Phytochemistry for a Sustainable Future: Bridging Nature, Innovation, and Health

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SPECIAL TALK

Computational Mass Spectrometry: Toward Discovery and Functional Metabolomics in Phytochemical Research

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Structural annotation of unknown metabolites has long been regarded as the central bottleneck of mass spectrometry (MS)-based untargeted metabolomics—a challenge that has persisted for over two decades. Recent advances in computational mass spectrometry, however, are dramatically improving annotation rates across diverse application domains. By decomposing complex metabolite mixtures into structural, substructural, and chemical class information, these tools enable not only the putative identification of key biomarker features but also the generation of mechanistically grounded hypotheses directly from annotation data.[1,2] Specialized metabolites, also known as natural products, exhibit immense chemical diversity shaped by the long course of evolution. Qualitative metabolomics, empowered by computational mass spectrometry, can offer insights into a wide range of questions surrounding natural products, including their biosynthesis, ecological function, and detoxification. In this presentation, I will highlight how state-of-the-art computational MS approaches can guide us toward causative hypotheses concerning plant specialized metabolites, drawing on two studies from my group. In the first case, we characterized the enzymatic function of a fungal UDP-glycosyltransferase with substrate promiscuity, where MS-based functional metabolomics played a key role in defining its catalytic activity.[3] In the second, I will describe our recent discovery of an evolutionary remodelling of the glucosinolate defence system in Brassicaceae, arising as a counter-counteradaptation against insect herbivores. Together, these cases illustrate how computational MS paves the way toward both discovery and functional metabolomics.

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INVITED LECTURES

Molecular Derivatization of Plant-Derived Compounds to Reverse Drug Resistance in Cancer

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Cancer drug resistance remains a major barrier to successful chemotherapy, contributing to treatment failure and tumor relapse. Plant-derived compounds are valuable sources of structurally diverse and biologically relevant scaffolds for the development of new anticancer agents. Molecular derivatization of these scaffolds offers a powerful strategy to expand chemical space and generate analogues with improved or complementary biological profiles.

Our recent studies highlight the relevance of this approach in anticancer drug discovery. By exploring diverse plant-derived scaffolds, including diterpenes, alkaloids, and flavonoids [1–5], targeted semi-synthetic modifications have enabled the generation of new derivatives with anticancer potential. These studies reinforce the value of natural product-derived compounds as starting points for the development of candidates against drug-resistant cancer phenotypes.

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Natural Phenylpropanoids, Phytocannabinoids, and Semisynthetic Derivatives as Modulators of the Aryl Hydrocarbon Receptor

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The aryl hydrocarbon receptor (AhR) is a ligand-activated transcription factor that regulates xenobiotic metabolism, immune responses, epithelial barrier function, and cellular homeostasis, making it an attractive pharmacological target [1]. While several naturally occurring phytochemicals have been identified as AhR ligands, the structural features governing receptor activation remain incompletely understood. In the present study, structurally diverse natural phenolic compounds, including coumarin derivatives, phenylpropanoids, phytocannabinoid cannbigerol (CBG) and a series of related semisynthetic derivatives, were evaluated to define the influence of specific chemical modifications on AhR activation. Natural compounds and newly synthesized mono- and disubstituted CBG derivatives, obtained through selective etherification and acylation of the phenolic hydroxyl groups, were prepared in high purity and assessed using an AhR-responsive luciferase reporter assay. The different classes of compounds exhibited distinct activation profiles, demonstrating that both the molecular scaffold and the nature, position, and degree of substitution critically influence receptor recognition and signaling. Among the natural products, selected oxyprenylated phenylpropanoids and coumarin derivatives displayed appreciable AhR agonistic activity, confirming the importance of lipophilic prenyl-type substituents. Phytocannabinoids also activated AhR, although with different potencies, while semisynthetic CBG derivatives showed marked variations in activity depending on the substitution pattern of the aromatic hydroxyl groups, revealing clear structure–activity relationships. Overall, the results demonstrate that subtle structural modifications profoundly affect the interaction of chemically diverse natural products with AhR and identify cannabinoid-, coumarin-, and phenylpropanoid-based scaffolds as promising templates for the development of novel receptor modulators. These findings expand the current knowledge of natural AhR ligands and provide a rational basis for the design of new bioactive compounds with potential applications in inflammatory, immune-mediated, metabolic, and skin disorders in which AhR signaling plays a pivotal role.

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From Phytochemistry to Mechanism of Action: Multi-Omics Investigation of Plant-Derived Bioactive Compounds in Prokaryotic Systems

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One of the most effective strategies to address the global threat of antibiotic resistance is the identification of new antimicrobial molecules with innovative mechanisms of action [1]. Plant specialized metabolism represents a valuable source of bioactive molecules, but translating phytochemical discoveries into drugs candidates requires integrating chemical characterization with functional and molecular approaches. In this context, our previous studies identified *Salvia tingitana* Etl. as a promising source of antibacterial compounds against gram-positive bacteria [2]. Bioactivity-guided isolation identified manool, a labdane diterpenoid, as a major active component, displaying MIC values ranging from 6.0 to 32.0 μg/mL against Gram-positive bacteria and a MIC of 6.0 μg/mL against *S. mutans*. Despite its promising antibacterial activity, the molecular mechanisms underlying manool antibacterial activity remain largely unexplored. In this study, we employed an integrated target identification and multi-omics strategy to link phytochemical characterisation and mechanism-of-action studies The Drug Affinity Responsive Target Stability (DARTS) chemical proteomics approach led to the identification of ATP-binding transporter proteins as candidate targets of manool [3]. Consistently, Manool increased the intracellular accumulation of ethidium bromide, indicating impaired efflux pump activity, and exhibited additive effects when combined with sub-MIC concentrations of the antibiotic kanamycin. Metabolomic analyses revealed alterations in amino acid uptake and extracellular metabolite profiles following treatment, providing further evidence of perturbations in bacterial transport and metabolism. Notably, manool showed high stability in simulated saliva and no cytotoxic effects on human gingival fibroblasts (HGF-1). Although manool did not significantly affect bacterial adhesion to HGF-1 cells, it markedly reduced bacterial invasion in a dose-dependent manner. Overall, these findings highlight how integrating phytochemistry, target identification, and multi-omics can provide mechanistic insights into plant-derived antibacterial compounds. Manool interferes with *S. mutans* transport and efflux processes, leading to metabolic alterations and reduced bacterial invasion, supporting its potential as a novel lead candidate against oral pathogens.

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Phytochemical Analysis and Artificial Intelligence in Quality Assurance and Evidence for Botanical Ingredients in Nutrition and Healthcare

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Botanical ingredients used in phytotherapy, supplements and other health products present persistent challenges for quality assurance and evidence generation: complex, variable matrices; batch-to-batch variability driven by agronomic and environmental factors; and the need to link analytical fingerprints to biological activity and clinical relevance. Established phytochemical methods — HPTLC fingerprinting, LC-HRMS/MS metabolite profiling, and bioassay-coupled analytics — remain the backbone of botanical quality control.

Artificial intelligence has become a ubiquitous buzzword, yet beyond large language models, AI has underpinned analytical and quality science for decades — it is time to connect the dots. This contribution examines how phytochemical analytics and AI can be integrated across the value chain, presenting original results from dry-lab models and the combination of novel tools within the EU GMP framework. It highlights current capabilities, regulatory constraints, and open questions for building trustworthy, auditable AI-supported quality and evidence systems for botanical ingredients.

A tale of “dead man’s fingers”!

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Xylaria polymorpha (Pers.) Grev. (family: Xylariaceae), a specific type of macabre woodland fungus that grows in stumps and buried deadwood of broadleaved trees, such as beech, is often referred to as ‘Dead man’s fingers’ because of its appearance that resembles burnt, black fingers poking up from the soil or moss.[1] However, other species of the genus *Xylaria Hill* ex *Schrank*, which comprises well over 100 species, do not exactly have a similar appearance to *X. polymorpha*.[2,3] *Xylaria* species are well known for producing bioactive compounds, belonging to chemical classes of alkaloids, lactones, polyketides, terpenoids, and simple alkylbenzene derivatives.[3] Many of these secondary metabolites from the genus *Xylaria* have been shown to possess anti-inflammatory, antimicrobial, antioxidant, cytotoxic, enzyme-inhibitory, and immunosuppressive properties. Thailand, with high biodiversity documented in both forest and agricultural ecosystems, is a global hotspot for *Xylaria* fungi, many of which are termite-nest-associated, unique, and endemic species.[4] As part of our exploration of the bioactivity and chemical diversity of fungal metabolites from *Xylaria* species, we have investigated several *Xylaria* species collected from different habitats in Thailand.[5-7] This talk will tell the tale of these investigations, highlighting key findings and relevant prospects.

