中国-泛巴尔干地区天然产物与药物发现联盟第六届年会
暨2025年联合国教科文组织天然产物化学安全与
福祉泛亚及太平洋区域网络研讨会

The 6th Annual Conference of Pan-Balkan Alliance of Natural Products and Drug Discovery Associations and the 2025 Seminar of UNESCO Regional Network of Natural Products Chemistry

Shanghai Institute of Materia Medica
Chinese Academy of Sciences
中国科学院上海药物研究所

26 - 29 October, 2025 | Shanghai, China

中国－泛巴尔干地区天然产物与药物发现联盟第六届年会暨 2025 年联合国教科文组织天然产物化学安全与福祉泛亚及太平洋区域网络研讨会

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Shanghai Institute of Materia Medica
Chinese Academy of Sciences
中国科学院上海药物研究所

26 - 29 October, 2025
Shanghai, China

Directed by

- Department of International Cooperation, Ministry of Science and Technology of China
- Bureau of International Cooperation, Chinese Academy of Sciences
- The Alliance of National and International Science Organizations
- Science and Technology Commission of Shanghai Municipality
- Chinese Academy of Sciences Shanghai Branch

Organized by

- Shanghai Institute of Materia Medica, Chinese Academy of Sciences (SIMM)
- Institute for Biological Research “Siniša Stanković”, National Institute for Republic of Serbia, University of Belgrade (IBISS)
- UNESCO Regional Office for East Asia
- State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences

INFORMATION

Theme

Cross-Disciplinary Dialogue: Natural Products Science and Global Health Well-being

Academic Committee

Prof. Abas, Faridah - Universiti Putra Malaysia, Malaysia
Prof. Abazi, Sokol - AAS-Advanced Analytical Solutions, Albania
Prof. Awakawa, Takayoshi - RIKEN Center for Sustainable Resource Science, Japan
Dr. Chooi, Yit Heng - University of Western Australia, Australia
Prof. Dalisay, Doralyn - University of San Agustin, Philippines
Dr. Fajriah, Sofa - Research Center for Pharmaceutical Ingredients and Traditional Medicine, National Research and Innovation Agency, Indonesia
Prof. Halabalaki, Maria - Department of Pharmacy, National and Kapodistrian University of Athens, Greece
Prof. Jenis, Janar - Research Center for Medicinal Plants of Al-Farabi Kazakh National University, Kazakhstan
Prof. Kukavica, Biljana - Faculty of Natural Sciences and Mathematics, University of Banja Luka, Bosnia and Herzegovina
Prof. Kurtán, Tibor - Department of Organic Chemistry, University of Debrecen, Hungary
Prof. Lazović, Biljana - Biotechnical Faculty, University of Montenegro, Montenegro
Prof. Lin, Ge - School of Biomedical Sciences, The Chinese University of Hong Kong, Hong Kong, China
Prof. Lin, Ligen - University of Macau, Macau, China
Prof. Normakhamatov, Nodirali - Tashkent Pharmaceutical Institute, Uzbekistan
Dr. Oidovsambuu, Sarangerel - Institute of Chemistry and Chemical Technology, Mongolian Academy of Sciences, Mongolia
Dr. Palamy, Sysay - Faculty of Pharmacy, University of Health Sciences, Laos
Dr. Soković, Marina - Institute for Biological Research “Siniša Stanković”, National Institute for Republic of Serbia, University of Belgrade, Serbia
Dr. Thongnest, Sanit - Chulabhorn Research Institute, Thailand
Prof. Trendafilova, Antoaneta - Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Bulgaria
Prof. Ye, Yang - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China

Organizing committee

Prof. Ye, Yang - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China
Dr. Soković, Marina - Institute for Biological Research “Siniša Stanković”, National Institute for Republic of Serbia, University of Belgrade, Serbia
Prof. Khan, Shahbaz - UNESCO Regional Office for East Asia
Dr. Sugiura, Ai - UNESCO Regional Office for East Asia
Mr. Wu, Yongzheng - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China
Ms. Li, Qing - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China
Ms. Yang, Tianyun - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China
Ms. Zhou, Yinuo - Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China
Ms. Hadžimurtović, Nađa - Institute for Biological Research “Siniša Stanković”, National Institute for Republic of Serbia, University of Belgrade, Serbia

GENERAL PROGRAM

Time	Activity	Location
26th October, Sunday		
Whole Day	Arrive in Shanghai, check-in at Parkyard Hotel	No. 699 Bibo Road
27th October, Monday		
08:20	SIMM Shuttle bus 1 and Registration	From Parkyard Hotel to the venue at SIMM Niudun Rd. Campus
08:40	SIMM Shuttle bus 2 and Registration	
09:00-09:20	Opening Addresses	Lecture Hall, FIRST FLOOR
09:20-09:35	PANDA New Member Admission Ceremony & Signing Ceremony	
09:35-09:50	Group Photo	Lecture Hall, FIRST FLOOR and the Lobby
09:50-12:30	Plenary & Invited Lectures in the Plenary Session	Lecture Hall, FIRST FLOOR
12:30-13:30	Lunch Break	SIMM Canteen, SECOND FLOOR
13:30-16:30	Invited Lectures & Oral Presentations in three Parallel Sessions	Room 403, 405 and 406, FOURTH FLOOR
16:30	SIMM Shuttle buses from SIMM Niudun Rd. Campus to Paulaner Wirtshaus@North Bund	No. 500 Dongdaming Road, North Bund, SECOND FLOOR
17:00-19:00	Conference Banquet at Paulaner Wirtshaus@North Bund	
Around 19:00	SIMM Shuttle buses from Paulaner Wirtshaus@North Bund to Parkyard Hotel	
28th October, Tuesday		
08:50	SIMM Shuttle bus 1 and Registration	From Parkyard Hotel to the venue at SIMM Niudun Rd. Campus
09:10	SIMM Shuttle bus 2 and Registration	
09:30-11:40	Invited Lectures & Oral Presentations in three Parallel Sessions	Room 403, 405 and 406, FOURTH FLOOR
11:40-13:00	Lunch break	SIMM Canteen, SECOND FLOOR
13:00-17:00	Plenary & Invited Lectures in the Plenary Session	Meeting Room 5, THIRD FLOOR
17:00-17:20	Closing Ceremony	
17:20	SIMM Shuttle buses from SIMM Niudun Rd. Campus to Shunfeng Restaurant	Shanghai No.1 Department Store, No. 500 Xizang Middle Road, SEVENTH FLOOR
17:50-19:50	Invited Dinner at Shunfeng Restaurant	
Anytime	Stroll around and return to Parkyard Hotel by subway or taxi	
29th October, Wednesday		
Whole Day	Depart from Shanghai	

SCIENTIFIC PROGRAM

Plenary Sessions

Time	Activity	Venue & Moderator
	27th October, Monday	
08:30-09:00	Registration	
09:00-09:20	Opening Addresses	Lecture Hall, 1F, SIMM Niudun Rd. Campus Moderator: Prof. Yang Ye
09:20-09:35	PANDA New Member Admission Ceremony & Signing Ceremony	
09:35-09:50	Group Photo in the Lecture Hall and in the Lobby	
09:50-10:20	Identification of bioactive compounds to treat metabolic disorders **Speaker:** Prof. Christian Wolfrum	Lecture Hall, 1F, SIMM Niudun Rd. Campus Moderator: Prof. Edward Kennelly
10:20-10:50	Synthesis, stereochemical analysis and bioactivity of isochroman derivatives **Speaker:** Prof. Tibor Kurtán	
10:50-11:00	Q&A	
11:00-11:20	Coffee Break	
11:20-11:40	Pyrrolizidine alkaloids, the phytotoxin responsible for a relevant human health problem **Speaker:** Prof. Ge Lin	Lecture Hall, 1F, SIMM Niudun Rd. Campus Moderator: Prof. Tibor Kurtán
11:40-12:00	Comparative Metabolomic and Bioactivity Analyses of American, Asian, and European *Aconitum* Species Speaker: Prof. Edward Kennelly	
12:00-12:20	Encapsulation as a tool for timely and targeted delivery of bioactives **Speaker:** Prof. Viktor Nedović	
12:20-12:30	Q&A	
12:30-13:30	Lunch break	SIMM Canteen 2F

28th October, Tuesday		
13:00-13:30	GPCR Structural Pharmacology and First-Principles Drug Design **Speaker:** Prof. H. Eric Xu	Meeting Room 5, 3F, SIMM Niudun Rd. Campus Moderator: Dr. Marina Soković
13:30-14:00	The olive tree (*Olea Europaea*), an invaluable source of bioactive molecules **Speaker:** Prof. Leandros Skaltsounis	
14:00-14:20	Myrrhasin is not present in myrrh but it is found in *Commiphora odurensis* **Speaker:** Prof. Ermias Dagne	
14:20-14:40	Fungal fruiting bodies – a valuable source for new (bioactive) secondary metabolites **Speaker:** Dr. Norbert Arnold	
14:40-14:50	Q&A	
14:50-15:10	Coffee Break	
15:10-15:40	Digitizing Pharmacognosy: From Natural Products Metabolomics to AI (Online Live Streaming / Pre-Recorded) **Speaker:** Prof. Jean-Luc Wolfender	Meeting Room 5, 3F, SIMM Niudun Rd. Campus Moderators: Prof. Leandros Skaltsounis
15:40-16:00	Integrating Traditional Chinese and Western Medicine: Clinical Outcomes in Chronic Pain and Advanced Lung Adenocarcinoma **Speaker:** Prof. Jan P. A. Baak	
16:00-16:20	Harnessing Nature's Potential: Natural Products as a Driving Force in Drug Discovery **Speaker:** Dr. Marina Soković	
16:20-16:50	The interactions of poxviruses with the host cell and immune system **Speaker:** Prof. Geoffrey L Smith	
16:50-17:00	Q&A	
17:00-17:20	Plenary Discussion & Closing Ceremony	Meeting Room 5, 3F, SIMM Niudun Rd. Campus Moderators: Prof. Yang Ye Dr. Marina Soković
17:20-19:50	Invited Dinner	Shunfeng Restaurant

Parallel Session 1

Time	Activity	Venue & Moderator
	27th October, Monday	
13:30-13:45	The hormetic mechanism of chrysanthemolide I in alleviating drug-induced liver injury: affinity-gated and saturation-enabled target engagement **Speaker:** Prof. Ligen Lin	Room 403, 4F, SIMM Niudun Rd. Campus Moderators: Dr. Sofa Fajriah Dr. Sysay Palamy
13:45-14:00	From Biodiversity to Health Solutions: The Philippines' National Program on Natural Products Discovery and Development **Speaker:** Prof. Doralyn Dalisay	
14:00-14:15	Comparative Phytochemical, Colloidal, and Antioxidant Profiling of Several *Artemisia* L. species: Potentials for Cosmeceutical and Nutraceutical Applications **Speaker:** Prof. Janar Jenis	
14:15-14:30	Synthesis of spiroketal natural products isolated from traditional Chinese medicines **Speaker:** Dr. Eilidh Young	
14:30-14:45	Total Synthesis of (–)-Cordycicadin D and 3,4-*trans*-Cordycicadins A & B: Entry to the 3,4-*trans*-Fused Cordycicadin Framework **Speaker:** Dr. Liam Hunt	
14:45-14:55	Q&A	
14:55-15:15	Coffee Break	
15:15-15:30	Explorations of Secondary Metabolites from Indonesian *Dysoxylum* Plants: Isolation, Structure elucidation, and Biological Activities Speaker: Dr. Sofa Fajriah	Room 403, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Janar Jenis Prof. Ligen Lin
15:30-15:45	Isolation and identification of phenolic compounds from the two Saussurea species from Mongolia **Speaker:** Mr. Purevdorj Erdenetsogt	
15:45-16:00	Investigation on Kazakhstani medicinal plants with special attention on *Rheum tataricum* L., *Artemisia albida* L. **Speaker:** Ms. Ayaulym Minkayeva	
16:00-16:15	Determination of Gallic Acid and p-Coumaric Acid in *Solanum indicum* L. Extract Using High-Performance Liquid Chromatography **Speaker:** Dr. Sysay Palamy	
16:15-16:30	Q&A	
16:30-19:00	Conference Banquet	Paulaner Wirtshaus@North Bund

28th October, Tuesday		
08:30-09:30	Registration	
09:30-09:45	Marine natural products as chemical probes for drug target identification **Speaker:** Prof. Xu-Wen Li	Room 403, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Antoaneta Trendafilova Prof. Biljana Kukavica
09:45-10:00	Bioactive Compounds from Medicinal Plants: Opportunities for Drug Development **Speaker:** Prof. Ipek Suntar	
10:00-10:15	Comparative analysis of the biological activity of *Hypericum perforatum* and *Centaurium erythraea* **Speaker:** Ms. Toda Ignjatović	
10:15-10:25	Q&A	
10:25-10:45	Coffee Break	
10:45-11:00	Chemical characterization and bioactivity of secondary metabolites in two *Scilla* species **Speaker:** Prof. Biljana Kukavica	Room 403, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Ipek Suntar Prof. Xu-Wen Li
11:00-11:15	Methods for detecting of adulterated *Arnicae flos* (*Arnica montana*) on the marketplace **Speaker:** Prof. Antoaneta Trendafilova	
11:15-11:30	Phytochemical Characterization and Antioxidant Potential of Stinging Nettle Leaves (*Urtica dioica* L.) **Speaker:** Ms. Nikica Lazarević	
11:30-11:40	Q&A	
11:40-13:00	Lunch Break	SIMM Niudun Rd. Campus Canteen 2F

Parallel Session 2

Time	Activity	Venue & Moderator
	27th October, Monday	
13:30-13:45	Finding the Oddballs: Genome Mining of an Unusual Fungal NRPS-PKS Hybrid Leads to the Discovery of Bicephalic Acid A with a Unique Biheterocyclic Scaffold **Speaker:** Dr. Yit Heng Chooi	Room 405, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Catur Sugiyanto Prof. Yanchuan Shi
13:45-14:00	Rational design and zebrafish validation of sulfonamide-chalcones as next-generation antiepileptic drug candidates **Speaker:** Dr. Siti Munirah Mohd Faudzi	
14:00-14:15	Detection of Sibutramine and Fluoxetine adulterated in dietary supplements and weight-loss products containing natural extracts sold in Vientiane Capital Lao PDR **Speaker:** Dr. Chithdavone Her	
14:15-14:30	Uncovering the Bioactive Potential of Malaysian Plants Through Metabolomics **Speaker:** Prof. Faridah Abas	
14:30-14:45	Computer assisted discovery of novel nicotinamide phosphoribosyltransferase agonists to combat muscle atrophy **Speaker:** Mr. Linxuan Li	
14:45-14:55	Q&A	
14:55-15:15	Coffee Break	
15:15-15:30	Does salt matter in metabolism? Insights beyond CVD Speaker: Prof. Yanchuan Shi	Room 405, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Faridah Abas Dr. Yit Heng Chooi
15:30-15:45	Advancing Metabolomics in Natural Products Science Through Spatial Mapping of Plant Nutraceuticals **Speaker:** Mr. Chuckcris Tenebro	
15:45-16:00	Extending the Potential of the Naturally Abundant Substance Anticopalic Acid for Drug Discovery Applications **Speaker:** Dr. Jutatip Boonsombat	
16:00-16:15	Opportunities and Challenges of Collaborating with Industry in Developing Marigold as a Food Colorant **Speaker:** Prof. Catur Sugiyanto	
16:15-16:30	Q&A	
16:30-19:00	Conference Banquet	Paulaner Wirtshaus@North Bund

