



Journal of Natural Products Discovery

ISSN 2755-1997, 2024, Volume 3, Issue 3

Conference Proceedings

PROCEEDINGS OF THE 5TH CNPD CONFERENCE

Centre for Natural Products Discovery (CNPD), 19-21 June 2024, Liverpool L3 3AF, United Kingdom.

D.O.I.

10.24377/jnpd.article2791

Received 2024-12-28

Accepted 2024-12-28

Published 2024-12-29

Keywords:

Natural Products

Conference

©2024 by the authors.

Licensee Liverpool John Moores Open Access, Liverpool, United Kingdom.

This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution.





Annual CNPD Conference Online 2024
Centre for Natural Products Discovery
School of Pharmacy and Biomolecular Sciences
Liverpool John Moores University
Liverpool, United Kingdom
19-21 June 2024



Conference website

<https://ysm2018.wixsite.com/cnpd2024>

Compiled by:

Dr Touraj Ehtezazi
Dr Alistair J. Fielding
Dr Francesca Giuntini
Prof Lutfun Nahar
Dr Ismini Nakouti

Welcome Message from the President of the Conference

Every journey has a beginning. Every beginning has a story to be told. The journey of the Centre for Natural Products Discovery (CNPD) formally began in March 2019 but the actual beginning was in late 2013 through the formation of the Natural Products and Medicinal Chemistry Research Group, where a group of like-minded academic researchers from the School of Pharmacy and Biomolecular Sciences got together to foster internal research collaborations within the 'drug discovery' area, working at the interface of chemistry and biology. This group gradually grew as one of the most productive research groups within the School, particularly having the main activities around various aspects of natural products, from simple isolation and identification of bioactive compounds from natural sources to complex mechanistic pharmacological evaluation, which prompted the need for the creation of a research centre, totally devoted to natural products discovery research; the CNPD was born.

The CNPD conducts externally funded and impactful natural products research to discover new high-value natural products that will contribute to tackling current and future societal and global challenges in health and well-being, socio-economic growth, natural conservation, and environmental sustainability. Most recently, the CNPD has now extended its reach to *in silico* natural products work, in addition to the research being carried out within the eight distinct divisions within the centre (visit the website for further details: <https://www.ljmu.ac.uk/research/centres-and-institutes/centre-for-natural-products-discovery>).

The first-anniversary conference of the CNPD was held in Liverpool in March 2020; it was at a time, when the pandemic just entered the UK, and universities started to close. Despite that adverse situation, the conference was a remarkable success, attended by people from various parts of Europe and beyond. The 2nd and 3rd-anniversary conferences had to be held online because of the pandemic, but we had the 4th-anniversary conference again face-to-face in Liverpool in 2023. At that point, we decided to organize the CNPD anniversary conferences online and face-to-face in alternative years. Therefore, we are having the 5th-anniversary conference online this year hoping that next year, we will be able to organize the 6th-anniversary conference face-to-face in Liverpool.

Since the establishment of the CNPD, we have expanded our activities with the launch of a new open-access (free-to-publish) journal (*Journal of Natural Products Discovery*, <https://openjournals.ljmu.ac.uk/JNPD>), and a brand new MSc programme in Natural Products Discovery (<https://www.ljmu.ac.uk/study/courses/postgraduates/36360-natural-products-discovery-msc>). So, the journey continues!

On behalf of the CNPD and the Conference Organising Committee, I cordially invite you to the 5th Annual CNPD Conference 2024 on 'Advances in Natural Products Research', which will be held online in Liverpool on 19-21 June 2024.

Like four previously organised successful annual CNPD conferences, this conference will also be a unique platform for highlighting the advances in natural products research covering cosmetics, food, medicine, and agricultural products. The conference will comprise invited talks (20 min) and short oral presentations (10 min) focusing on what matters most, to be delivered by global leaders

in natural products research as well as by young scientists (PhD students and postdocs). This conference will offer individual sessions dedicated to open, interactive and participatory discussions with selected panel members and the audience on various issues and challenges around natural products research.

The CNPD is based in the School of Pharmacy and Biomolecular Sciences at LJMU, the second oldest Pharmacy education provider in the UK and has a rich history of world-leading natural products research. This conference also forms a part of the celebrations of the 175th anniversary of Pharmacy education at LJMU.

I welcome you to this exciting conference and hope you have a great time with the CNPD family!



Professor Satya Sarker

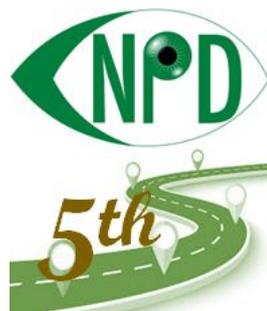
President of the CNPD Conference Organizing Committee

Founding Head of the CNPD

Director of the School of Pharmacy and Biomolecular Sciences at LJMU

Editor in Chief, *Phytochemical Analysis*

Programme



Annual CNPD Conference Online 2024

Centre for Natural Products Discovery

School of Pharmacy and Biomolecular Sciences

Liverpool John Moores University

Liverpool, United Kingdom

19-21 June 2024

Day 1

19 June 2024

9.30 – 10.00

Conference opening and welcome

Professor Satya Sarker, Founding Head of CNPD.

Professor Laura Bishop, Pro-Vice Chancellor of Science

10.00 – 12.00

Session 1:

Chairs: Professor Satya Sarker and Dr Fyaz Ismail

Prof Mingquan Guo

Ningbo Cixi Institute of Biomedical Engineering, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201, China

Potential phytochemicals and their biological activities of three Euphorbiaceae species explored by bio-affinity ultrafiltration LC-MS with multiple drug targets

Prof Sk Jamal Uddin

Pharmacy Discipline, University of Khulna, Khulna, Bangladesh

Ethnopharmacological Evaluation of Sundarban Plants: A Treasure of Natural Bioactive Molecules

Prof Syed Ghulam Musharraf

HEJ Research Institute of Chemistry, University of Karachi, Karachi, Pakistan

Fetal Hemoglobin (HbF) Inducers for the Treatment of Beta-thalassemia: Few Interesting Stories

Prof Eman Shawky

Department of Pharmacy, Alexandria University, Egypt

Metabolomics Unleashed: Untangling Nature's Chemical Diversity in Medicinal Plants Systems

13.30 – 14.30

Session 2: Panel discussion

Chairs: Professor Amos Fatokun and Dr Francesca Giuntini

14.30 - 16.00

Session 3: Short Talks

Parallel Session A

Chairs: Dr Kenny Ritchie and Dr Ismini Nakouti

Habib Emran

Mazandaran University of Medical Sciences, Iran

Effect of polysaccharide rich hot water extract of *Trametes versicolor* on blood factors in diabetic patients. A double-blind, randomized clinical trial

Reham Ibrahim

Alexandria University, Egypt

Chemometrics-aided standardization of Egyptian propolis using an integrated UV-TLC/MS-image analysis strategy for unravelling potential antidiabetic markers

Aminu Mohammed

University of KwaZulu-Natal, South Africa

Antioxidative effect and inhibition of key enzymes linked to type 2 diabetes of various solvent fractions from fruit ethanolic extract of *Xylopia aethiopica* in vitro

Gamal Abdelfattah

Alexandria University, Egypt

Treatment of HFD-induced diabetes mellitus by combination of metformin and natural products in rats

Sibu Sen

National Institute of Pharmaceutical Education & Research (NIPER), India

Repurposing of Unani polyherbal formulation in obese diabetes using network pharmacology, molecular docking and simulation approach

Parallel Session B

Chairs: Dr Stefan Roesner and Dr Francesca Giuntini

John Anyam

Joseph Sarwuan Tarka University Makurdi, Nigeria

Cycloartanes from the bulbs of *Crinum bulbispermum*

Al-Masum Hossain

Comilla University, Bangladesh

Phytochemical screening and in-vivo evaluation of analgesic and antidiarrheal effects of *Crateva unilocularis* L. leaf extracts

Dina A Selim

Alexandria University, Egypt

Implementation of metabolomics in conjunction with chemometrics to identify the distinguishing chemical markers of various grades of Sri Lankan white, green, and black tea (*Camellia sinensis* L.)

Anggra Paramita

King Abdullah University of Science and Technology, Saudi Arabia

Metabolomic approach to tackle adulterations in medicinal plants

Laura Grauso

Università degli Studi di Napoli Federico II, Italy

Diarylheptanoids from the seagrass *Zostera marina*

16.00 – 17.00

Session 4:

***Chairs:* Prof Amos Fatokun and Dr Ismini Nakouti**

Prof Lucie Cahlíková

Department of Pharmacognosy and Pharmaceutical Botany, Hradec Kralove, Czech Republic

Amaryllidaceae alkaloids as inspiration for medicinal chemistry

Prof Mirek Strnad

Institute of Experimental Botany of the Czech Academy of Sciences, Olomouc, Czech Republic

Brassinosteroids, their analyses, biological and medical activities

Day 2

20 June 2024

9.30 – 10.30

Session 5: Plenary talks

Chairs: Dr Garry McDowell and Dr Touraj Ehtezazi

Dr Babatunde Samuel

Faculty of Pharmacy, University of Ibadan, Nigeria

Structural elucidation and *in-silico* studies of antimalarial principles isolated from *Combretum racemosum* leaf extract

Prof Robert Nash

Phytoquest Ltd, Aberystwyth, Wales, UK

The benefits of natural imino-sugars

11.00 – 13.00

Session 6: Plenary talks

Chairs: Dr Mosharraf Sarker and Dr Pat Rahman

Dr Greg Leach

Antylia Scientific, UK

A technology presentation (the title will be revealed on the day)

Dr Touraj Ehtezazi

CNPD, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, UK

Formulation challenges for paediatric 3D printed personalised medicines

Prof Anca Miron

University of Medicine and Pharmacy Grigore T Popa, Iasi, Romania

Plant-derived agents in non-melanoma skin cancer: Current landscape and future perspectives

Prof Virginia Lanzotti

University of Naples Federico II, Naples, Italy

Advances of plant metabolomics in the study of self-DNA inhibition

14.00 – 15.00

Session 7: Panel discussion

Chairs: Dr Jose Prieto and Professor Khalid Rahman

15.00 – 16.00

Session 8: Short talks

Chairs: [Dr Stefan Roesner](#) and [Dr Francesca Giuntini](#)

Pitchapa Thongsuwan

Srinakharinwirot University, Thailand

Antimicrobial activities and TLC profiles of *Xylaria* spp. associated with termite nests in Thailand

Attilio Anzano

Università di Napoli Federico II, Italy

Chemical analysis and antimicrobial activity of *Moringa oleifera* Lam. leaves and seeds

Pat Rahman

Liverpool John Moores University, UK

Applications of biosurfactants in pharmaceuticals

Georgiana Gavril

National Institute of Research and Development for Biological Sciences,
Romania

Natural compounds: An alternative for safe packaging

Day 3

21 June 2024

9.00 – 10.30

Session 9: Plenary talks

Chairs: Dr Kenny Ritchie and Professor Lutfun Nahar

Dr Alessandro Maugeri

Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Mesina, Italy

A flavonoid-rich extract of white grape juice hampers seizures in different rodent models of epilepsy

Professor Mansurah Abdulazeez

Centre for Biotechnology Research, Bayero University, Kano, Nigeria

Cytotoxic activities of some plants used in Nigerian ethnomedicine for the treatment of cancer

Dr Evelyn Wolfram

ZHAW University of Applied Sciences, Zurich, Switzerland

Quality from source to benefit: Monographs and phytochemical analysis as the basis for evidence-based natural health products and phytotherapy

11.00 – 12.30

Session 10: Short talks

Parallel session C

Chairs: Professor Amos Fatokun and Dr Kenny Ritchie

Yemi Adekunle

University of Ibadan, Nigeria

Triterpenoid glycosides of *Olax subscorpioidea* Oliv. root: isolation, characterization, and anticancer evaluation

Waed Alsheikh

Liverpool John Moores University, UK

Cancer chemopreventive potential of *Ruta chalepensis* L. (Rutaceae) growing wild in Syria

Chuanchom Khuniad

Liverpool John Moores University, UK

Phytochemistry and *in vitro* cancer chemopreventive effect of *Leea indica* leaves on AREc32 Cells

Tolulope Oyedeji

University of Lagos, Nigeria

Cytotoxic effects of *Adenopus breviflorus* fruit extracts on prostate cancer cells

Shehla Adhami

Jamia Hamdard, India

***In vitro* antioxidant and cytotoxicity activity of extracts from *Chlorophytum comosum* (Thunb.) Jaques**

Parallel session D

***Chairs:* Professor Satya Sarker and Dr Fyaz Ismail**

Bruna Del Falco

Università degli Studi di Napoli Federico II, Italy

Stereostructure elucidation of *Euphorbia myrsinites* diterpenes and their anti-inflammatory properties

Nabarun Mukhopadhyay

National Institute of Pharmaceutical Education and Research (NIPER), India

Understanding molecular mechanisms behind the anti-inflammatory effects of *Machilus macrantha* (Gulmavu) in the arachidonic acid metabolic pathway by network pharmacological approach

Afaf El Baakili

Mohammed V University in Rabat, Morocco

Phytochemical investigation and antioxidant activity of *Salvia officinalis* aerial parts

Subrata Das

Assam University, India

Effect of acetone fraction of *Ottelia alismoides* on the G2/M cell cycle arrest and apoptosis in the human carcinoma cell lines

Tanveer Alam

Sabancı University Nanotechnology Research and Application Center

Orta Mahalle, Turkey

Natural food colors vs. synthetic food colors

Caterina Russo

University of Messina, Italy

Mechanism underlying the anti-inflammatory effects of oleacein from *Olea europaea* L. in LPS-exposed macrophages

14.00 – 15.00

Session 11: Plenary talks

Chairs: Professor Satya Sarker and Dr Fyaz Ismail

Prof Carlos Leonardo Armando Céspedes Acuña

Department of Basic Sciences, Faculty of Sciences, Campus Fernando May-
Chillan, Chile

Awaiting the title

Dr James Downing,

School of Pharmacy and Biomolecular Sciences, Liverpool John Moores
University, UK

Multiple smooth muscle relaxant activities of berberine chloride identified using *in vitro* rat model of viral-mimetic-induced motility changes underlying miscarriage

15.00 – 15.45

GOSS Best short presentation award

Closing remarks



Invited Plenary Speaker's Profiles

Prof Carlos L. Cespedes-Acuña

Professor Cespedes-Acuña is a full Professor in Chemistry and a Senior Researcher at the Department of Basic Sciences, Faculty of Sciences, University of Bio Bio, Chile. He obtained his PhD degree in Chemistry in 1994 from the University of Concepción, Concepción City, in Chile. In 1996 he moved to Mexico City (UNAM) for a postdoctoral position and worked there until 1998. During 1999 - 2000 he was appointed an Associated Researcher, and from 2001 to 2005 he worked as a Titular Researcher step A in the Chemistry Institute at UNAM. From January to December 2006, he served as a Professor and Titular Researcher step B at FES-Iztacala, UNAM. He joined the Basic Sciences Department, at the University of Bio Bio, Chillan, Chile in 2007 and has been working there since then. He is the Editor-in-Chief of *Natural Resources for Human Health* and has been on the editorial board of several other journals. He has published over 180 research publications, 12 book chapters and three books, and has a total citation of about 5,000 (h-index 36, i-10 index 113) to date.