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Challenging organic synthesis inspired by nature: from natural products chemistry to drug discovery

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The molecular modelling is widely recognized as a fast, efficient and cost-effective method by which to identify putative small molecule hits to submit to biological assays. At Sapienza University of Rome, we settled up an in silico screening procedure to filter a unique library of 1000 natural products (NP), mainly isolated, over the years, from plant belonging to different countries, with the aim to boost the drug discovery-oriented pipeline towards the identification of new NP leads for the treatment of several disease. In recent applications of this strategy, a number of potential NP hits/leads acting on several target proteins and disease were identified. The innovation of this approach is the opportunity to identify at the same time new potential therapeutic agents acting on different targets. For istance, we identified two NP, active against antibiotic resistance and as anticancer respectively. Antibiotic resistance limits our ability to treat lung infections in cystic fibrosis (CF). Old antibiotics, such as colistin, have been reintroduced to treat multidrug resistant gram-negative infections, which his has inevitably led to the spread of colistin-resistant strains.[1] Colistin is a cationic peptide that interacts with the lipid A moiety of the lipopolysaccharide (LPS), causing membrane destabilization and cell death. Strong experimental evidence demonstrated that in P. aeruginosa colistin resistance depends on the covalent addition of 4-amino-4-deoxy-L-arabinose (Ara4N) to lipid A, which reduces colistin affinity for LPS.[2,3] On the basis of the resolved crystallographic structure of ArnT,[4] the last enzyme of the pathway leading to lipid A aminoarabinosylation, we performed an in silico molecular docking approach that allowed to identify a compound capable to potentiate colistin activity against a colistin-resistant P. aeruginosa tester strain at relatively low concentrations. Based on computational and organic chemistry studies, some analogues have already been synthesized.

The toxicity and efficacy of synthesized compounds will be assessed in different in vitro and in vivo model systems. Hedgehog signaling is essential for tissue development and stemness and its deregulation has been observed in many tumors. Aberrant activation of Hedgehog signaling is the result of genetic mutations of pathway components or other Smo-dependent or independent mechanisms, all triggering the downstream effector Gli1. For this reason, the identication of novel molecules blocking the pathway at a downstream level, represents a critical goal in tumor biology. We clarified the structural requirements of the pathway effector Gli1 for binding to DNA and identify Glabrescione B as the first small molecule binding to Gli1 zinc-finger and impairing Gli1 activity by interfering with its interaction with DNA.

Remarkably, as a consequence, Glabrescione B inhibited the growth of Hedgehog-dependent tumor cells in vitro and in vivo as well as the self-renewal ability and clonogenicity of tumor-derived stem cells. The identification of the structural requirements of Gli1/DNA interaction highlights their relevance for pharmacologic interference of Gli signaling.[5]

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Bioactivity-correlated analytical techniques used for studying bioactive drug leads in desert-loving *Eremophila* spp.

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Eremophila is a genus of draught-tolerant plants endemic to Australia, and the entire genus is rich in structurally diverse natural products with multiple pharmacological activities.[1] We have established a collection of more than 300 *Eremophila* samples, and the use of bioactivity-correlating omics and other state-of-the-art analytical technologies are needed for accelerated drug discovery from such a collection. Thus, molecular phylogenetics combined with computational metabolomics were used to pinpoint intraspecies relationships,[2] whereas high-resolution inhibition profiling[3] and polypharmacology-labelled molecular networking[4] were used for pinpointing metabolites correlated with multiple bioactivities. The results from these explorative studies enabled us to identify *Eremophila* species and/or individual metabolites correlated with (poly)pharmacological bioactivity – and extracts of these species were subsequent analysed by hyphenated HR-inhibition inhibition profiling/HPLC-PDA-HRMS-SPE-NMR. This resulted in isolation of more than 120 new natural products, including e.g., structurally diverse serrulatane, cembrane, and viscidane diterpenoids[3,4] and a new class of dimeric branched-chain fatty acids formed by Diels Alder reactions.[5] Pharmacological activities included antibacterial, antihyperglycemic, and cancer resistance-reversing properties.

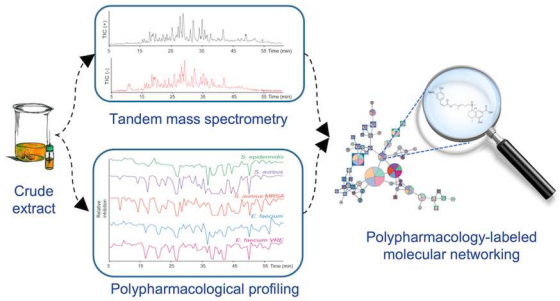

Figure 1. Graphical principle of polybioactivity-labeled molecular networking

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Medicinal Plants as Network-Level Regulators in Neurodegenerative Disorders

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Neurodegenerative diseases arise from many small problems occurring together. Stress increases, inflammation grows, mitochondria lose energy, proteins fail to maintain their shape, and gene control becomes unstable [1]. These linked changes weaken brain cells over time, and single-target drugs often show limited benefit. Medicinal plants offer a broader type of support. Their bioactive compounds act gently on several pathways at once. They help reduce oxidative stress through nuclear factor erythroid 2-related factor 2 (Nrf2) [2]. They ease inflammation by lowering nuclear factor kappa light chain enhancer of activated B cells (NF-κB). They support mitochondrial quality control and help maintain energy balance. They help proteins retain their proper shape and stabilise long-term gene activity through epigenetic pathways. Omics studies show a consistent pattern. Bioactive compounds influence key systems across genes, proteins, and metabolism, suggesting a network-level mode of action [3]. This presentation explains how medicinal plants help the brain by acting on many connected systems at the same time. Instead of targeting a single pathway, they support stress control, inflammatory balance, energy stability, protein maintenance, and long-term gene regulation. These combined effects help the whole system remain stable. As a result, stress declines, inflammation reduces, energy remains balanced, proteins stay functional, and brain cells survive longer. Overall, medicinal plants help regulate the entire network rather than a single target.

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Innovating Sesquiterpene Lactones for Sustainable Weed and Parasitic Plant Management

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Sustainable weed management requires agrochemical strategies inspired by nature that combine efficacy, selectivity and environmental compatibility. Allelopathy provides a valuable framework, as plant-plant chemical interactions reveal phytotoxins that may serve as lead structures for the development of new bioherbicidal agents. This lecture will focus on sesquiterpene lactones, a structurally diverse family of natural products widely distributed in the plant kingdom that comprises thousands of reported compounds.[1] For more than four decades, our group has investigated allelopathy of sesquiterpene lactones in natural and agricultural ecosystems through natural product chemistry, structural elucidation, synthesis, phytotoxic bioassays, SAR/QSAR analysis and mode-of-action studies.

First, this communication will address sesquiterpene lactones isolated from *Helianthus annuus* using allelopathic extraction approaches based on aqueous maceration at room temperature and supercritical CO_2 extraction. These studies illustrate how complementary strategies recover bioactive metabolites and support the identification of phytotoxic lead compounds.

The discussion will then focus on eudesmanolides and guaianolides from *Cynara cardunculus*. Bio-guided fractionation, structural modification and structure-activity relationship studies have identified molecular features associated with phytotoxicity and selectivity, while enriched active fractions provided practical starting points for formulation development.

A further application concerns sesquiterpene lactones and their derivatives for the control of parasitic plants. Through the honeypot strategy, these compounds may selectively stimulate parasite seed germination in the absence of a host, offering a promising route to deplete soil seed banks, fitting within a complex context of bioactive, species-specific metabolites.[2]

Finally, the design of bioactive hybrids and dimers incorporating sesquiterpene lactone motifs with complementary pharmacophores will be presented. Their potential applications, together with nanoencapsulation systems and nanoemulsions containing pure phytotoxins or enriched active fractions, illustrate how improved solubility, stability, delivery and biological performance may help translate allelopathic knowledge into innovative tools for sustainable weed and parasitic plant management.

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Phytochemicals in the forest: phenolics in conifer-bark beetle interactions

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Conifer trees produce large quantities of phytochemicals in their bark and outer sapwood that are thought to protect against insect herbivores, including bark beetles. Terpene resin components are toxic to bark beetles, while the resin as a whole forms a physical barrier to invasion. Conifer bark also contains abundant phenolic compounds, but their role in defense against bark beetles has received comparatively little attention, both with respect to the beetles themselves and to the numerous free-living fungi that bark beetles introduce into trees during invasion. Bark beetle-associated fungi are thought to provide nutrients to beetles and detoxify conifer defenses.