28th October, Tuesday		
08:30-09:30	Registration	
09:30-09:45	Integrated system can accelerate drug research and tech transferring **Speaker:** Prof. Jingshan Shen	Room 405, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Sokol Abazi Prof. Olga Gigopulu
09:45-10:00	Diversity of Cardiac Glycosides in Digitalis Taxa from the Balkan Peninsula: Phylogenetic Insights into Chemical Variation **Speaker:** Dr. Danijela Mišić	
10:00-10:15	Natural molecules for industrial application **Speaker:** Prof. Sandrina Heleno and Prof. Márcio Carocho	
10:15-10:25	Q&A	
10:25-10:45	Coffee Break	
10:45-11:00	Synthesis and antiproliferative activity of novel condensed heterocyclic ring systems **Speaker:** Dr. Sándor Balázs Király	Room 405, 4F, SIMM Niudun Rd. Campus Moderators: Dr. Danijela Mišić Prof. Sandrina Heleno
11:00-11:15	Loading Eugenol In Polymethylmethacrylate Discs Using Dense Carbon Dioxide **Speaker:** Prof. Sokol Abazi	
11:15-11:30	Integrating Spectroscopic Approach for Juniper and Blueberry Natural Resource Assessment in North Macedonia: Integrating Remote Sensing with GIS and Ground-Based Data **Speaker:** Ass. Prof. Olga Gigopulu	
11:30-11:40	Q&A	
11:40-13:00	Lunch Break	SIMM Niudun Rd. Campus Canteen 2F

Parallel Session 3

Time	Activity	Venue & Moderator
	27th October, Monday	
13:30-13:45	Creation of herbal preparations based on Uzbekistan medicinal plants according to the recipes of Abu Ali Ibn Sina using innovative technologies **Speaker:** Prof. Nodirali Normakhamatov	Room 406, 4F, SIMM Niudun Rd. Campus Moderators: Prof. Yongzhuo Huang Dr. Sarangerel Oidovsambuu
13:45-14:00	Polysaccharide-based macromolecular systems for cancer drug delivery **Speaker:** Prof. Bahtiyor Muhitdinov	
14:00-14:15	Biosynthsis of β-NAD-derived natural products **Speaker:** Prof. Takayoshi Awakawa	
14:15-14:30	The distinctiveness of (pre)formulation studies with natural products **Speaker:** Prof. Snežana Savić	
14:30-14:45	$GABA_A$ receptors in drug discovery of natural products **Speaker:** Prof. Miroslav Savić	
14:45-14:55	Q&A	
14:55-15:15	Coffee Break	
15:15-15:30	Antitumor activity of natural daphnane diterpenoids in EGFR-TKI resistant NSCLC cells Speaker: Dr. Sang Kook Lee	Room 406, 4F, SIMM Niudun Rd. Campus Moderator: Prof. Takayoshi Awakawa Dr. Sanit Thongnest
15:30-15:45	Advanced delivery of natural product compounds **Speaker:** Prof. Yongzhuo Huang	
15:45-16:00	Cytotoxicity of 114 Mongolian plant extracts on liver, colon, breast and cervix cancer cell lines **Speaker:** Dr. Sarangerel Oidovsambuu	
16:00-16:15	Polyoxygenated Cyclohex(a/e)ne Diterpene Esters identified in Thai *Kaempferia* subgen. *Protanthium* **Speaker:** Dr. Sanit Thongnest	
16:15-16:30	Q&A	
16:30-19:00	Conference Banquet	Paulaner Wirtshaus@North Bund

28th October, Tuesday		
08:30-09:30	Registration	
09:30-09:45	Artemisinin full industry chain research and industrialization **Speaker:** Dr. M. May Zhang and Dr. L. Ray Zhou	Room 406, 4F, SIMM Niudun Rd. Campus Moderators: Dr. Antonios Chrysargyris Dr. Nikolaos Tzortzakis
09:45-10:00	Domestication and Phytochemical Potential of *Sideritis cypria*: A Strategy for Conservation and Climate-Resilient Agriculture **Speaker:** Dr. Antonios Chrysargyris	
10:00-10:15	Tailoring nutrient needs for selected Medicinal and Aromatic plants and responses to climate changes challenges **Speaker:** Dr. Nikolaos Tzortzakis	
10:15-10:25	Q&A	
10:25-10:45	Coffee Break	
10:45-11:00	*In vitro* evaluation of supernatants of probiotic microorganisms against the causative agent of Lyme borreliosis **Speaker:** Miss. Kristina Jevremović	Room 406, 4F, SIMM Niudun Rd. Campus Moderators: Dr. Antonios Chrysargyris Dr. Nikolaos Tzortzakis
11:00-11:15	Integrating Chemical Ecology and Bio-Entrepreneurship in Drug Discovery **Speaker:** Prof. Sameh Soliman	
11:15-11:30	Chemical Investigation of *Commiphora* and *Boswellia* Resins **Speaker:** Ass. Prof. Olga Gigopulu	
11:30-11:40	Q&A	
11:40-13:00	Lunch Break	SIMM Niudun Rd. Campus Canteen Canteen 2F

PANDA Secretariat Shanghai and URSWAP Secretariat Shanghai Information:

Address: No. 555 Zu Chong Zhi Road, Zhang-Jiang High Tech Park, Pudong, Shanghai, China
Tel: +86 21 6807 7888, +86 18930490805

Hotel Information: Parkyard Hotel

Address: No. 699 Bibo Road, Zhang-Jiang High Tech Park, Pudong, Shanghai
Tel: +86 21 6162 1168

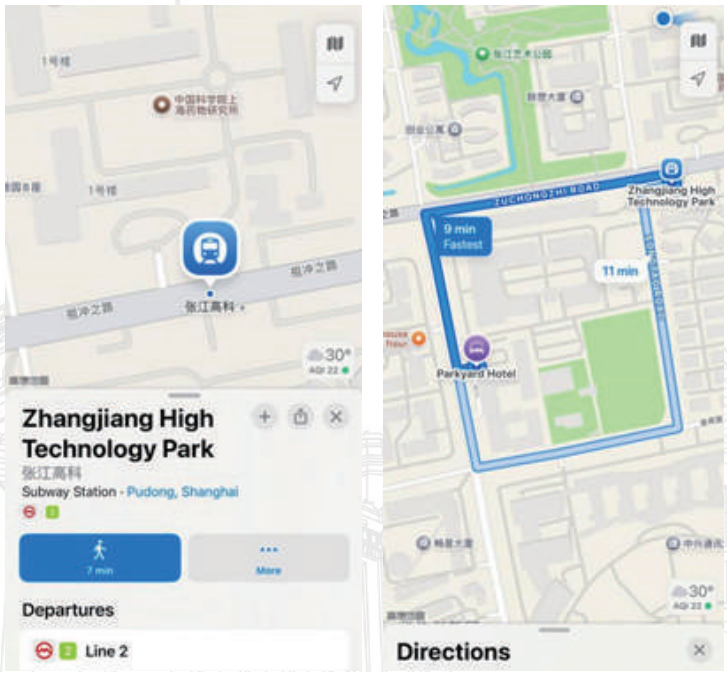
Venue Information: Shanghai Institute of Materia Medica, Chinese Academy of Sciences (Niudun Road Campus)

Address: No. 333 Niudun Road, Zhang-Jiang High Tech Park, Pudong, Shanghai
Plenary Session on 27th Oct Morning: Lecture Hall, 1F
Plenary Session on 28th Oct Afternoon: Meeting Room 5, 3F
Parallel Session 1: Room 403, 4F
Parallel Session 2: Room 405, 4F
Parallel Session 3: Room 406, 4F

Restaurant Information

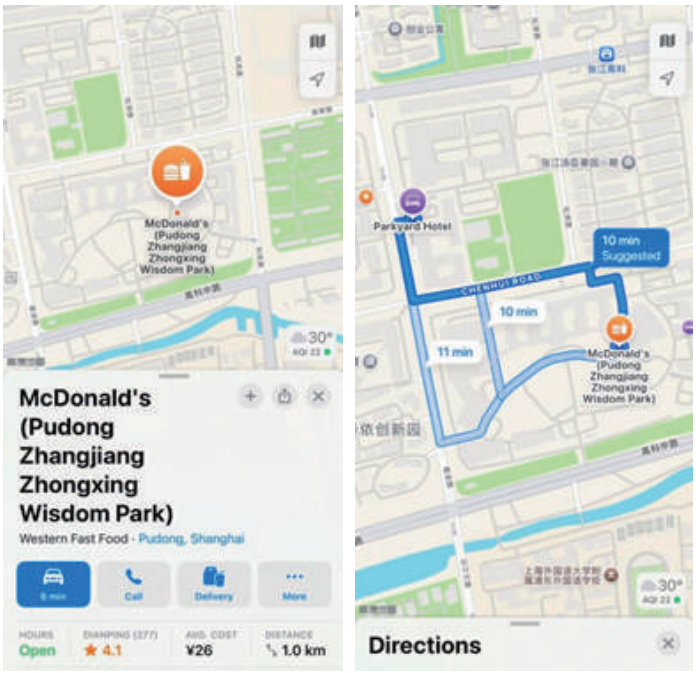
27th Oct Evening: Paulaner Wirtshaus@North Bund
Address: 2F, No. 500 Dongdaming Road, North Bund, Hongkou, Shanghai
28th Oct Evening: Shunfeng Restaurant
Address: 7F, Shanghai No.1 Department Store, No. 500 Xizang Middle Road, Huangpu, Shanghai

Nearest Subway Station: Zhangjiang High Technology Park Station (Line 2)

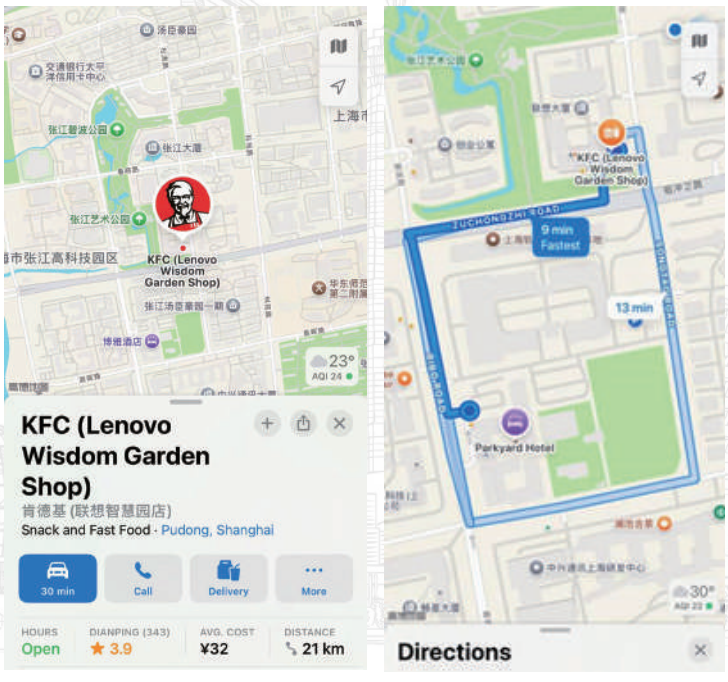


Fast Food near the Hotel

McDonald's (Pudong Zhangjiang Zhongxing Wisdom Park)
Opening Hours: 07:00-22:00
Address: 1F, No. 09-10, ZTE Building G, Pudong, Shanghai



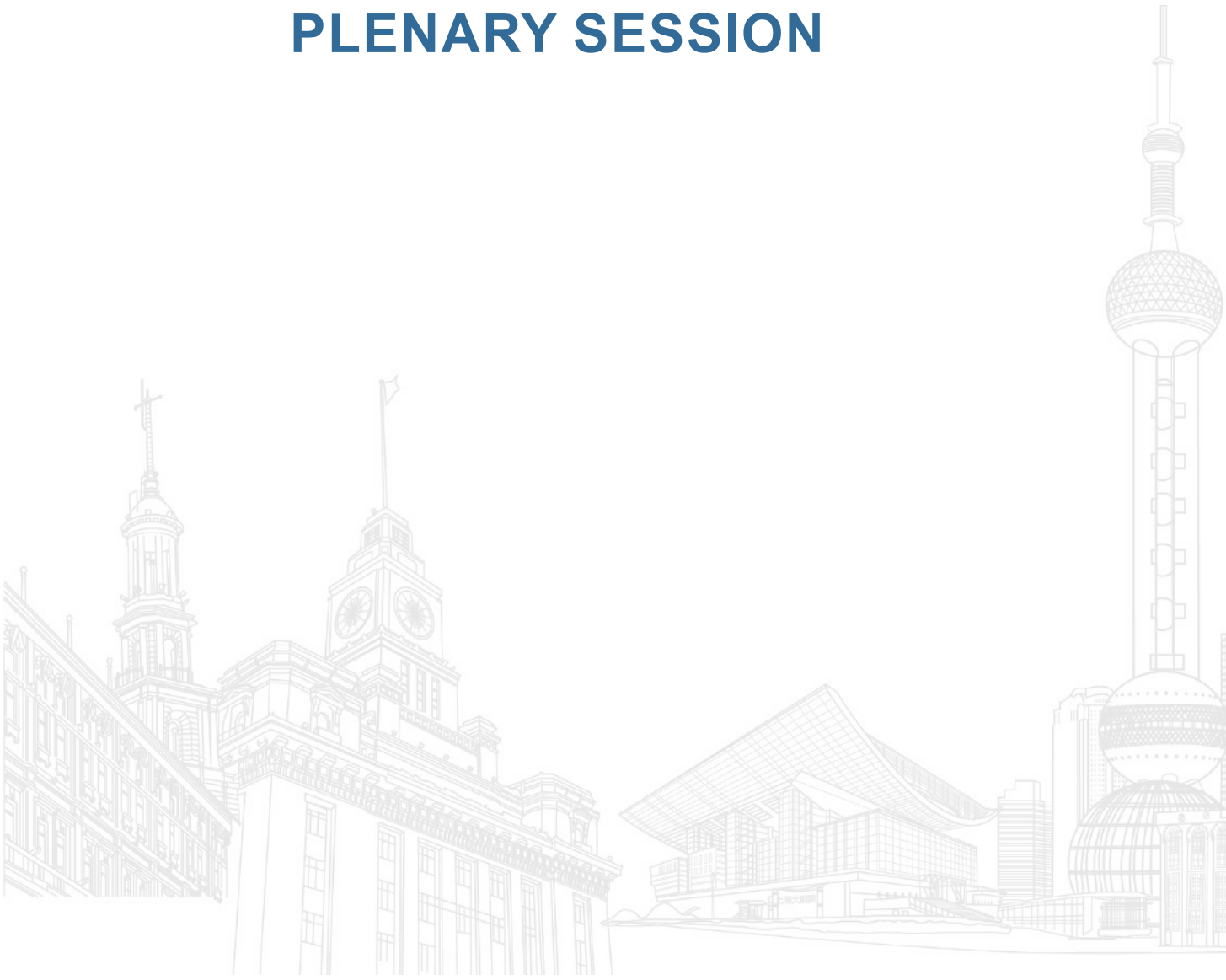
KFC (Lenovo Wisdom Garden Shop)
Opening Hours: 06:00-22:00
Address: No. 105, Building 3, No. 696 Songtao Road, Pudong, Shanghai



Guwu House of Flour (Zhangjiang Branch)
Opening Hours: 08:30-20:30
Address: 1F, Building 2, No. 690 Bibo Road, Zhangjiang Micro-electronics City, Pudong, Shanghai

ABSTRACTS

PLENARY SESSION



Name: Christian Wolfrum
Institution: Nanyang Technological University
Position: Deputy President and Provost
Email: christian.wolfrum@ntu.edu.sg

Research Field Chemistry of Natural Compounds

Title **Identification of bioactive compounds to treat metabolic disorders**

Abstract

Natural remedies are often used as stand-alone or additive treatments to modern medicine. Especially in the area of type 2 diabetes and prediabetes, several plant-based approaches exist, however the active compounds which mediate the effect are not known. The presentation will focus on the potential of the Palauan traditional leaf decoction of Phaleria nisidai (PNe) and its capacity to alleviate insulin resistance. PNe improves insulin sensitivity in mice and humans by regulating adipose tissue basal glucose uptake. Using a reverse pharmacology approach, we were able to identify several of PNe's active principle(s), by bioactivity-guided fractionation experiments. Especially the aglycone genkwanin (GE) improves insulin resistance to a comparable extent to metformin. These data demonstrate the possibility to identify new lead structures which could be employed in the management of type 2 diabetes.

