles and their pathways associated with CRF responsiveness to continuous endurance training (ET) or high-intensity interval training (HIIT) programs. Forty-three serum and 70 intramuscular (vastus lateralis) metabolites were characterized by Proton Nuclear Magnetic Resonance based metabolomics. CRF and metabolomics profile were measured in 70 sedentary healthy young men (23.7±3.0 years), at the baseline and Post 8-weeks of ET, HIIT and Control (CO) period. The pathways similarly enriched in serum or muscle between ET and HIIT programs were arginine and proline metabolism, glycine, serine and threonine metabolism, and glyoxylate and dicarboxylate metabolism. Individuals likely to be non-responders to the training programs were identified based on their baseline serum O-acetylcarnitine (accuracy=78.0%, P=0.006) and intramuscular creatinine (accuracy=72.3%, P=0.028) levels. These results highlight the potential of serum and intramuscular metabolites as biomarkers for CRF responsiveness and for understanding exercise response variability.

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OP-13

Targeted analysis of gut microbiota-derived metabolites in colonic fermentation models: Investigating the impact of food ingredients

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Keywords: Gut microbiota, food, LC-MS/MS, targeted analysis

The gut microbiota is composed of various bacteria that play a crucial role in human health, influencing processes such as digestion, immune function, and protection against pathogens[1]. This growing recognition of its importance has sparked interest in investigating its interactions with diet. However, to decipher the interactions between food and the microbiota in humans, sophisticated experimental models are required that can accurately reproduce the dynamic processes of the gastrointestinal environment, simulating the stomach, small intestine, and colon under controlled conditions[2]. Microbiota produces a wide range of bioactive compounds that are essential in the selection of microbes and the construction of metabolic signaling networks. Metabolomics is a fundamental technique for characterizing and quantifying the molecules produced by intestinal microbes, facilitating the study of interactions between the microbiota and the host[3]. In this work, *ad hoc* methodologies were developed for the targeted analysis of metabolites involved in key microbial metabolic pathways, such as trimethylamine-related metabolites, short-chain fatty acids, and bile acids, using HPLC-QqQ-MS.

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OP-14

Metabolomics for neuropsychiatric diseases differentiation and potential novel treatments study

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Keywords: metabolomics, mass spectrometry, bipolar disorder, ayahuasca, cannabis

Neuropsychiatric disorders are highly complex both clinically and biochemically, with multifactorial etiologies. Two critical challenges associated with these disorders are the diagnosis, which relies solely on clinical observations, and the treatment, which is empirically tailored to each patient based on clinical responses. Understanding the molecular mechanisms underlying the pathophysiology of these diseases, as well as the mode of action and efficacy of the treatments, is therefore of utmost importance. Omics strategies, including metabolomics, can provide valuable insights into the metabolic alterations caused by these disorders and/or their treatments, potentially identifying biomarkers that can aid in diagnosis and treatment evaluation within the context of personalized medicine. In this presentation, we will discuss studies on the molecular bases of bipolar disorder and the potential of ayahuasca and cannabis in developing novel treatments for depression and Alzheimer's disease. These studies aim to explore the efficacy of these alternative treatments by analyzing their impact on metabolic pathways, which may offer new insights into the development of targeted therapies.

OP-15

Geographical Indication Area Expansion for Aroeira Honey Supported by Untargeted Metabolomics

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Keywords: special honey, Myracrodruon urundeuva, liquid chromatography, chemical profile, metabolomics approach

Aroeira tree (*Myracrodruon urundeuva*), which grows naturally in the semi-acid region of Minas Gerais (Brazil), bear flowers that are used by bees to produce a special honey with recognized medicinal properties.[1] The aim of this study was to compare the chemical profile of aroeira honey from Vale do Jequitinhonha with the one produced in Norte de Minas, which is currently the established Geographical Indication origin of aroeira honey. An untargeted metabolomics approach was performed by liquid chromatography-mass spectrometry to evaluate the overall chemical composition of honeys originated from these two locations (n=44). Multivariate statistical analysis showed a considerable similarity between the groups, supported by univariate analysis, which indicated only nine significantly different compounds from a total of 3334 metabolic features under comparison (FDR p-value < 0.05 and fold-change > 2). Therefore, except for very few specific compounds, aroeira honeys from the two regions (Vale do Jequitinhonha and Norte de Minas) could not be differentiated based on their chemical profiles, which supports their compositional similarity throughout the semi-arid region of Minas Gerais.

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OP-16

Plasma metabolome signatures to predict responsiveness to neoadjuvant chemotherapy in breast cancer

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Keywords: Breast cancer; Cancer biology; Drug resistance; Metabolomics; Neoadjuvant chemotherapy response.

Neoadjuvant chemotherapy (NACT) has emerged as a treatment option for breast cancer (BC), though response to NACT remains unpredictable and varies by cancer subtype. Metabolomics offers a tool for identifying biomarkers and predicting chemotherapy response. In this study, plasma metabolomes from BC patients were analyzed before NACT to correlate with treatment response. Using liquid chromatography coupled with high-resolution mass spectrometry (LC-MS), pre-NACT plasma samples from 75 patients were examined. Extracted metabolites were used to build an SVM model to classify responsiveness, with data split into training (75%) and validation (25%) sets. The 19 identified metabolites predicted patient response with high sensitivity (95.4%/93.3%), specificity (91.6%/100.0%), and accuracy (94.6%/94.7%) for the training/validation sets, respectively. Remarkably, 95% of resistant and 94% of sensitive patients were correctly classified. Lipids and amino acids linked to chemoresistance pathways were identified. This metabolome-based model successfully predicted NACT response, offering potential for precision medicine in BC treatment.

OP-17

Zika Virus in Extracellular Vesicles: Insights from Integrated Proteomic and Metabolomic Dependent Regulation of B Cell and PI3K/AKT/mTOR Signaling Pathway

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Clinics are increasingly integrating metabolomics and proteomics. This research focused on children with Congenital Zika Syndrome CZS+ (n=15) and control children CZS- (n=15), utilizing gas chromatography-mass spectrometry (GC-MS) for metabolite identification (total n =30). Vesicles were isolated using Izon qEV columns, quantified, and characterized by nanoparticle tracking analysis and transmission electron microscopy. The results pointed to 12 metabolites and 18 proteins used in the construction of a classifier model by machining learning. Metabolite analysis indicated involvement in the PI3K-AKT-mTOR pathway and suggested a role in Angiotensin inhibition in CZS+. Upstream of mTOR, Akt is the central signaling molecule in the PI3K pathway and plays critical roles in brain development and synaptic plasticity important for Zika Virus. The study provides insights into molecular mechanisms associated with CZS+. The study pinpointed valuable possible biomarkers in Zika virus (ZIKV) infection, specifically proteins and metabolites. We have submitted our methods to the EV-TRACK knowledgebase, Human Metabolome Database, and Comite de ética CAAE: 86696618.7.0000.5467.

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OP-18

Metabolomics with Q-Orbitrap and Q-Linear Ion Trap – New Solutions for Targeted and Untargeted Analysis

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Keywords: Quadrupole-Orbitrap, Exploris series, untargeted metabolomics

The LC-MS/MS systems based on Quadrupole-Orbitrap mass analyzers from the Thermo Scientific Exploris series offer unique capabilities for the identification and quantification of metabolites and biological markers, making them a valuable analytical tool in untargeted metabolomics. To bridge the gap between the discovery and validation of thousands of biomarkers in translational studies, the latest LC-MS/MS^n Quadrupole-Ion Trap system from Thermo Scientific delivers unmatched capabilities in targeted analyses, achieving sub-single-cell sensitivity with throughput of hundreds of samples per day. This brief talk presents some of the advantages of using these technologies.

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OP-19

Separation technique hyphenated with mass spectrometry for improved metabolome coverage, from conventional to miniaturized approaches.

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Keywords: Bioanalysis, Metabolomics, µLC-MS, Sensitivity

Several analytical setups are required to provide a broad coverage of complex samples in metabolomics. A chemical library containing 597 metabolites was used as a benchmark to evaluate several separation modes (i.e. RPLC, HILIC, SFC, CE, etc.) hyphenated to high resolution MS. A scoring approach allowing to compare the performance of different separation techniques was used, taking into account both chromatographic and MS attributes (i.e. retention/migration, signal-to-noise ratio, peak intensity and shape). The scores not only allowed to evaluate each analytical platform, but also to optimize the number of analytical methods needed. The sensitivity could be drastically improved with miniaturized set-up due to the conventional analytical flow regime of 0.2-1 mL/min commonly used with LC. A far higher sensitivity can be obtained with nanoelectrospray thanks to a better ionization efficiency. Therefore, we explored microflow regime (i.e. 1-5 µL/min) with a novel microfabricated monolithic multinozzle electrospray emitter. The latter allows for flow splitting to obtain multiple stable nanosprays. This setup was compared to the protocol employed in our laboratory.