We have demonstrated that one of the major phenolic compounds in spruce bark, the flavan-3-ol (+)-catechin, is toxic to spruce bark beetles but is metabolized by bark beetle-associated fungal symbionts, thereby facilitating beetle invasion. Another group of spruce bark phenolics, the stilbenes, is also metabolized by these fungi. Stilbene glycosides are hydrolyzed and subsequently converted into methylated derivatives that we found to be toxic to other microorganisms, including the entomopathogenic fungus *Beauveria bassiana*. Thus, bark beetle-associated fungi may protect their beetle partners from one of their natural pathogens through the metabolism of host tree-derived stilbenes.

Under some conditions, however, the microbial metabolism of spruce bark phytochemicals may benefit the tree rather than the bark beetles. We found that spruce trees harbor an endophytic fungus, *Chaetomium globosum*, that suppresses bark beetle-associated fungi and thereby reduces bark beetle success. This endophyte converts stilbenes into *O*-sulfated derivatives, reducing their toxicity. CRISPR/Cas9-mediated knockout of the responsible endophyte sulfotransferase reduced stilbene sulfation and abolished suppression of the bark beetle-associated fungi. Thus, stilbene metabolism can be essential for the suppression of bark beetle-associated fungi.

Taken together, our results demonstrate that phenolic compounds in conifer trees play an important role in determining the outcome of bark beetle attacks, but that their effects depend strongly on the presence and metabolic activities of specific microorganisms.

Plant associated bacterial glycans

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Microbial cell surface molecules, such as the lipopolysaccharide, are very important cell wall glycoconjugates that act as microbe associated molecular patterns in eukaryotic/microbe recognition. Besides their general architectural principle, a number of subtle chemical variations are at the basis of the dynamic host-guest recognition that in case of pathogens is followed by the innate response and in case of symbiosis is followed by its suppression. Microbes differently from Eukaryotes have at their disposal an enormous array of monosaccharide structures/derivative by which they built up their external cell surface and drive their recognition by any eukaryotic host. Therefore, the chemical study of such glycoconjugates involved either as virulence or beneficial factors in plant interactions is a pivotal pre-requisite for the comprehension at molecular level of the (innate) immunity mechanisms.[1]

Viral glycoproteins are usually meant to carry on eukaryotic glycans. Indeed, typically, viruses use host-encoded glycosyltransferases and glycosidases to add and remove sugar residues from virus glycoproteins. However, the more recently discovered large and giant viruses broke from this paradigm. Instead, these viruses code for an (almost) autonomous glycosylation pathway. Virus genes include the production of activated sugars, glycosyltransferases and other enzymes able to manipulate sugars at various levels.

Within this frame, a new class of glyco-molecules has been discovered with a novel and original architecture only belonging to giant viral world.[2]

By this communication, I will also show that structural Glycoscience of microbial world is a fascinating travel through astounding chemical structures with no parallel in any other kingdom.

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Seeing the Whole: Pattern Recognition in Plant Metabolomics

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Plant specialized metabolism is characterized by remarkable chemical diversity and plasticity, shaped by genetic and developmental processes and by interactions with the biotic and abiotic environment.[1] Metabolomics provides a powerful means to explore this complexity, but its value extends beyond the detection and quantification of large numbers of metabolites. Multivariate data analysis and pattern-recognition approaches[2] can help identify coordinated chemical variation and extract biologically meaningful information that may remain hidden when metabolites are considered individually.

Drawing on selected case studies, this lecture will illustrate how a pattern-oriented perspective has been applied to address different phytochemical and biological questions in plant metabolomics. The selected examples will illustrate how metabolic patterns can be interrogated at different levels, from quality control and authentication of botanical materials to the characterization of phytochemical variation in Mediterranean plant species across different geographical and environmental conditions. Finally, the particular complexity of Cladonia lichen metabolomes will provide an example of how pattern-based approaches can help explore chemically intricate biological systems.

Rather than presenting pattern recognition as an end point of metabolomic analysis, these examples will highlight its role as a tool for moving from sample discrimination towards biological interpretation. By integrating phytochemical fingerprints with biological and environmental information, plant metabolomics can provide a broader view of phytochemical diversity and help formulate new hypotheses about the processes underlying the observed patterns.

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Plant chemophenetics – Comparative phytochemistry in the DNA-phylogenetic era

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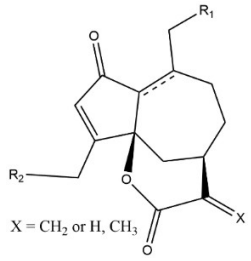
Plant chemosystematic or chemotaxonomic studies based purely on the profiles of small molecules have become obsolete as tools to study phylogenetic relationships of higher plants due to the advent of the much more powerful (macro-)molecular techniques and new methods of data analysis established in parallel to these techniques. Plant chemophenetics is thus proposed as a new term for the field of studies aimed at the exploitation of characteristic arrays of specialized natural products of plant taxa. Chemophenetic studies as defined here are studies aimed at describing the array of specialized secondary metabolites in a given taxon. Chemophenetic studies contribute to the phenetic description of taxa, similar to anatomical, morphological, and karyological approaches, which have already been recognized as of major importance for establishing "natural" systems, and which continue to be of the utmost importance for the description of organisms classified with the help of modern molecular methods. This approach, chemophenetics, allows characterizing species and clades based on their array of specialized metabolites, aids in deducing the evolution of biosynthetic pathways and coevolution, and can serve in identifying new sources of rare and economically interesting natural products.[1]

In my presentation, I will highlight some chemophenetic results on hypocretenolide type sesquiterpene lactones (Fig. 1) in the genus *Leontodon*, showing how chemophenetics can help in characterizing morphologically not characterizable systematic groups.[2] In another example from the Gnaphalieae tribe of the Asteraceae family, the focus will be on finding new sources for rare caffeoyl-D-glucaric acid derivatives (Fig. 2) originally described from a hard to cultivate alpine plant species, *Leontopodium alpinum*.[3]



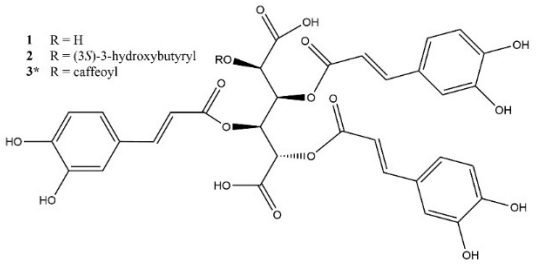


Fig 1. Hypocretenolides from *Leontodon* s.str. Fig. 2. Caffeoyl-D-glucaric acid derivatives from the Gnaphalieae.

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Seasonal Chemical Signals in *Rhododendron tomentosum* Harmaja: Phenolic and Terpenic Dynamics in a Coniferous Swamp Forest

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Coniferous swamp forests are acidic, water-saturated, and nutrient-limited habitats where evergreen plants face strong environmental constraints. In these conditions, secondary metabolites may contribute to stress tolerance, defence, seasonal adaptation, and plant–environment interactions [1]. *Rhododendron tomentosum* Harmaja, an evergreen Ericaceae species characteristic of swampy coniferous forests, is a valuable source of bioactive compounds from stress-adapted forest plants [2]. This study evaluated the seasonal variation of phenolic and triterpenic compounds in *R. tomentosum* leaves collected from a natural population in Lithuania over a full annual phenological cycle. The phenolic profile included phenolic acids, flavan-3-ols, procyanidins, flavonoids, and coumarin derivatives. The triterpenoid compounds were composed of several structural classes, including phytosterols and neutral pentacyclic triterpenoids of ursane-, oleanane-, lupane-, friedelane-, fernane-, and hopane- related types. The highest total phenolic and triterpenic content was observed during autumn–winter dormancy. In contrast, flowering was associated with increased accumulation of flavonol glycosides, particularly quercetin derivatives, suggesting metabolic changes during reproductive development. Triterpenic compounds may contribute to protective surface barriers, defence responses, and adaptation to environmental stress. Principal component analysis demonstrated clear phytochemical grouping of samples and revealed a distinction between dormancy-associated and flowering-associated phytochemical profiles.

These findings indicate that phenological stage is a key factor shaping the chemical profile of *R. tomentosum*. Seasonal variation in phenolic and triterpenic compounds may reflect adaptive strategies of evergreen Ericaceae species and contribute to the molecular language of swamp forest ecosystems. Furthermore, the phenolic and triterpenic profiles of certain Ericaceae plants contribute to their medicinal value, which has great potential for pharmaceutical, cosmeceutical, nutraceutical, and wellness products.