Name: Tibor Kurtán
Institution: Department of Organic Chemistry, University of Debrecen
Position: Department Chair
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Research Field Organic chemistry, Stereochemistry

Title **Synthesis, stereochemical analysis and bioactivity of isochroman derivatives**

Keywords *isochroman, biaryl natural products, chiroptical spectroscopy, stereochemistry, bioactivity*

Abstract

Our optically active synthetic isochroman-2*H*-chromene conjugate JE-133 was found to prevent SH-SY5Y neuroblastoma cells from hydrogen peroxide (H_2O_2)-induced cell death. Recently, anti-inflammatory activity of our conjugate was also observed on microglia cells and we prepared all the eight stereoisomers and provided 2.0 g enantiopure sample for in vivo testing in a novel stroke model. Motivated by our stereochemical analysis of isolated axially chiral *bis*-isochromans, we achieved the first synthesis of optically active biaryl-type heterodimeric bis-isochromans containing both axial and central chirality elements. Some of the target compounds showed good antibacterial activity against methicillin-resistant Staphylococcus aureus, and the synthesis and antibacterial activity of *bis*-isochromans were disclosed in a patent.

The configurational assignments of natural products containing isolated blocks of chirality were achieved by a combination of electronic (ECD) and vibrational circular dichroism (VCD), and optical rotation (OR) calculations aided by DFT-NMR analysis. The absolute configurations (AC) of the tetracycline antibiotics chelocardin and amidochelocardin were revised by revisiting its configurational assignment with TDDFT-ECD and DFT-NMR calculations. The AC of the chlorinated cyclotetrapeptides, omnipolyphilins A and B were determined by a combination of advanced Marfey's method, ROE correlation aided by conformational analysis, and TDDFT-ECD calculations. The ACs of the two remote chirality centers of asperphenalenones F-M were determined by the combination ECD and OR calculations using both truncated models and the original structures.

Name: Ge Lin
Institution: School of Biomedical Sciences, The Chinese University of Hong Kong
Position: Professor
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Research Field Chemistry of Natural Compounds

Title **Pyrrolizidine alkaloids, the phytotoxin responsible for a relevant human health problem**

Keywords *pyrrolizidine alkaloid*

Abstract Pyrrolizidine Alkaloids (PAs) are common plant constituents and present in various medicinal herbs. PAs are also found as contaminants in some foodstuffs such as teas and honey with varied but lower levels. After exposure, mediated by hepatic cytochrome P450 enzymes, PAs are metabolically activated in the liver into an unstable toxic metabolite which interact with proteins or DNAs to form PA-protein or PA-DNA adducts causing acute hepatotoxicity, typically hepatic sinusoidal obstruction syndrome (HSOS), and/or chronic DNA damage followed by potential liver cancer development. In the present presentation, the biochemical mechanism of PA-induced hepatotoxicity, especially the metabolic activation of PAs to generate toxic metabolites leading to formation of hepatotoxic PA-protein adducts will be introduced, followed by the illustration of various factors affecting the hepatotoxic potency of PAs in different animal models. In addition, some cases of PA-induced human liver disease, including acute HSOS caused by relatively high-level exposure to PA-producing herbs and liver disease triggered by chronical low-level exposure of PA-contaminated foods will be discussed.

Name: Edward Kennelly
Institution: Lehman College, The City University of New York
Position: Professor and Chair
Email: edward.kennelly@lehman.cuny.edu

Research Field Metabolomics

Title **Comparative Metabolomic and Bioactivity Analyses of American, Asian, and European *Aconitum* Species**

Keywords *Metabolomics, Aconitum, medicinal plants, cardiotoxicity*

Abstract

Aconitum species have been used to treat rheumatism, heart failure, fatigue, pain and other conditions for thousands of years in Asia. These therapeutical effects are mainly due to the pharmacologically active diterpenoid alkaloids. In North America, there are few records of Aconitum native species being used medicinally, even though they are phylogenetically close with the medicinally important Asian species. Since Aconitum diterpenoid alkaloids have chemotaxonomic significance, we hypothesize that these compounds account for part of the bioactivity observed in American Aconitum species. The chemical profiles of three American Aconitum, A. *columbianum*, A. uncinatum, and A. *delphiniifolium*, were obtained using UPLC-qTOF-MSE and compared with Asian and European Aconitum species. With the help of an in-house database, compounds were tentatively identified.

PCA results shows that the three American species clustered closely, and were distinct from the Asian and European species, indicating they possess unique compounds. OPLS-DA analysis was used to identify unique marker compounds for the American species. American Aconitum species contain relatively low concentrations of cardiotoxic diester diterpenoid alkaloids. Therefore, the zebrafish embryo assay was used to compare cardiotoxicity of American species with A. *carmichaelii,* the most used Asian species used in traditional Chinese medicine. American Aconitum species are chemically distinct from Asian and European species, but produce bioactive diterpenoid alkaloids. Some of the most characteristic cardiotoxic alkaloids are present in lower levels in America Aconitum species, as compared to A. *carmichaelii*.

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Research Field AI for Drug Discovery

Title **Encapsulation as a tool for timely and targeted delivery of bioactives**

Keywords *Encapsulation, bioactive moleculs, food industry*

Abstract

This paper is aiming to present the potential benefits resulting from the use of encapsulated ingredients and cells in the food industry. The role of food nowadays is more oriented to the prevention of nutrition-related diseases and improvement of the physical and mental well-being of consumers than to fulfil basic nutritional needs. The current industrial production of foods involves the addition of functional ingredients to increase process efficiency, tailor flavor, color, texture, or preservation properties, while recent trend is the inclusion of bioactive compounds with potential health benefits, such as vitamins, probiotics, minerals, polyphenols, omega-3-fatty acids, and phytosterols. In this regard, encapsulation is a powerful tool that can be applied for a variety of reasons, including delayed, targeted release, stability, thermal protection, and suitable sensorial profile of bioactives.

Encapsulation may be also used to immobilize cells or enzymes in food processing applications, such as fermentation processes and metabolite production processes. Immobilization of microbiological cells by entrapment within natural or synthetic polymers or by adsorption onto solid (in)organic carrier materials has become an increasing research area with high potential for industrial applications.

The usefulness of encapsulation is going to be illustrated via several case studies developed in our lab, such as targeted delivery of bioactive molecules, aroma stabilization, protection of natural colorants, enriched beverages, beer, wine, cider and raspberry wine fermentations as well as active food packaging.

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Research Field Pharmacology and drug design

Title **GPCR Structural Pharmacology and First-Principles Drug Design**

Keywords *First-Principles, drug design, GPCR*

Abstract

This presentation explores advanced strategies in drug discovery, divided into two parts: GPCR signaling mechanisms and first-principles design of a novel FXR agonist.

The first part addresses key questions in GPCR signaling: selective coupling with G proteins, arrestins, and GRKs. For G protein selectivity, building on the 2011 GPCR-Gs structure, our team resolved the first GPCR-Gi complex and multiple peptide hormone receptor structures (Nature 2018; Science 2019; Cell 2021). These revealed conformational changes enabling subtype-specific G protein selection and small-molecule agonist activation of peptide receptors. For arrestin recruitment, after a decade of effort using X-ray free electron laser technology, we solved the first GPCR-arrestin complex (Nature 2015) and decoded the C-terminal phosphorylation code for arrestin specificity (Cell 2017), illuminating signaling precision. For GRK assembly, our “Nanohook” technology stabilized unstable complexes, yielding over 100 GPCR structures and advancing the field. This enabled high-resolution GPCR-GRK structures, showing how biased intracellular agonists modulate signaling (Nature 2023).

The second part introduces CS0159, a pioneering FXR agonist for non-alcoholic steatohepatitis (MASH), where no effective therapies exist. As bile acid metabolism’s master regulator, FXR is pivotal. CS0159’s design mimics the body’s ~0.5-hour bile acid cycle, unlike long-half-life competitors (12-24 hours). Structure-guided optimization yielded a novel scaffold with superior pharmacokinetics, liver/intestine targeting, and efficacy in animal models. Phase I trials confirmed exceptional safety—no adverse events—versus rivals like OCA and Tropifexor. CS0159 is 300-fold more potent than OCA, with a >20,000-fold safety margin, absent LDL elevation or pruritus. This underscores designing drugs aligned with physiological rhythms for safer, superior outcomes.

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Research Field Chemistry of Natural Compounds

Title **The olive tree (*Olea Europaea*), an invaluable source of bioactive molecules**

Keywords *Olive oil, Olea europaea, Oleuropein, Oleoside, Oleocanthal*

Abstract Extra virgin olive oil (EVOO), the main product of *Olea europaea* and the key ingredient of Mediterranean diet, is characterized by substantial nutritional and health beneficial value. However, despite olive oil's economic and health impact, its industry is associated with environmental problems derived from the vast quantity of by-products, such as vegetation waters, olive cake, olive pulp and olive branches and leaves. The amount of olive leaves produced every year exceed 18 million tons and mostly are used as animal feed, compost production or simply are burned, causing serious environmental damage. In a recent study was found that burning of olive tree branches is a major organic aerosol source in the Mediterranean region. However this material still contains high value-added compounds such as triterpenoids, secoiridois, flavonoids, phenolic alcohols, phenolic acids, lignans which are known as olive polyphenols. All these constituents have a strong antioxidant profile and there is an increased industrial interest in possible nutraceutical, cosmetic and pharmaceutical applications. Our work is focused on finding alternative strategies to manage the residues of olive oil industry following two axes. Firstly, the isolation of these compounds in multi gram scale. Secondly the use of these compounds as starting material for the hemi-synthesis of new bioactive analogues.

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Research Field Natural Products Chemistry

Title **Myrrhasin is not present in myrrh but it is found in *Commiphora odurensis***

Keywords *Commiphora myrrha,Commiphora oddurensis, myrrh, Tao Shen myrrhasin*

Abstract

Tao Shen et al. studied a resin and reported a new triterpene compound to which they gave the name myrrhasin, believing that the investigated resin was the well-known myrrh from *Commiphora myrrha*. However, we have now established that myrrhasin is not present in genuine myrrh, a significant finding given that no triterpene compound has previously been reported from this species and considering the extraordinary cultural, medicinal, commercial, and biological importance of myrrh. Fortunately, we discovered myrrhasin in a resin from Ethiopia, specifically *Commiphora oddurensis Chiov.*, collected in the Ogaden region. This study therefore reports the isolation of the known triterpenoid myrrhasin from the EtOAc/MeOH (1:1, v/v) extract of C. *oddurensis* resin, together with its structural elucidation, and provides only the second verified account of myrrhasin's occurrence in nature. The first report, by Tao Shen et al., from C. *myrrha* thus appears to have been based on misidentified source material. In addition to its isolation, this study describes the preparation of functional group modifications of myrrhasin (1), yielding its epoxide (1a/b) and acetate (1c) derivatives. Furthermore, anticancer activity assays of the crude extract, compound 1, and derivatives 1a/b against cervical cancer cells (HeLa) revealed IC50 values of 33, 29, and 35 µg/mL, respectively, highlighting their potential therapeutic applications. These results not only clarify the true natural source of myrrhasin but also underscore the importance of accurate botanical identification in phytochemical studies, while pointing to new prospects for drug discovery from *Commiphora* species.

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Research Field Secondary metabolites from fungal fruiting bodies; biosynthesis; bioactivity

Title **Fungal fruiting bodies – a valuable source for new (bioactive) secondary metabolites**

Keywords *Mushrooms, Cortinarius, Hygrophorus, secondary metabolites*

Abstract

Fungi are among the least well-known organisms on Earth. It is estimated that there are between 1.5 and 10 million species of fungi. However, of these, only around 148,000 have been described. The Basidiomycota class, which includes well-known mushrooms and puffballs as well as microfungi such as yeasts, smuts, and rusts, comprises over 50,000 species. When investigating mushrooms, meaning fungi characterized by a visible fruiting body, it is important to distinguish between saprophytic and mycorrhizal species. The former feed on dead organic material, while the latter form symbiotic relationships with tree roots. The plant produces organic molecules through photosynthesis and provides the fungus with sugars or lipids in exchange for water and mineral nutrients taken from the soil. Consequently, mycorrhizal fungi are a valuable source of secondary metabolites, whereas saprophytic mushrooms contain various enzymes.

The talk will focus on the diverse new chemical structures and bioactivity of secondary metabolites isolated from mushroom species belonging to the mycorrhizal genera *Hygrophorus* and *Cortinarius*. Several new Cortinarius species were also described using a polythetic approach combining chemical analysis of secondary metabolites, microscopic and morphological characteristics, and molecular phylogeny.

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Research Field Metabolomics and Natural product chemistry

Title **Digitizing Pharmacognosy: From Natural Products Metabolomics to AI**

Keywords *Metabolomics , knowledge graph, AI*

Abstract

The integration of omics, digital technologies and artificial intelligence (AI) is gradually leading to a transformative change in pharmacognosy, enabling unprecedented insights into the plant and microorganisms chemodiversity through detailed metabolome profiling. In this context modern LC-MS platforms deliver extensive qualitative insights into natural extracts, yet key challenges remain unresolved. These include ensuring accurate metabolite annotations, linking spectral data to bioactive compound quantities, and deriving 3D molecular structures critical for predicting bioactivity. Our research leverages metabolomic datasets from thousands of biodiverse plant and fungal extracts. We are trying to understand how the massive amount of information collected and the taxonomic links can be used to answer questions about confidence/redundance in MS annotation. Managing this flood of data requires innovative solutions, such as semantic web-based knowledge graphs (KGs), which organize complex relationships and enable advanced querying for pattern discovery. This work addresses practical hurdles in automating chemical composition assessment and highlights the synergistic potential of KGs and AI in natural products metabolomics. By combining digitised data with the traditional roots of pharmacognosy, we aim to streamline NP research, accelerate new natural ingredient development and open up new paths for drug discovery

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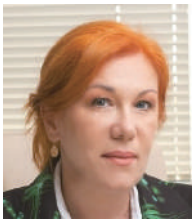
Title **Integrating Traditional Chinese and Western Medicine: Clinical Outcomes in Chronic Pain and Advanced Lung Adenocarcinoma**

Keywords *Traditional Chinese Medicine (TCM), Lung Adenocarcinoma, Integrated Medicine, Prognosis, Moxibustion*

Abstract

Stage IV lung adenocarcinoma (LUAD-IV), a leading cause of cancer mortality, often presents at an advanced stage. While genomic biomarkers guide Western treatments, patient outcomes remain heterogeneous. This research summarizes collaborative clinical studies demonstrating that integrating Traditional Chinese Medicine (TCM) with conventional Western therapy improves outcomes in LUAD-IV. Specifically, TCM herbal treatment provided a significant prognostic benefit for patients receiving platinum-based chemotherapy (PBC), with one prospective study showing TCM alone yielded superior survival outcomes compared to PBC alone. Furthermore, moxibustion therapy, combined with Western and herbal treatments, improved survival in a dose-dependent manner. Beyond efficacy, analyses of Astragali Radix in Western markets revealed significant variability in bioactive compounds, underscoring an urgent need for mandatory quality standards for TCM herbs in the US and EU. Despite promising results, key questions remain regarding the independent prognostic value of TCM interventions, the applicability of moxibustion to other lung cancer types, and the optimization of dosage and administration routes. Future research should prioritize large-scale, prospective, multicenter trials to validate these findings and explore additional metabolic and host-immune biomarkers to better integrate TCM response with clinical outcomes, ultimately advancing the personalized integration of TCM and Western medicine for advanced lung cancer.



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Research Field Metabolomics

Title **Harnessing Nature’s Potential: Natural Products as a Driving Force in Drug Discovery**

Keywords *Natural products, Plant and fungal species, Chemical analysis, Biological activity, Drug discovery*

Abstract

Natural products derived from plants, fungi, and other organisms represent a key driver of innovation in modern drug discovery. Their exceptional chemical diversity and long-standing use in traditional medicine offer a strong foundation for developing novel therapeutics to address pressing global health challenges.