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OP-20

Metabolomics in practice: The IonMedicine experience

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Keywords:Metabolome, Biomarkers, precision medicine, nutrition

IonMedicine is a company dedicated to advancing precision health through metabolomics. Its mission is to provide innovative solutions for private companies and universities, spanning human, veterinary, and agricultural sciences. Specializing in both targeted and untargeted metabolomics, IonMedicine leads several key initiatives. These include the development of a nutrimetabolomics test through IonNutri, designed to create personalized nutrition plans, and precision medicine projects focused on identifying biomarkers for various health conditions. Through IonVet, veterinary science efforts focus on monitoring health, evaluating therapeutic responses, and optimizing animal nutrition across all species. In agriculture, metabolomics is applied to discover novel metabolites and investigate intricate biochemical pathways in plants. Comparative analysis helps unravel metabolic responses, generating hypotheses on metabolite functions. In conclusion, IonMedicine's expertise is driving transformation in critical areas while promoting the potential of metabolomics across Brazil and Latin America, making this cutting-edge technology more accessible to a broader audience.

OP-21

ExpoSomics and Emerging Contaminants: A Brief Contribution to Understanding the Pharmaceutical Exposome and Antimicrobial Resistance

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Keywords: expossome, antimicrobial resistance, surface water, TFME-HPLC

Exposomics is a concept used to describe the cumulative impact of environmental exposures throughout our lives and how these exposures affect our health. Exposure to sub-therapeutic doses of antibiotics present in water may create selective pressure favorable to the development and survival of resistant bacteria. In this study, a TFME-HPLC method was developed and optimized for the evaluation of predicted and prioritized antibiotics, and the diversity of resistant bacterial species in surface waters was also determined. Thin film microextraction (TFME) was used to preconcentrate the water samples. PAN/PS-DVB showed the best recovery using ACN:H_2O (25:75) as desorption solvent. Antimicrobial susceptibility tests were performed using disk diffusion, and the selected bacterial species were identified by MALDI-TOF. Approximately 196 gram-negative microorganisms were isolated and identified. This approach optimized efforts for monitoring antibiotics in water, as their presence can increase the rate of horizontal transfer of resistance genes between different bacterial strains, allowing sensitive bacteria to rapidly acquire resistance.

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OP-22

Determination of allergenic proteins in food by on-line aptamer affinity solid-phase extraction capillary electrophoresis-mass spectrometry

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Keywords: aptamer, capillary electrophoresis, in-line; on-line; solid-phase extraction, food.

Today, it is widely accepted that high-performance separation techniques coupled to MS, such as LC-MS and CE-MS, are the preferred techniques for reliably analyzing protein biomarkers, at the intact level or after enzymatic digestion for bottom-up peptide mapping. However, in many cases, protein biomarkers are found at very low concentration in highly complex samples, such as food contaminated with allergenic proteins. Various strategies have been described to enhance sensitivity in LC-MS and CE-MS, including the on-line coupling of SPE for sample clean-up and analyte preconcentration from large sample volumes. On-line SPE-CE-MS is particularly advantageous, as it can be easily automated using valve-free microseparation set-ups in commercial CE instruments [1]. Here, I will provide an overview of our latest advancements in SPE-CE-MS for analyzing allergenic proteins at the intact level in food using aptamer-based sorbents [2-3]. The combination of aptamer affinity and selectivity, electrophoretic separation, and MS detection allows high-selectivity, high-sensitivity, and accurate quantification, with no possibility of false positives due to the unequivocal identification.

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OP-23

Advances on the integration of electrochemical and optical detectors to 3D-printed microfluidic devices

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keywords: 3D printing, microfluidic devices, electrochemical detection, fluorescence detection, lab on a chip

Our research group has been contributing to the establishment of methods and strategies of microfabrication of microfluidic devices using two 3D printing techniques, named Fusion Deposition Modeling (FDM) and Stereolithography (SLA) and its variation Digital Light Processing (DLP). Here, we address the integration of electrochemical and optical detectors to directly 3D-printed microfluidic channels. Contactless Conductivity Detection (C^4D) was implemented in both FDM- and DLP-made microdevices. Particularly, multi-material FDM is an interesting option to build devices containing embedded electrodes for C^4D, since conductive filaments can be acquired from many suppliers. We also developed microdevices by DLP with spiral channels printed around a 40 µm separation channel. Afterwards, the spiral channels were filled with Gallium in order to integrate the electrodes. Microchip electrophoresis with C^4D has been used mostly to the separation and detection of inorganic ions. Electrodes for amperometric detection were prepared with carbon black and commercial photoresins and used without the need of alignment tools. Potentiometric detection has also been implemented in our group in the Extended-Gate Field Effect Transistors setup. This strategy has been applied on the detection of anions and creatinine in biological fluids. Fluorescence detectors have also been successfully implemented in DLP-printed microfluidic channels. A multichannel optical detector and LED light sources were closely mounted to the microfluidic channel for the detection of Fluorescein and Rhodamine B. Recently, we developed a DLP multi-material 3D printer that allowed the preparation of objects up to four materials, including microfluidic devices containing embedded electrodes for C^4D and microchannels as narrow as 42 µm.

OP-24

3D Printing with Conductive Polymers in Capillary Electrophoresis and Microchip: Characteristics, Possibilities, and Limitations

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Keywords: 3D Printing, conductive filament, detection, high voltage, instrumentation

Although the most commonly used materials in 3D printing are insulators, it is also possible to find conductive materials (CMs), which further expands the possibilities of 3D printing. The opportunities for this combination of materials in capillary electrophoresis and microchip applications are numerous. For instance, it is possible to envision the use of CMs for connecting to the high-voltage source and even in the fabrication of electrodes at the ends of the devices. For the first purpose, the relatively low conductivity of a typical CM is not a limiting factor, but their inferior electrochemical behavior compared to platinum is certainly worth considering. When using conductive materials in the implementation of detectors such as C^4D, amperometric detection, or even in connecting a photodetector, it is crucial to consider both conductance and susceptance, as the material's behavior at high frequencies is important. Results on admittance, dielectric rigidity, contact resistance, voltammetric behavior, and thermal effects of carbon black-PLA and other materials will be presented and discussed, as well as possible applications and limitations of CMs in CE and microchips.

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OP-25

How low can we go? – A novel preconcentration strategy for the characterization of intact glycoproteins

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Keywords: Sheathless capillary electrophoresis, mass spectrometry, preconcentration, erythropoietin, intact protein

Erythropoietin (EPO) is a hormone which, in its recombinant form, is used for the treatment of anemia. The glycosylation of EPO is very important for in vivo biological activity and half-life and is considered a critical quality attribute (CQA). Sialylation is generally determined by CE-UV, however, information on other CQAs such as LacNAc repeats is not attainable. CE-MS provides a detailed overview of the glycosylation of EPO proving itself a powerful alternative for the characterization of EPO biopharmaceuticals.
Assessment of glycosylation during production is important to take informed decisions on the fermentation process. However, the concentration of EPO in fermentation supernatant is often very low limiting the application of most analytical approaches including CE-MS. We developed a novel CE-MS preconcentration strategy based on pH junction which allowed to increase the injection volume in the capillary up to 40% while maintaining a good separation profile. To further boost the sensitivity a sheathless CE-MS interface permitting nano-ESI was applied. The method allowed to analyze EPO at the intact level at low concentrations permitting to analyze several fermentation timepoints.

Abstracts – Poster Communications

PP-01

N-glycan biomarkers for early screening of type 2 diabetes: Sugars against sugar

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Keywords: type 2 diabetes, biomarker, N-glycan, capillary electrophoresis

Diagnosis of type 2 diabetes in its early stages is currently a major challenge, emphasizing the need for rapid, simple, and reliable methods for the screening of the disease. Our research aimed to develop a novel capillary electrophoresis-based analytical method suitable for the identification of potential N-glycan biomarkers from human blood before the disease appears and causes comorbidity. To obtain comprehensive profile information, the samples were treated with organic reagent (protein precipitation), enzymatically digested, fluorophore labelled and analyzed by capillary electrophoresis. Our results revealed detectable differences between the N-glycan profiles of close relatives who were healthy but later one became diabetic, and the other did not. The method may allow the prediction of diabetes before the onset of the disease, creating a new early screening method that can be easily integrated into routine diagnostics. In addition, clinical information from specific glycoprotein N-glycosylation profiles in diabetes may help to shed light on the underlying inflammatory pathophysiological processes and lead to new drug targets.

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PP-02

Determination of Glycerol in Biodiesel by Micellar Electrokinetic Chromatography

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Keywords: biodiesel, glycerol, micellar electrokinetic chromatography, fuel, derivatization

Biodiesel is synthesized from natural resources like vegetable oils, animal fats, and recycled cooking oil. It is a fuel that reduces greenhouse gas emissions and supports sustainable practices. Glycerol, a primary contaminant in biodiesel, can disrupt engine performance even in trace amounts. The European Union and the American Society for Testing and Materials have established standards for permissible glycerol levels in 0.24 and 0.25 %w/w, respectively.
To simplify this process, a robust method using MEKC is proposed. This method is based on glycerol reaction with iodate to produce formaldehyde which reacts with 3-methyl-2-benzothiazolinone hydrazone as a derivatizing to generate an adduct with adequate characteristics to be separated by MEKC. Under optimal conditions a linear range from 0.06 to 0.30 %w/w with a limit of detection of 0.02 %w/w, repeatability and reproducibility below 6.0% was obtained. The proposed methodology was applied to real biodiesel samples and the results obtained were similar (α=0.05) to those obtained using the reference methodology. MEKC is a competitive alternative for biodiesel quality assessment.