Prof Mansurah Abdulazeez

Professor Abdulazeez studied Biochemistry at Ahmadu Bello University, Zaria, Nigeria, and graduated in 2002 with a second-class upper degree, after which she was retained as a Graduate Assistant. She obtained her MSc in Biochemistry in 2008 and a PhD in Biochemistry in 2013 in the same department. She was at the Faculty of Pharmacy, Chiang Mai University, Thailand, as a visiting PhD student, and later at the Centre for Natural Products Discovery (CNPD), Liverpool John Moores University, UK, as a postdoctoral fellow working with Prof Amos Fatokun on the anticancer effects of some plants of African origin and their molecular mechanisms of action. In 2020 she was awarded the Science by Women (Fundación Mujerespor Africa) Fellowship (first winner from northern Nigeria), held at the Institute of Neurosciences, University Miguel Hernandez, Alicante, Spain, where she studied the molecular mechanisms of therapy resistance in triple-negative breast cancer (TNBC) cells, under the tutelage of Prof Angela Nieto, a pioneer and world-renowned leader in the field. Prof Abdulazeez transferred her services to the then newly established Centre for Biotechnology Research, Bayero University, Kano, in 2014, and rose through the ranks to become the first female Professor of Biochemistry at Bayero University, Kano, Nigeria, in 2021. She currently leads a research group focused on the discovery of novel compounds from medicinal plants with potentials for the treatment of non-communicable diseases, particularly, cancer and hypertension. She has secured significant funding for her research, published many scientific papers, and supervised BSc, MSc and PhD students. Her contribution to research, and particularly to cancer research, has won her several awards. She is a fellow of several associations, including the Nigerian Society of Biochemistry and Molecular Biology, International Union of Biochemistry and Molecular Biology, and the Nigerian Cancer Society. As a female academic in northern Nigeria, where girl-child education is still faced with significant challenges, Mansurah is considered a role model. She provides direct mentoring services to women and girls in her community. She also encourages and responds to requests for

support, advice and guidance from high school students at various symposia to ensure positive youth development.

Prof Lucie Cahlíková

Prof Cahlíková is the Head of the Department of Pharmacognosy and Pharmaceutical Botany at the Faculty of Pharmacy in Hradec Králové, Charles University, Prague, Czech Republic. She has studied at the University of Chemistry and Technology in Prague with a specialization in the Chemistry of Natural Products. After graduation in 2001, she continued with doctoral studies at the Institute of Organic Chemistry and Biochemistry in Prague. During her studies, she spent two years in Switzerland working for Novartis Pharma AG in the Department of Arthritis & Bone Metabolism. In 2004, she entered the Faculty of Pharmacy in Hradec Králové as a member of the Department of Pharmaceutical Botany, and since 2014 she has been head of the Department of Pharmacognosy and Pharmaceutical Botany and of the Research group “Natural products as potential drugs”. In 2020, she became a full professor in Pharmacognosy. She has published more than 90 scientific papers and supervised ten PhD students. The topics of her research are secondary metabolites from plants, with a focus on alkaloids and their biological activities connected with the potential treatment of neurodegenerative, oncological, and microbial diseases. She is also interested in modification of the structure of isoquinoline alkaloids, and total synthesis of minor compounds from the plant family Amaryllidaceae. She is involved in various projects and collaborates with national and international research institutions.

Dr James Downing

Dr Downing is a Senior Lecturer in Pharmacology at the School of Pharmacy and Biomolecular Sciences, LJMU. He has been teaching on several programmes including Masters in Pharmacy, and Pharmaceutical and Cosmetic Sciences. His current research interests include the following: tocolytic actions of natural products, using *in vitro* model of pathogen-induced motility disorder; *in vitro* methods for studying drug entry across blood-brain barrier; functional organisation of the thymus, including nitrergic system for deletional tolerance; the role of endothelial disorder in thymic involution and potential of natural products as regenerative agents.

Dr Touraj Ehtezazi

Dr Ehtezazi is a Reader in Pharmaceutics at Liverpool John Moores University. He is a pharmacist by training, having graduated from the University of Tabriz, Iran. He obtained his PhD from the University of Nottingham in 1997, studying mathematical modelling of drug release from polymeric microspheres. Dr Ehtezazi conducted postdoctoral studies at the University of Nottingham, and he was employed as a lecturer at the University of Leicester in 2000, investigating the interaction of pharmaceutical inhalers with the respiratory tract. He employed three-dimensional printing to produce live oropharyngeal models. He joined Liverpool John Moores University in 2002. He has

studied the application of 3DP in the formulation of pharmaceutical dosage forms since 2016. He has published papers (2018-2024) on the application of 3DP in manufacturing fast-dissolving oral films. He has continued to work on 3DP in the preparation of gummies for children to enhance their medication adherence. He has conducted two surveys with children and their parents about the acceptability of 3D-printed gummy bears. He has completed a special issue in the *Pharmaceuticals* journal (2023) on 3DP of pharmaceutical dosage forms and contributed a book chapter to "3D Printing: Fundamentals to Emerging Applications," a CRC book. Dr Ehtezazi is preparing a book on the application of 3D printing in pharmaceutical dosage forms with the title "3D Printing in Pharmaceuticals."

Prof Ming-Quan (Mark) Guo

Professor Guo is currently a professor at Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences (CAS). His current research interests include but are not limited to medicinal biological chemistry and food chemistry, and especially involve the development of a variety of chemical-biology and bio-affinity ultrafiltration-based strategies for the quick screening of bioactive small molecules against various drug targets from natural products in the context of targeted new drug discovery and development. By far, he has published over 100 SCI articles with some highly cited ones and has been acting as PIs for over 20 national or provincial scientific projects. He has also been invited to serve as Guest Editor or Editorial Board Member for several internationally renowned journals, such as the *Journal of Pharmaceutical Analysis (SCI)*, *Chinese Medicines (SCI)*, *Journal of Analysis and Testing (EI, ESCI)*; *Phytochemical Analysis (SCI)*, *Current Analytical Chemistry (SCI)*, *Phytochemical Analysis (SCI)*, *Frontiers in Nutrition (SCI)*, etc. In addition, he has presented over 50 keynote or invited talks at various international/national conferences since 2012.

Prof Virginia Lanzotti

Prof Lanzotti is a full professor of Organic Chemistry at the University of Naples Federico II, Italy. After the degree in Chemistry, she received a post-doctoral fellowship at the University of Bonn, joining the prof. Breitmaier group, where she became familiar with the use of NMR for structure elucidation of natural products. Later, she joined the group of prof. Cornelis Altona, the University of Leiden, working on conformational studies of DNA oligomers. Her research interests are focused on the stereostructure of natural compounds, drug discovery, food chemistry and metabolomics. She is the author of more than 180 papers in international journals. Winner of the 2003 Phytochemical Society of Europe (PSE) – Pierre Fabre Award for excellence in Phytochemistry, she has been in charge as President of the PSE from 2016 to 2018. Since 2012 she has been the ERASMUS and International Relationships Delegate for the Department of Agricultural Sciences, the University of Naples Federico II. 1997, University of Nottingham, Nottingham, United Kingdom, PhD, 1988, University of Tabriz, Tabriz, Iran, Pharm D.

Dr Alessandro Maugeri

Dr Maugeri is a Lecturer in Biochemistry at the Department of Veterinary Sciences of the University of Messina, Italy. He obtained his PhD from the University of Messina in 2021 and he worked there as a Research Fellow before securing his Lectureship. His research focuses on flavonoid-based natural compounds for different therapeutic applications. Dr Maugeri published 35 papers (*h*-index: 16) and delivered 43 presentations at congresses. He is a Topical Advisory Panel Member for the International Journal of Molecular Sciences (IJMS) and he acted as Guest Editor and Guest Co-Editor for special journal issues. His teaching activities focus on the veterinary structural and metabolic biochemistry for the course in Science, Technologies and Safety of Animal Production.

Prof Dr Anca Miron

Prof Miron got her PhD degree in Pharmaceutical Sciences from *Grigore T. Popa* University of Medicine and Pharmacy Iasi, Romania in 1998. In 2003-2004 she was awarded a NATO Fellowship for post-doctoral studies at the Department of Pharmacognosy, University of Oslo. In 2008 she became a professor in the Department of Pharmacognosy, Faculty of Pharmacy, *Grigore T. Popa* University of Medicine and Pharmacy Iasi, Romania. Prof Miron's main areas of interest are plant polyphenols and volatiles. Her major research activities include isolation, chemical characterization and biological evaluation of plant extractives/constituents with antioxidant, antigenotoxic and antitumor effects. A new direction in her research focuses on the identification of plant extractives/constituents exhibiting synergistic interactions with antibiotics. She published over 70 peer-reviewed articles in international journals and has co-authored four books and five book chapters. She was principal investigator in several national and international research grants and co-author of four national patents. Prof Miron received three national scientific merit awards. She was a guest editor for the *International Journal of Molecular Sciences* (special issue, 3rd International Symposium on Phytochemicals in Medicine and Food, Kunming 2018). Currently, she is a Professor at the Department of Pharmacognosy, Faculty of Pharmacy, *Grigore T. Popa* University of Medicine and Pharmacy Iasi, Romania.

Prof Syed Ghulam Musharraf

Prof Musharraf is working as a Professor at H.E.J. Research Institute of Chemistry, University of Karachi, Pakistan. His field of interest is phytochemical analyses and disease-based biomarker research particularly in beta-thalassemia using mass spectrometry-based metabolomic and proteomic approaches. Currently, he is the author of over 250 research publications (journal cumulative impact factor over 1000), several book chapters, Edited books, patents including a US patent and Editor of many journals including Scientific Reports. A total of 37 students have completed their PhD under his supervision. Due to his scientific contribution, he has been recognized by several international/national awards and honours such as selected member of the

Globe Young Academy from Pakistan; selected as a TWAS Young affiliate by the World Academy of Sciences (TWAS); Recipient of Pakistan Civil Award, Tamgha-e-Imtiaz, Gold Medal Awards (two times) in Chemistry from Pakistan Academy of Sciences, Fellow Chemical Society of Pakistan, and Executive Board Member of Asian Federation of Biotechnology (AFOB), Pakistan.

Prof Robert Nash

Prof Nash heads two natural product companies based in Wales, PhytoQuest Ltd and Sugars for Health Ltd. He has over 250 refereed publications on compounds and their activities and several granted patents related to oncology, immunology, metabolic syndrome and inflammation. His PhD at RBG Kew/King's College London with Professor Arthur Bell was on anti-HIV iminosugars from *Castanospermum australe* and as head of chemistry at a BBSRC institute (IGER) he continued to have a niche focus on iminosugars for new applications related to carbohydrate biology with most new iminosugar structures having been reported from his team and collaborators. Iminosugars occur in many foods and herbal supplements but are rarely noticed by analytical labs as they resemble common sugars and amino acids on analysis. They can have very potent and specific biological activities. Discovering and developing better cancer treatments is his main goal as well as improving ageing. The main focus of the companies has recently been commercializing food supplement products containing iminosugars for inflammatory disorders and priming immune responses but pharmaceutical and animal health uses are still the longer-term goal. He is an honorary professor at the Faculty of Science and Engineering at Swansea University. He was awarded the 1st Pierre Fabre Award of the Phytochemical Society for his work on iminosugars.

Dr Babatunde Samuel

Dr Samuel obtained a Bachelor's degree in Pharmacy from the University of Ibadan where he graduated as the best graduating student in Pharmaceutical Chemistry. He further got his Masters in Pharmaceutical Chemistry as the best graduating student in the department; and subsequently obtained his PhD in Natural Product Chemistry from the University of Ibadan [2006]. He commenced his career as a Research fellow at the National Institute for Pharmaceutical Research and Development, Abuja, Nigeria where he served for 15 years [1995 -2010]. It was there he developed with other scientists a phytopharmaceutical product that was patented in 46 countries [USA and UK inclusive] by the United Nations Development Organization. After his PhD, he engaged in two Postdoctoral Fellowships; first at the University of Pretoria, South Africa [NRF] and the second at the Indian Institute of Integrative Medicine, Jammu, India [TWAS]. He later moved to the University of Ibadan for Academic/Research activities in 2010. At the University of Ibadan, he was a Team member of CDDDP Research team that won a One Million Dollar MacArthur Research Grant for research and training of scientists in drug discovery. He has obtained several Travel Fellowships which enabled him to conduct research or attend conferences in the United States, Italy, and South Africa, among others. He holds a US Patent and he has co-authored about 50 publications in

reputable journals. In the last four years, he has expanded his natural products research studies to embrace Computer Aided Drug Design [*in-silico*] to facilitate his exploration of natural products. This approach has allowed him to explore thousands of compounds within a short time. He currently lectures and conducts research at the Pharmaceutical Chemistry Department of the University of Ibadan where he has supervised several Postgraduate students [MSc and PhD].

Prof Dr Eman Shawky

Prof Shawky, an academic from Egypt, is engaged in the field of pharmacognosy and natural products. Prof Eman's expertise shines brightly in her dedication to unravelling the complexities of metabolomics, quality control, and the mechanisms of action of herbal drugs as well as natural products drug discovery. With a genuine passion for research and teaching, she has authored more than 80 publications and overseen the supervision of more than 30 theses during her research career over the past 20 years. Currently serving as a Professor in the Pharmacognosy Department at the Faculty of Pharmacy, University of Alexandria, Prof Eman remains committed to advancing scientific knowledge. Prof Eman has been listed in the Top 2% scientists of in the world in the report prepared by Stanford University in 2021 and 2022. Alongside her academic pursuits, she humbly contributes as a reviewer and editorial board member for esteemed journals, reflecting her steadfast commitment to the field's growth.

Prof Miroslav Strnad

Prof Strnad is a professor in the Laboratory of Growth Regulators, Institute of Experimental Botany ASCR & Palacký University in Olomouc, Czech Republic (rustreg.upol.cz). Strnad's current focus is on the research and development of a new generation of compounds with anti-viral, anti-proliferative, anti-angiogenic and anti-senescence properties, the molecular mechanisms of their action and the potential combinatory therapies based on these compounds, new phytohormone derived cosmetic as well as plant growth regulators for plant biotechnology and agriculture. He graduated in Phytotechnologies from the Faculty of Agronomy, Mendel University, Brno, in 1982 (Ing.). In 2001 was promoted to Professor of the Palacký University in Olomouc, Czech Republic. In 1998, he was awarded the Rhone-Poulenc Rorer Award by the Phytochemical Society of Europe (PSE), in recognition of his work on the identification, analysis and biochemistry of phytohormones topolins. In 1999, he received the award of the City of Olomouc and honorary residency of Olomouc; in 2004 the prize of the Learned Society of the Czech Republic in recognition of his scientific achievements. Prof Strnad has been widely publishing (11 chapters in books; more than 480 papers in recognized journals; 3 books; 38 Czech and 43 international patents; citations >17, 000; *h*-index: 70). He was PSE president (2014-2016), and between 2012-2014, 2016-2018 vice-president.