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Efficacy of Phytocomplexes from Mediaterranean Plants to Ectoparasiticides

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The prevention and management of ectoparasite infestations are crucial for maintaining the health and well-being of companion animals. Reflecting this necessity, antiparasitic treatments constitute the second-largest sector of the global animal health industry. However, recent decades have seen several factors restricting the development of new solutions, even as dogs and cats continue to pose potential risks of zoonotic infection to humans[1].

A number of plants can synthesize secondary metabolites, which are used by the plants for their protection against pathogens and pests[2]. Several essential oils (EOs)—particularly those rich in phenolic compounds like thymol, carvacrol, eugenol, and cinnamaldehyde—show promising in vitro insecticidal and acaricidal efficacy. By targeting neuronal, respiratory, and cuticular functions simultaneously, their multi-target mechanisms not only ensure high effectiveness but also significantly hinder the rapid development of resistance[3].

The objective of this study was: i) to characterize the phytocomplex derived from plants of *Citrus* spp., peculiar of the Mediterranean region; ii) to determine the potential acaricidal effect of EOs in pest control. Lemon oil demonstrated extreme activity against AIT even at the lowest concentration tested and sweet orange oil showed 78% mortality at the lowest concentration tested in the AIT. All the EOs showed low toxicity at the lowest concentrations (≤0.01%, i.e., 100 μg/mL), with cytotoxic effects evident only at higher concentrations (≥0.025%) (Exposure of H9c2 cardiomyocytes). Lemon EO was the most active against this cell line while orange and bergamot EOs exhibited a milder cytotoxic profile. The diversity in biological profiles observed among the various species of the genus *Citrus* reflects the qualitative and quantitative variation of their respective phytocomplexes.

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ORAL COMMUNICATIONS

O1: From Waste to Value: Bioactivities, Mechanisms, and Molecular Targets of Chlorophyll Metabolites

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Phyllobilins (PBs) are bilin-type linear tetrapyrroles formed during chlorophyll breakdown, most notably during leaf senescence. First isolated in 1991,[1] they comprise a structurally diverse group generated via a regulated metabolic pathway. Their detection and annotation are usually accomplished by HPLC-DAD using characteristic UV-Vis signatures,[2] alongside MS and NMR.[3]
Once viewed solely as detoxification end-products, PBs are increasingly recognized for potential bioactivities. *In vitro* and cellular studies report antioxidative effects, with additional evidence for anti-inflammatory actions. Some PBs, particularly colored phylloxanthobilins (PxBs) and phylloroseobilins (PrBs), show anti-proliferative and anti-migratory effects in cancer cell lines. Indeed, the cytoskeletal protein actin was identified as molecular target of these colored PBs, suggesting a link between PBs, cytoskeletal dynamics, and cancer cell migration.[4] Structure–activity trends point to oxidation state and side-chain modifications as contributors to these effects.
Overall, current data support PBs as a chemically varied natural product class with emerging biological relevance. Ongoing efforts combine mass spectrometry-based identification with functional and target-based assays to clarify mechanisms, and evaluate their potential utility in phytochemistry, nutrition, and biomedical research.

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O2: Natural Deep Eutectic Solvents for the Sustainable Valorization of Comfrey (*Symphytum officinale* L.) Roots

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Symphytum officinale L. (comfrey, Boraginaceae) is a traditional medicinal plant widely used in topical preparations for inflammatory and traumatic conditions, including rheumatic pain, swellings, hematomas, wounds, and skin ulcers. Its therapeutic relevance has been associated with mucilage, allantoin, and phenolic constituents, particularly caffeic acid oligomers such as rosmarinic acid, rabdosiin, and globoidnans A and B. However, the valorization of comfrey roots requires careful balancing of efficacy and safety, due to the presence of toxic pyrrolizidine alkaloids.[1] In this study, (natural) deep eutectic solvents (NADES) were investigated as greener alternatives for the extraction of bioactive metabolites from comfrey roots, with further assessment of phytochemical composition, cytotoxicity, antioxidant activity, and inhibition of skin-related enzymes.[2,3] More than 30 DES were screened for the ultrasound-assisted extraction of comfrey roots. A design of experiments (DoE) was performed using a Box-Behnken design and response surface methodology. The extracts were characterized by LC-UV for the quantification of rosmarinic acid, rabdosiin, and globoidnans A and B, and by LC-HRMS/MS for the profiling of phenolic compounds and pyrrolizidine alkaloids. Among the tested systems, choline chloride-based DES, especially those containing hydroxy acids, showed the highest extraction efficiency. The comfrey DES extracts displayed relevant antioxidant activity and inhibition of skin-related enzymes, while showing low cytotoxicity in keratinocytes and fibroblasts. Overall, this work supports DES-assisted extraction as an efficient and sustainable strategy for obtaining phenolic-rich comfrey root extracts, while integrating phytochemical profiling and biological evaluation. This approach may contribute to the development of greener and standardized comfrey-derived ingredients for topical pharmaceutical and cosmeceutical applications.

Acknowledgements

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O3: Development of Biomimetic Porous Scaffolds Based on Marine Biopolymers for Bone Tissue Regeneration

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Porous scaffolds, fabricated from natural or synthetic polymers, as well as various inorganic materials, play a pivotal role in tissue engineering and regenerative medicine. In this context, biopolymers have emerged as highly promising materials for tissue engineering and regeneration owing to their biocompatibility, biodegradability, diverse functionalities, and tunable physicochemical properties.

Marine biopolymers have been used for the development of such scaffolds due to the wide spectrum of biological activities they exhibit, as well as their biocompatibility, biodegradability, chemical tuning ability, osteoinductivity and sustainability. So far, various seaweed polysaccharides, as well as gelatin, have been employed for the preparation of porous scaffolds and studied as extracellular matrix-compatible materials.

In this study, we rationally designed, fabricated, and characterized a series of novel porous hybrid scaffolds composed of crosslinked ulvan, ι-carrageenan, chondroitin sulfate, and gelatin, both with and without the addition of marine-derived nanohydroxyapatite. The influence of the constituents on the morphology, porosity, water-uptake, in vitro degradation ability and thermal stability of the scaffolds was subsequently assessed and selected compositions were further evaluated in respect to their biocompatibility and osteogenic differentiation potential. Overall, it was found that all constructed sponge-like scaffolds efficiently promoted the adhesion, proliferation, and osteogenic differentiation of osteoblast precursor cells, demonstrating their strong potential for bone tissue engineering applications.

O4: NMR-based metabolomics of *Astragalus* L. species from Türkiye to investigate potentially bioactive cycloartane-type saponins

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Historically, plant-derived natural compounds have long served as a significant source of therapeutic agents, proving highly effective as "leads" or model molecules for drug design, semisynthesis and synthesis. Driven by the success of phytochemicals as chemotherapeutic alternatives, contemporary research is increasingly focused on underexplored secondary metabolites.[1]

In this context, saponins have gained considerable research interest in the biopharmaceutical sector due to their remarkable biological and pharmacological properties, most notably anticancer potential.[2] Indeed, earlier phytochemical investigations on *Astragalus* L. species led to the isolation of cycloartane-type saponins, which have demonstrated outstanding antitumor activity both *in vitro* and in animal models.[3]

Based on these insights, extensive 1D and 2D NMR analyses (COSY, TOCSY, HSQC, HMBC, H2BC, HSQC-TOCSY) were carried out on fifty-two extracts from selected *Astragalus* species from Türkiye, with the aim to identify novel potentially bioactive cycloartane-type glycosides. This preliminary NMR-based profiling allowed to efficiently screen and target the species producing the cycloartane saponins of interest.

Since a modest 7% of Turkish *Astragalus* species have been comprehensively investigated for their secondary metabolite profiles, early efforts have focused on the elucidation of cycloartane saponins within these selected mixtures, highlighting the value of NMR spectroscopy-based metabolomics as a highly successful tool for structural characterization of complex natural mixtures. The project will then progress to purification strategies aimed at achieving a deeper understanding of the precise composition of the chosen extracts, involving a combination of chromatographic techniques and 2D NMR analyses. Ultimately, in order to prove the biological potential of cycloartane-type saponin-rich mixtures, an anti-cancer bioassay-guided screening was carried out on them.