As part of our research, comprehensive investigations were conducted on great number of plant and fungal species. Chemical analyses and biological activity assessments were performed on extracts, fractions, and isolated compounds, leading to the identification of numerous bioactive agents with potential antimicrobial, anticancer, anti-inflammatory, and immunomodulatory properties and food ingredients.

Advancements in metabolomics and analytical chemistry have significantly enhanced the identification and optimization of natural compounds, enabling a more efficient and targeted approach to drug discovery. Natural products are increasingly valued not only as direct drug candidates or food additives, but also as templates for synthetic and semi-synthetic modification.

Sustainability plays a crucial role in this field, ensuring responsible sourcing and preservation of biodiversity. Integrating traditional knowledge with modern biotechnological tools supports both innovative research and environmental stewardship.

This presentation will highlight our results and underline the importance of interdisciplinary and international collaboration. By connecting academic, industrial, and clinical perspectives, natural product research fosters the translation of basic discoveries into real-world applications, helping to bridge the gap between the laboratory and patient care.

Aligned with the United Nations Sustainable Development Goals, this work contributes to SDG 3 (Health), SDG 9 (Innovation), SDG 12 (Sustainable Production), and SDG 15 (Life on Land). By combining tradition, science, and sustainability, natural products remain central to the development of safer, more effective therapies and the building of healthier societies.

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Research Field Poxviruses

Title **The interactions of poxviruses with the host cell and immune system**

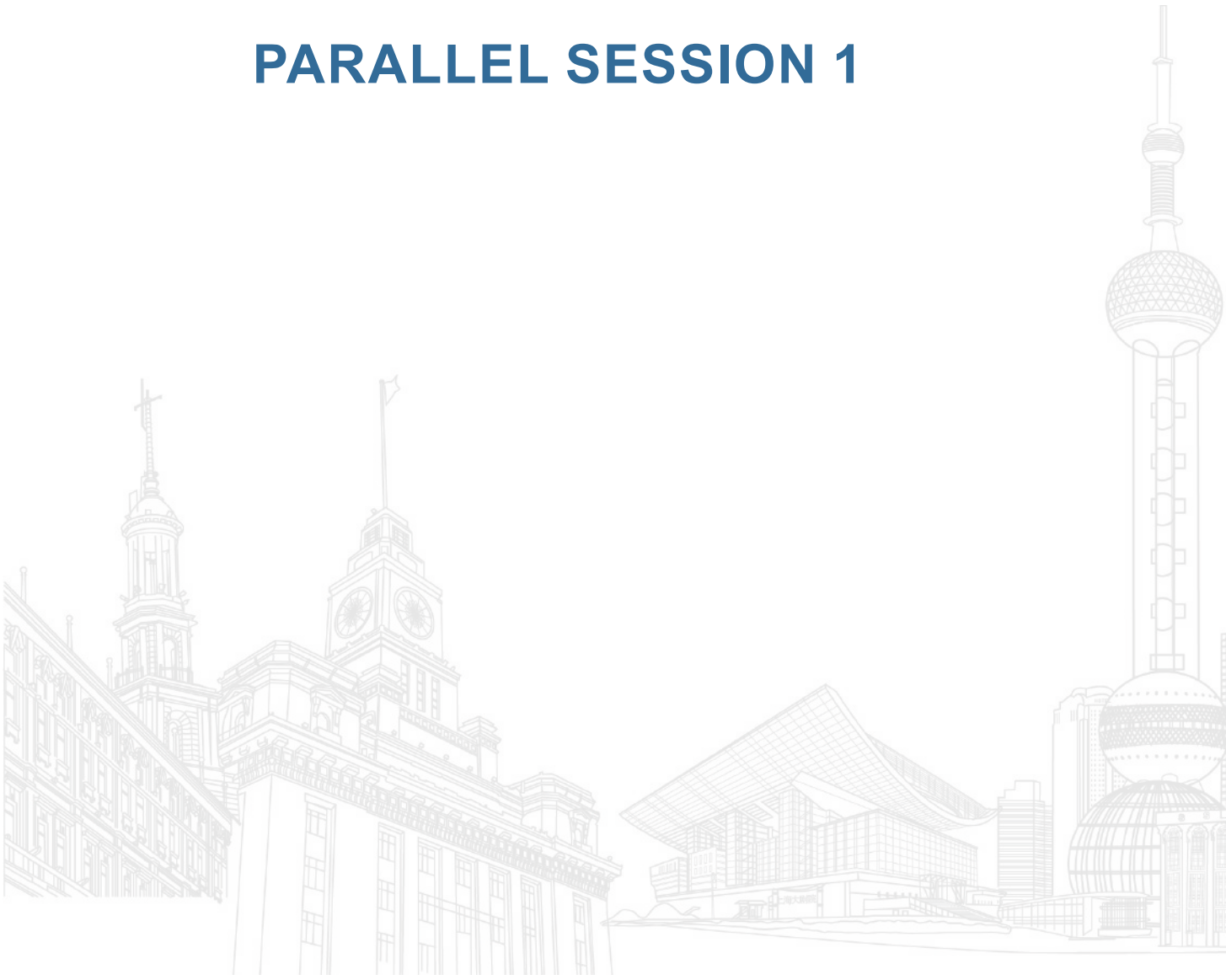
Keywords *Poxvirus, monkeypox, vaccinia, evasion of innate immunity, interferons*

Abstract

Poxviruses are complex viruses that replicate in the cytoplasm. The most notorious poxvirus was called variola virus (VARV) and caused smallpox, a disease declared eradicated by the WHO in 1979 following widespread vaccination with vaccinia virus (VACV). After smallpox eradication, poxviruses caused little human disease until 2022, when clade IIb monkeypox virus (MPXV) spread from its natural reservoir in west Africa to cause a worldwide mpox epidemic that WHO designated a Public Health Emergency of International Concern (PHEIC). Subsequently, a second mpox epidemic started in central Africa caused by the more dangerous clade Ib MPXV, and this also spread to many nations within and outside Africa and was designated a PHEIC by WHO. VARV, VACV and MPXV are all orthopoxviruses and have dsDNA genomes of ~ 200 kbp and encode about 200 proteins. Many of these proteins aid evasion of the innate immune response to infection and contribute to virus virulence. Studying these proteins is increasing understanding of how viruses cause disease and also how our innate immune system detects and responds to virus infection. This information is useful in designing safe and immunogenic poxvirus vaccines and therapies to treat poxvirus infections.

The talk will illustrate how orthopoxvirus proteins inhibit innate immune signalling pathways that regulate the production and action of interferons. Strategies include, binding to cellular proteins to inhibit their function, modifying cellular proteins to alter their function, mimicking cellular proteins to retain their function, and degrading cellular proteins to eliminate their function. A remarkable feature of these evasion strategies, is that a single pathway may be targeted by many different virus proteins and that deletion of an individual viral inhibitor still gives an in vivo phenotype despite the presence of the remaining inhibitors of the same pathway.

PARALLEL SESSION 1



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Research Field Chemistry of Natural Compounds

Title **The hormetic mechanism of chrysanthemolide I in alleviating drug-induced liver injury: affinity-gated and saturation-enabled target engagement**

Keywords *hormesis, AMPK, drug-induced liver injury, mitochondrial homeostasis, STK11, PP2Ac*

Abstract Hormesis, characterized by low-dose stimulation and high-dose inhibition, is closely linked to drug discovery and the Yin/Yang philosophy of traditional Chinese medicine; however, its underlying mechanisms remain unclear. Herein, chrysanthemolide I (CI), isolated from Chrysanthemum *indicum*, alleviated drug-induced liver injury (DILI) in vitro and in vivo in hormetic manners. Through drug affinity responsive target stability-mass spectrometry (DARTS-MS) and functional validation, we uncovered an intriguing mechanism: at low doses, CI binds directly to ALA-205 and ARG-301 within the kinase domain of STK11 with high affinity, enhancing its kinase activity and thereby activating AMP-activated protein kinase (AMPK); at middle doses, binding of CI to STK11 reaches saturation, leading to peak AMPK activity; at high doses, CI additionally binds to SER-261 within the C-terminal domain of PP2Acα with low affinity, activating its phosphatase activity and subsequently reducing AMPK activation. Furthermore, CI alleviates DILI by attenuating mitochondrial oxidative stress and enhancing mitochondrial biogenesis and mitophagy through the activation of the AMPK/GSK-3β/Nrf2, AMPK/PGC-1α/Nrf1, and AMPK/ULK1/PINK1/Parkin signaling pathways, respectively. Taken together, our findings describe an affinity-gated and saturation-enabled target engagement mechanism that provides a universal framework for elucidating the relationships among drug concentration, target binding, and pharmacological effect.

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Research Field Chemistry of Natural Compounds, Biosynthesis and Synthetic Biology, Metabolomics

Title **From Biodiversity to Health Solutions: The Philippines' National Program on Natural Products Discovery and Development**

Keywords *Philippines, Tuklas Lunas Program, Bioprospecting, Natural Products Discovery, Functional Foods, Metabolomics, Drug Discovery, marine actinomycetes*

Abstract

The Philippines is endowed with immense biodiversity that provides a foundation for natural products research and drug discovery. Building upon centuries of traditional medicine and ethnopharmacology, the Department of Science and Technology (DOST) launched the *Tuklas* Lunas Program to systematically explore, harness, and develop the country's rich biological resources into safe and effective therapies and functional foods. *Tuklas* Lunas, from *tuklas* (discovery) and *lunas* (remedy), represents the integration of indigenous knowledge, modern science, and nationwide collaboration in natural products research. At the University of San Agustin, the Center for Chemical Biology and Biotechnology (C2B2) and the Center for Natural Drug Discovery and Development (CND3) have advanced this vision by bioprospecting marine sediment–derived actinomycetes and Philippine plants. Through metabolomics, genomics, mass spectrometry imaging, bioinformatics, and bioassay-guided screening, our teams have identified bioactive metabolites with antibacterial, antiviral, and anticancer activities, while also validating nutraceuticals in functional foods such as ginger, pineapple, cacao, and pigeon pea. Importantly, these discoveries have been translated into prototypes and partnerships with local industries, bridging science and innovation. This report highlights achievements, challenges, and future directions of the Philippine Tuklas Lunas initiative, demonstrating how investment in capacity building and collaborative networks can transform biodiversity into health solutions for national and regional well-being.

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Research Field Chemistry of Natural Compounds

Title **Comparative Phytochemical, Colloidal, and Antioxidant Profiling of Several Artemisia L. species: Potentials for Cosmeceutical and Nutraceutical Applications**

Keywords *Artemisia species, antioxidants, DNA oxidation protection, hydrolates, sun protection factor*

Abstract Plants remain to this day one of the most important sources of bioactive compounds and continue to provide new medical preparations. Three Artemisia L. species native to Kazakhstan (A. *albida* Willd., A. *leucodes* Schrenk., and A. *scopaeformis* Ledeb) remain underexplored with respect to their phytochemical constituents and therapeutic potential. A detailed chemical, colloidal, and biological investigation of three *Artemisia* L. species was undertaken as the central objective for obtaining unique hydrolates derived from these medicinal plants. To achieve this objective, a comprehensive scientific study was conducted on the phytochemical composition, antioxidant potential, and colloidal properties of hydrolates obtained from three Artemisia L. species growing in different geographical regions of Kazakhstan. Qualitative and quantitative analyses of bioactive compounds were performed. Antioxidant activity was assessed through the DPPH and FRAP assays, while additional evaluations included sun protection factor, DNA protection against oxidative damage, and molecular docking to examine interactions between active compounds and biological targets. The colloidal characteristics of the hydrolates were evaluated, including surface tension, pH, and membrane permeability, along with their emulsifying and foaming capacities. The results obtained are considered in the context of their practical application in the development of cosmetic and therapeutic formulations, such as creams and ointments.

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Research Field Chemistry of Natural Compounds

Title **Synthesis of spiroketal natural products isolated from traditional Chinese medicines**

Keywords *Total synthesis, natural products, traditional Chinese medicines*

Abstract

The spiroketal moiety is well established as a 'privileged scaffold' in drug discovery. The spiroketal motif is ubiquitous in biologically-active natural products isolated from traditional Chinese medicine, with the scaffold arising from diverse biosynthetic and phylogenetic origins, implicating an evolutionary driving force towards the construction of this privileged scaffold.

Herein, we report the synthesis of three such spiroketal natural products, lycibarbarines A–C. Key features of the total synthesis include N-alkylation of a tetrahydroquinoline with an α-bromoketone, acid-mediated spiroketalisation, and late-stage formylation of an aryl bromide. Through this work it was established that the spiroketal unit of lycibarbarines A–C exhibits unusually high resistance to acid-mediated isomerization, likely due to the proximal basic nitrogen atom. As such, lycibarbarines A–C denote a notably more acid-stable N-heterocyclic spiroketal scaffold, and present an interesting case study in the isolation and synthesis of new privileged bioactive pharmacophores from traditional medicine sources.

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Research Field Chemistry of Natural Compounds

Title **Total Synthesis of (–)-Cordycicadin D and 3,4-*trans*-Cordycicadins A & B: Entry to the 3,4-*trans*-Fused Cordycicadin Framework**

Keywords *Total synthesis, Natural Products, Polyketides*

Abstract We report a total synthesis of (–)-cordycicadin D and two anticipated natural products 3,4-*trans*-cordycicadin A & B. Our routes feature a divergent-convergent strategy, taking advantage of the target's inherent symmetries. This strategy was enabled by an enzymatic resolution and a late-stage bioinspired dimerization. The routes afford (–)-cordycicadin D in 14 steps and 3,4-*trans*-cordycicadin A & B in 13 steps. The synthesis confirms the structure of the (–)-cordycicadin D and gives indication as to why the anticipated natural products are yet to be isolated. We hope our synthesis of 3,4-*trans*-cordycicadin A & B may aid in their isolation from biological sources.

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Research Field Chemistry of Natural Compounds

Title **Explorations of Secondary Metabolites from Indonesian Dysoxylum Plants: Isolation, Structure elucidation, and Biological Activities**

Keywords *Dysoxylum, sesqui- and sesquiterpenoid dimers, DP4+ algorithm, immunomodulatory based TLR4*

Abstract In our continuing study of Indonesian medicinal plants, we have successfully isolated, identified, and reported secondary metabolites from Indonesian *Dysoxylum* plants including sesqui- and sesquiterpenoid dimers, triterpenoids, limonoids, and macrolides. Some were established as new compounds. The structure determination was performed using an extensive spectroscopy method, quantum chemical calculations, as well as supplemented by the DP4+ algorithm. The identified compounds were tested their biological activity as cytotoxic compounds against human cancer cells, and immunomodulatory based TLR4. The best results are moderate activity for cytotoxic and anti-inflammatory agents, and paraxyline B as a strong agonist TLR4 can be further investigated for vaccine adjuvant development. The diversity of structures and biological activities of the identified compounds has resulted in a SAR study. A continuing phytochemical study on Indonesian *Dysoxylum* species is pursuing.

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Research Field Phytochemistry, Pharmacology

Title **Isolation and identification of phenolic compounds from the two Saussurea species from Mongolia**

Keywords *Saussurea, isolation, phenolic compounds, flavonoids*

Abstract

We investigated the phenolic composition of the aerial parts of two Saussurea species from Mongolia, *S.schanginiana* and *S.alpina*, to characterize their bioactive compounds.

From *S.schanginiana*, thirteen compounds were isolated, including simple phenols and phenolic acid derivatives such as syringin (75.0 mg), salidroside (3.2 mg), picein (5.9 mg), and chlorogenic acid (125.6 mg), as well as flavonoid derivatives including quercetin (16.3 mg), kaempferol (31.7 mg), apigenin (2.7 mg), hispidulin (5.3 mg), hispidulin-7-O-β-D-glucopyranoside (15.5 mg), apigenin-7-O-β-D-galactopyranoside (6.4 mg), isorhamnetin-3-O-rutinoside (67.9 mg), quercetin-3-O-rutinoside (58.9 mg), and kaempferol-3-O-β-D-glucopyranoside (13.3 mg).