Prof Shaikh Jamal Uddin

Prof Uddin has been a Professor in Pharmacy Discipline at Khulna University, Bangladesh since 2019. Currently, he is also serving as an Associate Fellow of Bangladesh Academy of Sciences. He started his academic career in 2005 as a Lecturer in Pharmacy Discipline at Khulna University. He completed BPharm (Hons.) from Khulna University in 2004 with the President and Prime Minister Gold Medal awards. To develop advanced research skills in natural products chemistry and pharmacology, he moved to the School of Pharmacy, Griffith University, Australia to pursue his PhD research, in the field of anticancer drug discovery from Bangladeshi medicinal plants through International Postgraduate Research Scholarship (IPRS) and completed his PhD in 2011. After returning to his discipline, he developed his research group and continued his teaching and research as an independent researcher. He also completed postdoctoral research in 2015 at the Division of Pharmacognosy, Uppsala University, Sweden, under the competitive EXPERT4Asia Erasmus Mundus fellowship. He also worked as an adjunct researcher for the Faculty of Pharmacy, Ton Duc Thang University, Vietnam from 2019 to 2020. He is the Executive Editor of Khulna University Studies (an official Journal of Khulna University, Bangladesh) and an Associate Editor in Frontiers in Pharmacology section Ethnopharmacology. He also acts as a reviewer of several reputed journals. Prof Uddin's main fields of interest are ethnopharmacology and drug discovery from natural sources. He has more than 20 years of research experience in the field of drug discovery from medicinal plants and developed an excellent research career in this field. As a principal and associate investigator, Prof Uddin has won over 25 million BDT (Bangladeshi taka) in research funding including from Khulna University Research Cell, Ministry of Science and Technology, Bangladesh, Ministry of Education, Bangladesh, University Grant Commission, Bangladesh and World Bank. He has developed several pharmacological methods to evaluate the therapeutic potential of different medicinal plant extracts in mouse models and discovered many bioactive novel compounds with different biological properties. He has published more than 100 papers in high-impact journals in his field of research, and he has an *h*-index of 38, *i10*-index of 69 and total citations >5000 (source: Google Scholar). For his excellent research record, he has been awarded the University Grant Commission Award by the President in 2014, United Group Best Paper Award in 2015 and Khulna University Vice Chancellor Award in 2020. He was also awarded different conference and travel awards. He has established collaborations within the university and with other national multidisciplinary research scientists as well as many scientists and research groups around the globe including Australia, UK, Arab, India, Malaysia, Jordan, Brazil, Pakistan, Poland and China. He regularly attends national and international conferences and symposia to present his work. Currently, Prof Uddin is involved in different University committees and works as an active member of different professional organizations.

Dr Evelyn Wolfram

Dr Wolfram obtained a degree in Environmental Engineering from Technical University Berlin and a Master of Science from the University of Massachusetts at Amherst. She pursued a PhD in Biotechnology at the Helmholtz Centre Jülich and the Technical University of Munich. She served in several R&D Management positions in the pharmaceutical, food and cosmetic supplement industry before she became a senior researcher and lecturer at ZHAW for phytopharmacy and natural products. She is currently the author of over forty peer-reviewed publications and the author of three patent applications and two book contributions. Since 2016, she works as an Associate Editor of the journal *Phytochemical Analysis*. In 2018, she co-founded planar4 GmbH, a ZHAW startup company focusing on commercialization of bioautographic assays and is working in applied science within the herbal health product industry. She is a senior scientific advisor of the global non-for-profit Empowered by Evidence initiative and a member of the board and scientific committee of ESCOP.



Abstracts of the Invited Plenary Talks

(In alphabetical order)

***Aristotelia chilensis* (Mol) Stunz, “Maqui” new advances in the search for bioactive molecules**

Carlos L. Cespedes-Acuña^{1*} and Julio Alarcon-Enos¹

¹Department of Basic Sciences, Research Group in Chemistry and Biotechnology of Bioactive Natural Products, Faculty of Sciences, University of Bio-Bío, Andrés Bello Avenue, Chillan, Chile

*E-mail: ccespedes@ubiobio.cl

Maqui-berry (*Aristotelia chilensis*) is an emerging Chilean superfruit with high nutraceutical value. Until now, the research on this commodity has focused on the formulations enriched with polyphenols from the pulp. Herein, the contents of tocopherols were compared in the seed oil of Maqui-berry obtained through different extraction methods followed by determining their antioxidative and enzyme inhibitions *in-vitro*. Firstly, oilseed was extracted with *n*-hexane (Soxhlet method), chloroform/methanol/water (Bligh and Dyer method) and pressing (industrial). These samples were analyzed for their effects against DPPH, HORAC, ORAC, FRAP, Lipid-peroxidation (TBARS), α -amylase, α -glucosidase, and pancreatic lipase. Newly, we report that the isomers of tocopherol, tocotrienol, and β -sitosterol show enzyme inhibition. Additionally, tocopherols, our extracts and isolated compounds from fruit and aerial parts of this super berry have shown activity against Ishikawa and colon cancer cells and in Alzheimer's disease enzymes such as acetylcholinesterase. Further, seed oil from Maqui berry and their tocopherols (α , β , γ , δ -tocopherols, tocotrienols, and β -sitosterol) warrant clinical investigation for their antioxidative and anti-obesity potential. Taken together, these findings provide relevant and suitable conditions for the industrial processing of Maqui-berry.

Cytotoxic activities of some plants used in Nigerian ethnomedicine for the treatment of cancer

Mansurah A. Abdulazeez^{1*}, Jiradej Manosroi², Yusuf Saidu³, Abdullahi B. Sallau⁴, Musa A. Tabari⁵, Abubakar Hafiz⁶, Muhammad Y. Gwarzo⁷, Shamsudeen Haruna⁷, Aminu IDI (AI)⁶, Musa Bashir⁸, Shamsudeen L. Pedro¹, Kamaludeen Babagana⁶, Aranya Manosroi², and Amos A. Fatokun⁹

¹*Centre for Biotechnology Research, Bayero University, Kano, Nigeria*

²*Department of Cosmetic Technology, Faculty of Science and Technology, North-Chiang Mai University, Chiang Mai, Thailand*

³*Department of Biochemistry, Usmanu Danfodiyo University, Sokoto, Nigeria*

⁴*Department of Biochemistry, Faculty of Life Sciences, Ahmadu Bello University, Zaria, Nigeria*

⁵*Department of Radiology, Barau Dikko Teaching Hospital (BDTH), Kaduna State University (KASU), Kaduna, Nigeria*

⁶*Department of Biochemistry, Faculty of Basic Medical Sciences, Bayero University, Kano, Nigeria*

⁷*Department of Medical Laboratory Science, Faculty of Allied Health Sciences, College of Health Sciences, Bayero University, Kano, Nigeria*

⁸*Centre for Dryland Agriculture, Bayero University, Kano, Nigeria*

⁹*Centre for Natural Products Discovery (CNPD), School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Liverpool L3 3AF, UK*

*E-mail: mabdulazeez.cbr@buk.edu.ng

Despite considerable efforts, cancer remains an aggressive killer worldwide: in Africa, approximately 573,653 deaths in 2022, and a projected one million deaths in 2030. Most cancer patients in Nigeria use medicinal plants for treatment, but the therapeutic efficacies of a majority of the plants are yet to be established. We, therefore, investigated the cytotoxic activities of fourteen (14) medicinal plants used in Nigerian ethnomedicine for the treatment of cancer. The leaves of *Acacia senegal*, *Ageratum conyzoides*, *Albizia chevalieri*, *Annona muricata*, *Borreria stachydea*, *Cassia singueana*, *Dicoma tomentosa*, *Guiera senegalensis*, *Heliotropium indicum*, *Peristrophe bicalyculata*, *Physalis angulata*, *Senegalia ataxacantha*, *Xeromphis nilotica*, and the stem bark of *Euphorbia hirta* were screened for cytotoxicity against the human cervical cancer (HeLa), breast cancer (MCF-7) and lung cancer (A549) cell lines, using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) assay. Bioactivity-guided fractionation of the most cytotoxic extracts was carried out and the mechanisms of cell death of the most active subfractions were investigated: LDH activity, mitochondrial membrane integrity, caspase activity, and DNA damage. Effects on migration and VEGF secretion were also analysed to provide insights into potential effects on metastases and

angiogenesis. Changes to mRNA expression were assessed using Quantitative Real-Time PCR. The plants were most cytotoxic against HeLa cells. Three subfractions, AMHE-S-1, AMHE-S-2, and AMHE-S-3, obtained from the ethyl acetate fraction of *A. muricata* (AMHE2), were most cytotoxic against HeLa, with IC_{50} values of 8.56 ± 1.36 , 15.35 ± 1.28 and $16.38 \pm 1.31 \mu\text{g/ml}$, respectively. AMHE-S-1 significantly induced LDH and caspase activity, inhibited migration, damaged mitochondrial membrane integrity, and caused DNA damage. AMHE-S-1 and AMHE-S-3 increased BAX and decreased BCL2 mRNA expression, while only AMHE-S-1 induced caspase 3 expression. Liquid chromatography-mass spectrometry (LC-MS) analysis of AMHE-S-1 identified bromosuccinic acid, 3-hydroxy-beta-ionone (a sesquiterpenoid) and 2-arylbenzofuran flavonoid. This study further established the therapeutic potential of *A. muricata* for the treatment of cervical cancer.

Amaryllidaceae alkaloids as inspiration for medicinal chemistry

Lucie Cahlíková*, Filip Pidaný, Jan Korábečný, Jana Křoustková, Negar Maafi

Secondary Metabolites of Plants as Potential Drugs Research Group, Department of Pharmacognosy and Pharmaceutical Botany, Faculty of Pharmacy, Charles University, Heyrovského 1203, 500 05 Hradec Králové, Czech Republic

*E-mail: cahlikova@faf.cuni.cz

Plants of the family Amaryllidaceae have a long history of being used as herbal remedies all over the world to cure different ailments and diseases. Since the isolation of the first Amaryllidaceae alkaloid (AA), lycorine, more than 600 AAs have been isolated and studied in terms of their biological activities. In the last decade, our research group has isolated more than 100 AAs of various structural types from the genera *Zephyranthes*, *Narcissus*, *Nerine*, and other species. Isolated compounds have been tested for biological activity connected with the potential treatment of neurodegenerative, oncological, and infectious diseases. Because several AAs can be isolated from plants in large quantities, they are also an interesting target for the preparation of semisynthetic derivatives. On the other hand, minor compounds can be used as inspiration for the development of fully synthesized compounds. The structural aspects of AAs (haemanthamine, ambelline, vittatine, and galanthamine) allowed us to prepare novel chemical entities by derivatizing their free hydroxyl groups and inspecting the structure-activity relationship of the novel derivatives. The hydroxy group was acylated with differently substituted benzoyl chlorides, 1- and 2-naphthoyl chlorides, and 2-furoyl chloride, affording the corresponding esters. Minor alkaloids isolated from *Narcissus pseudonarcissus* cv. Carlton have been used as structural scaffolds for the design of synthetic compounds inspired by their structure. We determined the structures of the newly synthesized compounds using MS, HRMS, and 1D- and 2D-NMR. An antimycobacterial assay was performed with fast-growing *Mycobacterium smegmatis* DSM 43465, *Mycobacterium aurum* DSM 43999, and an avirulent strain of *Mycobacterium tuberculosis* H37Ra ITM-M006710. The technique used for activity determination was the microdilution broth panel method using 96-well microtitration plates. Modified Elmann's method has been used for the determination of the inhibition activity of cholinesterases. Cytotoxicity has been tested using an MTT assay on a panel of 10 cancerous cell lines. In several recent studies, it has been shown that semisynthetic derivatives of AAs and synthetic compounds inspired by their structure have promising pharmacological potential for further exploration and structure optimization as new drugs against various diseases.

Multiple smooth muscle relaxant activities of berberine chloride identified using *in vitro* rat model of viral-mimetic-induced motility changes underlying miscarriage

James EG Downing*, Fikayo Mary Fadiran

*Centre for Natural Product Discovery (CNPD), School of Pharmacy and Biomedical Sciences,
Liverpool John Moores University, James Parsons Building, Byrom Street, Liverpool L3 3AF,
United Kingdom*

Maternal immune response to infection triggers cytokines which evoke smooth muscle activity leading to miscarriage. Up to 26% of pregnancies are estimated to result in spontaneous abortion. Pathogen-induced motility disorder can be modelled *in vitro* using pathogen-associated molecular pattern (PAMPs) such as the viral mimetic polyinosinic:polycytidylic acid (PIC). Subsequently, the therapeutic potential of Natural products can be investigated from their efficacy in modifying either cytokine- or neurotransmitter-induced motility. Berberine chloride (BBCl) is reported to be effective at averting experimental abortion in response to the bacterial PAMP, lipopolysaccharide, but it is not known whether BBCl is effective against PIC. The aim was to assess the tocolytic potential of BBCl (20 μ M) *in vitro* on rat smooth muscle preparations. To determine whether PAMP-evoked motility, once initiated in uterine strips, could be attenuated by BBCl, it was applied (20 μ M, over 60m) after PIC (10 μ g/ml, over 120m). Second, to determine whether PAMP-evoked motility was limited by prior exposure to BBCl, it was applied (20 μ M, over 90m) before PIC (10 μ g/ml, over 120m). Third, to determine whether 20 μ M BBCl affects the pharmacodynamics of prokinetic (acetylcholine, Ach; serotonin, 5HT) and relaxant (noradrenaline, NA) neurotransmitters affecting smooth muscle motility of gut ileal strips (and therefore likely also the uterus), dose-response to transmitters were collected in the absence, presence then again in the absence of BBCl. It was found that, although BBCl itself induced changes in uterine motility, its tocolytic potential of BBCl was evidenced by both anti-inflammatory and pharmacodynamic modifying effects on transmitters. BBCl reduced uterine motility not only once triggered by PIC, but also prevented motility when administered preceding PIC. In addition, BBCl competitively antagonised prokinetic Ach and 5HT; while potentiating stasis induced by NA. In conclusion, some authors have recognised the potential for natural selection to endow natural products with multiple coordinated target efficacies (Sánchez-Rodríguez *et al.*, 2017). Berberine has multiple activities that may be relevant to reproductive health, including anti-microbial, anti-inflammatory and transmitter modifying activity. Our findings suggest the efficacy of BBCl on several mechanisms, each of which would favour tocolysis in the face of viral sepsis.