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PP-03

Determination of corticoids in cosmetic cream samples by micellar electrokinetic chromatography

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Keywords: corticosteroids, cosmetic, creams, electrophoresis, MEKC.

Illegal addition of corticosteroids to cosmetic products has been described with the aim of obtaining a whitening and/or rejuvenating effect on the skin causing harmful consequences to health. In this sense, it is important to have methodologies that allow their analysis in complex matrix.

Corticosteroids are generally found in their neutral form, so their electrophoretic analysis was performed using MECK, the analytes were detected at 254 nm using methylprednisolone as internal standard. The optimal background electrolyte composition was: sodium phosphate (25 mM), sodium dodecyl sulfate (5.0 mM) and sodium taurocholate (30.0 mM), adjusted to pH 7.0. Solid phase extraction was employed for sample treatment and the SPE-MEKC combination was applied to spiked cream samples. Under optimal conditions, it was obtained a linear range of 8.0-48.0 mg kg^{-1}, with limits of detection of 2.0-2.4 mg kg^{-1}. Repeatability and reproducibility were < 10.0 % (n=3) with recoveries values around 100.0 %. A total of 12 samples (cosmetic creams) were analyzed using the proposed methodology, in all cases the concentrations found were <LOD.

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PP-04

Application of Fe_3O_4@SiO-LDH/DS^- as an efficient adsorbent for the removal of tetracyclines from milk samples by capillary electrophoresis

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Keywords: Layered double hydroxides, tetracyclines, capillary electrophoresis, large volume sample stacking

Antibiotics are chemical compounds commonly used in human and veterinary medicine. Tetracyclines (TCs) as tetracycline (TC), chlortetracycline (CT), oxytetracycline (OT), and doxycycline (DT) are examples of antibiotics. Nevertheless, they might be used as growth promoters, and, in consequence, the TCs could be presented in animal origin food, such as milk, which can enter the human body and cause health problems. International organizations have established maximum residue limits (MLR) to regulate the presence of antibiotics in animal origin food (300 g kg^{-1} for the combined residues of TC, OT, and CT).
This work shows a layered double hydroxide (LDH) coupled to magnetic particles (Fe_3O_4@SiO-LDH/DS^-, where DS^- is the interlayer anion) as an alternative for the removal of four tetracyclines. We used large volume sample stacking capillary electrophoresis (LVSS-CE) to achieve LODs around the MRL. Under optimal LDH synthesis (reaction time of 30 min, Mg^{2+}/Al^{3+} molar ratio 7:1, and DS^- as interlayer anion), and magnetic solid phase extraction (MSPE) conditions (pH 6, 5 min of contact time, 10 mg of adsorbent) percentage removal of 99.0% for each tetracycline were obtained.

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PP-05

Simple and low-cost platform for fluorescence measurements integrated with microcontrollers.

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Keywords: fluorescence, microcontrollers, 3D printed,

The fluorescence spectroscopy is a technique that allows for extremely low limits of detection, high selectivity, and fast results [1]. However, portable and low-cost devices usually lack automation and adaptability to different applications [2].
In this work we present a device capable of performing fluorescence assays in the visible spectrum range and also allows the controlled injection of different reagents. This device was created using a commercial multispectral light sensor, homemade syringe pumps, commutative valves, a microfluidic channel to mix reagents, and a microcontroller that integrate all parts. Due to the multispectral functionality of the selected sensor, this simple system can be used with a variety of fluorescent probes, which is a major advantage compared to other portable fluorometers that use photodiodes as detectors. We estimate that the cost to produce the whole device is less than 60 USD.
As proof of concept, rhodamine B and fluorescein were used to create analytical curves. Without any optimization, we obtained a limit of detection of 79 nmol L^{-1} with linear range from 0.25 to 100 µmol L^{-1} for Rhodamine B. For fluorescein the limit of detection was 229 nmol L^{-1} with linear range from 0.68 to 10 µmol L^{-1}.

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PP-06

Determination of cocaine residues and metabolites in breast milk: a special approach for milk banks

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Keywords: breast milk, cocaine determination, gas chromatography, mass spectrometry, human milk banks

Breast milk is essential for newborn nutrition, but drugs such as cocaine (COC) can be transferred through it, posing potential risks to infants. In Brazil, human milk banks currently use self-reported questionnaires for drug screening. This study aims to develop a GC-MS method to detect COC residues and metabolites in breast milk and apply it to milk bank samples to estimate the prevalence of these substances. The sample preparation involved acidifying the milk (spiked or blank), vortex mixing, centrifugation, transferring the aqueous phase, using solvents and NaCl for cleaning, transferring the organic phase, drying under nitrogen, and resuspension in ethyl acetate before GC-MS analysis. Validation studies on drug-free samples showed linear ranges from 2.5 to 250 ng/mL, with LOQs starting at 2.5 ng/mL. Precision (RSD%) and accuracy (Bias%) were up to 12.8% and 14.6%, respectively (n=15, 4 concentration levels, 3 days). Stability studies demonstrated samples remained stable for at least one week in the freezer and 2 days at room temperature. The results indicate that this work can contribute to the already rigorous safety standards for breast milk donation in Brazilian milk banks.

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PP-07

Determining major Capsaicinoids in pepper by capillary electrophoresis with UV detection using dual-surfactant in BGE: method development and validation

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Keywords: Electrophoresis, Capsaicin, Capsicum, Pungency, Figures of Merit

Peppers are globally consumed primarily for their spicy flavor, with capsaicinoids (CAP) being key due to their pungency[1]. A study was conducted to identify major CAP in real pepper samples using capillary electrophoresis with UV detection. The method was developed by optimizing the chemical composition and pH of the background electrolyte (BGE) along with instrumental parameters. A dual-surfactant system was utilized for the baseline separation of Capsaicin (C) and Dihydrocapsaicin (DC) ($R > 1.5$), detected at 214 nm; CAPs were confirmed by the spiking method and UV spectra analysis. Sample preparation involved a simple methanolic extraction of dried pepper through dynamic maceration. The optimized method showed good precision (RSD < 5% for peak areas; intra- and interday tests) and accuracy (recovery over 80%). Linearity was assessed by ANOVA, revealing no lack of fit (p-values of 0.07 and 0.27 for C and DC, respectively), with limits of detection at 8.48 mg L^{-1} for C and 5.53 mg L^{-1} for DC. This validated method was applied to three different pepper species.

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PP-08

Multivariate data analysis for carbohydrate profiling in isothermal wort

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Keywords: Beer, Wort composition, Fermentable sugar, Principal Component Analysis, Hierarchical Cluster Analysis

Aiming to optimize the process of beer production and improve quality, the changes in the fermentable sugar composition during the mashing process of Pilsner malt wort were studied.[1,2] Our research introduces a novel approach, utilizing capillary electrophoresis with UV detection to analyze key sugars—glucose, maltose, maltotriose, fructose, and sucrose—across mashing temperatures ranging from 61°C to 75°C.[3] Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) revealed distinct groupings based on mashing time and temperature, highlighting enzyme activity patterns. The distribution of samples in the PC1 versus PC2 scores plot indicated the limit of activity to dextrinase (61°C), beta-amylase (61-67°C), and alpha-amylase (65-75°C). Samples mashed at similar temperatures clustered together in the HCA, reflecting enzyme activity patterns, with alpha-amylase activity evident from 71 to 75°C. These insights provide valuable information for optimizing mashing conditions and introduce an analytical technique that significantly improves the accuracy, efficiency, and environmental sustainability of carbohydrate analysis in brewing.

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PP-09

CE-ICP-MS on the hunt for liposomal rejuvenation potion

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Keywords: CE-ICP-MS/MS, hyphenated techniques, liposomes, tripeptide copper complex (GHK-Cu)

The tripeptide copper complex (GHK-Cu) exhibits exceptional regenerative and anti-inflammatory properties [1], making it a valuable ingredient in modern cosmetic formulations that support skin renewal. However, its limited skin permeability and relatively high price pose some obstacles. Encapsulation of GHK-Cu in liposomes offers a potential solution by facilitating its effective penetration into deeper skin layers and providing prolonged release [2]. In this work, the CE-ICP-MS/MS optimized method was used to characterize liposome-GHK-Cu suspensions obtained by ethanol injection method and to study their permeation through human skin mimicking membranes. The lipid composition of the vesicles was optimized for efficient encapsulation of GHK-Cu and its effect on liposome permeability was evaluated. Liposomes containing GHK-Cu with a size below 200 nm were stable for at least 2 weeks, and *in vitro* tests showed their improved permeability compared to non-encapsulated GHK-Cu. The results obtained demonstrate the applicability of liposomes as a biocompatible delivery system that could enhance the therapeutic effect of the anti-aging complex and promote its use in cosmetic formulations.