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O5: New Stilbene Glycosides from *Prospero autumnale* and their Anti-inflammatory Activity

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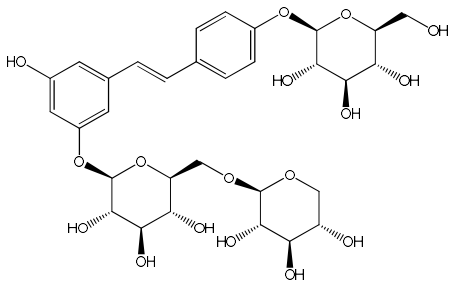
Prospero autumnale (L.) Speta (Asparagaceae), a Mediterranean bulbous herb[1], represents a promising yet largely unexplored source of bioactive secondary metabolites. Our previous phytochemical investigation of this species revealed structurally diverse phenolic compounds in the EtOAc fraction of the EtOH extract, highlighting its significant but still underexplored chemical potential[2]. In the present study, we aimed to further characterize secondary metabolites from the *n*-BuOH fraction and evaluate their anti-inflammatory activity in LPS-induced HMC3 microglial cells. Phytochemical analysis led to the isolation of two new stilbene glycosides (**1** and **2**), along with three known analogs, resveratrol 3,4′-*O,O*′-di-β-D-glucopyranoside (**3**), lysidiside L (**4**), and resveratrol 3,5-*O*-β-diglucoside (**5**). Structures were elucidated using comprehensive 1D and 2D NMR spectroscopy and HR-MS analysis. Compound **2** features an unusual *tert*-butyl substituent on a glucopyranose unit, representing a rare structural motif among natural stilbene glycosides; however, its absence in the crude extract suggests it may originate as an isolation artifact. Biological evaluation using the DHR123 assay revealed that compounds **3** (50 μM) and **4** (10 and 50 μM) significantly attenuate LPS-induced oxidative stress in HMC3 cells. These findings further highlight *P. autumnale* as a valuable source of structurally unique stilbene derivatives with potential relevance for neuroinflammatory conditions.



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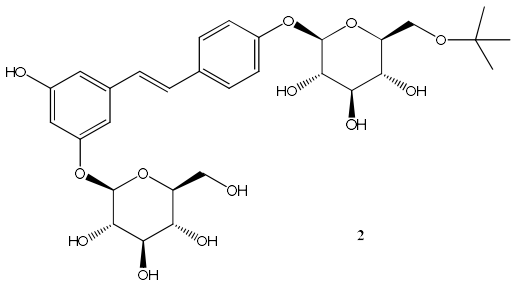

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O6: From extreme environments to sustainable applications: the multifaceted profile of C-phycocyanin from *Galdieria spp.*

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C-phycocyanin (C-PC) is a water-soluble blue phycobiliprotein used in food, nutraceutical, cosmetic and fluorescence-based applications and investigated for antioxidant, anti-inflammatory and antiproliferative activities[1]. Its technological relevance was reinforced in 2025, when the U.S. FDA listed *Galdieria sulphuraria* extract as a food colour additive. While previous studies focused on *G. phlegrea* and *G. sulphuraria*, exploring strains from distinct acidothermal sites is essential to fully understand the genus biotechnological potential. To establish a comprehensive comparison, this study characterises C-PC from a newly investigated extremophilic red microalga, *G. daedala*.
To elucidate evolutionary context, the C-PC α- and β-subunit sequences were phylogenetically analysed. For biotechnological applications, C-PC was extracted from lyophilized biomass and enriched through multistep purification. Structural integrity and purity of the pigment were verified by UV–Vis spectrophotometry and SDS-PAGE. Environmental resilience was assessed through pH (1.5-9.0) and thermal (20-70 °C) stability assays. Bioactive potential was also investigated via cytotoxicity profiling on HepG2 cells (0.01-0.5 µM for 48 h) using the XTT assay[2]. Phylogenetic analyses placed both subunits within a monophyletic *Galdieria* clade showing closest affinity to *G. sulphuraria*. Purification yielded a highly pure C-PC extract (purity index 0.90; 20 mg g^{-1} dry biomass), with major SDS-PAGE bands at ~15 and 20 kDa, confirming optimal structural preservation. Stability assays highlighted robust environmental tolerance: C-PC maintained 84-100% relative concentration across pH 3.0-9.0, though it degraded at highly acidic conditions. It demonstrated moderate thermostability, retaining 83.9% concentration at 30 °C, before gradually degrading at 60-70 °C[3]. Functionally, the enriched fraction induced a concentration-dependent reduction in HepG2 cells metabolic activity with an apparent IC_{50} of 0.13 µM (~15.1 µg mL^{-1}). Compared to established species, *G. daedala* showed broad pH tolerance, moderate thermal stability, and preliminary bioactivity against HepG2 cells, expanding the diversity of potentially valuable C-PC sources within *Galdieria*.

Keywords: C-Phycocyanin; *Galdieria daedala*; phylogenetic analysis; HepG2

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O7: Spatiotemporal Changes in Central Metabolism Control Scent Volatiles Emission in *Morinda citrifolia* Petals

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Floral scent emission physiology is a tightly regulated process that ensures efficient resource utilization for enticing pollinators and which in turn maximize reproductive success of the plants. The central metabolic networks branch out into the specialized metabolic routes to produce these volatile scent molecules[1]. A tight regulation in the central metabolic pathways is not only necessary for efficient release the volatile cues, but also enables flowers to spend energy on other cues such as floral display or visitation rewards[2]. *Morinda citrifolia* L. is an evergreen tree, cultivated mostly for its fragrant flowers and nutritious fruits. The flowers show a nocturnal rhythm of scent volatiles emission, with peak emission between 8.00 p.m. to 2.00 p.m. The emitted scent volatiles are dominated by phenylpropanoid/benzenoid compounds such as benzoic acid, benzyl acetate, benzyl nitrile etc. Significant emission of terpenoids such as linalool were also observed. Histochemical and GC-MS based studies show the adaxial epidermal cells are the primary sites of floral volatile accumulation and emission. We observed specialized inverted urn-shaped epidermal cells only towards the adaxial surface indicating the petals are anatomically adapted for scent emission from the upper surface of the petals. These upper epidermal and subepidermal layers also show higher metabolic sugar and organic acid accumulation, indicating elevated metabolic activity in the adaxial petal surface. Spatial metabolomic studies further revealed a higher turnover of Krebs cycle in the upper cell layers of the petals, suggesting an enhanced energy production probably for supporting emission physiology. Temporal metabolic profiling during flower opening showed an increase in metabolic sugar content, which likely provide precursors for volatile biosynthesis and fuel the energy-intensive emission process. Our study reveals that the adaxial cell layers of petals in fully bloomed flower enter into a high-energy-state to support scent volatiles biosynthesis and emission.

Key words: Central metabolism, floral volatiles, histochemistry, *Morinda citrifolia*, spatial metabolomics.

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O8: Colour Transition Influences Scent Emission in *Gardenia carinata* Flowers

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Gardenia carinata commonly known as 'golden gardenia', is a rubiaceous shrub commonly found in South-East Asian countries. The species has got wide popularity as ornamental plant for their colour-changing fragrant flowers[1]. The flowers exhibit a gradual colour transition from white to golden through a span of three to four days. We identified crocin, a carotenoid-cleavage product, as the major pigment responsible for petal colouration. GC-MS analysis of *G. carinata* floral headspace revealed that the scent bouquet is dominated by benzenoid and terpenoid compounds such as isoeugenol, chavicol, β-ocimene etc. Temporal volatilomics showed the flowers predominantly follow a nocturnal pattern of scent emission. However, we observed a constitutive emission of terpenoid volatiles from the pigmented flowers. The non-rhythmic emission of terpenoids is probably associated with the constitutive upregulation of carotenoid-synthesizing methylerythritol phosphate pathway, which also provides precursors to the volatile terpenoid biosynthetic routes. Furthermore, our studies on floral colour change demonstrated that air temperature of the environment is the key regulator of colour change in *G. carinata* flowers. Higher temperatures significantly upregulate pigment synthesis, whereas the lower temperatures showed reduced pigment accumulation. Correspondingly, flowers undergoing colour transition in higher temperature regimes exhibited enhanced emission of terpenoid volatiles and a few carotenoid-cleavage volatiles viz. β-cyclocitral, a byproduct of crocin metabolism. In contrast, experiments conducted in lower temperature regimes were devoid of such compounds in their floral headspace. The emission physiology of benzenoid volatiles did not show any dependence on the floral colour change. Thus, our experiments revealed that colour changes in *G. carinata* petals indeed influence the terpenoid volatiles synthesis and emission from the flowers. The outcome of this study might help to understand the impact of climate change in altering the cues for plant-pollinator interaction.

Keywords: carotenoid-cleavage product, crocins, *Gardenia carinata*, floral volatiles.