Formulation challenges for paediatric 3D printed personalised medicines

Touraj Ehtezazi,* Alice McCloskey, Satyajit D Sarker

*Centre for Natural Product Discovery, Liverpool John Moores University, Byrom Street,
Liverpool, L3 3AF, UK*

*E-mail: t.ehtezazi@ljmu.ac.uk

Over seven billion population and the increase in average age require a different type of supply chain and production for medicines, which has been referred to as personalised medicine. This type of therapy plays an important role in the prevention, diagnosis, treatment, and prognosis of several diseases such as cancer. The current pharmaceutical production processes and regulatory aspects have been optimised to provide a limited variety of pharmaceutical dosage forms. Additive manufacturing has emerged as a promising technology to meet the demand for personalised medicine. This technology allows us to adjust the drug amounts in the dosage form, and combine different drugs and excipients (both natural and synthetic compounds) to achieve desired targeted drug release profiles. 3D printing (an additive manufacturing technology) of gels allows to production of gummies with attractive shapes and flavours. The gel formulation should follow certain viscoelastic behaviour during printing, allowing for printing objects with minute details. In theory, 3D printing allows production of gummies with different flavours; and this must be maintained to ensure adherence to medication in children. However, this becomes challenging in practice as changing the flavouring agents may completely change the rheological behaviours of gels. Therefore, the formulation components should be adjusted/changed to achieve certain rheological properties for 3D printing of objects with desired details. This presentation covers the formulation optimisations in 3D printing of pharmaceutical gels and a survey of acceptance of 3D printed gummy bears by children.

Potential phytochemicals and their biological activities of three Euphorbiaceae species explored by bio-affinity ultrafiltration LC-MS with multiple drug targets

Ming-Quan (Mark) Guo*, Tojofaniry Fabien Rakotondrabe², Min-Xia Fan²

*Ningbo Cixi Institute of Biomedical Engineering, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201, China

²Wuhan botanical Garden, Chinese Academy of Sciences, Wuhan, 430074, China

*Email: guomingquan@nimte.ac.cn

Euphorbiaceae species have been used worldwide as remedies for an array of animal and human ailments. Among them, *Acalypha australis* L., *Euphorbia maculata* L., and *Euphorbia humifusa* Willd are traditionally used for managing multiple diseases and express similar pharmacological activities. However, very limited research has been conducted on their bioactive compounds responsible for potential anti-inflammatory, antidiabetic, antiproliferative, and hemostatic effects, and their possible mode of action also remained elusive. This talk will highlight the innovative methodologies and technological advances in exploring the potential bioactive compounds of each species underlying their empirical activities, and further reveal their possible mode of action. An integrative approach combining different in vitro activity assessments followed by fast screening strategies through the bio-affinity ultrafiltration coupled with ultraperformance liquid chromatography connected to a quadrupole time of flight mass spectrometer (UF-LC/MS), and in silico study was also adopted. The multiple key enzymes participating in inflammation (Cyclooxygenase 2: COX-2), diabetes (α -Glucosidase: α -Glu), cancer (Topoisomerase I: Topo I, and Topoisomerase II: Topo II), and bleeding disorders (urokinase plasminogen activator: uPA) were selected as drug targets to screen for their respective ligands with UF-LC/MS. As a result, 9 potential candidates were screened out and validated, which consisted of the anti-inflammatory compound aurantiamide from *A. australis*; the double-acting anti-inflammatory and antiproliferative DHM and guaijaverin, from *E. maculata*; the antidiabetic and anti-inflammatory compounds astragaloside and vitexin, from *E. humifusa*; as well as the hemostatic compounds isoquercetin, orientin, BCA, and rutin from the three Euphorbiaceae species. These outcomes may serve as scientific sources and open up new perspectives for further pharmaceutical research.

Advances of plant metabolomics in the study of self-DNA inhibition

Virginia Lanzotti*

Dipartimento di Agraria, Università di Napoli Federico II, Via Università 100, 80055 Portici, Italy

*E-mail: lanzotti@unina.it

Extracellular DNA (exDNA) widely occurs in the environment due to release by either cell lysis or active secretion. The role of exDNA in plant-soil interactions has been investigated in the past years. An inhibitory effect on the growth of conspecific individuals by their self-DNA has been recently reported. This effect was first discovered in plants and then demonstrated in the model organisms: *Arabidopsis thaliana* (plants), *Coenorabtidis elegans* and *Drosophila melanogaster* (animals), and *Saccharomyces cerevisiae* (fungi). Transcriptome analysis in the model plant *A. thaliana* showed a clear recognition by the plant roots of self- and nonself-exDNA, with inhibition occurring only after exposure to the former. Untargeted NMR and LC-MS metabolomics followed by chemometrics were used to assess at molecular level the plant reactions to self and nonself-exDNA exposure. Results evidenced that self-DNA significantly induces the accumulation of RNA constituents (nucleobases, ribonucleosides, dinucleotide and trinucleotide oligomers). Interestingly, AMP and GMP are found along with their cyclic analogues cAMP and cGMP, and in the form of cyclic dimers (c-di-AMP and c-di-GMP). Also, methylated adenosine monophosphate (m6AMP) and the dimeric dinucleotide *N*-methyladenylyl-(3'→5') cytidine (m6ApC) increased only in the self-DNA treatment. Such striking evidence of self-DNA effects highlights a major role of exDNA in plant sensing of its environment. This discovery opens a new scenario of pharmacological applications integrating metabolite profile assessment with specific inhibitory effects by self-DNA.

Cryogenic milling

Greg Leach*

Antylia Scientific, UK

*E-mail: Greg.Leach@antylia.com

Cryogenic milling is a means of efficient, effective & safe sample preparation for a wide spectrum of materials. The use of liquid nitrogen (a cryogen) is used to embrittle the sample and pulverize it to a powder. The sample preparation of solid sample materials represents a challenge for many areas of scientific analysis. For decades, traditional milling was done using a mortar and pestle. It is still widely used for a variety of materials and is often defined as a good sample preparation method. However, the criteria for a well-ground sample should yield good analytical results and be easily reproducible. The homogenisation and particle size reduction process must be efficient, effective, reproducible, and safe. The Cole-Parmer Freezer/Mills offers the opportunity for safe, reliable, and reproducible results when milling a wide range of sample materials into a fine analytical powder. Since the vial is securely closed the integrity of its contents is maintained, hazardous or critical samples are easily controlled, and cross-sample contamination is eliminated. The sample chemical composition is preserved as a result of the vials being immersed in liquid nitrogen at cryogenic temperatures throughout the grinding process. Furthermore, using the Freezer/Mill preserves volatile analytes which can degrade during traditional milling methods with a mortar and pestle. The Cole-Parmer Freezer/Mills are the “mills of first choice” for many materials, or samples whose composition or structure cannot be ground using conventional grinding methods.

Plant-derived agents in non-melanoma skin cancer: Current landscape and future perspectives

Iolanda Alca Iliescu Toma¹, Liliana Verestiuc¹, Ina Albert², Evelyn Wolfram², Anca Miron^{1,*}

¹Grigore T. Popa University of Medicine and Pharmacy, Universitatii Str. 16, 700115, Iasi, Romania

²Zürich University of Applied Sciences, 8820 Wädenswil, Switzerland

*E-mail: anca.miron@umfiasi.ro, ancamiron@yahoo.com

Non-melanoma skin cancer (NMSC) is the most common type of cancer, mainly caused by overexposure to UV radiations. Other contributing factors include the frequent use of artificial tanning sunbeds, immunosuppressive medication, exposure to mutagens, viral infection and genetic propensity. Chemoprevention is an essential approach for decreasing the incidence of NMSC. But the most used chemopreventive agents (retinoids, difluoromethylornithine, cyclooxygenase-2 inhibitors, DNA repair enzymes, inhibitors of hedgehog pathway) show disadvantages associated with lack of expected efficacy and adverse reactions. Other treatment options (cryotherapy, radiotherapy, chemotherapy, photodynamic therapy) also have drawbacks such as recurrence and side effects. The present limits in the prevention and treatment of NMSC support the need for novel prophylactic and/or therapeutic agents. This presentation, including also own studies, focuses on plant-derived agents (extracts, phytochemicals) affecting NMSC through various pathways (down-regulation of fibroblast growth factor receptors, mechanistic target of rapamycin and beta-catenin pathways, inhibition of ornithine decarboxylase, DNA damage repair, reduction of inflammation and oxidative stress, induction of apoptosis). Relevant drug delivery systems to boost the topical bioavailability of plant extracts/phytochemicals are discussed. The latest research supports the ability of some plant extracts/phytochemicals to prevent, suppress or reverse processes involved in NMSC. Undoubtedly, plant-derived agents represent an emerging strategy in NMSC prevention and treatment but evidence from more animal and human trials reinforcing their efficacy and safety is strongly needed.

A flavonoid-rich extract of white grape juice hampers seizures in different rodent models of epilepsy

Alessandro Maugeri^{1*}, Caterina Russo², Rita Citraro³, Giovambattista De Sarro³,
Michele Navarra²

¹*Department of Veterinary Sciences, University of Messina, Viale G. Palatucci, 98168 Messina, Italy*

²*Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Viale F. Stagno d'Alcontres, 98166 Messina, Italy*

³*Department of Health Sciences, University "Magna Græcia" of Catanzaro, Viale Europa, 88100 Catanzaro, Italy*

*E-mail: amaugeri@unime.it

The beneficial properties of natural products to manage neurological diseases are acknowledged by the whole scientific community. On this line, flavonoids have been suggested to possess anticonvulsant properties, which can be exploited as tools in novel strategies against epilepsy. Therefore, this study aimed to investigate the effects of a flavonoid-rich extract of white grape juice (WGJe) in different rodent models of epilepsy, as well as to explore its putative mechanism of action. Our results showed that the administration of WGJe exerted anticonvulsant effects in pentylenetetrazole (PTZ)-induced seizures in ICR-CD1 mice, in which only tonic seizures were significantly hindered ($p < 0.01$). In WAR/Rij rats, a genetic model of absence epilepsy with comorbidity of depression, WGJe did not alter the number and/or duration of the spike-wave discharges in comparison to untreated rats. In genetically audiogenic seizures (AGS)-susceptible DBA/2 mice, WGJe was able to significantly hamper both clonic and tonic seizures ($p < 0.01$). Moreover, WGJe showed to possess anxiolytic effects, as assessed through the open-field test. Interestingly, the co-administration of WGJe with flumazenil in DBA/2 mice restored both clonic and tonic seizures, as well as did not protect mice against wild running in comparison to WGJe administered alone, thus suggesting that GABA_A receptor mediates the observed results. This study demonstrated the antiepileptic activity of WGJe, thus supporting its potential role in the management of epilepsy as a novel complementary therapy in the frame of a multitarget pharmacological strategy.

Fetal Hemoglobin (HbF) Inducers for the Treatment of Beta-thalassemia: A Few Interesting Stories

Syed Ghulam Musharraf ^{a, b}

^aH.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan.

^bDr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan

E-mail: musharraf1977@yahoo.com, musharraf@iccs.edu

Beta-thalassemia is an inherited autosomal recessive blood disorder, characterized by the complete absence or reduction of β -globin chain of haemoglobin (Hb). The imbalance in α and β -globin chains synthesis causes precipitation of unbound α -globin chains in erythroid cells, which results in dyserythropoiesis. Pharmacological induction of γ -globin production (production of fetal haemoglobin HbF) can ameliorate the severity of the disease and is a promising way the management of beta-thalassemia. In continuation of our research work in understanding beta-thalassemia at the molecular level, we have also worked on treatment strategies. In our research group, we have used two important strategies to identify potent HbF inducers, 1-Screening of a large number of FDA-approved drugs to evaluate their potential for HbF induction and thus can be used for repurposed 2-Scientific evaluation and validation of indigenous medicinal plants that are used in the treatment of blood disorders particularly in beta-thalassemia. Based on the above-mentioned screening strategies, a large number of experiments are performed using different *in-vitro* and *in-vivo* models including the Erythroleukaemia K562 cell line, CD34⁺ progenitor cells and β -YAC transgenic mice model. Different molecular and analytical techniques were used for sample analysis and data generation such as γ -globin gene expression by RT-qPCR, estimation of fetal haemoglobin production by flow cytometry and immunofluorescence microscopy, and metabolomics and proteomics analysis using advanced mass spectrometry tools. Different classes of compounds from synthetic and natural products were identified as HbF inducers, Similarly, three FDA-approved drugs were identified as potent HbF inducers. Interestingly, two medicinal plants *Fagonia indica* and *Adhatoda vasica* were extensively studied and we have identified their potential for use in the treatment of beta-thalassemia. Details will be discussed in the lecture.

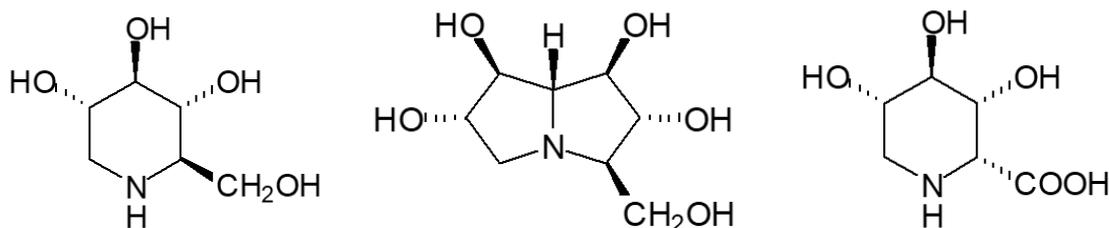
The benefits of natural imino-sugar

Robert J. Nash* and Yana B. Penkova

PhytoQuest Limited, Aberystwyth SY23 3EB, UK

*E-mail: robert.nash@phytoquest.co.uk

The presentation will focus on our research on iminosugars in human and animal foods. Iminosugars are common plant components but are rarely detected or identified. The iminosugars are analogues of common metabolites such as monosaccharides, disaccharides or amino/imino acids and can have potent biological activities via receptor interactions or enzyme inhibition or promotion. They are orally available, not toxic, not incorporated into larger molecules and are eventually excreted unchanged in urine although the effects can be long-lasting.



DNJ from mulberry casuarine from certain honeys idoBR1 from some cucumbers

1-deoxynojirimycin (DNJ) was one of the first of the iminosugars to be discovered in 1970 from Chinese herbal medicines and is the basis of drugs for controlling blood glucose levels (e.g. Glyset). More recently iminosugars have aroused great interest as potential new medicines for a wide range of ailments related to their ability to modulate carbohydrate biochemistry without necessarily being glycosidase inhibitors. For example, idoBR1, an iduronic acid analogue from some cucumbers is anti-inflammatory and has shown to be of benefit in osteoarthritis at $\mu\text{g}/\text{daily}$ per person; it reduces the production of TNF-alpha. There are well over a hundred natural iminosugars now known but few are commercially available due to the special expertise needed to isolate, identify or synthesise them. They are common in foods and herbal medicines and may be the elusive highly active components of many of them.