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PP-10

Capillary electrophoresis for the determination of carbohydrates in lignocellulosic biomass through acid hydrolysis

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Keywords: Syngonium podophyllum, Electrophoresis, Saccharification, Xylose, Glucose

Lignocellulosic biomass is a valuable renewable resource for biofuels and chemicals. Pre-treatment, especially acid hydrolysis, is crucial for converting cellulose and hemicellulose into fermentable sugars, such as pentoses and hexoses.[1] This study applied dilute sulfuric acid under reflux to *Syngonium podophyllum* hydrolysis, a lignocellulosic urban residue, aiming to assess its potential as a feedstock without competing with food-derived biomass sources.[1] Capillary Zone Electrophoresis was applied to the determination of glucose and xylose, using a background electrolyte consisting of 5 mmol L^{-1} phthalic acid and 0.4 mmol L^{-1} CTAB at pH 12.5.[2] Linearity was verified in the range of 20.0 to 1800.0 μg mL^{-1}, using sucrose as the internal standard, and a limit of detection of 6.3 μg mL^{-1} were found for both analytes. The results revealed the saccharification of the biomass under reflux pre-treatment, with xylose content measured at 36.6 ± 3.4 mg g^{-1}. Glucose was detected, but its value was below the limit of quantification. The study of saccharification of *Syngonium* biomass provided valuable information on the efficiency of the hydrolysis method for carbohydrate extraction.

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PP-11

Simultaneous separation of artesunate and mefloquine in fixed-dose combination tablets by CZE-UV

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Keywords: mefloquine, artesunate, capillary zone electrophoresis, Box–Behnken, quality control

A novel method was proposed for simultaneous determination of artesunate (ATS) and mefloquine (MFQ) in fixed-dose combination tablets by capillary zone electrophoresis with simultaneous direct and indirect detection by ultraviolet (CZE-UV). The background electrolyte, consisting of 30/15 mmol L^{-1} TRIS/3,5-dinitrobenzoic acid buffer at pH 8.2, a chromophore buffer, was selected taking into account a detailed study involving the effective mobility vs. pH curves of the analytes and electrolyte compounds in association with the very low molar absorptivity of ATS. Suitable separation conditions, considering voltage, temperature and buffer concentration as factors, were achieved through the 3^3 Box–Behnken design investigation. The optimum baseline separation conditions were: injection pressure of 30 mbar for 10 s, cartridge temperature of 22.5 ºC and positive voltage of +30 kV. The method proved to be rapid (5 minutes), simple, selective, linear ($r^2 > 0.98$), precise (relative standard deviation (RSD): ATS < 2.9% and MFQ < 2.2%) and accurate (recoveries: ATS 98.13–102.96% and MFQ 98.75–106.77%), proving to be suitable for routine quality control analysis.

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PP-12

Primaquine analysis in pharmaceutical formulation using multiple and short end injections by capillary zone electrophoresis with UV detection

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Keywords: primaquine, capillary electrophoresis, multiple injections, short-end injection, degradation

Novel methods were proposed for determining primaquine (PQN) in tablets by multiple-injection capillary zone electrophoresis (MICZE) and by capillary zone electrophoresis by short-end injection procedure (CZE-SEIP) with UV detection. The background electrolyte (BGE), consisting of 20/30 mmol L^{-1} Tris/HCl at pH 2.0, was selected considering a comprehensive study involving the effective mobility versus pH curves of the analytes and BGE components. Experimental designs were applied in methods developments, showing chemometric tool's applicability in achieving suitable electrophoretic conditions. A baseline resolution in the separation of adjacent peak pairs was obtained by injecting a spacer electrolyte for 18 s, with a voltage of +15 kV, and the sample can be injected six consecutive times in a single run in less than 3 min, in the MICZE-UV method. For the CZE-SEIP-UV method, the migration time of PQN was 0.6 min, and the method was applied to a demonstrative forced degradation study. Some validation parameters were evaluated for both methods, and all results were satisfactory, indicating that they can be implemented for PQN determination in routine quality control analyses.

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PP-13

UHPLC-MS/MS Analysis on *Brachyotum naudinii* Triana Composition and its Toxic and Antimicrobial Activities

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Keywords: Brachyotum naudinii Triana*, LC-MS/MS, anthocyanins, antioxidant potential.*

Brachyotum naudinii Triana (*Melastomataceae*), grows in the high Andean areas of South America. This species shows purple and violet flowers which are potential source of natural dyes, phenolic and anthocyanin compounds. This work aims to evaluate the chemical composition of *B. naudinii* T. flowers using ultra high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) as well as the *in vitro* anthocyanin antioxidant potential study, preliminary toxicity against *Artemia salina* Leach and the antimicrobial activity. Twenty-eight compounds were identified by UHPLC-MS/MS (flavonoids, tannins, anthocyanins, lipids, disaccharides, coumaric acids and organic acids). The extract showed antimicrobial activity against *Staphylococcus aureus*, moderate toxicity against *Artemia salina* L. (LC_{50}=106.9±9.9 µg mL^{-1}), antioxidant capacity by inhibiting $DPPH^{\bullet}$ and $ABTS^{\bullet+}$ radicals and reducing power in the FRAP test. This study has expanded the knowledge of the chemical composition and bioactive properties of *B. naudinii* T. flowers, underscoring its potential for future biotechnological and pharmaceutical applications and establishing a solid foundation for further research in this field.

PP-14

Fast Stability-Indicating RP-HPLC Method for Determination of Antiarrhythmic Drug Amiodarone in Pharmaceutical Formulation

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Keywords: RP-HPLC, amiodarone, method validation

Amiodarone is a potent antiarrhythmic drug used to treat and prevent various types of cardiac arrhythmias by stabilizing heart's electrical activity. The aim is to develop and validate a rapid stability-indicating reverse-phase high performance liquid chromatographic method for determination of amiodarone in tablets and its separation from degradation products. Chromatographic analysis was performed using a Symmetry C8 (150 × 4 mm, 3.5 µm) column, mobile phase acetonitrile:sodium hydrogen phosphate buffer, pH 2.2 adjusted with orthophosphoric acid (70:30, v/v), flow rate of 1.5 mL min^{-1}, and detection at 240 nm. Samples were subjected to alkaline, acidic, thermal and oxidative stress conditions. Amiodarone was separated from its alkaline and oxidative degradation products within 2.1 min. Proposed method exhibited linearity with R^2 value of 0.9974. Limits of detection and quantitation were 4.9 and 14.9 µg mL^{-1}, respectively. Recovery ranged from 99.80 and 102.00%. Proposed method was effectively applied to the determination of amiodarone in tablet preparations without interference from degradation products and excipients. The method is suitable for routine analysis of amiodarone.

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PP-15

Lifelong Exercise and Metabolic Health: Differential Serum Metabolite Responses in Young and Master Athletes

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Keywords: metabolomics, athletes, physical exercise, keyword4, keyword5

Physical exercise modulates numerous metabolic and signaling pathways, yet the specific pathways linked to enhanced immune function in lifelong exercisers remain largely unexplored. A key question is whether immunometabolic responses to exercise are preserved during healthy aging. Here, we investigated the impact of lifelong athletic training on serum metabolite profiles following a 30-minute cycling exercise at the ventilatory threshold, comparing master and young athletes. Master (51.8±8.97 years, n=12) and young (22.0±4.06 years, n=7) athletes performed a maximal aerobic test on a cycle ergometer to determine their peak oxygen uptake ($\dot{V}O_2$) and ventilatory threshold (VT). After 24 hours, they completed a 30-minute steady-state cycling session at an intensity 5-15% above their VT. Blood samples were collected immediately after, and serum metabolome assessment was performed using 2D NMR experiments. Data were analyzed using multivariate statistical models, including PCA and OPLS-DA, to identify key metabolites (VIP > 1) driving group differences, followed by pathway enrichment analysis via MetaboAnalyst 5.0. Partial segregation between young and master athletes groups was observed. Eight metabolites emerged as key contributors to groups

differentiation, including Alanine (p=0.029), Glutamine (p=0.043), Leucine (p=0.039), Betaine (p=0.039), Glucose (p=0.008), Glycerol (p=0.0003), Ethanol (p=0.006), and Succinate (p=0.013). Four metabolic pathways—ammonia recycling, phenylalanine and tyrosine metabolism, valine, leucine, and isoleucine degradation, and the transfer of acetyl groups into mitochondria—were similarly enriched. However, carnitine synthesis and branched-chain fatty acid oxidation were differentially enriched. Lifelong exercise seems to help preserve essential metabolic functions (e.g., amino acid metabolism, mitochondrial energy production) while promoting adaptations that improve fat oxidation and energy efficiency, thereby contributing to the maintenance of metabolic health with aging.

PP-16

Determination of Sucralose Using Capillary Electrophoresis with Capacitively Coupled Contactless Conductivity Detection

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Keywords: artificial sweetener, electromigration, separation methods, electrochemical detection

Due to its intense sweetness, sucralose, a zero-calorie sweetener, has gained popularity as a sugar substitute. However, extensive research has been conducted to fully comprehend its potential impact on human health and in the environment. This study developed a new method to determine sucralose in commercial sweeteners using capillary electrophoresis (CE) with capacitively coupled contactless conductivity detection (C^4D). A homemade CE-C^4D system was used with a bare fused silica capillary and a background electrolyte composed of NaOH and Na_2HPO_4. Galactose was used as an internal standard. The method showed high separation efficiency, with limits of detection (LOD) and quantification (LOQ) of 4.9 mg/L and 16.4 mg/L, respectively. Recovery tests demonstrated good accuracy, with recovery percentages ranging from 82% to 119% for two different commercial samples of tabletop sweeteners. The original sucralose concentrations found in the two samples were (20.7 ± 0.8) mg/mL and (25.6 ± 0.6) mg/mL. The proposed CE-C^4D method was considered simple and reliable for quantifying sucralose in commercial samples of sweeteners.