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O9: Antiadipogenic and prolipolytic coumarins in Greek lemons and their risk of cytochrom P450 enzyme inhibition

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In our on-going studies on antiadipogenic coumarins from lemon peels, 5-geranyloxy-7-methoxycoumarin proved to have a similar mode of action as bergamottin[1,2] whereas limettin has a prolipolytic activity in 3T3-L1 cells[3]. However, furanocoumarins of *Citrus* fruits, especially bergamottin and 6′,7′-dihydroxybergamottin, are under discussion due to their inhibitory effects on cytochrome P450 (CYP) enzymes[4]. In order to explore the quantities of coumarins in lemon varieties from Greece, we recently analysed 6 accessions, separated into flavedo, albedo, pulp and juice fractions.

By far the highest concentrations of bergamottin were found in the flavedo layers of all accessions (0.68 ± 0.26 mg/g dry material, 0.25 - 1.02 mg/g), whereas albedo, pulp and juice contained only 0.06 – 0.10 mg/g. 6′,7′-dihydroxybergamottin could not be detected. The second coumarin with significant antiadipogenic effects, 5-geranyloxy-7-methoxy-coumarin was cumulating in the flavedo layer too (0.36 ± 0.19 mg/g vs. 0.06 – 0.13 mg/g in other parts). The same trend was found for the prolipolytic citropten (0.25 ± 0.16 vs. 0.03 – 0.04 mg/g in other parts). Among further furanocoumarins, byakangelicin and 8-geranyloxypsoralen were present in relevant amounts (0.04 – 0.17 mg/g and 0.03 – 0.16 mg/g, respectively).

For bergamottin an IC_{50} value for CYP3A4 of 4.48 µM in human liver microsomes was published[5]. Consumption of 1 g dried lemon zest (flavedo) will lead to an approximate intestinal concentration of up to 12 µM (based on 250 ml intestinal liquid volume). For comparison, total concentration of bergamottin and 6′,7′-dihydroxybergamottin in grapefruit juices was found up to 113.76 µM in a study of VanderMolen et al.[6] As a conclusion, further development of herbal medicines or nutraceuticals from lemon peels should focus on reduced bergamottin levels.

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O10: Microplate Liquid and Solid Matrix Volatilization Assays for Antimicrobial Susceptibility Testing of Plant-Derived Volatile Agents and Their Combinations in Vapour Phase

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Evaluating antimicrobial activity of volatiles in the vapour phase is challenging due to their volatility and hydrophobicity. Standard assays do not provide accurate results, and methods developed for testing in the gaseous phase yield only qualitative results while requiring large amounts of material and labour[1]. The main aim of this work was to develop quantitative and cost-effective methods for testing plant-derived volatiles in the vapour phase suitable for high-throughput screening.
As a result, broth microdilution volatilization[2], broth volatilization checkerboard[3], and microplate disc volatilization assays[4] were designed. With the aim of improving handling, manipulation safety, reproducibility, and sensitivity of the developed assays, we invented a new microplate sealing lid (SLIM-V®) with 96 flanges designed to snap-fit into conventional microplate wells[5].
Among all volatiles tested using above-mentioned methods, the vapours of thymoquinone and 8-hydroxyquinoline were the most effective against *Haemophilus influenzae* and *Staphylococcus aureus* with MIC 2 μg/cm³. In the case of complex mixtures of volatiles, the essential oil of *Alpinia oxymitra* pericarp was the most effective against *H. influenzae*, with MIC 8 μg/ cm³, and the supercritical CO_2 extract obtained from *Neolitsea cassia* bark was the most active against *Listeria monocytogenes* with MIC 64 μg/ cm³. The best combinatory anti-staphylococcal effect was found in the vapour phase against *S. aureus* ATCC 25923 for the combination of carvacrol and thymol (ΣFIC=0.51). Chemical structure-activity relationship analysis of 31 monoterpenoids identified the critical role of hydroxyl, ketone, and isopropyl groups on six- or seven-membered rings containing double bonds for their antibacterial potency in the vapor phase[6].
Microplate liquid and solid matrix volatilization assays allow for a cost- and labour-effective high-throughput screening of volatile agents in the vapour phase. In the future, these methods can be used for the development of new agricultural, food, pharmaceutical, and medicinal applications.

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O11: Comparison of traditional and contemporary approaches to identify chemophenetic markers in leaves of *Verbascum* species

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Verbascum (mullein) is a genus of the Scrophulariaceae family distributed throughout Europe, occupying habitats ranging from coastal areas to mountainous regions. Several *Verbascum* species are used in traditional medicine: flowers are employed to relieve sore throat and cough, whereas leaves are traditionally applied for the treatment of skin disorders [1].

Although the phytochemical profiles of *Verbascum* leaves are generally characterized by the presence of phenylethanoid glycosides and flavonoids, no established chemophenetic markers are currently available to discriminate among species, which may differ in their medicinal properties and commercial value [2].

The present study compares a conventional phytochemical approach with an untargeted metabolomics workflow to identify chemophenetic markers in the leaves of four *Verbascum* species (*V. thapsus*, *V. nigrum*, *V. sinuatum*, and *V. phlomoides*).

Methanolic leaf extracts were initially profiled by TLC and LC–MS. This targeted phytochemical investigation indicated phenylethanoid glycosides as the most informative metabolite class for species discrimination. To characterize these compounds in more detail, extracts of *V. sinuatum* and *V. phlomoides*, selected as representative species, were subjected to chromatographic fractionation and purification. This led to the isolation of verbascoside and several less abundant, species-specific phenylethanoid glycosides, whose structures were elucidated by 1- and 2D-NMR spectroscopy.

In parallel, methanolic extracts were analysed by UHPLC-ESI-HRMS/MS, and the resulting dataset processed using MZmine and visualized as feature-based molecular network. PCA revealed subtle differences between *V. thapsus*, *V. sinuatum*, and *V. phlomoides*, whereas all three species are clearly distinct from *V. nigrum*, in contrast to the relationships inferred from the targeted phytochemical workflow. The untargeted analysis further identified flavonoids, in addition to phenylethanoid glycosides, as the metabolites contributing most strongly to species discrimination and, therefore, as promising marker compounds.

These findings demonstrate that conventional phytochemical investigation and untargeted metabolomics address different aspects of chemical diversity, providing complementary perspectives on chemophenetic differentiation in *Verbascum*.

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O12: Metabolite Profiling Of The Invasive Aquatic Plant *Pontederia crassipes* Mart.: Insights Into Biomass Valorisation

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Invasive alien species represent a major threat to biodiversity, ecosystem integrity, and socioeconomic stability worldwide[1]. *Pontederia crassipes* (water hyacinth) is considered one of the most problematic invasive plants globally, severely impacting freshwater ecosystems[2,3] and generating large amounts of biomass during mechanical removal, for which sustainable strategies for biomass management remain limited.

In this study, HPLC-DAD-MS-based metabolomic profiling was applied to leaves, roots, rhizomes, and flowers of P. *crassipes* collected from three Portuguese freshwater systems. The aims were to characterise the phytochemical composition of the species, evaluate organ- and site-dependent variations, and assess its potential for resource recovery.

A diverse phenolic profile was observed, including hydroxycinnamic acid derivatives, caffeoylquinic acids, flavonols, flavones, flavan-3-ols and organic acids. Kaempferol-derived flavonols were the predominant metabolites detected. Quantitative analysis revealed significant organ-specific differences, with flowers exhibiting the highest total flavonoid content (4.3–11.0 mg/g DW), whereas leaves, roots, and rhizomes contained lower levels. Flavonols accounted for approximately 75–85% of total flavonoids in flowers. Site-dependent differences were also observed, indicating that environmental conditions may influence secondary metabolite accumulation.

Overall, these findings highlight the potential of *P. crassipes* as a source of phenolic compounds with reported bioactive properties, providing a basis for future biological activity studies and sustainable biomass valorisation strategies.