Structural elucidation and *in-silico* studies of antimalarial principles isolated from *Combretum racemosum* leaf extract

Babatunde B. Samuel^{1*}, Wande M. Oluyemi², Lisolette Krenn³

¹*Pharmaceutical Chemistry Department, Faculty of Pharmacy, University of Ibadan, Nigeria*

²*Pharmaceutical Chemistry Department, Faculty of Pharmacy, Afe Babalola University, Ekiti State, Nigeria*

³*Department of Pharmacognosy, University of Vienna, Althanstrasse 14, A-1090 Vienna, Austria*

*E-mail: bb.samuel@mail.ui.edu.ng

Combretaceae species are widely applied locally for the treatment of various diseases including malaria. Our study screened ten Combretaceae plants extracts selected based on their use in ethnomedicine for antimalarial activity. Methanol and acetone leaf extracts of the plants were screened by applying the inhibition of β -hematin synthesis colourimetric assay. *Combretum racemosum* (methanolic extract) which had the most significant inhibitory activity from the colorimetric assay was subjected to further studies. The crude methanolic extract and solvent fractions of *Combretum racemosum* were investigated for antiplasmodial activities against D10 and W2 strains of *Plasmodium falciparum* in a lactate dehydrogenase (LDH) enzymatic assay. Repeated chromatographic separations were conducted on the chloroform fraction to isolate bioactive compounds for further antiplasmodial activity tests. The characterization of the isolated compounds was performed by applying NMR and MS techniques. An *in-silico* study was thereafter carried out on the isolated compounds to investigate their potential allosteric inhibition of pflDH by targeting the substrate-binding site. Eight bioactive compounds were isolated and characterized as; 19 α -hydroxyasiatic acid, 6 β ,23-dihydroxytormentic acid, madecassic acid, nigaichigoside F1, arjungenin, combrogenin, terminolic acid, arjunglucoside I. Madecassic acid was identified as the most active compound (D10: IC₅₀=28 \pm 12 μ g/mL and W2: IC₅₀=17.2 \pm 4.3 μ g/mL). The docking studies also confirmed that madecassic acid had the highest binding affinity (-33.40 kcal/mol) as observed in the energy calculations, indicating that madecassic acid exhibited profound inhibitory activity. This study has provided a scientific basis for the use of *C. racemosum* leaf for the treatment of malaria in ethnomedicine.



Metabolomics Unleashed: Untangling Nature's Chemical Diversity in Medicinal Plants Systems

Eman Shawky

*Pharmacognosy Department, Faculty of Pharmacy, Alexandria University, Egypt,
Alexandria 21521, Egypt*

E-mails: shawkyeman@yahoo.com, eman.m.shawky@alexu.edu.eg, shawkyeman@yahoo.com

For centuries, medicinal plants have served as the foundation of traditional medicine, yet unlocking their full potential necessitates a deeper dive into their intricate chemical makeup. This talk explores the evolving field of metabolomics and its transformative power in revolutionizing our understanding of medicinal plants. This talk highlights the innovative methodologies and technological advances driving the field of plant metabolomics forward, including mass spectrometry, nuclear magnetic resonance spectroscopy, and high-throughput profiling platforms. Metabolomics offers a comprehensive analysis of a plant's entire metabolite profile, encompassing small molecules with diverse functions. This empowers researchers to discriminate between closely related species with similar appearances by analyzing unique metabolite fingerprints, ensuring the authenticity and quality of herbal products. Furthermore, metabolomics allows for pinpointing the specific metabolites responsible for a plant's therapeutic effects, streamlining the drug discovery process and leading to the identification of novel bioactive compounds with immense pharmaceutical potential. By shedding light on the complex biochemical pathways involved in a plant's therapeutic action, metabolomics unravels the mechanism of action, enabling researchers to design more targeted and efficacious herbal remedies. Ultimately, harnessing the power of metabolomics empowers the development of standardized herbal products, personalize treatment plans based on the interplay between plant metabolites and the body, and discover novel drug leads from previously unknown bioactive compounds – paving the way for a new era of botanical drug discovery and optimization, leading to more effective and personalized therapeutic strategies.

Brassinosteroids, their analyses, biological and medical activities

Miroslav Strnad^{a,*}, Jana Okleštková^a, Lucie Rárová^b, Gabriel Gonzalez^b, Miroslav Kvasnica^a, Danuše Tarkowská^a

^aLaboratory of Growth Regulators, Palacký University Institute of Experimental Botany ASCR, Šlechtitelů 27, Olomouc, Czech Republic

^bDepartment of Experimental Biology, Palacký University, Šlechtitelů 27, Olomouc, Czech Republic

*E-mail: miroslav.strnad@upol.cz

Brassinosteroids (BRs) are a group of phytohormones occurring naturally in extremely low endogenous concentrations (fg-pg/g FW). We therefore developed several sensitive mass spectrometry-based methods for the simultaneous profiling of eighteen brassinosteroids including biosynthetic precursors and most biologically active metabolites. The extraction procedure and one-step purification based on solid phase extraction (SPE) were optimized in combination with subsequent ultrahigh performance liquid chromatography (UHPLC) analysis coupled to positive electrospray ionization tandem mass spectrometry ((+)ESI-MS/MS). The detection limit for most analysed BRs ranged between 0.05 and 40 pg using only 50 mg of plant tissue. These analyses showed that not all BRs known from described biosynthetic pathways are present in plant tissues. In vitro and in vivo experiments have also demonstrated that they can also have diverse effects on animal cells and tissues. The molecular and cellular effects of natural BRs were examined in different human cancer cell lines and primary endothelial cells in vitro. BRs caused growth inhibition, cell cycle arrest and initiation of apoptosis in many different cancer cell lines. The inhibition of proliferation and migration of human endothelial cells by BRs was also demonstrated. The observed inhibition of migration and tube formation demonstrated the antiangiogenic activity of BRs. Investigation of the BR mechanisms of action in human cancer and endothelial cells indicated the possible involvement of steroid receptors in BR action. However, BRs were shown not to bind directly to steroid receptors which demonstrates that BRs act via steroid receptor-independent pathway(s). Our results suggest that tested BRs are promising leads for the development of a new generation of potential anticancer drugs.

Ethnopharmacological Evaluation of Sundarban Plants: A Treasure of Natural Bioactive Molecules

Shaikh Jamal Uddin*

Pharmacy Discipline, Life Science School, Khulna University, Khulna-9208, Bangladesh

*Email: uddinsj@pharm.ku.ac.bd/ uddinsj@yahoo.com

Sundarbans is the world's largest mangrove forest consisting of dynamic environments and diverse terrestrial and aquatic flora and fauna. Mangrove and mangrove associates have long been widely used for medicinal or non-medicinal purposes. The coastal people around the Sundarbans are directly or indirectly dependent on the mangrove habitat for their livelihood. Plants of Sundarbans origin have been used in traditional systems of medicine and act as a rich source of several bioactive compounds. This study demonstrated the ethnomedicinal uses and ethnopharmacological evaluation of plant extracts of Sundarbans origin as well as further identification of bioactive chemical constituents from different Sundarbans plants. This study highlights the ethnomedicinal importance of some Sundarbans plants including *Xylocarpus muluccensis*, *Xylocarpus granatum*, *Avicennia officinalis*, *Cereops decandra*, *Aegicerus corniculatum*, *Heritera fomes*, *Acrostichum aureum*, *Bruguiera gymnorrhiza*, *Cuscuta reflexa*, *Excoecaria agallocha*, *Sonneratia alba*, etc. to confirm their ethnomedicinal uses and further explore their potential in drug discovery.

Quality from source to benefit: Monographs and phytochemical analysis as the basis for evidence-based natural health products and phytotherapy

Evelyn Wolfram^{1, 2, 3}

Zürich University of Applied Sciences, Institute for Chemistry and Biotechnology, Natural Products and Phytopharmacy Research Group, CH-8820 Wädenswil, Switzerland

Planar4 GmbH, ZHAW Startup Company, 8712 Stäfa, Switzerland

Bioheme GmbH, Consulting Agency, 8712 Stäfa, Switzerland

Board member of ESCOP.com, Exeter UK

*E-mail: wola@zhaw.ch

The development of evidence-based natural health products hinges on rigorous quality control from the initial sourcing of raw materials to the final consumer benefits. This process is underpinned by monographs (PhEur, HMPC, ESCOP) and meticulous phytochemical analysis, which serve as critical tools in ensuring consistency, efficacy, and safety. PhEur monographs provide detailed descriptions and standards for botanical identification, composition, and processing methods, establishing a benchmark for quality assurance. Phytochemical analysis further validates these standards by identifying and quantifying bioactive compounds, thus verifying the presence and potency of key constituents. HMPC assessment reports and monographs, as well as ESCOP monographs, both provide a comprehensive collection of the state of science and evidence. They differ by perspective—HMPC from a regulatory standpoint and ESCOP from academic, pharmaceutical, and medical practice viewpoints. By integrating these knowledge bases, producers can substantiate health claims with scientific evidence, fostering consumer trust and advancing the credibility of natural health products in the marketplace. This structured approach not only enhances product reliability but also supports regulatory compliance and facilitates the advancement of natural health products and phytotherapy as legitimate health-promoting modalities.



Abstracts of the Short Oral Presentations

(In alphabetical order)

Treatment of HFD-induced diabetes mellitus by combination of metformin and natural products in rats

Nadia Zaki. Shaban, Nihal M. Elguindy, Gamal Abdelfattah*.

Biochemistry Department, Faculty of Science, Alexandria University, Alexandria, Egypt

E-mail: jimmymostafa@yahoo.com

Asphodelus microcarpus (fam: Asphodelaceae) is widely distributed over the coastal Mediterranean region. It is traditionally used in the treatment of diabetic conditions. The aim of this investigation was to evaluate the antioxidant, anti-hyperlipidemic, and anti-diabetic activity of ethyl acetate extract of this plant. Ethyl acetate extract was obtained from *Asphodelus microcarpus* (AM) tubers. Chemical tests of different extracts, diabetic profiles, lipid profiles, kidney and liver functions, and antioxidant and anti-inflammatory parameters were performed. Diabetes was induced in rats by HFD feed for 10 weeks. The rats were divided into the following groups: Group-I: Normal control, Group-II (vehicle): Diabetic control, Group-III: Diabetic rats (AM 10 mg/kg), Group-IV: Diabetic rats (AM 10 mg/kg + MET 100 mg/kg), Group-V: Diabetic rats (AM 20 mg/kg), Group-VI: Diabetic rats (AM 20 mg/kg + MET 100 mg/kg), and Group-VII: Diabetic rats (MET 100 mg/kg). The body weight of each rat in the different groups was recorded daily. Biochemical and antioxidant enzyme parameters were determined on day 16. The ethyl acetate extract of AM showed better glucose utilisation and insulin resistance improvement. Oral treatment of different doses of AM tuber extract alone and/or with metformin decreased the level of serum glucose, activity of liver alpha-glucosidase, activity of pancreatic alpha-amylase, MDA, CRP and leptin. Treatment showed an increased level of plasma insulin, Catalase, glutathione peroxidase, liver GSH, and total antioxidant capacity. HFD-induced diabetic rats treated with different doses of AM tubers extract and metformin significantly increased muscle glucose transporter 4 (GLUT4) and remarked regenerative effects on the liver, kidney, and pancreas. The antioxidant, anti-hyperlipidemic, and antidiabetic effects of ethyl acetate extract from *A. microcarpus* suggest a potential therapeutic effect to treat diabetic conditions.

***In vitro* antioxidant and cytotoxicity activity of extracts from *Chlorophytum comosum* (Thunb.) Jaques**

Shehla Adhami¹, Humaira Farooqi,^{*1} and Malik Z. Abdin

¹Department of Biotechnology, School of Chemical and Life Sciences, Jamia Hamdard, New Delhi
110062, India

*E-mail: hfarooqi@jamiahamdard.ac.in

Cancer is a complex cellular disorder hijacking normal cellular machinery and creating an outlaw by continuous activation and aggressive invasion of the malignant cells into the healthy microenvironment. It is the second major cause of death worldwide after cardiovascular diseases. Modern treatment of cancer involves toxic chemotherapeutic drugs and personalized therapies involving immunotherapy that help in combating cancer. However, serious side effects during the treatment perturb the quality of life of cancer patients and are a major challenge to reflect on. Inclination towards natural products for their apoptotic potential has been seen and researched extensively to find novel chemotherapeutic active molecules from nature's pharmacy. The aim involves combating and promoting cancer cell death with minimized drug toxicity and improved quality of life. *Chlorophytum comosum* (Thunb.) Jaques commonly known as Spider Ivy is a world-popular ornamental plant widely recognized for its phytoremediation properties. It has an Ethnomedical background in Traditional Chinese Medicine (TCM) and African Traditional Medicine (ATM), however, still underexplored on scientific grounds. In the present study, we aimed to explore the antioxidant and cytotoxic effects of the extracts of *Chlorophytum comosum* against human lung (A549 & NCI-H1299) and breast cancer (MCF-7) cell lines. Dose-dependent percent cell inhibition along different concentrations (10 µg/ml-320 µg/ml) was significantly observed in all the cancer cell lines with IC₅₀ values ranging from 55.72 µg/ml – 90.78 µg/ml; while no cytotoxic effects were seen against normal L-132 human lung cell line. Antioxidant assays revealed significant free radical scavenging potential of the extracts.