PP-17

The Evaluation of Galectin-1 – Glycopeptide Interactions by Affinity Monolith Chromatography

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Keywords: affinity chromatography, frontal analysis, monolith, galectin-1, glycopeptide

Weak affinity chromatography on monolithic support is a powerful technique for quantification of the specific interactions between immobilized ligand and its target. This approach is convenient for weak-to-moderate binding strengths with typical dissociation constant of the complex falling to the range of mM to µM. Recently, the staircase frontal affinity experimental setup was introduced to increase throughput of the affinity screening [1]. Here, the monolithic support consisted of poly(GMA-co-EDMA) acrylate grafted with streptavidin by reductive amination. Then, the biotinylated target protein was attached to the monolithic column through the streptavidin-biotin linkage [2-3]. In our case, a protein of interest was galectin-1 stemming from a group of galectins, which have affinity for beta-galactosides. A set of specifically designed glycopeptides was evaluated as ligands for galectin-1. Typically, the glycopeptides consisted of 8 amino acids with 0-2 saccharide moieties, glucose or thiolactose, attached to the side-chain by an appropriate linker. The dissociation constant K_d values of the ligands were then calculated from a double reciprocal plots displaying the amount of ligand captured on the monolithic column vs. the ligand concentration [2-3]. The values obtained varied from 10 µM for the compound with the highest affinity, to 100 µM for the thiodigalactoside standard.

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PP-18

Determination of amino acids in retina of the chicken embryo through capillary electrophoresis

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Keywords: Central nervous system, Retina cells, Neurotransmitter Amino Acids, Chemical Derivatization

Amino acids play crucial roles in neurochemical processes and can serve as key biomarkers for understanding biological phenomena.[1,2] This study introduces a novel analytical method utilizing capillary zone electrophoresis for the determination of amino acids involved in neurochemical activities. The developed and validated electrophoretic method allowed the selective quantification of arginine, citrulline, glutamate, and aspartate, along with eight other amino acids—lysine, ornithine, tryptophan, valine, serine, alanine, glycine, and tyrosine—in solutions containing a total of 22 amino acids. Chemical derivatization was performed with ortho-phthalaldehyde (4 mmol L^{-1}) and tert-butyl mercaptan (5 mmol L^{-1}), and the method exhibited a linear concentration range from 0.2 to 10 µg mL^{-1}, with detection limits between 0.06 and 0.15 µg mL^{-1}. A simple aqueous extraction method was employed for the preparation of chicken embryo retina samples, preserving the integrity of water-soluble proteins without compromising the method's selectivity. This study proves to be robust and reliable for determining amino acids in biological samples, offering valuable insights into neurochemical processes.

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PP-19

Chemical profiling of Amazonian Propolis using a metabolomics approach

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Keywords: propolis; mass spectrometry; bees; liquid chromatography; untargeted metabolomics.

Propolis is a resinous mixture produced by bees by mixing plant resins with salivary enzymes and beewax [1]. Propolis extracts have been used in folk medicine due to their antioxidant, antibacterial, and antiviral properties. While Brazil is a global leader in propolis research, studies on the chemical composition of Amazonian propolis remain limited. This pilot study aimed to characterize the chemical profile of four Amazonian propolis samples, produced by different bee species, using an untargeted metabolomics approach. The samples were extracted using methanol and analyzed by UPLC-ESI-QTOF-MS. Several bioactive compounds were tentatively identified, including terpenoids, flavonoids and polyphenols, which are known for their antioxidant, antiviral, and antibacterial effects. The compounds were identified based on their exact mass, precursor ion fragmentation, and isotopic patterns. Results showed that all propolis samples contained bioactive compounds with health-beneficial properties, although the composition varied among the bee species. Therefore, this study provides a basis for future research on Amazonian propolis and supports local propolis-producing communities.

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PP-20

Determination of multiclass antibiotics by capillary electrophoresis using the AQbD approach

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Keywords: CZE, TFME, antibiotics, AQbD

The use of antibiotics in human health and livestock farming has led to the contamination of surface waters, contributing to the rise in antimicrobial resistance. Antibiotics have been detected in low concentrations (ng L^{-1}) in water bodies, and their analysis has typically been conducted using LC-MS/MS, which incurs high costs. The development of alternative and more accessible methods is important for the environmental agencies monitoring these compounds. In this study, a capillary electrophoresis method was developed to determine two classes of antibiotics (beta-lactams and quinolones) in surface water. Analytical Quality by Design (AQbD) was used with the objective of achieving the shortest separation time. An experimental design (DOE) was defined by the evaluation of voltage, buffer concentration, and additives. The optimized conditions were 20 mM sodium tetraborate, 20 kV voltage, 10 s injection, and detection at 254 nm. The antibiotics were separated in less than 6 min, with high resolution. Thin film microextration was used to preconcentrate samples. This developed approach can be used for low-cost monitoring of antibiotics in surface waters, while also being considered a 'green' method.

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PP-21

Low-Resolution CZE-MS screening data of urine samples associated with deep learning modeling for discriminative classification of COVID-19

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Keywords: CZE-MS, Machine Learning, COVID-19

Aiming at a focused study involving a "segmented untargeted metabolomics" of key groups of biomarker candidates for COVID-19 diagnosis, a dataset containing low-resolution mass spectra information was collected by using a CZE-QQQ system followed by deep learning processing. Knowing that amino acids are a fundamental group of chemicals present in human urine as final products of metabolic pathways, an analytical method was developed based on the intrinsic selectivity that features CZE analysis combined with effectiveness of mass spectrometry on finding fingerprinting information for registering low-weighted cations with amino acid-like structures. A hundred urine samples of volunteers that were submitted to the RT-PCR test for COVID-19 were analyzed as a part of a Test Group (38) and a Control Group (62) in an Agilent 7100 CE triple Quadrupole system operated in ESI (+) at scan mode with *m/z* range from 20 to 500. The CZE component was operated under normal polarity applied in a pH 3 BGE with hydrodynamic injection. The raw mass spectra dataset was modeled through Randon Forest algorithm considering a variable selection strategy where only differentiated *m/z* among positive and negative cases, faced against an average spectrum, were indeed modeled resulting in 80 % accuracy and 0.612 MCC. Despite not reaching the accuracy standards for diagnostic applications yet, the study provides valuable insights into using capillary electrophoresis coupled with low-resolution MS under an investigative metabolomics perspective useful for gathering valuable information about health-related issues or any complex analytical environment.

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PP-22

3D-Printed Porous Microstructures and their Role in Electromambrane extraction

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Keywords: Electromembrane extraction, 3D printing, porous structure

Sample preparation is increasingly relevant due to the ongoing need to isolate target analytes in complex matrices. Electromembrane extraction (EME) is a microextraction technique in which analytes electrically migrate from an aqueous donor to an acceptor solution. This migration is generated by an electric field applied across an immiscible liquid membrane supported on a porous membrane. Usually, EME is conducted using a porous hollow fiber (HF) impregnated with an organic solvent that has low polarity and suitable selective to the target compound[1]. EME can provide quick and efficient microextraction of several ionic and ionizable compounds with minimal use of organic solvents, great sensitivity, and selectivity.
In this work, we have developed a new and innovative fabrication method of porous membrane for EME, utilizing 3D Printing and TPMS (Triply Periodic Minimal Surfaces) method[2]. A custom photopolymerizable resin was formulated to 3D print the porous with suitable sizes to support a liquid membrane to pre-concentrate emerging pollutants using EME. This novel process showed the potential to fabricate EME membranes to replace commercial HF.

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PP-23

Synergic effect evaluation of antiplatelets and statins on infarcted patients: a targeted metabolomics approach

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Keywords: Metabolomics, Cardiovascular Diseases, TMAO, Adenosine, L-Carnitine

Coronary artery disease (CAD) is related to metabolites changes in biofluids [1]. Metabolites as Trimethylamine-N-Oxide (TMAO), L-Carnitine and Adenosine have been related to CAD, statins, and antiplatelets administration [2-6]. Thus, this study aimed to inspect the concentration changes of these three metabolites in urine of infarcted patients treated with four therapeutic strategies. The patients (n=80, 20 per arm) were randomized to be treated with rosuvastatin+clopidogrel (G1), simvastatin+clopidogrel (G2), rosuvastatin+ticagrelor (G3) and simvastatin+ticagrelor (G4). The urine samples were collected within 24 h, 30 and 180 days after administration. No therapeutic strategy was efficient in decreasing TMAO and L-Carnitine levels, even after 180 days of treatment. Adenosine levels were significantly increased in all groups after 180 days, especially in G4 with an increase of 32% (p-value < 0.001). Patients of G4 presented increased Adenosine levels in 5% (p-value = 0.003) after 180 days when compared to patients of G2. These results suggests that simvastatin+ticagrelor was the most efficient treatment, once the highest increase of Adenosine levels in urine was observed.