From *S.alpina*, nine compounds were isolated: syringin (32.7 mg), salidroside (8.2 mg), chlorogenic acid (15.6 mg), quercetin-3-O-β-D-glucuronide (18.6 mg), luteolin (12.6 mg), luteolin-7-O-β-D-glucuronide (7.9 mg), luteolin-7-O-rutinoside (18.2 mg), luteolin-7-O-β-D-glucopyranoside (2.6 mg), and kaempferol-3-O-neohesperidoside (28.8 mg). The structures of all isolated compounds were elucidated using detailed spectroscopic analyses, including MS and NMR techniques.

Our results indicate that these two Saussurea species differ considerably not only in their morphology but also in the composition of their phenolic compounds, with chlorogenic acid and flavonol derivatives being abundant in S.schanginiana, and S.alpina being rich in flavones, particularly luteolin derivatives.

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Research Field Chemistry of Natural Products

Title **Investigation on Kazakhstani medicinal plants with special attention on *Rheum tataricum* L., *Artemisia albida L.***

Keywords *Bioactive constituents, GC-MS, HPLC, antioxidant, pharmacological activity*

Abstract *Rheum tataricum* L. is a potential medicinal plant growing up in Kazakhstan that represent a valuable source of anthraquinones, tannins, flavonoids and mineral elements. This study investigates the phytochemical composition and biological activity of *Rheum tataricum* with the aim of evaluating its pharmacological potential. The plant's extract fractions were analyzed by gas-chromatography method with mass-spectrometric detection (petroleum ether fraction) together with high performance liquid chromatography (EtOAc, BuOH fractions). GC-MS analysis of the lipophilic fractions of R. *tataricum* revealed 18 distinct compounds. The major constituents were an anthracene derivative, 9,10-Anthracenedione, 1,8-dihydroxy-3-methyl- (35.1%) and 3,4-dihydro-8-hydroxy-3-methyl-1H-2-benzopyran-1-one (17.9%), a flavonoid-like structure, may contribute to the plant's antioxidant effect. HPLC analysis revealed that the highest concentration was found for phlorizin (1214.7 μg/g), with catechin also present in significant amounts (409.5 μg/g) in the EtOAc fraction. For BuOH part, relatively high levels of gallic acid (64.6 μg/g) and epicatechin (66.9 μg/g) were observed. The antibacterial activity of different fractions were comparatively evaluated. Fluorescence measurements were performed according to previously published methods to perform bacterial neurominidase (BNA) assays. The inhibition rate against BNA shows 88.21% for EtOH crude extract and 91.67% for EtOAc which indicates the polarity of bioactive compounds.

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Research Field Chemistry of Natural Compounds

Title **Determination of Gallic Acid and p-Coumaric Acid in Solanum indicum L. Extract Using High-Performance Liquid Chromatography**

Keywords *Phenolic Compounds, Solanum indicum L, High Performance Liquid Chromatography*

Abstract Bitter eggplant (*Solanum indicum L.*), locally known in Laos as Mak Khaeng Khom, is a medicinal plant commonly used in traditional medicine. It contains phenolic compounds such as gallic acid, p-coumaric acid, and ferulic acid, which are well-known for their important biological and pharmacological activities. The objective of this study was to determine the content of gallic acid, p-coumaric acid and ferulic acid in S. *indicum* extracts using High-Performance Liquid Chromatography. Plant material was extracted using ethanol maceration and Supercritical Fluid Extraction (SFE). HPLC analysis showed that ethanol maceration contained 224.00 ± 0.8 µg/ml of gallic acid, 56.25 ± 0.57 µg/ml of p-coumaric acid, and 131.68 ± 0.18 µg/ml of ferulic acid. SFE with 3% ethanol contained 209.55 ± 1.23 µg/ml of gallic acid, 13.30 ± 0.04 µg/ml of p-coumaric acid, and 275.18 ± 0.79 µg/ml of ferulic acid. SFE with 5% ethanol contained 219.32 ± 1.60 µg/ml of gallic acid, 15.06 ± 1.06 µg/ml of p-coumaric acid, and 277.14 ± 1.09 µg/ml of ferulic acid. The findings indicate maceration provides higher p-coumaric acid, while SFE enhances ferulic acid extraction.

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Research Field xwli@simm.ac.cn

Title **Marine natural products as chemical probes for drug target identification**

Keywords *Marine invertebrates, Marine natural products, Drug target*

Abstract

Marine natural products have long been recognized as a valuable source for drug discovery. However, transforming these complex molecules into functional tools for mechanistic studies and therapeutic exploration remains a central challenge. Our group work on the interface of marine natural product chemistry and chemical biology. Focusing on representative bioactive marine metabolites, and by integrating chemical proteomics and AI-assisted compound–target interaction prediction, we successfully identified the molecular targets of several marine-derived compounds and uncovered novel mechanisms in inflammation and cancer. For instance, by employing chemical proteomics approaches such as photoaffinity labeling combined with activity-based protein profiling (PAL-ABPP), we performed target fishing for a marine polyketide with anti-ischemic stroke activity and a marine alkaloid with anti-acute lung injury activity. Key molecular targets PKM2 and CSE1L were identified, respectively, and their functions were validated both in vitro and in vivo, providing valuable insights for the development of related therapeutics. Recently, we employed an AI-guided and pathway-informed perturbation transcriptomics strategy to have identified a marine bromotyrosine alkaloid as the first WRN Degrader for MSI-high cancer therapy. These studies not only expand the application of marine natural products in target discovery but also provide a paradigm for establishing a “natural product–chemical probe–disease mechanism” research framework.

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Research Field Chemistry of Natural Compounds, Pharmacognosy

Title **Bioactive Compounds from Medicinal Plants: Opportunities for Drug Development**

Keywords *Biological activity, phytochemistry, natural compounds*

Abstract

Natural products continue to provide an invaluable reservoir for modern pharmaceutical research. Plants produce a wide spectrum of secondary metabolites, including flavonoids, phenolic acids, lignans, alkaloids, terpenoids, and steroids, that exhibit remarkable structural diversity, ranging from simple molecular skeletons to highly complex compounds that are often impossible to synthesize artificially. These metabolites exert highly specific biological effects through distinct mechanisms of action. Research on medicinal plants is increasingly focused on identifying the phytochemicals responsible for their pharmacological effects. Ethnopharmacological approaches provide a valuable framework for recognizing potential natural agents and linking ethnomedical knowledge to modern applications. Preclinical and clinical investigations of medicinal plants have received considerable attention, elucidating their mechanisms and providing scientific support for traditional uses. In our recent studies, the biological activities of various medicinal plant species were systematically investigated through both in vitro and in vivo models, yielding significant findings. Active principles responsible for these activities were further isolated and structurally characterized using advanced instrumental techniques. This presentation will discuss our preclinical research on medicinal plants, with particular emphasis on bioactivity-guided fractionation and isolation techniques, demonstrating their potential as sources of new drug candidates.

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Research Field Chemistry of Natural Compounds

Title **Comparative analysis of the biological activity of Hypericum perforatum and Centaurium erythraea**

Keywords *phenolic compounds, antioxidative, α-amylase, α-glucosidase, anti-inflammatory*

Abstract *Hypericum perforatum* L. and *Centaurium erythraea Rafn* are highly valued plant species in Balkan traditional medicine. H. *perforatum* is widely recognized for its wound-healing, anti-inflammatory, and antidepressant properties. *C. erythraea* is known for its bitterness, which stimulates appetite, improves digestion, and supports liver function. This study aimed to evaluate the antioxidative, anti-inflammatory, and antidiabetic potential of leaf and aerial part (herba) extracts of both species collected in Bosnia and Herzegovina. Antioxidant activity of ethanol extracts was assessed spectrophotometrically, antidiabetic activity was determined by the ability of the extracts to inhibit α-amylase and α-glucosidase, and anti-inflammatory activity was evaluated through inhibition of protein denaturation. Extracts of H. *perforatum* showed higher total phenolic content and stronger antioxidative activity in the ABTS assay. Anti-inflammatory, antidiabetic, and trace metal reducing activities were also significantly higher in H. *perforatum* extracts. These findings highlight the remarkable biological activity of both species, especially H. *perforatum*, and suggest their potential application in the treatment of diseases associated with inflammation and oxidative stress.

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Research Field Chemistry of Natural Compounds

Title **Chemical characterization and bioactivity of secondary metabolites in two *Scilla* species**

Keywords *phenolic compounds, saponins, antioxidative activity, Scilla lakusicii, Scilla litardierei*

Abstract *Scilla lakusicii* and S. *litardierei* are unique plants from karst ecosystems. As Balkan endemics, they reflect the ecological diversity of the Dinaric karst, with S. *litardierei* found in wet meadows of karst fields, while S. *lakusicii* grows on the surrounding rocky limestone habitats. In this study, we analyzed the secondary metabolites and biological activity of their leaf extracts. The chemical profile was determined by UHPLC-Orbitrap MS, while antioxidant capacity was assessed using EPR spectroscopy and spectrophotometric assays. Saponins were identified as the dominant group of compounds, along with hydroxycinnamic acids, flavonoid glycosides, flavonoid aglycones, and homoisoflavonoids. Both extracts exhibited pronounced antioxidant effects, demonstrated through •OH and DPPH radical scavenging, Fe chelation, and reduction of transition metals. This strong antioxidant activity is likely related to their unique chemical composition and may contribute to the species' ecological resilience in karst habitats. Furthermore, the results highlight the potential therapeutic relevance of *Scilla* species in conditions associated with oxidative stress. However, further studies are required to fully characterize the extracts and evaluate possible adverse effects linked to saponins.

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Research Field Chemistry of Natural Compounds

Title **Methods for detecting of adulterated Arnicae flos (Arnica montana) on the marketplace**

Keywords *Arnica montana, Heterotheca inuloides, differentiation*

Abstract

Arnica montana is distributed in the mountainous parts of Europe from southern Iberia to southern Scandinavia and Carpathians. The flower heads (*Arnicae flos*) are widely used in phytopreparations such as ointments, creams and gels for topical treatment of bruises and sprains, due to their anti-inflammatory properties. Due to the high market value of wild-collected raw material and the cultivation challenges, the genuine plant material is often adulterated or substituted with cheaper or more widely available plants. Some of the known adulterants are other Arnica species, Mexican arnica (*Heterotheca inuloides*), or other yellow-flowering species from the family Asteraceae (*Calendula officinalis L, species from genera Inula, Dorinicum, etc.*).

In this study we applied different methods (IR, HTLC, HPLC, and LC/MS) for differentiation of A. *montana* and H. *inuloides* and for analysis of raw "*Arnicae flos*" sold in drug stores in Bulgaria, Serbia and Spain. The obtained results showed that the tested samples are H. *inuloides* or *Pulicaria* sp. This investigation emphasizes the critical need for systematic monitoring and regulation of herbs in trade.

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Research Field Chemistry of Natural Compounds

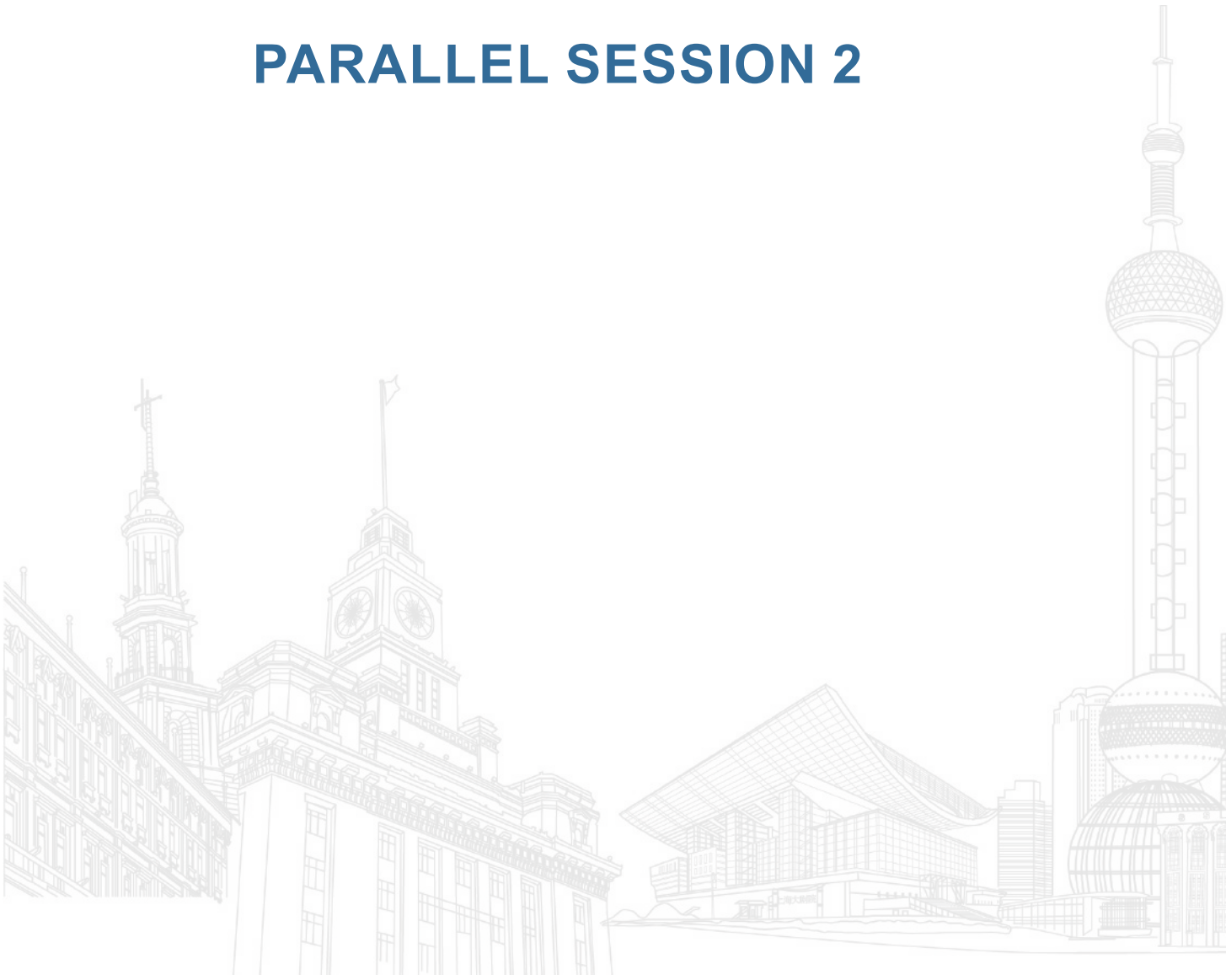
Title **Phytochemical Characterization and Antioxidant Potential of Stinging Nettle Leaves (*Urtica dioica* L.)**

Keywords *Urtica dioica; Antioxidant capacity; Polyphenolic compounds; Maceration; Ultrasonication; Soxhlet extraction; Montenegro*

Abstract The antioxidant potential of plants is attributed to secondary metabolites that neutralize reactive oxygen and nitrogen species generated by metabolism and environmental stressors. Despite the widespread use of *Urtica dioica* L. (stinging nettle), data on the antioxidant capacity of Montenegrin populations remain scarce. We quantified bioactive constituents and antioxidant activity in leaves collected at two ecologically distinct sites, Herceg Novi (south) and Pljevlja (north; n = 8 per site). Extractions employed maceration, Soxhlet, and ultrasonication with methanol, ethyl acetate, or water. Total phenolics, flavonoids, and tannins were measured; antioxidant activity was assessed by DPPH, FRAP, and ABTS.