Triterpenoid glycosides of *Olox subscorpioidea* Oliv. root: isolation, characterization, and anticancer evaluation

Yemi A. Adekunle^{1,2,3}, Babatunde B. Samuel¹, Amos A. Fatokun², Nahar Lutfun⁴,
Satyajit D. Sarker²

¹Pharmaceutical Chemistry Department, University of Ibadan, Ibadan, Nigeria

²School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street,
Liverpool L3 3AF, United Kingdom

³Pharmaceutical & Medicinal Chemistry Department, Afe Babalola University, Ado-Ekiti, Nigeria

⁴Laboratory of Growth Regulators, Palacký University and Institute of Experimental Botany, The
Czech Academy of Sciences, Olomouc, Czech Republic

*E-mails: y.a.adekunle@2022.ljmu.ac.uk; adekunleya@abuad.edu.ng

Cancer is a leading cause of global death, killing about 10 million people every year. An ethnobotanical survey of plants used to treat breast cancer in Nigeria's Ogun State revealed that *Olox subscorpioidea* Oliv. (Olacaceae) is included in the cancer recipe. This study aims to isolate, characterise, and evaluate the cytotoxic compounds from *O. subscorpioidea* root extract. The methanol extract of *O. subscorpioidea* root was fractionated using solid-phase extraction. The most active fraction was subjected to separation using preparative and semi-preparative high-performance liquid chromatography affording three oleanane-triterpenoid compounds that had not been previously described. They include oleanolic acid 3-*O*-[α -L-rhamnopyranosyl-(1 \rightarrow 3)- β -D-glucopyranosyl-(1 \rightarrow 2)-6-*O*-methyl- β -D-glucuronopyranoside]-28-*O*- β -D-glucopyranosyl ester (**1**); oleanolic acid 3-*O*-[β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranosyl-(1 \rightarrow 3)- β -D-glucopyranoside] (**2**); and oleanolic acid 3-*O*-[β -D-glucopyranosyl-(1 \rightarrow 4)-6-*O*-methyl- β -D-glucuronopyranoside] ester (**3**). Three known compounds were also isolated: oleanolic acid 3-*O*-[β -D-glucopyranosyl-(1 \rightarrow 4)-6-*O*-methyl- β -D-glucuronopyranoside]-28-*O*- β -D-glucopyranosyl ester (**4**); oleanolic acid 3-*O*-[β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-glucuronopyranoside] (**5**); and oleanolic acid (**6**). Their chemical structures were established by spectroscopy (1D- and 2D-NMR) and spectrometry (HR-ESI-MS). All isolated compounds were screened against three human cancer cell lines (cervical, HeLa; colorectal, Caco-2; and breast, MCF-7) using the colorimetric 3-[4,5-dimethylthiazole-2-yl] 3,5-diphenyltetrazolium bromide (MTT) assay. Vincristine was used as the positive control. The results showed that compounds **2** and **3** exhibited significant cytotoxic effects against the HeLa cell line (IC₅₀: 7.42 \pm 0.34 μ M and 10.27 \pm 1.26 μ M) and moderate effects against the MCF-7 cell line (IC₅₀: 36.67 \pm 1.23 μ M and 43.83 \pm 0.65 μ M) and the Caco-2 cell line (IC₅₀: 35.83 \pm 0.55 μ M and 39.03 \pm 4.38 μ M, respectively). The active compounds were also more selective than vincristine against the tested cancer cell lines when compared with cytotoxicity against the normal lung cell line MRC5. This study provides support for the use of *O. subscorpioidea* in breast cancer treatment.

Natural food colors vs. synthetic food colors

Tanveer Alam*

Sabancı University Nanotechnology Research and Application Center Orta Mahalle, Üniversite Caddesi No. 27 Tuzla, 34956, Istanbul, Republic of Turkey

*E-mail: tanveer.alam@sabanciuniv.edu

A substance which imparts colour to a food, drug, cosmetic, or the human body comes under the category of a colour additive. Colour additives can be either manufactured (synthetic) or sourced from natural sources such as plants and animals (natural). Colour, whether manufactured (synthetic) or natural, has always had an important implication on the minds of people as far as food is concerned. Cuisines served in vibrant colours have lured men from all over the world. As a result, it is important to maintain the natural or characteristic colour of a food product while it is being prepared or preserved for future use. A non-attractive colour, on the other hand, makes the food look unfresh and is more likely to be rejected. This has led to the manufacture of synthetic food colours, which are commonly known as artificial food colours. As the name indicates, synthetic food colours are produced chemically and require extensive research to ensure that they meet international food quality standards. Many synthetic food colours are believed to cause cancer, asthma, lethargy, and hyperactivity (particularly in children). Tartrazine is known to cause asthma and allergy responses due to its nitrous derivatives. Scientists at Southampton University investigated synthetic food colours, specifically Azo dyes, and discovered that they have adverse effects on children. Natural colours are food additives obtained from natural sources that are used to colour food and beverages. Natural colours come from several sources, including fruits, vegetables, seeds, leaves, animals, and minerals. These pigments, often known as exempt colours, are considered safe for human consumption by the FDA. There is no GRAS exception for color additives. All colour additives must be certified by the FDA, except for natural colours. These are labelled "exempt colours" and must be derived from natural sources. The best option is to use natural food colouring rather than synthetic colour in food applications.

Cancer chemopreventive potential of *Ruta chalepensis* L. (Rutaceae) growing wild in syria

Waed Alsheikh^{a*}, Lutfun Nahar^{a,b}, Kenneth J. Ritchie^a, Satyajit D. Sarker^a

*E-mail: w.alsheikh@2020.ljmu.ac.uk

^aCentre for Natural Products Discovery (CNPD), School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Liverpool L3 3AF, United Kingdom

^bLaboratory of Growth Regulators, Palacký University and Institute of Experimental Botany, The Czech Academy of Sciences, Šlechtitelů 27, 78371 Olomouc, Czech Republic

The growing incidence of cancer cases and deaths is a substantial health challenge. The preferable approach to reducing cancer prevalence aims to prevent the carcinogenesis process. Published literature highlighted the potential of phytochemicals as cancer chemopreventive agents. This study investigated the chemopreventive potential of *Ruta chalepensis* L. (Rutaceae). Three extracts were obtained from the dried and ground aerial parts of this plant by Soxhlet extraction, sequentially, using *n*-hexane, dichloromethane (DCM) and methanol (MeOH). The concentration that does not cause more than 10% cell death was determined by MTT cytotoxicity assay against AREc32 cells. The chemopreventive activity was studied by applying the luciferase reporter gene assay to assess the potential of the extracts to activate the Nrf2 pathway. The *n*-hexane extract was found to be highly toxic to AREc32 cells and was excluded from the chemoprevention assessment. The DCM and MeOH extracts demonstrated a chemoprevention potential with 3.56- and 2.82-fold induction in the luciferase assay. The active MeOH extract was then fractionated using solid-phase extraction (SPE) into four fractions. The SPE fractions were subjected to the aforementioned bioassays to determine the most active fraction(s). Reversed-phase analytical and preparative high-performance liquid chromatography (HPLC) were employed to isolate compounds from the active SPE fractions. The structures of the isolated compounds were elucidated by 1D and 2D nuclear magnetic resonance (NMR) analysis. The SPE fraction 3 showed the highest induction of luciferase activity (9.2-fold) at a nontoxic concentration (0.05 mg/mL), and this fraction contained chalepin, chalepentin, and rutamarin as the major compounds.

Cycloartanes from the bulbs of *Crinum bulbispermum*

John Vershima Anyam^{1,2*}, Asenge Silas Terdoo¹, Naphthali Musa¹, Victoria Ihotu Adah¹, John Ogbaji Igoli¹

¹Phytochemistry Research Group, Joseph Sarwuan Tarka University Makurdi, Nigeria

²Centre for African Medicinal Plants Research, North Eastern University, Gombe, Nigeria

*E-mail: johnversh@gmail.com

Crinum bulbispermum is an herbal remedy used extensively for treating venereal diseases, especially syphilis, in some form, throughout Sub-Saharan Africa. The root bulbs of *C. bulbispermum* were extracted using *n*-hexane, ethyl acetate, and methanol. The ethyl acetate extract was then subjected to silica gel column chromatography. Fractions obtained were analysed using nuclear magnetic resonance spectroscopy. Importantly, this investigation led to the isolation of three cycloartanes—24-methylene-cycloartan-3 β -ol, cycloartenol, and cycloeucalenol and the alkaloid hippadine. While hippadine and other lycorine-type alkaloids are frequently reported in this plant and members of the *Amaryllidaceae*, this marks the initial isolation of the cycloartanes from this plant. This research provides valuable insights into the chemical composition of *Crinum bulbispermum*, establishing a foundation for both its conservation and potential applications in herbal medicine and beyond.

Chemical analysis and antimicrobial activity of *Moringa oleifera* Lam. leaves and seeds

Attilio Anzano¹, Bruna de Falco¹, Mohammad Ammar², Annarita Ricciardelli³, Laura Grauso¹, Mohammed Sabbah², Rosanna Capparelli¹ and Virginia Lanzotti^{1*}

¹*Dipartimento di Agraria, Università di Napoli Federico II, Via Università 100, 80055 Portici, Italy*

²*Department of Nutrition and Food Technology, Faculty of Agriculture and Veterinary Medicine, An-Najah National University, Nablus P.O. Box 7, Palestine*

³*Dipartimento di Biologia, Università di Napoli Federico II, Complesso di Monte Sant'Angelo-Via Vicinale Cupa Cintia, 21, 80126 Naples, Italy*

E-mail: lanzotti@unina.it

Moringa oleifera is a traditional food crop widespread in the Asiatic, African, and South American continents. The plant, able to grow in harsh conditions, shows a high nutritional value and medicinal potential evidencing cardioprotective, anti-inflammatory, antioxidant, and antimicrobial properties. The purpose of this study was the phytochemical analysis of *M. oleifera* leaves and seeds and the identification of antimicrobial compounds by combining a chemical approach with in vitro tests. The metabolite profile of *M. oleifera* polar and apolar extracts of leaves and seeds were investigated by using Nuclear Magnetic Resonance spectroscopy (¹H-NMR) and Gas Chromatography-Mass Spectrometry (GC-MS). The antimicrobial activity of all of the obtained extract was evaluated against four bacterial pathogens (*Staphylococcus aureus*, *Staphylococcus epidermidis*, *Pseudomonas aeruginosa* and *Salmonella enterica*). The chemical analysis provided a wide set of metabolites that were identified and quantified. Moreover, apolar extracts from seeds showed a significant concentration-dependent antimicrobial activity against *S. aureus* and *S. epidermidis*, (4 mg/mL reduced the viability up to 50%) that was associated with the content of specific fatty acids. Our results noted the advantages of an integrated approach for the identification of plant metabolites and its use in association with biological tests to recognize the compounds responsible for bioactivity without compound purification.

Effect of acetone fraction of *Ottelia alismoides* on the G2/M cell cycle arrest and apoptosis in the Human Carcinoma cell lines

Subrata Das^{a*} and Anupam Das Talukdar^b

^aDepartment of Botany, Karimganj College, Karimganj, Assam, India, 788710

^bDepartment of Life Science & Bioinformatics, Assam University, Silchar, Assam, India, 788011

*E-mail: subrata555das@gmail.com

In recent times, with the technological advancement and modernization of the medical systems, cancer treatment is getting much appreciation. However, lung carcinoma persists among the fatal category of diseases. High rates of proliferation and metastasis, and drug resistance with non-specific target activity are important challenges in the management and treatment of lung carcinoma. Hence, finding novel therapeutic targets and lead molecules to treat lung cancer progression is needed to enhance the patient's survival with treatment. In the present study, the acetone extract of *O. alismoides* (OA-AC) was evaluated and found as a potential anticancer agent with induction of apoptosis in lung cancer (A549) cells. The cell cycle phase distribution analysis in A549 at 24hrs exposure with 10 µg/mL and 25 µg/mL of OA-AC showed a potent arrest or blockage at the G2/M phase of the cell cycle with reduced expression of cyclin B and p-Cdc2. At 48hrs exposure, apoptosis was observed in these cancer cells with elevated expression of Bax and cleaved caspase 3 and reduced expression of the Bcl2. AO-EtBr staining of these cancer cells reveals that the death induced by OA-AC were apoptotic. The HRLC-MS-QTOF analysis of OA-AC depicted 14 major isolable compounds and molecular docking analysis with these compounds displayed 4 compounds that might act as an inhibitor of cyclin B for G2/M phase arrest that leads to apoptotic induction in the cells.

Stereostructure elucidation of *Euphorbia myrsinites* diterpenes and their anti-inflammatory properties

Laura Grauso,^a Bruna de Falco^{*},^a Giuseppe Lucariello,^b Raffaele Capasso^a and
Virginia Lanzotti^a

^aDipartimento di Agraria, Università degli Studi di Napoli Federico II, Portici, Napoli

^bDipartimento di Farmacia, Università degli Studi di Napoli Federico II, Napoli

*E-mail: bruna.defalco@unina.it

The *Euphorbia* genus includes a wide variety of plants, ranging from leafy herbaceous species to succulent spurges, with a global distribution. Extracted compounds from *Euphorbia* species exhibit diverse pharmacological activities, with phytochemical investigations revealing unique diterpenes, serving as taxonomic markers. This study focuses on the chemical analysis of *Euphorbia myrsinites* specimens from Italy, leading to the isolation and characterization of a novel atisane diterpene named myrsatisane, alongside four previously identified tetraester derivatives of myrsinol, three ingenol derivatives, and a euphane skeleton triterpene. Structural elucidation of myrsatisane was performed by high-resolution mass spectrometry (HR-MS) and 1D and 2D-NMR experiments, establishing its relative configuration via ROESY and absolute stereochemistry through quantum-mechanical density functional theory (DFT) studies. While atisane diterpenes are common in *Euphorbia* species, this is the first report of such a compound isolated from *E. myrsinites*. The subsequent evaluation of the anti-inflammatory property of the isolated terpenes on J774A.1 macrophages stimulated with lipopolysaccharide revealed a dose-dependent activity (0.001-3 μ M) in the three ingenol derivatives, suggesting their potential as candidates for the development of anti-inflammatory drugs.

Phytochemical investigation and antioxidant activity of *Salvia officinalis* aerial parts

Aafaf El Baakili¹, Souad El Hajjaji²

¹Mohammed V University in Rabat, LPCMIO, Materials Science Center (MSC), Ecole Normale Supérieure, Rabat, Morocco

²Centre Eau, Ressources Naturelles, Environnement et Développement Durable (CERNE2D), Mohammed V University, Rabat 10090, Morocco

Salvia officinalis L., also known as sage, is mostly used in local cuisines, as ornamental plants, and in folk medicine for their diverse therapeutic properties. Sage plants are aromatic, and their phytochemistry is rich since they contain several phenolic acid derivatives, flavonoids, also terpenes in high amounts.

This study comprises the phytochemical characterization, the evaluation of the total phenolic content (TPC) and antioxidant activity (AA), and the investigation of the antioxidant of fractioned extracts derived from *Salvia officinalis* L. aerial parts as well as essential oil. GC-MS was used for the characterization of the essential oil and the determination of the major ingredients. Afterwards, the TPC and TFC were determined. Moreover, its antioxidant potential was assessed using different assays DPPH, FRAP and ABTS. Since then, our ongoing work with *Salvia officinalis* L aerial parts revealed that the essential oil comprises numerous metabolites, with oxygenated monoterpenes notably α -terpineol being the major compound. It had a high value of TPC and TFC and exerted significant AA as shown by the results of the Ferric Reducing Antioxidant Power (FRAP) and Radical Scavenging Activity by DPPH assays.