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PP-24

Untarget analysis of human skin derived fibroblast cells exposed to phthalates by GCxGC-Q-TOFMS/MS

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Keywords: phthalates, HDFa, metabolomics, GCxGC, QTOF

Plastics are often modified with additives to improve properties like thermal stability, elasticity, and antistatic capabilities. However, these substances can leach into the environment alongside plastic degradation products. Phthalates, commonly used as additives, are harmful to human health. Dermal exposure to these contaminants is particularly concerning since the skin is the first barrier against chemical agents. This study aimed to investigate the exposure of human skin derived fibroblast cells to a 1:1 mixture of dimethylphthalate (DMP) and diethylphthalate (DEP), both frequently found in cosmetics. Fibroblast cells were cultured until they reached 80% confluence, and then exposed to 0.42 g L-1 DMP:DEP 1:1 for 24 hours. After exposure, cells were quenched, and the metabolites were extracted, lyophilized, and stored at -80ºC. For analysis, the dry extracts were derivatized and injected using GCxGC-Q-TOFMS/MS. Comparing control and exposed sample color plots, 613 and 442 compounds were identified, respectively, suggesting potential metabolic changes from phthalate exposure that warrant further investigation into their health effects.

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PP-25

Metabolomic fingerprint of cytotoxic extract from Gram-positive bacteria recovered from Itaguaré Beach (SP, Brazil)

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Keywords: Metabolomics, GNPS, Chemical diversity, Streptomyces sp., Itaguaré Beach

Using a metabolomics approach, this study investigated the chemical diversity of cytotoxic extracts obtained from Gram-positive bacteria recovered from sediments at Itaguaré Beach on the southeastern coast of Brazil. This method allows for comprehensive analysis of small molecules produced by these bacteria, essential for annotating novel bioactive compounds. The bacteria were prepared in A1 media with reconstituted seawater for 7 days, and the extracts were obtained using ethyl acetate. The extracts underwent metabolomic fingerprinting via HPLC-MS/MS, while spectral analysis was conducted using the Global Natural Products Social Molecular Networking (GNPS) platform. GNPS annotated a diverse range of compounds, including diketopiperazines, lipopeptides (surfactins), and desferrioxamine siderophores, along with many unidentified compounds. The use of DEREPLICATOR+ (a GNPS tool) enabled the annotation of the cyclodepsipeptide Neoantimycin D, a highly cytotoxic compound found in the extract of *Streptomyces sp.* BRB-094. These findings underscore the potential of marine-derived Gram-positive bacteria as a rich source of novel bioactive compounds for future pharmaceutical applications.

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PP-26

Untargeted metabolomic evaluation of the mefloquine for *Leishmania amazonensis* treatment

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Keywords: Leishmaniasis, mefloquine, metabolomics, mass spectrometry, analytical multiplatform.

Leishmaniasis is a neglected disease affecting millions of people worldwide, and its treatment consists of highly toxic drugs associated with adverse side effects, and parasite resistance. To circumvent such issues, repurposing drugs have been used. In this sense, this work evaluated by multiplatform untargeted metabolomics the mechanism of action of mefloquine, initially used to prevent and treat malaria, against *Leishmania amazonensis*. Two groups of *L. amazonensis* promastigotes were studied: with mefloquine (at IC50 8.4 µM) and without the drug (control group). Metabolites were extracted with methanol 50% and analyzed by LC-ToF-MS and GC-MS. Normalized data demonstrated adequate multivariate model quality parameters and grouping of QCs (quality controls). Significant *m/z*'s were searched in online databases, in which metabolites belonging to the class of amino acids, fatty acids, and lipids derivatives are highlighted. The changes in metabolism demonstrate that mefloquine acts on the cell membrane and energy pathways, essential for parasite maintenance and survival, and may be an interesting alternative for treating leishmaniasis.

PP-27

Understanding feline mammary carcinoma by untargeted metabolomics

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Keywords: GC-MS, Breast cancer, Veterinary, Amino-acids, Metabolomics.

Cancer is essentially a metabolic disease, as carcinogenic cells present distinct metabolic phenotypes[1]. Many studies have explored human metabolic alterations, but there is little understanding of the disorder in the veterinary field. Thus, there is a need for more information on the metabolic changes caused by cancer. In this work, we applied untargeted metabolomics in serum samples collected from cats with breast cancer compared to a control group (healthy animals). The samples were subjected to protein precipitation by adding cold methanol and then derivatized by silylation with a previous oximation step. The derivatized extracts were then analyzed by GC-MS. A total of 64 metabolites were annotated, of which 29 were considered significant according to univariate and multivariate statistical methods. The cancer group presented decreased levels of amino acids, indicating alterations in several pathways, such as alanine, aspartate, and glutamate metabolism, precursors of important metabolic pathways, like the TCA cycle, fundamental for energy production. This type of change is similar to that found in humans[2-3], indicating similarities between the organisms.

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PP-28

Experimental design applied to the optimization of sample plasma preparation for untargeted metabolomic analysis

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Keywords: GC-MS, Extraction Solvent, Optimization, Metabolomics.

This work aimed the optimization of extraction solvent to prepare blood plasma samples for untargeted metabolomics studies. An experimental design was used based on a triangle of mixtures using methanol, water, and acetonitrile as extractants, varying in binary, ternary, and pure compositions. The supernatants were dried and derivatized for GC-MS analysis. The design included 14 experiments, with the central point analyzed in triplicate to reduce the number of experiments without losing relevant information. Metabolite annotation was performed based on fragmentation pattern spectra and retention time of the compounds. The results showed around 60 metabolites annotated, including essential amino acids, carbohydrates, organic acids, and fatty acids. In general, extracts containing high concentrations or 100% methanol showed the most ability to precipitate proteins and extract metabolites. Despite the consistency with the instrument used, methanolic extracts can be applied to other analytical platforms with high compatibility, broadening the application and metabolic coverage of a single extract.

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PP-29

Clinical metabolomics in the study of acute kidney injury (AKI)

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Keywords: Acute Kidney Injury, Metabolomics, Biomarkers

AKI is defined as an abrupt reduction in kidney function and it is one of the main complications in the intensive care unit (ICU). One of the main limitations in the treatment of AKI is the lack of early diagnosis tools. The aim of this research is to identifying discriminating metabolites as candidates for early biomarkers of AKI.
Urine samples from patients who developed AKI (group 1) and those who did not (group 2) in an ICU environment were analyzed by GC-MS using untargeted metabolomics approaches. It was observed that there is an overlap of samples within each group, when clinical criteria were considered for group classification. After cluster analysis, new groups are now classified based on similarities of the metabolome of the individuals under investigation and not on pre-established clinical criteria. The generated model showed high correlation and high predictability, with sugars as the main metabolites identified as discriminants between these two new groups. These results suggest that for spectral diseases, such as AKI, clinical criteria as classification of individuals into categorical groups may not necessarily be aligned with the metabolic status of the individual.

PP-30

Molecular Signatures of Wilms Tumor issued by Metabolomic and Transcriptomic Integrative Analysis

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Keywords: Wilms tumor, Bioinformatics, Chemoresistance, Metabolomics, Transcriptomics

Wilms tumor is the most common renal embryonic tumor comprising triphasic histology including blastemal, epithelial, and stromal. High-risk patient or those who present disease relapse have a decrease in their life span. A better risk classification process and new prognostic biomarkers can improve the treatment and the course of the disease. In this study, tumoral kidney tissue (WT; n=20) and adjacent tissue free of tumor (NK; n=20) were collected from 20 infant research participants. Mass spectrometry (MS)-based metabolomics was assisted by machine learning algorithms. WT and NK tissues were differentiated with a 96.8% accuracy in a support vector machine (SVM) model. Metabolic signatures of NK samples enabled the differentiation of risk. Altogether, altered pathways indicated by multi-omic integrated analysis pointed to glutathione metabolism as an important route in the phenotype changes altered by tumor onset. The metabolic profile of WT can be used for tumor detection and correlates to a patient's risk of relapse, retrieved from adjacent tissue analysis. Altered metabolites are part of biological pathways validated using transcriptomics and can elucidate tumor progression.

PP-31

Comparative metabolomic evaluation of cisplatin and synthetic tellurium compounds in search of drug candidates for lung cancer treatment

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Keywords: lung cancer, metabolomics, cisplatin, tellurium compounds.

Lung cancer has the highest incidence and mortality rates worldwide among all cancers. The suitable treatment selection is of great importance, being surgery, radiotherapy and/or systemic therapy the most used strategies. Cisplatin is one of the most used drugs worldwide for the chemotherapy treatment of lung cancer and other types of solid cancer, but it has several disadvantages, such as frequent recurrence, resistance and high toxicity, with several side effects. Therefore, the importance of searching more efficient alternative therapies is unquestionable. The aim of this work is to conduct a comparative metabolomic evaluation of cisplatin and synthetic organic tellurium compounds in search of drug candidates for non-small cell lung cancer treatment. For this purpose, a human non-small cell lung cancer line, H1299, was used. Four experimental conditions were contrasted (control, cisplatin, Te18 and Te24) with 15 replicate samples of each group, totaling 60 samples containing 10^6 live cells each. After exposure and cellular activity interruption, intracellular metabolites were extracted. The samples were derivatized and analyzed using a GC-MS equipment with a quadrupole mass analyzer. Data were processed and discriminant metabolites identified using the MSDial software. Statistical analysis was performed in MetaboAnalyst. The statistical models used for comparisons proved to be satisfactory, showing differences between the metabolism of cells in response to the treatment. Preliminary results indicate that tellurium compounds metabolic action differs from cisplatin, showing potential for treating lung cancer.