Keywords: invasive species; metabolite profiling; phenolic compounds; biomass valorisation

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O13: Phytochemical characterization of volatile and non-volatile fractions of oleogum resins from *Commiphora* species of Socotra Island

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Many species belonging to the genus *Commiphora* Jacq. (Burseraceae) produce an aromatic resin, generally called myrrh, important for its traditional and medicinal uses[1].
In the island of Socotra, a UNESCO World Heritage Site known for its botanical biodiversity, five species of the genus *Commiphora* grow: *C. kua* (R.Br. ex Royle) Vollesen, *C. ornifolia* (Balf.f.) J.B.Gillett, *C. planifrons* Engl., *C. parvifolia* Engl., and C. *socotrana* Engl. With the exception of *C. kua*, the other four species are endemic to the island of Socotra[2].
Despite their traditional use for medical purposes, these species remain poorly studied. For this reason, the present research investigated the volatile and non-volatile fractions of oleogum resins of *Commiphora* species from Socotra. The phytochemical analysis of the volatile compounds was carried out using headspace solid-phase microextraction coupled with gas chromatography–mass spectrometry (HS-SPME-GC-MS)[3], while non-volatile constituents were studied using high-performance liquid chromatography coupled with high resolution mass spectrometry (HPLC-HRMS), high-performance thin-layer chromatography (HPTLC), and nuclear magnetic resonance (NMR) spectroscopy[4].
The obtained results highlighted that the volatile fractions are rich in monoterpenes and sesquiterpenes, which followed a different trend among the studied species in accordance with the ecology of the collection areas of the species.
In the non-volatile fraction of the oleogum resin of *C. ornifolia* we identified (+)-yangambin, a furofuran lignan known for its vasorelaxant and cardiovascular activities[5], reported for the first time in this species. The analysis of the hydrolyzed polysaccharide fraction revealed the presence of arabinose, rhamnose, galactose, and galacturonic acid.
Overall, these findings expand the known chemical diversity of the genus *Commiphora* and suggest that these plants may produce other bioactive compounds of pharmaceutical interest.
Further studies will aim to isolate and characterize additional compounds from the *Commiphora* species endemic to Socotra Island and to evaluate their biological activities.

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O14: Unlocking Hidden Monoterpene Indole Alkaloids in *Picralima nitida* through pH-Zone-Refining Centrifugal Partition Chromatography

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Monoterpene indole alkaloids (MIAs) represent one of the most structurally complex groups of plant specialized metabolites. Their biosynthesis yields numerous closely related analogs that differ only by subtle changes in stereochemistry, molecular connectivity, or ionization properties, making their chromatographic resolution particularly challenging. These challenges are especially pronounced in complex botanical matrices such as the seeds of *Picralima nitida* (Stapf) T. Durand & H. Durand (Akuamma, Apocynaceae). For such cases, conventional chromatographic techniques often provide insufficient selectivity to separate compounds with similar polarity and pKa values, thereby restricting comprehensive chemical and biological investigations.

In this work, pH-zone-refining centrifugal partition chromatography (pHZR-CPC) was evaluated as a preparative strategy to explore the residual complexity of Akuamma alkaloids. Dichloromethane seed extracts were fractionated in ascending mode using an ethyl acetate/water biphasic solvent system, with triethylamine in the mobile phase as the eluter and hydrochloric acid as the retainer in the stationary phase. The separation process was followed by online UV detection and offline TLC analysis, whereas structural characterization of the isolated constituents was achieved by LC-HRMS/MS together with one- and two-dimensional NMR spectroscopy. Optimization of the pHZR-CPC protocol was accomplished by systematically adjusting the injected sample load, the concentrations of the retainer and eluter, and by implementing a stepwise eluter gradient. Under the optimized conditions, 16 MIAs were successfully isolated. Purity evaluation by LC-UV indicated an average purity of approximately 95%, while qHNMR yielded an average purity of about 88%. Overall, these results highlight the capability of pHZR-CPC to achieve high-capacity, high-resolution isolation of structurally similar alkaloids, providing improved access to low-abundance metabolites and enabling a more realistic assessment of the chemical complexity of bioactive natural products.

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O15: Thiocanthal and thiocanthol: a green route for the synthesis and isolation of two novel sulfur-containing anti-inflammatory secoiridoids from extra-virgin olive oil

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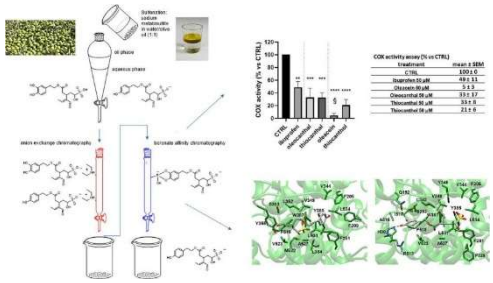
Oleocanthal and oleacein are the two major secoiridoids exclusively found in extra virgin olive oil (EVOO), and exert relevant pharmacological activities, including anti-inflammatory, anti-tumoral, neuro- and cardiovascular protective effects.[1] Their anti-inflammatory action is largely ascribed to the inhibition of cyclooxygenases (COX). Despite their therapeutic potential, obtaining these compounds in appreciable amounts is hampered by the high reactivity of their aldehydic functions and by extraction and purification procedures that are expensive, low-yielding, and reliant on organic solvents harmful to both the environment and operators. Here we describe a fully green strategy to obtain and purify two novel EVOO-derived compounds, named thiocanthal and thiocanthol. By mixing EVOO with a dilute sodium metabisulfite solution, a sulfonate group is regioselectively introduced at the C-3 aldehyde of oleocanthal and oleacein, inverting their polarity and yielding water-soluble products while protecting the aldehydes from hydration and acetalization. The two derivatives were isolated from the aqueous phase through a two-step, organic-solvent-free chromatographic strategy exploiting anion-exchange and boronate-affinity resins, and were fully characterized by HR-MS, MS/MS, FT-IR and NMR.[2] The COX-inhibitory activity of thiocanthal and thiocanthol, assessed in vitro, proved comparable to that of their precursors and markedly higher than that of the reference NSAID ibuprofen (≈50 % inhibition at 50 μM). At the same concentration, thiocanthal inhibited COX activity by ≈60 %, as did oleocanthal, while thiocanthol reached ≈87 % inhibition, close to that of oleacein. Molecular docking studies further predicted a preferential binding to COX-2 for both derivatives, suggesting a potentially favourable selectivity profile. This inexpensive and eco-friendly process represents a novel route for the sustainable production of secoiridoid derivatives, making thiocanthal and thiocanthol attractive both as bioactive compounds *per se* and as lead compounds for the development of new selective COX-2 inhibitors.



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O16: Preventive Blood Pressure Control with Oleuropein-Standardized Olive Leaf Extract and Potassium

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Elevated blood pressure is a leading modifiable driver of cardiovascular risk and often develops gradually before pharmacological treatment becomes necessary. Preventive nutritional strategies that support early blood pressure control are therefore of particular interest. Olive leaf extract (OLE), standardized for the secoiridoid oleuropein, has been associated with vasoprotective, antioxidative, and antihypertensive effects, while potassium contributes to normal blood pressure maintenance through natriuretic and vascular mechanisms. Their combined use may offer a complementary approach to early cardiovascular prevention. In a randomized, double-blind, placebo-controlled trial, 70 adults with untreated mildly to moderately elevated blood pressure received OLE (1000 mg/day, ≥160 mg oleuropein) plus potassium (300 mg/day) or placebo for 12 weeks. Seven-day home blood pressure monitoring revealed consistent treatment effects in favour of the active combination. Morning systolic blood pressure decreased by 5.4 mmHg in the verum group, with a significant between-group advantage versus placebo; evening home measurements further supported systolic and diastolic improvements. In addition, the combination reduced total cholesterol by 11.1 mg/dL and LDL-cholesterol by 6.9 mg/dL, lowered triglycerides by approximately 22 mg/dL at Week 6 and decreased oxidized LDL by about 23%. The intervention was well tolerated, with no product-related serious adverse events and no evidence of electrolyte imbalance. These findings support oleuropein-standardized OLE plus potassium as a safe, mechanistically plausible nutraceutical strategy for preventive blood pressure control and early cardiovascular risk reduction.[1]

No conflicts of interest have to be declared.

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O17: Stem and Root Decoctions of Cucumis prophetarum L. Improve Insulin Sensitivity and Metabolic Dysfunction in Experimental Models of Insulin Resistance and Type 2 Diabetes

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Type 2 diabetes mellitus (T2DM) is a metabolic disorder characterized by progressive pancreatic β-cell dysfunction and systemic insulin resistance driven by chronic metabolic stress, ultimately leading to the loss of functional β-cell mass and impaired glycemic control. Despite the availability of pharmacological treatments, their limited long-term efficacy and associated adverse effects have stimulated growing interest in plant-derived bioactive compounds as complementary or alternative strategies for metabolic diseases management. In this context, the present study investigated the metabolic potential of decoctions prepared from the leaves, stems, and roots of *Cucumis prophetarum* L., using both combined in vitro and in vivo approaches. Phytochemical characterization by UV–Vis, ATR-FTIR, and UHPLC-ESI-QqTOF HR-MS/MS analyses revealed distinct organ-specific metabolite profiles. In an in vitro model of palmitic acid-induced insulin resistance in L6 rat myoblasts, stem and root decoctions significantly reduced intracellular lipid accumulation and restored insulin signaling through modulation of the IRS1/PI3K/AKT and AMPKα/mTOR pathways, with the root decoction exhibiting the strongest biological activity. Based on these in vitro findings, the stem and root decoctions were selected for further evaluation in a rat model of T2DM. Treatment with both decoctions attenuated diabetes-induced body weight loss and mitigated alterations in metabolically active tissues by reducing liver mass, preventing skeletal muscle wasting, and preserving pancreatic mass, indicating an overall improvement in metabolic status. Moreover, both treatments significantly enhanced insulin sensitivity and glucose tolerance, as demonstrated by the Insulin Tolerance Test (ITT) and Intraperitoneal Glucose Tolerance Test (IPGTT). Given the central role of pancreatic β-cell dysfunction in T2DM pathogenesis, pancreatic function was also assessed: both decoctions improved pancreatic function while reducing oxidative stress and inflammation in diabetic animals. Collectively, these findings identify stem and root decoctions of Cucumis prophetarum L. as promising candidates for the management of T2DM and support their further investigation as phytochemical-based strategies.