Natural compounds: An alternative for safe packaging

**Georgiana-Luminita Gavril^{1*}, Magdalena Wrona², Davinson Pezo³, Anis Bertella⁴,
Lutfun Nahar⁵, Cristina Nerin²**

¹*Department of Bioinformatics, National Institute of Research and Development for Biological Sciences, 296 Splaiul Independentei, sector 6, 060031, Bucharest, Romania*

²*Department of Analytical Chemistry, Aragon Institute of Engineering Research I3A, CPS-University of Zaragoza, Torres Quevedo Building, María de Luna 3, 50018 Zaragoza, Spain*

³*Faculty of Health Sciences, San Jorge University, Villanueva de Gállego, Autovía A-23 Zaragoza-Huesca Km. 299. C.P: 50830, Spain*

⁴*Department of Molecular and Cellular Biology, Faculty of Life and Nature Sciences, Abbes Laghrour Khenchela University, BP 1252 Road of Batna, Khenchela 40004, Algeria*

⁵*Laboratory of Growth Regulators, Palacký University and Institute of Experimental Botany, The Czech Academy of Sciences, Šlechtitelů 27, 78371 Olomouc, Czech Republic*

*E-mail: georgiana.gavril@incdsb.ro

Medicinal and aromatic plants (MAPs) show a broad spectrum of bioactivities and because of their importance MAPs are used in various fields such as food, for safe packaging used to store products, in nutrition to preserve food in an antiseptic medium, in medicine, as adjuvants in the phytotherapy of some diseases, in cosmetics (perfumery), in agriculture (biopesticides), etc. In the production of food, phyto-preparations and medicinal plant products, a great number of techniques are prohibited that are related to obtaining, maintaining, preserving, handling, and incorporating food additives for manufacturing the healthiest products. In food production, especially in pre-packaged foodstuffs (for a short period), inadequate conditions of packaging and storage could increase the risk of microbial development, also the reduction of shelf life and may affect the product quality in terms of taste, texture and sensory aspects, not fulfilling the consumer expectations. A solution in this regard could be the medicinal and aromatic plants which are accepted as natural ingredients in food, due to the content of secondary metabolites with antimicrobial and antioxidant activity. In this sense, we chose two species of medicinal plants *Melissa officinalis*, *Salvia officinalis* that have a good antioxidant and antimicrobial capacity due to bioactive compounds and can represent a good alternative to be used for storage and packaging food.

Funding. This work was supported by the Romanian Ministry of Research, Innovation and Digitization (MCID) through, Subprogram 1.2-Institutional Performance-Projects for Excellence Financing in RDI–grant number 2PFE/2021 and by Core Program within the National RDI Plan 2022–2027– grant number 7N/2022-23020101(SIA-PRO).

Diarylheptanoids from the seagrass *Zostera marina*

Laura Grauso^{*},¹ Yan Li,² Paola De Cicco,³ Francesca Borrelli,³ Christian Zidorn,²
Alfonso Mangoni³

¹*Dipartimento di Agraria, Università degli Studi di Napoli Federico II, Portici (NA), Italy*

²*Pharmazeutisches Institut, Christian-Albrechts-Universität zu Kiel, Kiel, Germany*

³*Dipartimento di Farmacia, Università degli Studi di Napoli Federico II, Napoli, Italy*

*E-mail:laura.grauso@unina.it

Natural products have always been a great source of inspiration for drug discovery because of the wide variety of specialized metabolites with pharmacological activity. This is even more convenient when their natural source is abundant and easily accessible. The widespread seagrass *Zostera marina* has been shown to contain a rich family of cyclic diarylheptanoids including two tetracyclic diarylheptanoids, zosteraphenols A and B, and three diarylheptanoids heterodimers, zosterabisphenones A, B and C. These compounds are structurally unique, featuring keto tautomers of catechol or rearranged benzene rings. Their structure elucidation was made intriguing by the coalescent NMR signals shown by all these compounds due to their slow conformational equilibria and was performed with the aid of quantum mechanical studies. In addition, zosterabisphenones are selectively cytotoxic against human colorectal cancer HCT116 cells, and this has encouraged us to further study their mechanism of action and in vivo antitumor effects using the murine xenograft model of colorectal cancer. The presentation will provide the complex structural determination of these compounds together with the results on their in vitro and in vivo antitumor activity in colorectal cancer.

Effect of polysaccharide rich hot water extract of *Trametes versicolor* on blood factors in diabetic patients. A double-blind, randomized clinical trial

Emran Habibi*, Ehsan Rajabi, Zahra Kashi, Adele Bahar, Majid Saeedi

Faculty of Pharmacy, Mazandaran University of Medical Sciences, Sari, Iran

*E-mail: Emrapharm@yahoo.com

Evaluation of the efficacies of natural compounds in the treatment of various diseases such as diabetes, is very important, so in this study, the effect of capsules containing polysaccharide extract of *Trametes versicolor* (a medicinal mushroom) on blood factors in diabetic patients was examined. The polysaccharide extract was prepared by boiling water from the mushroom and turned into a fine-dried powder. The resulting powder was inserted into the capsule according to pharmaceutical criteria. Finally, a randomized double-blind clinical trial study was performed on patients who met the inclusion criteria. A total of 66 patients including the intervention group (33 patients) and the control group (33 patients) were included in the study. In addition to the usual treatment, the patients received 5 capsules of 220 mg containing mushroom extract daily in the intervention group and 5 placebo capsules containing Avicel in the control group (2 in the morning, 2 at noon, 1 at night) for 2 months. In the present study, anthropometric indices including height, weight, BMI, waist circumference were measured at the beginning and end of the study. Intravenous blood samples were taken from patients at the beginning and end of the study and the levels of HbA1c, BS (2hr p.p), fasting blood sugar, two-hour postprandial blood sugar, Cholesterol, Triglyceride, LDL, HDL, ALT, AST, ALP, Creatinine and Urea was assayed. There was a statistically significant difference between HbA1c, BS (2hr p.p) and AST in the intervention group after consumption of mushroom extract compared to the control group ($P < 0.05$). There was a statistically significant difference between BMI, waist circumference, and fasting blood sugar at the beginning of the study and two months after taking the drug ($P < 0.05$). Regarding ALT indices, ALP also showed a general decrease in mean and standard deviation, but this decrease was not significant ($P > 0.05$). Also, no significant changes in lipid profile and renal factors were observed at the expressed dose of mushroom polysaccharide extract ($P > 0.05$). Based on the findings of this study, administration of *T. versicolor* extract controlled blood sugar in type 2 diabetic patients as much as possible.

Phytochemical screening and in-vivo evaluation of analgesic and antidiarrheal effects of *Crateva unilocularis* L. leaf extracts

Al-Masum Hossain, Sumaia Aktar, Tonema Tabassum Prova, Jannatul Fardous*

^aDepartment of Pharmacy, Comilla University, Cumilla-3506, Bangladesh

E-mail: fardousj11@cou.ac.bd

Crateva unilocularis L. is a deciduous plant of the Capparaceae family, domestically known as the Borun tree and is popular among the local population for its nutritional and medicinal values. The current study aims to determine the phytochemical constituents of *C. unilocularis* leaves followed by pharmacological activity evaluation at different doses *in vivo*. Leaf extract was collected by reflux extraction process using ethanol followed by phytochemical screening tests and evaluation of analgesic and antidiarrheal activity in mice. Results showed that *C. unilocularis* leaves are rich in alkaloids, steroids, flavonoids, glycosides, terpenoids, while carbohydrates and saponins were absent. The analgesic effect of *C. unilocularis* was similar to that of naproxen for both 200 mg/kg and 400 mg/kg doses with a maximum reaction time of ~ 5 sec during the tail immersion test. Interestingly, the onset of the analgesic effect required a shorter time (1 h) than naproxen (2 h). Similarly, acetic acid-induced writhing test also confirms the analgesic activity of *C. unilocularis* leaves for the same doses with a significant decrease in writhing number (65-70% inhibition) after 30 min and was similar to that of etoricoxib. Moreover, *C. unilocularis* leaves exert antidiarrheal effect for both 100 mg/kg and 200 mg/kg doses with significant inhibition of defecation of about 34% and 46%, respectively. Therefore, *C. unilocularis* leaf extract has potential analgesic and antidiarrheal effects which may result from the presence of different phytochemicals. Further studies are needed to confirm the possible pharmacological action of *C. unilocularis* leaves that could emerge a new dimension in the field of natural medicine.

Chemometrics-aided standardization of Egyptian propolis using an integrated UV-TLC/MS-image analysis strategy for unravelling potential antidiabetic markers

Reham S. Ibrahim^{a, *}, Ahmed A. Nada^a, Iman H. Nour^b, Aly M. Metwally^a, Aya M. Asaad^a, Safa M. Shams Eldin^a

^a*Department of Pharmacognosy, Faculty of Pharmacy, Alexandria University, 21521, Alexandria, Egypt*

^b*Botany and Microbiology Department, Faculty of Science, Alexandria University, Alexandria 21511, Egypt*

*E-mail: reham.abdelkader@alexu.edu.eg

The current study implemented an integrated technique for standardizing propolis by combining chromatographic, spectroscopic, palynological, and biological analyses. Digitally-optimized HPTLC photographs were examined using a dual visualization technique with four image analysis software packages that applied distinct digitalization procedures, namely Sorbfil TLC View[®], ImageJ[®], JustTLC[®], and Gel Analyzer[®]. ImageJ[®] and Gel Analyzer[®] demonstrated outstanding figures of merit for flavonoids and phenolic acids quantification, respectively. Unsupervised and supervised multivariable pattern recognition models were developed to distinguish between three varieties of propolis (blue, orange, and green) collected from diverse regions throughout the world. Subsequently, HPTLC-ESI-MS was used to precisely identify the discriminating constituents. An Orthogonal Projection to Latent Structure (OPLS) multivariate model was used to analyze the fingerprint-efficacy connection and identify bio-efficient indicators for inhibiting α -glucosidase and α -amylase as primary targets. As a result, 3,4-Dimethoxycinnamic acid, caffeic acid, isoferulic acid, rosmarinic acid, and quercetin were identified as the most important health indicators. A supplementary rapid, simple, and widely accessible UV spectroscopic approach employing aluminium chloride as a bathochromic shift reagent was employed as an alternative method for predicting the aforementioned biomarkers using a validated Partial Least Squares Regression (PLSR) model. In addition, the botanical origin of Egyptian propolis was determined for the first time using palynological study. Twenty-eight pollen types belonging to 13 families were found, with Asteraceae being the most represented. The studied samples lacked dominating pollen types, reflecting Egyptian propolis' multifloral origin. The identification of plant sources for propolis, which has a direct impact on its chemical composition and, as a result, biological efficacy, is an essential component of its standardization.

Phytochemistry and *in vitro* cancer chemopreventive effect of *Leea indica* leaves on AREc32 cells

Chuanchom Khuniad^{1,2*}, Lutfun Nahar^{1,3}, Kenneth J. Ritchie¹ and Satyajit D. Sarker¹

¹Centre for Natural Products Discovery (CNPD), School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Liverpool L3 3AF, United Kingdom

²Department of Thai Traditional Medicine, Faculty of Health and Sports Science, Thaksin University, 93210 Phatthalung, Thailand

³Laboratory of Growth Regulators, Palacký University and Institute of Experimental Botany, The Czech Academy of Sciences, Šlechtitelů 27, 78371 Olomouc, Czech Republic

*E-mail: C.Khuniad@2020.ljmu.ac.uk

Leea indica (Burm. f.) Merr. (Vitaceae) is a Thai medicinal plant used traditionally to treat fever, diarrhoea, pain, gastric ulcer, leucorrhoea, viral infections and cancer. Previous studies of this species revealed the presence of alkaloids, flavonoids, polyphenolics and terpenoids along with a wide range of bioactivities such as analgesic, antidiabetic, anti-inflammatory, antimicrobial, antioxidant and antiproliferative activities. This study aimed to identify phytoconstituents of *L. indica* leaves and investigate their chemopreventive effect following a bioassay-guided isolation procedure. Three crude extracts (*n*-hexane, dichloromethane and methanol) of *L. indica* leaves were screened for Nrf2 induction activity using a luciferase reporter assay in the AREc32 cell line. The active crude extracts were fractionated by solid-phase extraction and vacuum liquid chromatography. The results showed that DCM (0.18 mg/mL) and MeOH extracts (0.2 mg/mL) increased luciferase activity by 3.7- and 2.8-fold relative to control, respectively. Therefore, both active extracts were fractionated. However, none of the DCM fractions displayed any significant luciferase induction. MeOH F2 (0.2 mg/mL) exhibited the highest luciferase induction with 4.2-fold, followed by F4 (0.2 mg/mL), with 2.94-fold and F3 (0.1 mg/mL), with 2.86-fold. The isolation and identification of major active compounds from the most bioactive MeOH F2, DCM F4+5, F6+7 and F8+9+10 fractions are underway. This talk will present the most up-to-date results from this project.

Antioxidative effect and inhibition of key enzymes linked to type 2 diabetes of various solvent fractions from fruit ethanolic extract of *Xylopia aethiopica* *in vitro*

Aminu Mohammed,^{1,3*} Neil Anthony Koorbanally² and Md. Shahidul Islam¹

¹Department of Biochemistry, School of Life Sciences, University of KwaZulu-Natal, (Westville Campus), Durban, 4000, South Africa

²Department of Chemistry, School of Chemistry and Physics, University of KwaZulu-Natal, (Westville Campus), Durban, 4000, South Africa

³Department of Biochemistry, Faculty of Science, Ahmadu Bello University, Zaria-Nigeria

*E-mail address: alamindagash27@gmail.com

Xylopia aethiopica (Dun.) A. Rich (Annonaceae) has been widely used in food preparations and is locally used in the treatment of various diseases. The present study was carried out to assess the anti-oxidative and anti-diabetic potentials of solvent-solvent fractions from crude ethanolic extract of *X. aethiopica* fruit using various *in vitro* models. Crude ethanolic extract was fractionated using hexane, dichloromethane, ethyl acetate and acetone. They were subjected and investigated for 1,1-diphenyl-2-picryl-hydrazyl (DPPH) radical scavenging activity, ferric reducing anti-oxidant power (FRAP), inhibition of haemoglobin glycosylation, α -amylase and α -glucosidase activities as markers of *in vitro* anti-diabetic effects at various doses (30-240 $\mu\text{g}/\text{mL}$). Possible bioactive compounds were analyzed using Gas Chromatography-Mass Spectrometry (GC-MS) analysis. The results indicated that acetone fraction exhibited significantly ($p < 0.05$) higher total polyphenols and flavonoids contents and recorded lower IC_{50} values in all the models used (DPPH: $84.47 \pm 0.71 \mu\text{g}/\text{mL}$; inhibition of haemoglobin glycosylation: $148.15 \pm 3.57 \mu\text{g}/\text{mL}$; α -amylase: $155.41 \pm 1.83 \mu\text{g}/\text{mL}$; α -glucosidase: $86.23 \pm 0.30 \mu\text{g}/\text{mL}$) compared to other solvent fractions. Possible phytochemicals present in the acetone fraction were mostly phenolics and fatty acid derivatives. This finding demonstrates that acetone fraction possesses anti-oxidative and anti-diabetic effects.