PP-32

Clinical metabolomics in the study of patients with COVID-19 and acute kidney injury (AKI)

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Keywords: Acute Kidney Injury, metabolomics, COVID-19

During the most critical phase of the COVID-19 pandemic, the high demand for hospitalizations led to a notable rate of renal function impairment in hospitalized patients. This correlation impairment is still not well understood. Thus, the present work seeks to use metabolomics as a tool to elucidate how biological pathways are affected when a patient with COVID-19 presents, whether as a pre-existing condition or not, acute kidney injury.

The study cohort includes about 600 patients from HC-FM-USP during the first phase of the COVID-19 pandemic. Plasma samples were collected and analyzed by liquid chromatography coupled with mass spectrometry (LC-MS) using an untargeted metabolomics approach, contrasting patients with COVID-19 and kidney injury from those with COVID-19 without kidney injury.

This separation using PCA or PLS-DA models, based on clinical data group classification, was not effective for distinguishing the two groups. Therefore, the data were analyzed using Self-Organizing Maps, which provide a separation based on the metabolic status of individuals. From this new reclassification, further analyses will be performed using classical multivariate analysis tools.

PP-33

LC-HRMS for prospecting secondary metabolites of aqueous extract of *Strychnos peckii* B.L.Rob.

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Keywords: LC-HRMS, Annotation, Natural Products, Strychnos L.

Herein liquid chromatography-high resolution mass spectrometry (LC-HRMS) was used for exploring the chemical profile of *Strychnos peckii* B.L.Rob., an endemic Amazonian species. To select the appropriate column and gradient elution conditions, an automated column and eluent scouting protocol monitoring from 190 to 800 nm was carried out. Four orthogonal columns were used with acetonitrile (B) and water (A) with 0.1% of formic acid at linear gradients of 2-100% of B in 18 min and of 10-50% of B in 22 min at flow rates of 300 µL min^{-1}. From the scouting experiments the ACQUITY® HSS T3 (100Å, 1.8 µm, 2.1 mm X 100 mm) column was selected and the gradient paraments (ΔB; *tG*) optimized to 10-30% and 16 min, respectively, for running the LC-HRMS analysis. Molecule annotation was achieved through molecular dereplication, employing MS^2 fragmentation experiments, the creation of an in-house database, comparisons with public data, and the propagation of the molecular network using *in silico* tools. As a result, 42 molecules were annotated in the extract, belonging to the classes of alkaloids (32), benzoic acid derivatives (8), and flavonoids (2).

PP-34

Cationic Dyes with High Molar Absorption Coefficients to be Used as Labels or Co-ions in Capillary Electrophoresis

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Keywords: Detection, microchip electrophoresis, limit of detection, limit of quantification

Dyes are used in Capillary Electrophoresis as labels for direct detection (absorption or fluorescence) of analytes, or as co-ions for indirect detection. There are thousands of water-soluble anionic dyes known in the literature (*Kist 2023*). These occurs mainly due to the high hydrophilicity of the sulfonic and carboxylic groups, which are negatively charged in wide pH ranges, conferring high water solubility to the dyes bearing these groups. However, the number of options of water-soluble cationic dyes with high molar absorption coefficients is much lower. Dyes bearing amine groups, responsible for the positive charges, are much less water soluble. In this work we tabulated dozens of cationic dyes (with a positive net charge in neutral aqueous solutions), their molecular structures, and respective photophysical properties (wavelength of absorption maximum and molar absorption coefficients). Examples of such dyes are: rhodamine 6G 2+, rhodamine 6G 3+, DAOTA 3, AI3, methyl green, nitrotetrazolium blue, and many pyridines, oxazines and thiazines, to mention a few.

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PP-35

Hypolipemiants and antiplatelets treatments in patients with ST-segment elevation myocardial infarction: Semi-targeted lipidomics of the BATTLE-AMI study

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Keywords: AMI, hypolipemiants, antiplatelets, semi-targeted lipidomics

Acute myocardial infarction (AMI) is the largest cause of mortality in the world. The 2023 ESC Guidelines for the management of acute coronary syndromes recommends the administration of an antiplatelet besides the conventional hypolipemiant therapy although the metabolic consequences of such simultaneous use are not yet fully explored. The objective of this work was to evaluate part of the metabolic mechanisms involved in different combination of treatments after cardiac ischemia, as part of a comprehensive study within the BATTLE-AMI clinical trial (1) by a semi-targeted lipidomics approach.

Plasma samples were collected from 145 patients, one day and six months after AMI. All patients received a combined treatment with one antiplatelet (Clopidogrel or Ticagrelor) plus one statin (Simvastatin or Rosuvastatin) at different doses combined or not with ezetimibe. Samples were analyzed by RPLC-MS in positive ionization mode. Besides mobile phase and gradient optimization, method's development included matrix effect study and data acquisition parameters d-MRM optimization for 116 lipids.

All compounds were quantified, and compared by means of nonparametrical analysis of longitudinal data. Significant differences could be seen between different therapies combinations. As expected, rosuvastatin was superior to simvastatin in terms of the number of altered compounds after six months of treatment. Interestingly, different trends of variation were found for tryglicerides (TGs) depending on the size of the carbonic chain and the number of double bounds presented in the structure of the compound. Short-chain TGs were altered only in rosuvastatin groups. Consequences of such differences will be evaluated in the context of the whole trial.

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PP-36

Untargeted metabolomics to reveal the mechanism of action of potential drugs against Chikungunya

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Keywords: Vero cells, GC-MS, metabolomics, Chikungunya

Chikungunya virus (CHIKV) is transmitted to humans by mosquitoes of the genus Aedes, causing the chikungunya fever disease. This disease poses a significant global public health challenge. In Brazil, over 380,000 cases of chikungunya have already been reported in 2024. Currently, there is no specific antiviral treatment available for chikungunya fever. Therefore, this study aims to investigate, via untargeted metabolomics, the mechanisms of action of potential drugs for treating chikungunya fever. Metabolic disturbances using mammalian cultured cells (Vero E6 - African green monkey kidney cells) as model were investigated. Samples of uninfected VERO CCL81 cells and VERO CCL81 cells infected with the CHIKV99/2016BR virus were prepared. The reference drug used was interferon alfa-2, while the candidate drug was a selenium compound derivative (Sl-Se-023). Analyses were conducted using gas chromatography coupled with mass spectrometry. The identified metabolites that showed significant differences between the groups include the following amino acids and derivatives: phenylalanine, β-alanine, L-alanine, L-tyrosine, norvaline, aspartic acid, DL-isoleucine, L-pyroglutamic acid, and L-glutamic acid. Identified carboxylic acids and derivatives are fumaric acid, L-lactic acid, pyruvic acid, 4-guanidinobutyric acid, 2-hydroxybutyric acid, and oxalic acid. Additionally, sugars and derivatives include D-glucose, thalose, sorbitol, ribitol, among others. It was observed that the most disturbed pathways in the study include tyrosine and tryptophan biosynthesis, phenylalanine metabolism, alanine, aspartate, and glutamate metabolism, glycine, serine, and threonine metabolism, phenylalanine, taurine, and hypotaurine metabolism, as well as pyrimidine metabolism.

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PP-37

Rationalizing solvent effects on the MEKC separation of natural and synthetic steroids using QSRR

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Keywords: solvent effect, MEKC, QSRR, steroids, hormones.

In this work, the retention of eleven steroids in eight aqueous borate/SDS electrolyte systems, modified by ethanol, acetonitrile and/or tetrahydrofuran, in single and/or different binary and ternary proportions, was rationalized by QSRR models involving log Pow, Abraham's solute parameters, as well as electrotopological and quantum chemical descriptors.
Despite the high hydrophobicity of the solute series, overall results reveal details of loci of incorporation in the micellar structure and important effects of the organic modifiers in the solute partition. Enhanced acidity of micellar surface by the presence of ethanol in the electrolyte system allows hydrogen bonding interactions with carbonyl and hydroxyl groups in the extremities of a rigid carbon skeleton, once ethanol intercalates into the micelle palisade. Therefore, solutes with structural OH groups interact with the basic sulfates at the micellar interface whereas those lacking OH groups interact via carbonyl oxygen with the ethanol at the palisade. For acetonitrile electrolyte systems, in the absence of ethanol, a smaller degree of micellar dissociation occurs due to the low bulk dielectric constant causing an increase of the surface acidity, producing similar effects of ethanol regarding the incorporation site which is the micellar surface too. Electrolytes containing small amounts of THF behave similarly to those with pure water as solvent, discriminating solutes by molecular interactions in different incorporation sites, depending on the presence of hydroxyl groups in the structure. For this series only progesterone and 21-hydroxyprogesterone acetate do not have hydroxyl groups and are more deeply incorporated in the micellar structures.

PP-38

Comparison of different Acquisition Modes - untargeted urinary metabolome analysis of COVID-19 patients

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Keywords: Mass Spectrometry, COVID-19, Metabolomics, Acquisition Mode, Urine.