Pljevlja samples exhibited higher total phenolics and ABTS inhibition, whereas Herceg Novi had greater flavonoid and tannin contents; FRAP values were comparable between sites. Under maceration, extraction efficiency followed methanol ≥ ethyl acetate □ water. Ultrasonication generally reduced DPPH IC□□ relative to maceration, most notably in water, while Soxhlet yielded good results in a solvent-dependent manner. Although water macerates were consistently weakest, water–ultrasonication in Pljevlja produced the lowest IC□□, consistent with ultrasound-enhanced recovery of polar phenolics. ABTS trends mirrored total phenolics, whereas FRAP more closely reflected flavonoids/tannins. These results guide solvent–method selection for the valorization of Montenegrin nettle in food and nutraceutical applications.

PARALLEL SESSION 2



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Research Field Biosynthesis and Synthetic Biology

Title **Finding the Oddballs: Genome Mining of an Unusual Fungal NRPS-PKS Hybrid Leads to the Discovery of Bicephalic Acid A with a Unique Biheterocyclic Scaffold**

Keywords *genome mining, natural products, polyketide synthase, nonribosomal peptide synthetase, fungi*

Abstract The continuous discovery of novel natural product scaffolds is vital for drug development, as their unique chemical diversity and biological activity can lead to new therapeutics for unmet medical needs. In search of new scaffolds, we employed a phylogenetic-guided approach to identify under-explored hybrid synthetases and uncovered a biosynthetic gene cluster encoding a nonribosomal peptide synthetase-polyketide synthase (NRPS-PKS) hybrid from *Aspergillus* sp. MST-FP2004, an Australian fungal isolate. This NRPS-PKS hybrid enzyme features an unusual domain organisation. Heterologous expression in *Aspergillus nidulans* led to the production of bicephalic acid A, a novel molecule with an unusual biheterocyclic scaffold comprising a pyrrole linked to a pyrrolidinedione. To elucidate its biosynthetic mechanism, we performed domain mutation and truncation studies. A point mutation in the methyltransferase domain abolished compound production, while truncation of the TE domain resulted in the formation of bicephalic acid B, a new dimeric pyrrolidinedione. Isotope feeding assays established the biosynthetic precursors of the pyrrolidinedione moiety, allowing us to propose a potential biosynthetic pathway for bicephalic acid A. Phylogenetic analysis suggests that *bicA* was likely acquired through horizontal transfer of a partial NRPS gene from an actinomycete donor and subsequently evolved new functions in fungi. Bioassays revealed that bicephalic acid A exhibits mild antifungal activity against Candida albicans (200 µg/ml) and cytotoxic activity against the NS-1 mouse myeloma cell line (100 µg/ml). This study highlights the potential of phylogenetic-guided approaches in uncovering novel natural product scaffolds.

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Research Field AI for Drug Discovery

Title **Rational design and zebrafish validation of sulfonamide-chalcones as next-generation antiepileptic drug candidates**

Keywords *Antiepileptic, design, computational, chalcones, zebrafish*

Abstract Epilepsy remains a major neurological disorder, with one- third of patients experiencing drug-resistant seizures and adverse effects of current antiepileptic drugs (AEDs). To address this unmet need, we applied a computational and zebrafish-based strategy to identify sulfonamide-chalcones as next-generation AED candidates. Thirty-six compounds were designed and screened using molecular docking and molecular dynamics (MD) simulations against the GABAA receptor, with compound **20** emerging as the most promising candidate due to its strong binding affinity (−10.3 kcal/mol), structural stabilization and persistent hydrogen bonding. The compound was synthesized and structurally confirmed using various spectroscopic techniques. A toxicity profile in zebrafish embryos confirmed a favourable safety margin [No Observed Adverse Effect Level (NOAEL) = 1.268 μM]. In vivo behavioural tests with pentylenetetrazole (PTZ)-induced seizures and zc4h2 knockout zebrafish models showed that compound **20** significantly reduced seizure-like hyperactivity at 0.39 μM and outperformed valproic acid at 100 μM. Overall, these results demonstrate the power of integrating computational and zebrafish-based platforms for early-stage drug discovery and highlight sulfonamide chalcones, particularly compound **20**, as promising AED candidates with potential translational value for safer and more effective epilepsy therapy.

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Research Field Food and Drug Safety

Title **Detection of Sibutramine and Fluoxetine adulterated in dietary supplements and weight-loss products containing natural extracts sold in Vientiane Capital Lao PDR**

Keywords *Sibutramine, Fluoxetine, Dietary supplement, weight-loss products, natural extracts*

Abstract In recent years, many countries have reported problems with adulteration of hazardous chemicals in dietary supplements and weight-loss products made with natural extracts. Although marketed as natural and safe, such products are often found to contain hidden substances like Sibutramine and Fluoxetine. Sibutramine, once prescribed for obesity, was banned due to serious health risks, while Fluoxetine, an antidepressant, has also been used in weight management. The presence of these drugs in natural supplements poses significant dangers to unsuspecting consumers. This study aimed to detect Sibutramine and Fluoxetine in dietary supplements and weight-loss products containing natural extracts sold in Vientiane Capital. A total of 40 samples were randomly collected from markets and shops. Analysis was performed using HPLC-UV. Validation showed LOD/LOQ values of 0.18/0.55 µg/mL for Sibutramine and 0.19/0.59 µg/mL for Fluoxetine, with recovery of 98.14 to 99.75%. Among the samples, Sibutramine was detected in 7 (17.5%) at 39.73-66.60 µg/g, Fluoxetine in 5 (12.5%) at 71.43 - 206.75 µg/g, and both in 3 (7.5%). These findings confirm that adulteration remains a risk, underscoring the need for stronger regulation and monitoring to ensure consumer safety.

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Research Field Metabolomics

Title **Uncovering the Bioactive Potential of Malaysian Plants Through Metabolomics**

Keywords *Metabolomics, 1H-NMR, LCMS, Biological activity*

Abstract Metabolomics is a systemic “top-down” approach that directly reflects cellular physiological states, as it represents the most downstream layer in the omics hierarchy. Conventional standardization of herbal materials typically relies on detecting one or a few predetermined marker compounds using high-performance liquid chromatography (HPLC) or thin-layer chromatography (TLC). However, this strategy is limited, since selected markers may not represent bioactive constituents, and therapeutic effects often result from the synergistic action of multiple compounds. Metabolomics therefore offers a holistic platform for the standardization of herbal medicines and for elucidating the scientific rationale behind traditional practices. Liquid chromatography–mass spectrometry (LC-MS) metabolomics has emerged as a powerful tool due to its high sensitivity, broad metabolite coverage, and capacity for both targeted and untargeted analyses. It enables detection of trace metabolites and provides valuable structural information for biological interpretation. Complementarily, nuclear magnetic resonance (NMR) metabolomics offers rapid, reproducible, and non-destructive analysis with minimal sample preparation. Together, LC-MS and NMR provide a comprehensive strategy for metabolite profiling, authentication, and quality control of herbal medicines. This presentation highlights our recent findings and progress using integrated LC-MS– and NMR-based metabolomic approaches to evaluate the bioactive potential and ensure the reproducibility of Malaysian plants.

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Research Field AI for Drug Discovery

Title **Computer assisted discovery of novel nicotinamide phosphoribosyltransferase agonists to combat muscle atrophy**

Keywords *NAMPT, high-throughput docking, molecular dynamics, allosteric activator, muscle atrophy*

Abstract NAD^+ is a crucial cofactor for maintaining cellular homeostasis, and its level is strictly regulated by the rate-limiting enzyme NAMPT. Small molecule NAMPT agonists hold great potential to boost NAD^+ level, while only few agonists were available currently. Herein, we established a rapid screening workflow for NAMPT agonists by integrating molecular docking and molecular dynamics simulations. In brief, the high-throughput docking was firstly performed on 1.3 million compounds from the ZINC20 Lead-like subset, and the top 20 candidates were further evaluated by all-atom molecular dynamics simulations and MM/GBSA assessments, ultimately identifying 3,4-dihydro-1H-isoquinolin-2-yl-[4-(2H-tetrazol-5-yl)phenyl]methanone (DIPM) as the most potent NAMPT activator. DIPM binds stably to NAMPT with a binding free energy of -30.86 kcal/mol. Its binding sites are located far from the catalytic active center of NAMPT and do not interfere with the substrate channel, indicating that DIPM activates NAMPT through an allosteric mechanism. DIPM elevated intracellular NAD^+ levels with no obvious toxicity in C2C12 myotubes. In a dexamethasone-induced C2C12 myotube atrophy model, DIPM restored myotube diameter, decreased the expression of atrophy markers Atrogin-1 and MuRF1, and increased MyHC expression. As a potent, low-toxicity, non-competitive allosteric NAMPT agonist, DIPM represents a promising lead compound for treating conditions involving muscle wasting.

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Research Field Metabolism, Obesity and Diabetes

Title **Does salt matter in metabolism? Insights beyond CVD**

Keywords *Dietary salt, metabolism, energy balance, neuropeptide Y (NPY)*

Abstract Obesity is a global epidemic and is a multifactorial disease associated with an increased risk of serious conditions, including type 2 diabetes, cardiovascular disease (CVD) and certain cancers. It arises from an imbalance between energy intake and energy expenditure. Gaining a deeper understanding of how energy balance is regulated under health and disease is essential for developing better therapeutics for obesity, diabetes and their comorbidities. While much research has focused on how sugar and fat disrupt energy homeostasis, the role of dietary salt, a common yet often overlooked dietary factor, remains poorly understood. In this talk, I will present our recent findings on how high salt intake modulates energy balance, with a particular focus on the critical involvement of the hypothalamic neuropeptide Y (NPY) system.

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Research Field Metabolomics, Mass Spectrometry Imaging

Title **Advancing Metabolomics in Natural Products Science Through Spatial Mapping of Plant Nutraceuticals**

Keywords *Metabolomics, Natural Products, Spatial Mapping, Nutraceutical*

Abstract Metabolomics-driven strategies enable the identification and quantification of nutraceuticals in natural products research. Compared to conventional MS, matrix-assisted laser desorption/ionization time-of-flight mass spectrometry imaging (MALDI-MSI) has emerged as a powerful tool for the rapid and sensitive mapping of specialized metabolites directly from intact tissues. MALDI-MSI has been successfully applied to reveal the spatial arrangement of metabolites across diverse plant tissues and organs. Here, we present the MALDI-MSI analysis of naturally occurring compounds in three functional foods: *Zingiber officinale* (ginger) rhizome, *Ananas comosus* (pineapple) fruit, and *Theobroma cacao* (cacao) seed. Plant tissues were cryosectioned, mounted on MALDI plates, and coated with 2,5-dihydroxybenzoic acid (DHB) matrix. The workflow was enhanced with ion mobility spectrometry (MALDI-HDMS Imaging), which enabled drift time separation and improved metabolite annotation through reference standard comparisons. The MALDI-HDMS Imaging analysis provided spatiotemporal snapshots of nutraceuticals such as low-molecular-weight (LMW) phenolics, ligands, and alkaloids in plant tissue samples. Notably, this research investigates the first spatial mapping of a LMW ligand in ginger rhizome that may help decode its physiological role in metal chelation. These results highlight spatial metabolomics as a transformative approach for functional food research, providing new perspectives for nutraceutical discovery and accelerating innovation in natural products science.

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Research Field Organic Synthesis, Natural Product, Medicinal Chemistry

Title **Extending the Potential of the Naturally Abundant Substance Anticopalic Acid for Drug Discovery Applications**

Keywords *Anticopalic acid, Kaempferia elegans, Derivatives, Total synthesis, Drug Discovery, Biological Activity*

Abstract The use of naturally abundant substances in drug discovery has long been explored, as they provide versatile molecular scaffolds for generating structurally diverse derivatives, serve as synthetic precursors for complex natural products, and enable access to rare metabolites in sufficient quantities for biological evaluation. Here, we report recent progress using anticopalic acid (ACP), a bicyclic diterpenoid obtained in high abundance from the rhizome extract of *Kaempferia elegans*, a cultivable plant in the ginger family. The carboxylic acid functionality of ACP was exploited to synthesize a series of derivatives. Evaluation of their anticancer activity against a panel of cell lines identified compounds with potent cytotoxic effects against leukemia cell lines HL-60 and MOLT-3, and a derivative that induced non-apoptotic programmed cell death in the triple-negative breast cancer cell line MDA-MB-231. In addition, ACP has been employed as a chiral pool starting material, enabling the total synthesis of complex meroterpenoid natural products. This presentation highlights the synthesis of habiterpenol from ACP, underscoring its potential as both a renewable precursor and a versatile scaffold for drug discovery applications.

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Research Field catur@ugm.ac.id

Title **Opportunities and Challenges of Collaborating with Industry in Developing Marigold as a Food Colorant**

Keywords *Marigold, Natural Food Colorant, Circular Economy, Institutional Economics, Inclusive Development*

Abstract

The global demand for natural food colorants continues to rise, driven by health concerns, restrictions on synthetic dyes, and the shift toward sustainable production. Marigold (*Tagetes erecta*) offers unique potential as a source of lutein and carotenoids, combining vibrant color with health benefits. In Indonesia, research by Universitas Gadjah Mada's Indonesia Natural Dye Institute (INDI UGM) and partnerships with PT Rumah Atsiri Indonesia (PT RAI) have transformed marigold from discarded waste into a promising food-grade ingredient. Opportunities include technological advances in extraction and stabilization, integration into circular economy models, and diversification of farmer and cooperative incomes. Moreover, women and youth can play central roles in processing and marketing, aligning with SDG 5 on gender equality.

However, challenges remain in ensuring pigment stability, designing effective contractual mechanisms, achieving cost competitiveness, and securing regulatory approvals from BPOM and international agencies. Institutional economics highlights the importance of contracts in reducing transaction costs, while the sustainable livelihoods framework demonstrates marigold's contribution to financial, human, and social capital. Drawing lessons from mangrove-based dye enterprises, marigold exemplifies how science–industry–community collaboration can create inclusive green growth. With robust governance and certification, marigold can become a strategic eco-friendly alternative to synthetic dyes and strengthen Indonesia's sustainability branding.

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Research Field Drug discovery and development for the treatments of diseases related to the central nervous system, reproductive health, and antivirals; Design and evaluation of green and sustainable route of synthesis for industrial application, based on the concept of “Control from Root Design”

Title **Integrated system can accelerate drug research and tech transferring**

Keywords *Integrated System, VV116, Xiannuoxin, Onvita, Control from Root Design*

Abstract

The ultimate goals of scientific research on medicine is to innovate advanced technologies and drugs that are beneficial to humanity and society. Integrated drug R&D and manufacturing system can accelerate operations across the entire process with high quality and efficiency, and enables the fast research, tech transferring and manufacturing of drugs and drug candidates. The system also can reserve candidate drugs and technologies in case of of emergency situations such as emerging and sudden spreading of viral infections.

Among the drug discovery projects from this system, VV116 (Mindvy®) and VV934 (Xiannuoxin®) are currently the only two regularly approved antiviral agents for COVID-19 in China, and VV116 also approved in Uzbekistan; TPN171 (Onvita®) were approved for the treatment of male erectile dysfunction in both Uzbekistan and China; The phase II clinical trial of VV116 for the treatment of respiratory syncytial virus (RSV) infection was completed.

The system also established an innovation platform for generating green and sustainable API production technology underpinned by a “Control from Root Design” strategy. This strategy prioritizes the design and evaluation of the reactions and synthetic routes from the very beginning of a project under the principle of green chemistry with the concepts of safety, environmental protection, operational simplicity, and low cost, etc.

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Research Field Horticulture, Vegetable Science, Aromatic/Medicinal Plants, Greenhouse Crops and Hydroponics, Soil and Substrate/Growing Media Evaluation, Abiotic Stress, Postharvest Science and Preservation

Title **Diversity of Cardiac Glycosides in Digitalis Taxa from the Balkan Peninsula: Phylogenetic Insights into Chemical Variation**

Keywords *Phylogeny, DNA barcoding, Metabolomics, Foxgloves, Cardiac glycosides*

Abstract

Among foxgloves (genus *Digitalis*, family Plantaginaceae), *D. purpurea L.* and *D. lanata* Ehrh. have well-documented history of medicinal use, particularly in the treatment of cardiovascular issues, owing to cardiac glycosides (CGs) they produce. In contrast, other species within the genus remain largely unexplored in terms of their chemical composition, thus being poorly exploited. This study aimed to genetically and chemically characterize five Digitalis taxa naturally growing across the Balkan Peninsula—one of the primary centers of the genus’ diversity—in order to establish a foundation for their potential future utilization.