Understanding molecular mechanisms behind the anti-inflammatory effects of *Machilus macrantha* (Gulmavu) in the arachidonic acid metabolic pathway by network pharmacological approach

Nabarun Mukhopadhyay¹, Sibun Sen³, Ashish Kumar², Rujuta Sandbhor¹, Srishti Singh³, Amol G Dikundwar³, Venkata Rao Kaki^{1*}

¹ Department of Chemical Sciences (Natural Products), National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, Telangana, India

² Department of Chemical Sciences (Medicinal Chemistry), National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, Telangana, India

³ Department of Pharmaceutical Analysis, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, Telangana, India

Machilus macrantha, also known as Gulmavu in Kannada, is an ethnopharmacologically important medicinal plant that is widely cultivated in the Indian states of Karnataka, Maharashtra, etc. Traditionally, this plant was used to treat a diverse range of diseases like asthma, arthritis, etc. Our current study explores the molecular mechanisms of *M. macrantha* underlying its anti-inflammatory effects in the arachidonic acid metabolic pathway and also predicts the main genes responsible for the same. IMPPAT 2.0, ScienceDirect, Google Scholar, and Pubmed databases were utilized to collect the information related to the phytochemicals of this plant and a total of five compounds named machiline, atheroline, machigline, β -sitosterol, and quercetin were found in the same. By using the SEA search server and Swiss target prediction tools, a total of 238 targets were predicted; out of that, 215 targets were selected for further studies. PPI interactions were predicted by using the STRING database and a total of 23 targets were obtained (High confidence > 0.7). The final networks were constructed by Cytoscape 3.10.1 software, and three topological parameters (degree, betweenness, and closeness) were employed for selecting the most potential targets named PTGS2, NF κ B1, CYP2C8, CYP2C9, and MAPK1 found in the constructed network. KEGG and GO enrichment analyses were performed using the SRPLOT database, and it was observed that the Arachidonic acid metabolism pathway exhibited the lowest p-value and highest number of enriched targets. The ADME properties and toxicity prediction of the mentioned phytochemicals have also been done by using SWISS ADME and ProTox-II softwares.

Cytotoxic effects of *Adenopus breviflorus* fruit extracts on prostate cancer cells

Tolulope A. Oyedeji^{1,2}, Satyajit D. Sarker² and Amos A. Fatokun^{2*}

¹Department of Biochemistry, Faculty of Basic Medical Sciences, College of Medicine, University of Lagos, Lagos, Nigeria

²Centre for Natural Products Discovery (CNPD), School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Liverpool L3 3AF, United Kingdom

*E-mail: A.A.Fatokun@ljmu.ac.uk

Traditionally, *Adenopus breviflorus* fruit decoction is used to treat prostate cancer. However, this claim has not been validated scientifically. Therefore, this study investigated the cytotoxic effects of *A. breviflorus* fruit extracts on two prostate cancer cell lines (PC3 and LNCaP). The dried fruit of *A. breviflorus* was extracted exhaustively with n-hexane and methanol. The effects of the extracts on cell viability were assessed using the 3-[4, 5-dimethylthiazol-2-yl]-2, 5-diphenyl tetrazolium bromide (MTT) assay while cellular Reactive Oxygen Species (ROS) levels were quantified using the 2',7'-dichlorofluorescein diacetate (DCFDA) dye. The n-hexane fruit extract up to 500 µg/mL had no significant effect ($p > 0.05$) on cell viability. In contrast, the methanol fruit extract significantly ($p < 0.05$) decreased cell viability in a concentration-dependent manner, with IC_{50} values of 209 µg/mL and 112.1 µg/mL, for PC3 and LNCaP cells, respectively. The methanol fruit extract at 100 µg/mL reduced the basal levels of ROS (compared to the negative control) in the PC3 cells (0.56 ± 0.14 fold) and the LNCaP cells (0.28 ± 0.06 fold), in contrast to ROS induction by the positive control, hydrogen peroxide (H_2O_2) (5.07 ± 0.69 and 2.57 ± 0.60 fold for PC3 and LNCaP cells, respectively). We conclude that the methanol extract of *A. breviflorus* possesses cytotoxic and anti-ROS properties. *A. breviflorus* fruit is, therefore, a potential source of chemotherapeutic compounds, and the traditional use of the plant is considered to have some scientific basis.

Metabolomic approach to tackle adulterations in medicinal plants

Anggra Paramita*

The BioActives Lab, Plant Science Program, Biological and Environmental Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

*Email: anggra.paramita@kaust.edu.sa

Plants have been used as a source of medicine for generations, and even recently, animals such as orangutans in Indonesia have also used plants to treat wounds. Various medicinal plants have been produced into herbal medicines based on these empirically known properties. However, with the increasing market demand, the adulteration of these medicinal plants is also increasing. For instance, the author has observed cases where the plants that were ordered were replaced with cheaper alternatives, or where plants of poor quality were mixed with those of good quality. These adulterations can cause various problems for both producers and consumers of herbal medicines. They can lead to the mismatch of plants that come with what is ordered, mixing with other plants so that the weight meets the target ordered by the company, and mixing medicinal plants of poor quality with those of good quality. All these adulterations will cause health problems because if people consume herbal medicines that have medicinal plant compositions that do not meet the requirements, they can provide different pharmacological effects. In this case, metabolomics can be used to overcome this problem by testing marker compounds from medicinal plants. A further step is creating a database and collecting the marker compounds in a database that various sectors can access but still have an authorized organization to control the information submitted into the database.

Applications of biosurfactants in pharmaceuticals

Pattanathu K.S.M. Rahman* and Abdullah Isreb

Centre for Natural Products Discovery, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, James Parsons Building, Byrom Street, Liverpool L3 3AF, United Kingdom

*E-mail: p.k.rahman@ljmu.ac.uk

Biosurfactants derived from microbial sources are highly valued in various industries, including food, cosmetics, and pharmaceuticals. Glycolipid biosurfactants, such as rhamnolipid and sophorolipid, stand out for their biodegradability and FDA approval, serving as greener alternatives to synthetic surfactants. Biosurfactants' self-assembling properties make them suitable for solubilizing hydrophobic drugs, presenting promising applications in pharmaceutical formulations. Moreover, encapsulating phytocompounds within biosurfactant micelles, structured at the nano level, demonstrates a suitable antimicrobial compound against Gram-positive and Gram-negative organisms. The use of glycolipid biosurfactants to solubilize hydrophobic phytochemicals like curcumin, by entrapping them within micelles creates new avenues for developing soluble curcumin-based systems, enhancing their bioavailability and therapeutic potential.

Mechanism underlying the anti-inflammatory effects of oleacein from *Olea europaea* L. in LPS-exposed macrophages

Caterina Russo^{1*}, Alessandro Maugeri², Martina Farina¹, Michele Navarra¹

¹Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Viale F. Stagno d'Alcontres 31, 98166 Messina, Italy

²Department of Veterinary Sciences, University of Messina, Viale G. Palatucci, 98168 Messina, Italy

*E-mail: carusso@unime.it

Inflammation arises as a protective response to tissue or organ damage caused by physical, chemical, or biological stimuli, with the aim of eradicating the harmful agent. However, when the organism fails to eliminate the pathogen, it develops a chronic inflammatory state, which can lead to different disorders. Plant polyphenols represent valuable allies for organisms since they can act as antioxidants and modulate key pro-inflammatory factors. *Olea europaea* L. (Oleaceae) has recently been investigated as a natural source of bioactive compounds, proving beneficial properties. Nevertheless, little research has targeted the biological effects of its most abundant secoiridoid, oleacein (OLC). The goal of this study was to investigate the potential antioxidant and anti-inflammatory properties of OLC in THP-1 macrophages exposed to lipopolysaccharide (LPS). In our experimental model, LPS significantly increased both the release and gene expression of pro-inflammatory cytokines (IL-6, IL-1, and TNF- α), while decreasing the release and gene expression of anti-inflammatory cytokines (IL-10), all effects reversed by pre-treatment with OLC. Furthermore, OLC reduced the production of COX-2, NO, and PGE₂, stimulated by LPS in THP-1 macrophages. Notably, OLC acted on inflammatory signalling pathways by inhibiting the CD14/TLR4/MyD88 axis and activating NF- κ B. Finally, OLC showed relevant antioxidant capability, assessed by abiotic assays, thus reducing the intracellular ROS levels, produced by exposure of THP-1 macrophages to LPS. The findings of this study suggest that the antioxidant properties and anti-inflammatory activity of OLC may contribute to determining its protective effect against inflammatory stressors, thus representing a potential alternative strategy to attenuate the inflammatory process.

Implementation of metabolomics in conjunction with chemometrics to identify the distinguishing chemical markers of various grades of Sri Lankan white, green, and black tea (*Camellia sinensis* L.)

Dina A. Selim^{1*}, Eman Shawky¹, Rasha M. Abu El-Khair^{1, 2}

¹*Department of Pharmacognosy, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt*

²*College of Pharmacy, Arab Academy for Science, Technology and Maritime transport, Alexandria, Egypt*

*E-mail: dinaselim2157@gmail.com

Orange pekoe, flowery pekoe, broken orange pekoe fannings, broken orange pekoe black tea, green tea, silver tips, and golden tips are the seven Sri Lankan tea grades that were included in the current study. A thorough metabolic profiling of white tea grades was conducted using UPLC-MS/MS in conjunction with chemometrics. The primary chemical markers of the black tea type were assensinin C and E, theaflavin, and theacitrin; the primary discriminatory markers of the green tea type were catechin, epicatechin, epigallocatechin, and methyl epigallocatechin; while the primary chemical markers of white tea type were theanine, oolongotheanine, and quercetin glycosides. The primary down-accumulated metabolites between whole and broken black tea leaf grades were theogalloflavin, epigallocatechin, and flavonoid glycosides; the primary up-accumulated metabolites were theaflavin gallate and N-ethyl pyrrolidinone epicatechin. The primary down-accumulated metabolites between broken and fanning black tea grades were puerin A and C and gallic acid; the primary up-accumulated metabolite was N-ethyl pyrrolidinone epicatechin gallate.

Repurposing of Unani polyherbal formulation in obese diabetes using network pharmacology, molecular docking and simulation approach

Sibu Sen¹, Nabarun Mukhopadhyay², Srishti Singh¹, Rujuta Sandbhor², Venkata Rao Kaki², Amol G. Dikundwar^{1*}

¹*Department of Pharmaceutical Analysis, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India*

²*Department of Chemical Sciences (Natural Products), National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India*

E-mail: sibsens7@gmail.com

Dawa-ul-kurkum (DK) is a well-known Unani polyherbal formulation which contains parts of 7 medicinal plants and is used to treat spleen disorders, liver dysfunction, anorexia, abdominal pain, ascites, and dropsy and also as a renal, liver, and urinary bladder tonic and carminative. As per the literature, phytoconstituents such as Crocin, β -gurjunene, chlorogenic acid, homovanillin, glutathione, rutin, catechin, geraniol, piperitone, Z-guggulsterone, dehydrocostus lactone, costunolide, cinnamaldehyde, crocetin, cinnamic acid, safranal and (E)-Cinnamyl acetate etc. are indicated to be present in this formulation. The current formulation is explored for activity against Diabetes owing to well-known anti-oxidant properties of its constituents e.g., polyphenolics (Rutin, cinnamic acid, cinnamaldehyde, and (E)-cinnamyl acetate) and terpenoids (crocin, Z-guggulsterone, dehydrocostus lactone, costunolide, crocetin and safranal). With the help of Network Pharmacology, the top 10 genes and enriched pathways were identified which can be targeted for treating diabetes. Rutin was found to be the top ranker in docking score among the other 18 compounds when docked against the top 10 genes found in network pharmacology. Rutin was found to be stable towards interaction with EGFR and SRC proteins as compared to the other 8 proteins as assessed by molecular simulation. The presence of two polyphenolics phytoconstituents namely, Cinnamic acid was confirmed in the polyherbal formulation by the Q-marker standardization method using HPLC. Hence, the present study can help to understand the mechanism lying behind the antidiabetic action of this Unani polyherbal formulation. The observations from this study need to be further validated by *in-vitro* and *in-vivo* studies for the concerned formulation.

Antimicrobial activities and TLC profiles of *Xylaria* spp. associated with termite nests in Thailand

Pitchapa Thongsuwan^{1,4*}, Cherdchai Phosri², Lutfun Nahar^{3,4}, George Sharples⁴,
Satyajit D. Sarker⁴ and Nuttika Suwannasai¹

¹Dept of Microbiology, Faculty of Science, Srinakharinwirot University, Bangkok, 10110, Thailand

²Dept of Biology, Faculty of Science, Nakhon Phanom University, Nakhon Phanom, 48000, Thailand

³Laboratory of Growth Regulators, Palacký University and Institute of Experimental Botany, The Czech Academy of Sciences, Šlechtitelů 27, 78371 Olomouc, Czech Republic

⁴Centre for Natural Products Discovery (CNPD), School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Liverpool L3 3AF, United Kingdom

*E-mail: Pitchapa.jang@g.swu.ac.th

The *Xylaria* is a genus of ascomycetous fungi classified in the Phylum Ascomycota, Order Xylariales, and Family Xylariaceae. These fungi are commonly found in decaying wood, fruits, seeds, leaves, petioles, and soil. Only species related to termite nests belong to *Pseudoxylaria*. This genus has a rich source of bioactive metabolites. However, there are only a few reports that present bioactive metabolites from the *Xylaria* subgenus *Pseudoxylaria*. Recently, two new species of *Xylaria thienhirunae* and *X. chaiyaphumensis* have been reported from termite nests in Thailand, and another one is *Xylaria* sp., for which there is no information on its bioactive compound production when cultured in different media. Therefore, this study aimed to cultivate and extract bioactive compounds from the novel species of *Xylaria* associated with termite nests in Thailand using five different media and evaluate their bioactive properties, including antibacterial activity. The mycelium of three new species was grown in five different media, including modified coconut medium, modified Norkrans's C (MNC), potato dextrose broth (PDB), SMYA, and yeast malt (YM), for six weeks. The culture broth was extracted with ethyl acetate three times. The crude extracts were evaluated for antimicrobial activity against *Bacillus subtilis* ATCC6633, *Escherichia coli* ATCC35218, *Pseudomonas aeruginosa* ATCC27853, and *Staphylococcus aureus* ATCC25923, using 96-well plates by the resazurin method. All crude extracts were effective in inhibiting and killing bacteria. *X. thienhirunae* cultured in YM medium, *X. chaiyaphumensis*, and *Xylaria* sp. cultured in MNC medium showed MIC and MBC better when cultured in other media. In addition, all extracts were checked by TLC using UV and spraying with reagents [i.e., anisaldehyde and 2,2-diphenyl-1-picrylhydrazyl (DPPH)] for screening the chemical profiles. Further studies will separate, purify, and identify chemical compounds from the crude extracts using preparative high-performance liquid chromatography (prep-HPLC) and nuclear magnetic resonance (NMR) spectroscopic techniques.



Annual CNPD Conference Online 2024
Centre for Natural Products Discovery
School of Pharmacy and Biomolecular Sciences
Liverpool John Moores University
Liverpool, United Kingdom
19-21 June 2024



Prof Lutfun Nahar designed the front and back covers