The most common acquisition methods for Untargeted metabolomics analysis are data-independent acquisition (DIA), data-dependent acquisition (DDA), and Full-scan. In this work, we compared the three data acquisition modes using the urine samples from patients with COVID-19 (n=21) and control (n=21). The samples were diluted and injected into a liquid chromatography mass spectrometry (LC-MS) system, using an HILIC column with each acquisition mode being acquired in positive and negative ionization modes. Full-scan mode is able to capture the largest number of metabolic features, followed by DIA and DDA. Comparing the MS2 spectra in DIA and DDA, spectra quality is higher in DDA with average dot product score of 83.1%. Moreover, a comparison of relative standard deviation distribution between modes shows consistency in the quantitative precision, with the exception of DDA showing a minor disadvantage (on average 19.8% and 26.8% fewer features in urine with RSD < 5% than full-scan and DIA, respectively). Amino acid pathways were altered in all modes. The method that returned the greatest number of altered metabolic pathways was DIA.

PP-39

Noncovalent Labeling of Proteins in Sodium Dodecyl Sulfate Capillary Gel Electrophoresis

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We introduce a new on-column labeling method for sodium dodecyl sulfate capillary gel electrophoresis (SDS-CGE) that utilizes propidium iodide, a dye traditionally used for nucleic acid analysis, to label proteins in real-time during the electrophoretic separation process. This approach eliminates the need for pre- or post-column derivatization, significantly simplifying the sample preparation workflow. Propidium iodide binds non-covalently to SDS-protein complexes, allowing for *in situ* labeling while avoiding the time-consuming fluorophore labeling steps required in most conventional multicapillary electrophoresis systems. The method was initially tested with a commercially available protein sizing ladder ranging from 6.5 to 200 kDa. It was then applied to the analysis of a therapeutic monoclonal antibody (mAb) and its subunits, including glycosylated and non-glycosylated heavy chains. By varying the concentration of propidium iodide in the gel-buffer system, we optimized the labeling conditions to achieve high sensitivity, resolution, and detection precision. The optimal concentration for maximum detection sensitivity of the intact monoclonal antibody was found to be 200 µg/mL, with a limit of detection (LOD) of 2 µg/mL and excellent detection linearity over three orders of magnitude. For the separation of glycosylated and non-glycosylated heavy chains, the best resolution was achieved at 100 µg/mL propidium iodide. This labeling strategy was shown to provide excellent peak efficiency and resolution across a range of ligand concentrations, allowing for flexible optimization depending on the sample composition. This method enhances the throughput and efficiency of SDS-CGE for biopharmaceutical applications, particularly in the analysis of therapeutic proteins such as monoclonal antibodies. The novel propidium iodide labeling approach offers a fast, reliable, and highly sensitive alternative to traditional labeling methods, making it a valuable tool for protein separation and analysis.

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PP-40

Metabolomics evaluation of the kynurenine pathway in COVID-19 associated to acute kidney injury by LC-MS

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Keywords: COVID-19, acute kidney injury, kynurenine pathway, LC-MS.

SARS-CoV-2 led to one of the largest pandemics in recent history.[1] COVID-19 symptoms are predominantly respiratory. However, association with other diseases have been revealed, such as acute kidney injury.[2],[3] The kynurenine metabolic pathway is the main tryptophan catabolism and its imbalance is related to several diseases.[4] Thus, the present study aims to differentiate metabolic mechanisms in severe COVID-19 patients with those who also had renal complications. A LC-MS method is being optimizaed for the quantification of four key metabolites: tryptophan; kynurenic acid; kynurenine, and picolinic acid (Pic) in blood plasma samples. The main parameters of the separation by RPLC-ESI-MS were evaluated. [5] Mobile phase was composed of: A - 0.1% formic acid (FA); B - acetonitrile + 0.1% FA. Due to high polarity of Pic, better chromatographic resolution was observed with isocratic elution at 40% of B. Ions *m/z* 106 and 78 were selected for MRM of Pic. However, the mobile phase gradient is under optimization for appropriate separation of all analytes, and decrease of the carry over effect. Method validation will be performed in a surrogate matrix for a trustworthy quantification.

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PP-41

Study of metabolic alterations linked to the SARS-CoV-2 virus and the use of low-level laser as anti-inflammatory therapy in zebrafish (*Danio rerio*).

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Keywords: Animal models for diseases, COVID-19, Chromatography, Metabolomics, Mass spectrometry

The most recent pandemic caused by SARs-CoV-2 virus killed more than 6.8 million people. The zebrafish (*Danio rerio*) animal model allowed the study of metabolic alterations linked to inflammation. The organism under study was exposed to SARS-CoV-2 spike protein and the low-level laser as an anti-inflammatory therapy was evaluated. Through metabolomics, 30 compounds were annotated for inflammatory changes caused by the spike protein. The inflammation is supported by the work of ours partners. These compounds belong to 12 different classes, correlated to nine biological pathways. The most affected pathway was glycerolipid metabolism. This route correlate with inflammatory mechanism and is related to adipose tissue endocrine function. The remaining compounds corelates with mechanisms of cell membrane integrity and cell health, hormonal regulation and protein degradation. The low-level laser showed a protective effect against the alteration in glycerolipid metabolism and protected partially the other pathways. These findings suggest that the laser can be helpful in the disease treatment and recovery. Overall, this work showed the capability of zebrafish as an inflammation model, the spike metabolic action and the potential of the laser as an anti-inflammatory therapy.

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PP-42

Refining Extraction Techniques for Alpha and Beta Acids in *Humulus lupulus*: Chemical Analysis via CD-MEKC-UV and HPLC-DAD

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Keywords: Humulus lupulus extracts, extraction methods, bioactive compounds, CD-MEKC-UV, HPLC-DAD

Numerous methods have been documented for extracting alpha acids, beta acids, xanthohumol and other prenylflavonoids from *Humulus lupulus*[1]. These approaches vary in efficiency and yield. This study aims to stablish an extraction procedure that optimizes both mass and target component yields. A range of extraction techniques and solvents were investigated. Preliminary methods by HPLC and CD-MEKC with diode-array detection are currently being employed to assess chemical profiles.

Pellets of the Columbus variety were crushed, and 0.500 g of plant material was extracted for three hours using static and dynamic maceration, ultrasound, and Soxhlet apparatus. Solvents included methanol, ethanol, acetonitrile and acetone.

Statistical analysis identified dynamic maceration with methanol as the most effective for maximizing mass yield. HPLC-DAD revealed differences in chemical profiles based on solvent choice while early CD-MEKC-UV results showed better peak separation and sensitivity for the target compounds. These initial findings offer valuable insights for the brewing and herbal industries in optimizing hop extract formulations.

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PP-43

Evaluating the mechanism of action of novel Te-based drugs for the treatment of Schistosomiasis with an untargeted metabolomics approach

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Keywords: metabolomics; GC, Schistosomiasis, myo-inositol.

Schistosomiasis is a neglected parasitic disease caused by helminths of the genus Schistosoma. Transmission occurs via contact with water sources contaminated by feaces and urine of infected individuals, containing parasite eggs, which hatch in water. Schistosomiasis is endemic to poor regions where proper sanitation and access to clean drinking water is lacking. The disease causes consequences for both public health and the country's socioeconomic sector. More than 700 million people live in endemic regions around the world, according to WHO. Despite the existence of an effective treatment, the exclusivity of such active pharmaceutical ingredient, praziquantel, is dangerous. There are reports of the drug's ineffectiveness in Senegal, which raised an alert about the possibility of resistant strains. In this context, research for new drugs is encouraged.

The untargeted metabolomics approach is very helpful to investigating mechanisms of action of drugs. In this work, gas chromatography coupled to mass spectrometry was applied to compare metabolic profiles of worms treated with reference drugs (praziquantel), worms treated with test drugs (Te compound derivatives) and warms not treated at all. Samples were prepared with 6 worms each, derivatized for GC-MS analysis and injected randomized. Chromatographic parameters were set as to follow Fiehn's method and library.

The results demonstrated striking changes in the myo-inositol profile for both reference drug and test drug in addition to changes in lactic acid and glutamic acid. Samples were too diluted to identify a significant number of metabolites. Therefore, a new test is under investigation with a larger amount of worms per sample. In addition, a different analytical technique will be explored, such as RPLC-MS, to improve metabolite coverage.

PP-44

Study of polysaccharide hydrolysis by capillary electrophoresis with direct UV detection

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Keywords: Capillary Electrophoresis, Monosaccharides, UV detection, Polysaccharides, Hydrolysis

Acid hydrolysis of glycosidic bonds is the most utilized method for polysaccharide analysis, process in which the detection of monosaccharides and other structures formed from further reactions, such as sugar dehydration [1]. This work intends to develop a method for polysaccharide hydrolysate analysis through capillary electrophoresis with direct UV detection (possible due to the background electrolyte's high pH value), based on existing works for sugar analysis [2,3]. Seven saccharides, namely sucrose, lactose, glucose, arabinose, fructose and xylose, as well as furfural and 5-hidroxymethylfurfural are currently being used in this investigation and some preliminary applications in lignocellulosic biomass have been performed.

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