Phylogeny, reconstructed based on plastid markers (*matK,* trnL-F, rbcL and *psbA-trn*H) and nuclear ITS regions, clustered the representatives of the sect. Globiflorae (*D. lanata, D. laevigata* Waldst. & Kit., and D. *ferruginea* L.) separately from the members of the sect. *Macranthae* (*D. viridiflora Lindl.* and *D. grandiflora Mill.*). Composition of CGs in five Digitalis species, was found highly conserved at the intra- and inter-species levels. Representatives of the sect. *Globiflorae* are recognized as high producers of CGs, with *D. lanata* being rich in digoxin, lanatoside C, and deslanoside. *D. ferruginea* leaves are abundant in tigonin, while *D. laevigata* is rich in furostanol derivatives. Phylogenetically distinct *D. grandiflora*, on the other hand, is highlighted as a low producer of CGs, possessing considerable amounts of digoxigenin di-deoxyhexoside. Projecting the diversity of CGs in Digitalis species within a phylogenetic framework offers novel insights into the chemical evolution of the genus. This lays the groundwork for future exploration of currently unknown molecular aspects of chemical diversity using advanced omics technologies. Such an approach holds promise for developing alternative strategies for the biotechnological production of bioactive CGs.

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Research Field Chemistry of Natural Products

Title **Natural molecules for industrial application**

Keywords *Natural compounds, Functional agents, industrial application, sustainability, circular economy*

Abstract

Distinct classes of compounds such as phenolics, quinones, organic acids, sterols and others, reported as strong bioactive agents, can be found in natural matrices, and applied in different industrial segments. Considering the global agendas, and in line with the strategy to promote circular economy, these molecules can also be extracted from raw material considered as biowaste, being possible to obtain highly valuable compounds and re-include them in the value chain. The Food&Biotech research group inserted in CIMO-IPB (Portugal) is dedicated to the extraction optimization, stabilization and application of natural compounds in different industries such as the food, the wine and vine, and the textile ones. The main applications include preservation, fungicidal, biostimulant properties, hypocholesterolemic activities, coloring pigments from fungi, within the financed projects: ChestWine, NatFoodCoating, Vitex, Subsus, Mush4Chol, Forswap, and Textblustyle. These projects contribute to the development of naturalalternatives to artificial ones, promoting health, sustainability and circular economy..

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Research Field Synthesis of heterocycles, Domino reactions, Stereochemistry

Title **Synthesis and antiproliferative activity of novel condensed heterocyclic ring systems**

Keywords *Heterocycles, antiproliferative, Diels-Alder reaction*

Abstract

While heterocyclic derivatives constitute a significant part of both natural products and API-s, only a small portion of their diversity is being utilized. Only 351 unique ring systems are present in drug molecules, and 6 new ring systems are introduced annually on average.

To increase chemical diversity, the synthesis of new ring structures, and the identification of their bioactivities is essential. To obtain complex heterocyclic ring systems, domino reactions were utilized, using five and six membered heterocycles as dienophiles in cycloaddition reactions. Using oxa-, aza- and thiadienes, the corresponding *O*-, *N*- and S-heterocyclic moieties were prepared in domino condensation-intramolecular cycloaddition reactions. Apart from the various hetero Diels-Alder cyclizations, alternative cyclization mechanisms were identified and studied. Altogether, 21 novel heterocyclic ring systems were identified, with over 200 representatives.

The antiproliferative effect of these compounds were tested on various human cancer cell lines, and a number of them showed promising in vitro effects with low micromolar IC50 values, even on aggressive cell lines like the U87 glioblastoma.

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Research Field Natural products, High pressure extraction

Title **Loading Eugenol In Polymethylmethacrylate Discs Using Dense Carbon Dioxide**

Keywords *Subcritical CO2, Eugenol, PMMA*

Abstract

PolyMethylMethAcrylate (PMMA) dental discs are used in computer aided manufacturing process of milling removeable dental protheses. Such provisional or permanent protheses are often provided to patients after placing dental implants when the risk of inflammation is high.

Carbon dioxide is reported to solubilize well in the PMMA, depending on its temperature and pressure, but up to now, no data have been reported on loading substances into PMMA.

The aim of this work is to study the possibility of eugenol loading into the PMMA dental discs via the high-pressure CO2 technique. The solubility of CO2 in PMMA was measured in a magnetic suspension balance (MSB–RUBOTHERM). Thermogravimetric analysis (STA 449 Jupiter, NETZSCH GB) was used to measure the eugenol loading of PMMA.

The solubilities of CO2 in PMMA disc were measured at temperatures of 301, 308 and 323 K and at pressures of 7, 8, 10, 16, 20 and 30 MPa, and the CO2 was released over 2 hours.

Eugenol loading of PMMA dental discs is possible through high pressure CO2 technique without any visual change in the form and shade, reaching the maximum value of 20 wt% at 338 K and the density of CO_2 of 375 g/cm^3..

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Research Field Remote Sensing and Smart Agriculture for Natural Products

Title **Integrating Spectroscopic Approach for Juniper and Blueberry Natural Resource Assessment in North Macedonia: Integrating Remote Sensing with GIS and Ground-Based Data**

Keywords *Juniperus communis; Vaccinium myrtillus; Multispectral imaging; Sustainable resource management*

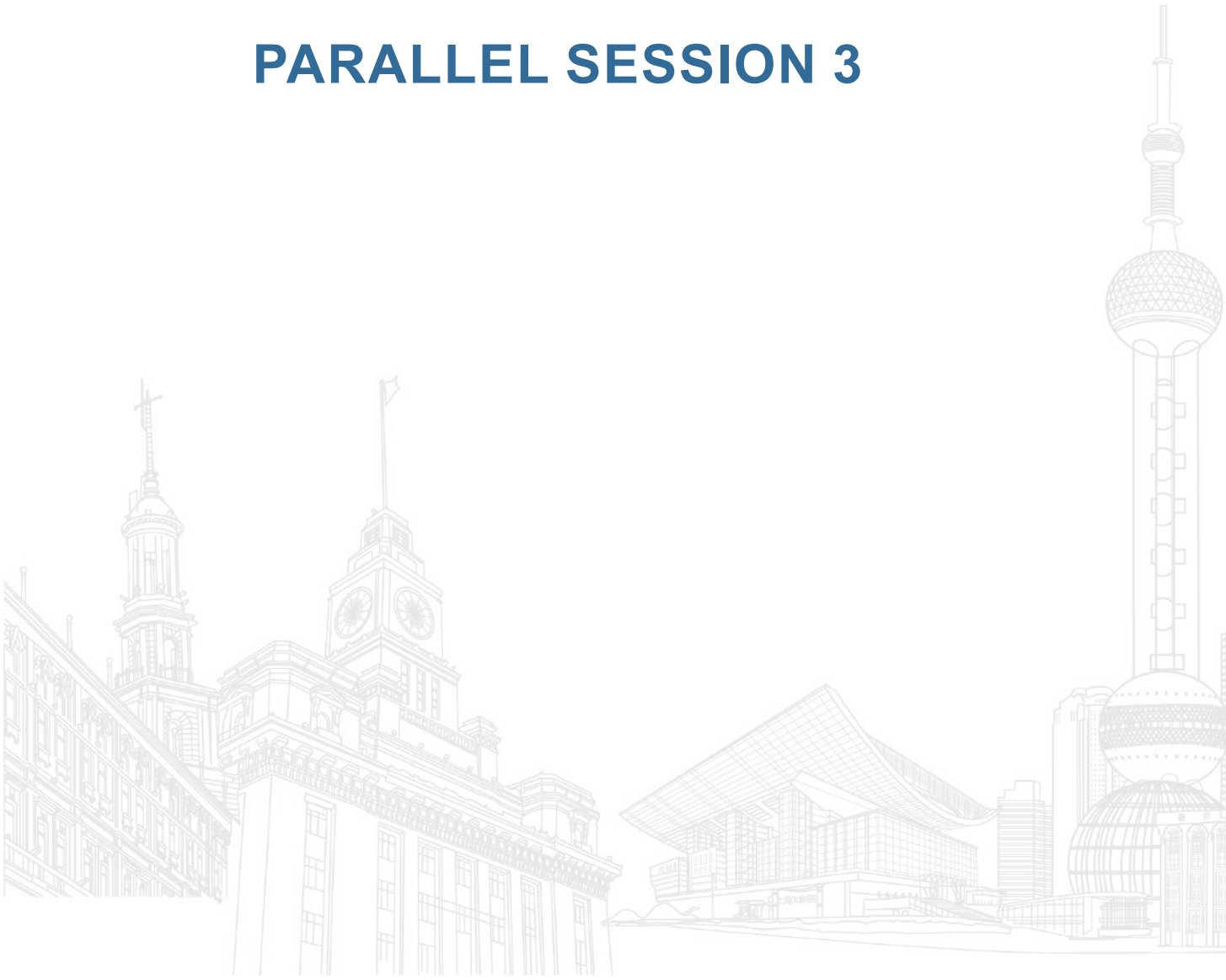
Abstract

Wild-growing Juniper (*Juniperus communis*) and blueberries (*Vaccinium myrtillus* L. and *Vaccinium uliginosum* L.) are recognized as valuable natural resources in North Macedonia, with significant ecological, nutritional, and economic importance. However, underdeveloped collection, licensing and monitoring systems result in unsustainable use.

In this study, an assessment of juniper and blueberry resources was conducted by applying integrated multiple approach. Drone-based remote sensing with multispectral and LiDAR cameras were utilized to capture high-resolution vegetation indices, and 3D terrain models. The remote sensing data were integrated into Geographic Information Systems (GIS) and combined with satellite imagery for regional-scale analysis. Ground truthing was carried out through field transect surveys, enabling validation of remote sensing and GIS outputs. Machine learning algorithms were applied for automated classification and prediction of blueberry distribution and biomass across diverse ecosystems.

The integration of drone-based spectral technologies with ground validation establishes a scalable methodology for accurate resource assessment, biodiversity monitoring, and ecosystem service evaluation. By providing a reliable knowledge base for sustainable harvesting, conservation planning, and value-chain development, this work demonstrates how smart integrated spectral tools can transform underutilized forest resources into drivers of green innovation.

PARALLEL SESSION 3



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Research Field Pharmaceutical Chemistry

Title **Creation of herbal preparations based on Uzbekistan medicinal plants according to the recipes of Abu Ali Ibn Sina using innovative technologies**

Keywords *Abu Ali Ibn Sina, herbal preparations, phytopharmacology, traditional medicine, innovative extraction technologies, standardization, drug development*

Abstract

Uzbekistan's flora, comprising more than 4,500 vascular plant species, represents a significant source of biologically active compounds, with over 500 species traditionally used in medicine. Many were systematically described by Abu Ali Ibn Sina (Avicenna) in The Canon of Medicine, which remains a cornerstone of herbal therapeutics. Despite this rich heritage, the integration of these plants into standardized modern phytopreparations remains limited.

This study aims to develop herbal preparations from indigenous medicinal plants based on Ibn Sina's formulations, applying innovative technologies to ensure reproducibility, efficacy, and safety. The research involves ethnopharmacological selection of species, phytochemical profiling using HPLC and LC-MS, and optimization of extraction by eco-friendly methods such as supercritical CO_2 and ultrasound-assisted extraction. Biological activities, including antioxidant, antimicrobial, and anti-inflammatory properties, are assessed through standardized in vitro assays, while cytotoxicity and safety evaluations follow international guidelines.

Preliminary findings highlight species such as *Gentiana Olivieri*, *Salbia Officinalis*, *Glycyrrhiza glabra* and *Ricinus communis* which demonstrate synergistic antioxidant and antimicrobial activity. The results confirm that combining Avicenna's traditional medical concepts with modern pharmaceutical technologies enables the creation of effective and culturally relevant herbal products. This approach supports both the preservation of medical heritage and the advancement of innovative phytopharmaceuticals for global application.

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Research Field Bioorganic Chemistry, Pharmaceutical Chemistry

Title **Polysaccharide-based macromolecular systems for cancer drug delivery**

Keywords *Polysaccharides, hyaluronan, galactomannan, tumor, antitumor activity, drug delivery*

Abstract

The incidence of cancer and its associated mortality are increasing worldwide. Today, chemotherapeutic drugs are widely used as an important element of treatment methods and in combination with other types of drugs or methods, such as surgery and radiotherapy, in order to increase therapeutic effectiveness. However, the main issues with the use of these cytotoxic drugs are their high toxicity, poor absorption, short half-life in the body, and serious side effects.

In this regard, polysaccharides (e.g., galacturonans, hyaluronans, and galactomannans are natural ligands of proteins highly expressed by cancer cells. The study of these polysaccharides derivatized with cytotoxic compounds may allow the development of safer and effective materials against cancer or postsurgical cancer recurrence.

In this direction, we developed macromolecular systems and biomaterials based on the ligand polysaccharide matrices for safer and specific delivery of the toxic drugs against cancer.

The results indicated that galactose residues and sulfate groups in the polysaccharide chain play an important role in the tumor-specific drug delivery of macromolecular systems. The polysaccharide-based macromolecular systems demonstrated less toxic and more effective antitumor properties than the free drugs. Preliminary findings highlight that the polysaccharide-based materials developed can be promising for cancer drug delivery.

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Research Field Natural Product Chemistry

Title **Biosynthsis of β-NAD-derived natural products**

Abstract

β-Nicotinamide adenine dinucleotide (β-NAD) is a pivotal metabolite for all living organisms and functions as a primary electron acceptor and carrier during central catabolic processes. In this study, we demonstrate the first example that β-NAD functions as a building block for the assembly of potent and structurally intriguing bacterial secondary metabolites, such as the anti-cancer compound altemicidin and the Ile-tRNA inhibitor SB-203208 from Streptomyces. Our biochemical analyses identified a PLP-dependent enzyme (SbzP) as a novel family of enzyme catalyzing the scaffold formation via (3+2)-annulation reaction at the pyridinium moiety of β-NAD, utilizing S-adenosyl methionine (SAM) as a co-substrate (Figure). Furthermore, we clarified the structural basis and reaction mechanism of the (3+2)-annulation reaction between β-NAD and SAM, based on cryo-electron microscopy analysis, biophysical analysis, and computational analysis. In this presentation, the enzymatic synthesis of unnatural β-NAD derived compounds and identification of the products from the SbzP homolog gene cluster will be also presented.

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Research Field Pharmaceutical technology and Cosmetology

Title **The distinctiveness of (pre)formulation studies with natural products**

Keywords *Low energy (LE)- and high energy (HE)-nanoemulsion systems, curcumin, essential oils, red raspberry seed oil, natural surfactants, eucalyptol, pinene, skin delivery, parenteral delivery, PEGylated nanoemulsion*

Abstract

In this overview, low and high energy (PEG-ylated) nanoemulsions (LE-NEs and HE-NEs) are presented in more detail as carriers for natural active ingredients: Curcumin (CU) and Red Raspberry Seed Oil (RRO) for: i) parenteral administration of CU (0.75 mg/ml), dermal administration (CU 3 mg/ml) in combination with penetration enhancers of monoterpenes (pinene (PIN) and eucalpitol (EUC) in medium chain trielicerides (MCT)) resp., and for cosmetic antioxidant care (RRO in LE-NEs stabilised with natural surfactants).

Spontaneous emulsification was the preparation method for curcumin-loaded LE-NEs, while a slightly modified phase inversion composition (PIC) method was used for cosmetic LE-NEs. PEGylated HE-NEs were prepared by high pressure homogenisation (HPH) varying PEG2000-DSPE and PEG5000-DPPE at concentrations of 0.1/0.3/0.6 % (m/m).

The results obtained showed that the CU-LE-NEs had an average droplet diameter of 102 nm to 132 nm, with the monoterpenes being significantly smaller compared to the MCT formulation.

This finding was investigated in detail using electron paramagnetic resonance spectroscopy, which proved that the presence of monoterpenes altered the interfacial environment of the nanoemulsions, leading to a reduction in droplet size. The CU-loaded HE-NEs prepared with HPH exhibited an average droplet size of about 105 nm, a polydispersity index <0.15, a zeta potential of ±40 mV and an acceptable osmolality of about 550 mOsm/kg. In addition, the results of the pilot pharmacokinetic study showed that the PEGylated HE-NEs improved the CU plasma residence time of 20 minutes after intravenous administration compared to the non-PEGylated NE (2-fold higher) or the CU solution (3-fold higher). Finally, Raman spectroscopy for the cosmetic NEs showed that the cold-pressed, unrefined, organic RRO with 6.62% saturated fatty acids and 92.25% unsaturated fatty acids was optimal for the LE-NEs prepared by the PIC method.

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Research Field Pharmacology

Title **$GABA_A$ receptors in drug discovery of natural products**

Keywords *inhibitory neurotransmission; $GABA_A$ receptor subtype-selectivity; positive allosteric modulation; negative allosteric modulation*

Abstract

More than half a century ago, natural products played a crucial role in elucidating the role of γ-aminobutyric acid (GABA) in regulating chloride flux across plasma membranes in nervous tissues. While muscimol and bicuculline act at the orthosteric site of the vast majority of $GABA_A$ receptors as agonist and antagonist, respectively, picrotoxin is a channel blocker at all receptors of this family. On the other hand, today's widely used drugs and various psychotropic substances of abuse act at the benzodiazepine site and other allosteric sites, which are thus more druggable than the orthosteric site itself. It is intriguing that data on the binding and electrophysiological activity of natural products at allosteric sites of $GABA_A$ receptors are sparse and fragmentary at best. In general, those natural products that have been studied to some degree for their modulatory action at the benzodiazepine binding site show modest potency and usually have additional targets as likely substrates for their pharmacological activity. Nonetheless, recent breakthroughs in structural biology, coupled with the abundance of receptor subpopulations and binding sites, herald a promising future for research to select natural products with selective action at $GABA_A$ receptors suitable for psychiatric and neurological indications with currently unmet needs.

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Research Field Natural products-bioactivity and molecular mechanism study

Title **Antitumor activity of natural daphnane diterpenoids in EGFR-TKI resistant NSCLC cells**

Keywords *Daphne genkwa, daphne diterpenoids, AXL, EGFR-TKI resistance*

Abstract

Although the first generation of epidermal growth factor receptor (EGFR) tyrosine kinase inhibitors (TKIs), such as gefitinib and erlotinib, have improved prognosis for NSCLC patients, their long-term efficacy is questionable due to the emergence of acquired resistance. A third generation EGFR-TKI osimertinib, a specific inhibitor of mutant EGFR, has been approved for clinical use. However, several resistant mechanisms of osimertinib were subsequently reported from patients' samples. AXL, a receptor tyrosine kinase, can promote many downstream signaling pathways regulating cell survival, growth, EMT, and metastasis in cancer cells. In our study, we demonstrated the involvement of AXL in the acquired resistance to gefitinib and osimertinib of EGFR-mutant NSCLC cells, and showed the combination effect of an AXL degrader and EGFR-TKIs to overcome EGFR-TKIs-driven resistance in EGFR-mutant NSCLC cells. Yuanhuadine (YD), a natural antitumor agent from Daphne *genkwa* (Thymelaceae), effectively suppressed the expression of AXL by accelerating protein degradation. YD combined with gefitinib or osimertinib synergistically inhibited the growth of resistant cells in *vitro* and suppressed tumor growth in *vivo* animal model. These findings suggest that the combination of YD with either gefitinib or osimertinib is a potentially effective treatment strategy for overcoming acquired resistance in NSCLC by targeting AXL degradation.

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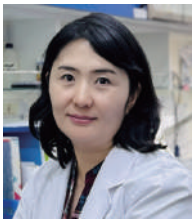
Research Field Chemistry of Natural Compounds, Pharmaceutics

Title **Advanced delivery of natural product compounds**

Keywords *Drug delivery, targeting delivery, formulation, immunoregulation*

Abstract Many natural product compounds are poorly water soluble and unstable. These unfavorable properties create big challenges for drug development. Our strategy is to apply advanced drug delivery technology (e.g., liposomal technology, smart hydrogels, microspheres, transdermal technology) to improve their druggability and therapeutic efficacy.



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Research Field Natural Product Chemistry, Pharmacology

Title **Cytotoxicity of 114 Mongolian plant extracts on liver, colon, breast and cervix cancer cell lines**

Keywords *Medicinal plant, cytotoxicity, cancer cell line, ethanolic extract*

Abstract

This research aims to build a library of extracts from Mongolian medicinal plants by screening them for anti-proliferative effects against various cancer cell lines. A total of 114 Mongolian plant species were subjected to cytotoxicity screening against liver (HepG2), colon (HCT116), breast (MCF7), and cervical (HeLa) cancer cell lines. Among them, ethanolic extracts of *Androsace incana*, *Artemisia rutifolia*, *Saussurea amara*, and *Inula salsoloides* exhibited remarkable cytotoxicity, with IC 50 values below 1.5 µg/mL against at least 2 tested cell lines when treated for 48 hours. *Erysimum flavum*, *Juniperus sibirica*, and *Stellaria dichotoma* demonstrated selective cytotoxicity against specific cancer cell lines. Extracts from 23 plant species, such as *Artemisia xerophytica*, *Ajania trifida*, *Melandrium brachypetalum*, *Brachanthemum mongolicum*, and *Rhinanthus songaricus*, showed moderate toxicity. Further research on the phytochemicals and biological activities of these species is crucial for a deeper understanding and potential applications. These screening results of the cytotoxic effects of numerous Mongolian plants could establish a foundational dataset for subsequent comprehensive studies on the screened plants.

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Research Field Natural Product Chemistry

Title **Polyoxygenated Cyclohex(a/e)ne Diterpene Esters identified in Thai *Kaempferia* subgen. *Protanthium***

Keywords *Kaempferia albiflora, Kaempferia aurora, Zingiberaceae, Cyclohex(a/e)ne diterpene esters, Albiflorenes, Auroranes, Antibacterial acitivty, Anti-inflammatory activity*

Abstract This study reports the isolation and structural elucidation of 19 compounds from the whole plants and rhizomes of two *Kaempferia* species. Twelve polyoxygenated cyclohex(a/e)ne diterpene esters, designated albiflorenes A–L, were obtained from the whole plants of *Kaempferia albiflora*, while seven related esters, designed auroranes A–G, were isolated from the rhizomes of *Kaempferia* aurora. These compounds present an unusual carbon skeleton in which a polyoxygenated cyclohex(a/e)ne derivatives is bound to either an isopimaric or abietic acid diterpenoid. Their structures and relative stereochemistry were determined by extensive spectroscopic analysis, and absolute configurations were assigned using NMR-based DP4+ calculations for some compounds and by ECD-TDDFT comparison for others. To our knowledge, this study represents the first report of these compounds from *Kaempferia* subgenus *Prothanthium* (family Zingiberaceae). Among them, albiflorene C showed antibacterial activity against Bacillus cereus, with MIC and MBC values of 3.13 and 6.25 μg/mL, respectively. Auroranes C and D displayed notable NO inhibitory activity, with IC50 values of 5.2 and 4.8 μM, respectively.


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Research Field Development of natural drugs

Title **Artemisinin full industry chain research and industrialization**

Keywords *Artemisinin;The entire industry chain; Research and industrialization*

Abstract Artemisinin is a specific drug for the treatment of malaria. Our team have carried out a lot of research on Artemisinia annua cultivation, artemisinin extraction and artemisinin derivative synthesis, forming a complete industry chain. In terms of production process, we have studied the green extraction process of artemisinin, high-efficiency synthesis of artemisinin derivatives, reducing the manufacturing cost. We also established production bases with annual capacity of 200 tons of artemisinin and artemisinin derivatives. In terms of cultivation, we have selected varieties of Artemisia annua (artemisinin content about 3%) through the application of heavy carbon ion irradiation, which guarantees the application artemisinin drugs at home and abroad.

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Research Field Floriculture; Under-exploded and endemic species; Aromatic/Medicinal Plants; Essential oil analysis and biocidal activity; Evaluation of natural products; Development of strategies for plant nutrition and response to abiotic stress; Hydroponics

Title **Domestication and Phytochemical Potential of Sideritis cypria: A Strategy for Conservation and Climate-Resilient Agriculture**

Keywords *Wild plant species, biological properties, mineral needs, hydroponics, climate change*

Abstract *Sideritis cypria*, an endemic and endangered species of Cyprus, represents a significant component of the island's botanical heritage and Mediterranean biodiversity. Adapted to extreme conditions (prolonged drought, high temperatures), it represents a promising candidate for climate-resilient agriculture. The species possesses notable antioxidant, antimicrobial, and anticancer properties, giving it both medicinal and commercial importance. However, natural populations are increasingly threatened by habitat loss, overharvesting, and climate change. Introducing S. *cypria* into cultivation systems is therefore essential for both conservation and sustainable exploitation. Cultivation would reduce pressure on wild populations while providing a stable, high-quality supply of raw material for standardized phytochemical and pharmacological applications. This research evaluated the nutritional and phytochemical profile of cultivated S. *cypria*, including essential oil composition, biological activities and mineral content. Findings confirmed that cultivated plants maintained a comparable phytochemical profile to wild populations, indicating that domestication does not compromise quality. Compared with other herbs (mint, oregano, thyme, sage) S. *cypria* was richer in minerals and demonstrated stronger antimicrobial and anticancer activity. Hydroponic cultivation was also investigated assessing the impact of nitrogen, potassium, and phosphorus to optimize fertilization strategies. Domestication thus ensures conservation, strengthens agroecosystem resilience and secures consistent, high quality material for scientific and commercial use.

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Research Field Natural Product Chemistry

Title **Tailoring nutrient needs for selected Medicinal and Aromatic plants and responses to climate changes challenges**

Keywords *nutrient solution, quality, antioxidants, essential oil, Lavandula angustifolia, Mentha spicata, soilless culture*

Abstract

Medicinal and Aromatic plants (MAPs) are exposed to climate change challenges and adapted mechanisms to withstand stress conditions. Drought and saline stress affect negatively plant growth and yield but might enhance several quality-attributes. Lavandula angustifolia and Salvia fruticosa plants decreased plant growth but enhanced essential oils (EOs) insecticidal properties under drought stress. Spearmint (Mentha spicata) decreased growth but increased phenolics and antioxidant capacity, following oxidative stress under salinity (0-25-50-100 mM NaCl). Carvone, EO main component, was decreased at high saline levels, whereas foliar K enrichment alleviated the saline-stress conditions, and brought carvone to the control levels.

Considering the various metabolic functions of minerals (N, K, P) and the lack of information on the mineral needs in MAPs, each species requires its own nutrient management. To that direction, hydroponics is a tool to fully control plant development for stable and reproducible growth, minerals, antioxidants and EO constituents. For example, spearmint biomass increased in N (200 mg/L) and K (325 mg/L) levels, but increased carvone (high oil quality) was observed in N ≤200 mg/L. Potassium ≤325 mg/L increased EO antioxidant and antibacterial activities. Custom-made recipes for each plant species can be recommended depending on the production needs (food, pharmaceuticals, cosmetics, plant protection).

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Research Field Microbiology

Title ***In vitro* evaluation of supernatants of probiotic microorganisms against the causative agent of Lyme borreliosis**

Keywords *Lyme borreliosis, Borrelia, susceptibility, supernatants, probiotic microorganisms, MICs*

Abstract

Lyme borreliosis (LB) is a multisystem disorder caused by bacteria from the *Borrelia burgdorferi* sensu lato complex, transmitted to humans through the bite of I*xodes* spp. ticks. Standard treatment relies on prolonged antibiotic therapy, while no topical product is currently available for prophylactic use following a tick bite.

The aim of the study was to investigate in vitro effects of probiotic supernatants derived from the microorganisms Saccharomyces *boulardii* and *Lactiplantibacillus plantarum* on the growth and motility of Borrelia afzelii, the most common cause of LB in Europe.

The susceptibility of B. *afzelli* to probiotic supernatants was assessed using a modified broth microdilution method adapted for *Borrelia*. Minimum inhibitory concentrations (MICs) were determined by evaluating both the number and motility of *Borrelia* cells after 72 hours of incubation with the probiotic supernatants under anaerobic conditions, compared to a positive control consisting of untreated B. *afzelii* culture.

The median MIC values were found to be 12.5% for the S. *boulardii* supernatant and 6% for the L. *plantarum* supernatant, demonstrating that both are effective in the eradication of the causative agent of LB.

These results support further investigation into the molecular mechanisms underlying the probiotic microorganisms activity against *Borrelia* species.

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Research Field Chemistry of Natural Compounds

Title **Integrating Chemical Ecology and Bio-Entrepreneurship in Drug Discovery**

Abstract

The antioxidant potential of plants is attributed to secondary metabolites that neutralize reactive oxygen and nitrogen species generated by metabolism and environmental stressors. Despite the widespread use of *Urtica dioica L.* (stinging nettle), data on the antioxidant capacity of Montenegrin populations remain scarce. We quantified bioactive constituents and antioxidant activity in leaves collected at two ecologically distinct sites, Herceg Novi (south) and Pljevlja (north; n = 8 per site). Extractions employed maceration, Soxhlet, and ultrasonication with methanol, ethyl acetate, or water. Total phenolics, flavonoids, and tannins were measured; antioxidant activity was assessed by DPPH, FRAP, and ABTS.

Pljevlja samples exhibited higher total phenolics and ABTS inhibition, whereas Herceg Novi had greater flavonoid and tannin contents; FRAP values were comparable between sites. Under maceration, extraction efficiency followed methanol ≥ ethyl acetate □ water. Ultrasonication generally reduced DPPH IC_{50} relative to maceration, most notably in water, while Soxhlet yielded good results in a solvent-dependent manner. Although water macerates were consistently weakest, water–ultrasonication in Pljevlja produced the lowest IC_{50}, consistent with ultrasound-enhanced recovery of polar phenolics. ABTS trends mirrored total phenolics, whereas FRAP more closely reflected flavonoids/tannins. These results guide solvent–method selection for the valorization of Montenegrin nettle in food and nutraceutical applications.

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Research Field Natural Products

Title **Chemical Investigation of Commiphora and Boswellia Resins**

Keywords *Resins, Polygamatin Lignan, Boswellia, Commiphora*

Abstract

Ethiopia is an important global source of resin producing plants, especially species from the genera *Boswellia* and *Commiphora* (which produce frankincense and myrrh, respectively), as well as Acacia (which provides gum arabic). These species are widely spread across the country's dryland ecosystems, particularly in the Borana zone and the nearby Somali region. This area has a high diversity of these valuable species, making it a key region for the production of oleo-gum resins used in many industries. Chemically, resins are complex mixtures of volatile and nonvolatile terpenoid and phenolic secondary metabolites.

As part of our ongoing research to identify novel compounds from *C. erlangeriana*, we have isolated additional known and new compounds from both polar and non-polar fractions. These include polygamatin type aryltetralin lignans, a limonoid type triterpene, and a unique lignan featuring a seven membered ring lactone.

Furthermore, we conducted a phytochemical investigation of *C. sphaerocarpa*, an adulterant of commercially traded myrrh, and isolated several known bioactive sesquiterpene lactones. We also analyzed the resin of B. *neglecta*, identifying known triterpenes, including canaric acid, epi-α-amyrin, α-amyrone, β-amyrone, lupenone, lupeol, epi-lupeol, and β-Boswellic acid in large quantities.

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