O18: Wound Healing and Antimicrobial Potential of *Agrimonia eupatoria* L.

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Agrimonia eupatoria L. is a perennial herbaceous plant traditionally used in European and Asian medicine. According to the European Union herbal monograph (EMA/HMPC/680597/2013), Agrimony herb is indicated for the symptomatic treatment of mild diarrhea, minor inflammatory conditions of the mouth, throat, and skin, and small superficial wounds. Experimental studies have shown enhanced re-epithelialization, extracellular matrix remodeling, and improved collagen maturation following treatment with *A. eupatoria* extracts[1]. The plant also exhibits antimicrobial and antibiofilm activity against clinically relevant pathogens, including *Staphylococcus aureus* and *Pseudomonas aeruginosa*[2].

In our experiments, *A. eupatoria* extract modulated fibroblast behavior in murine 3T3 cells and primary human dermal fibroblasts, promoting fibroblast-to-myofibroblast differentiation. Antimicrobial activity was evaluated by broth microdilution using aqueous, methanolic (MeOH), and 50% MeOH extracts and their butanol and aqueous fractions. Isothermal microcalorimetry was used to confirm bacterial growth inhibition.

The highest antimicrobial activity was observed against *Staphylococcus aureus* (MSSA and MRSA), with MIC values ranging from 0.62 mg/mL for the butanol fraction of the MeOH extract to >20 mg/mL for the aqueous fraction. *Enterococcus faecalis* showed moderate susceptibility, whereas Gram-negative bacteria were less susceptible. *Escherichia coli* was resistant (MIC >20 mg/mL), while moderate activity was observed against *Pseudomonas aeruginosa* and *Proteus mirabilis*. *Candida albicans* was not susceptible to the tested extracts. Overall, antimicrobial activity decreased in the order: MeOH extract > 50% MeOH extract > aqueous extract.

These findings demonstrate that antimicrobial activity depends on the extraction solvent, extract fraction, and target microorganism, with Gram-positive bacteria generally showing greater susceptibility.

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O19: Natural Products in the Search for Novel Anticancer Agents: Bridging Discovery and Mechanistic Insights

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Natural products have consistently represented one of the most prolific and enduring sources of anticancer drug discovery. A substantial proportion of the chemotherapeutic agents used in modern oncology—including vincristine, vinblastine, irinotecan, paclitaxel and its analogues, as well as etoposide derivatives—originate directly from plant-derived natural products or have been developed as semisynthetic derivatives. Likewise, soil-dwelling microorganisms have yielded numerous clinically important anticancer agents, including the anthracyclines doxorubicin (Adriamycin), daunorubicin, and dactinomycin, the glycopeptide bleomycin, and the macrolide rapamycin.

The remarkable contribution of natural products to oncology is further underscored by the fact that, among the 184 small-molecule anticancer drugs approved by the U.S. Food and Drug Administration between 1981- 2019 (excluding biological macromolecules and vaccines), 155 (84%) are natural products, their derivatives, or agents inspired by natural product scaffolds[1].

Our research has focused on the discovery and mechanistic characterization of anticancer natural products from diverse botanical and fungal sources, including *Juncus heldreichianus* subsp. *heldreichianus*, *Achillea multifida* Griseb., and *Ganoderma lucidum* Karst. Beyond evaluating their cytotoxic potential, we have isolated and structurally characterized bioactive secondary metabolites responsible for the observed activities and elucidated the molecular mechanisms underlying their anticancer effects.

In this presentation, the anticancer potential of selected plant and fungal extracts, together with their bioactive constituents, will be highlighted, and the mechanistic pathways through which they exert their anticancer activities will be discussed.

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O20: Phytochemical Investigation and Anti-inflammatory Activity of Bachtiari Savory (*Satureja bachtiarica* Bunge) Root.

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Satureja bachtiarica Bunge is an endemic plant from Lamiaceae family, growing in the Zagros mountain range of Iran.[1,2] Even if numerous reports highlighting the biological activities of *S. bachtiarica*,[3] the chemical composition of its roots remains essentially unexplored. For this reason, in the present research, a phytochemical investigation of this species and specific tissue was carried out.

Air-dried plant material was extracted by maceration at room temperature using EtOH/H_2O (7:3, v/v). The extract was then partitioned between *n*-butanol and water to remove free sugars. To have a preliminary metabolite profile of *S. bachtiarica* roots, the *n*-BuOH extract was analyzed by LC-ESI/LTQOrbitrap/MS/MS in negative ion mode, allowing the identification of specialized metabolites belonging to flavonoid, monoterpene, phenylpropanoid, phenolic, fatty acid, and triterpene classes. The LC-MS/MS analysis guided the isolation of compounds and their structures were characterized by spectroscopic methods including 1D- and 2D-NMR experiments and $HRMS^n$ analysis. Furthermore, antioxidant activity of the extract by DPPH and TEAC assays have been carried out. Moreover, given the presence of triterpenes structurally related to tormentic acid, which are known for their anti-inflammatory properties, the anti-inflammatory activity of the extract, the enriched fraction, and selected pure compounds was evaluated. All of the samples were tested at a concentration of 100 µg/mL for their ability to inhibit cyclooxygenase enzymes (COX-1 and COX-2) using a colorimetric assay, with meloxicam used as the reference inhibitor. The results indicate that the EtOH extract of *S. bachtiarica* roots exhibited moderate inhibition of COX-1 but no inhibitory activity toward COX-2. In contrast, several fractions and isolated triterpenes obtained from the extract showed markedly higher COX-2 inhibition. Consequently, the roots of *S. bachtiarica* may represent a promising natural source of bioactive compounds with potential health benefits, warranting further clinical investigations to explore their pharmaceutical applications.

Keywords*: Satureja bachtiarica* Bunge; LC-HRMS/MS; NMR analysis; Anti-inflammatory activity, COX-1 and COX-2 activity

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O21: Bioactivity-Linked Profiling of Plant Extracts with Inhibitory Effects on Photosystem II and Early Seedling Growth

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The progressive loss and regulatory restriction of conventional herbicidal active substances are narrowing the range of compounds available for weed management. The demand for more sustainable crop-protection strategies is increasing,[1] and plant natural products offer a structurally diverse and largely underexplored source of bioactive compounds. An established target for compounds affecting plant growth and development is the photosystem II, a central component of photosynthetic electron transport.[2]

In this study, selected plant extracts were investigated for the effects on photosystem II-mediated electron transport and early plant development. The extracts from aerial parts of different plant species, including *Artemisia* and *Plantago*, were prepared using 80% aqueous ethanol. The ability to inhibit light-dependent electron transport was evaluated using isolated chloroplasts and the Hill reaction assay. The inhibitory effects of extracts were compared with those of selected synthetic herbicides. Extracts having a pronounced effect were further investigated by chromatographic fractionation and bioactivity-linked chemical profiling using LC-HRESIMS and GC-MS. Linking observed bioactivity to the metabolite profiling represents a useful strategy for prioritizing potentially relevant lead structures in plant extracts, without requiring prior isolation of individual compounds.[3] Selected extracts were additionally evaluated in whole-plant bioassays using *Arabidopsis thaliana*. Effects on seed germination and short-term seedling growth were assessed by determining germination, primary root length, and fresh biomass after eight days of exposure.

Several extracts caused a concentration-dependent inhibition of photosystem II-mediated electron transport, with IC_{50} values ranging from approximately 23 µg/mL to 470 µg/mL. Selected extracts also showed extract-dependent effects on early seedling growth, reducing primary root length by 53%–82%.

These findings highlight selected plant extracts as promising sources of natural products affecting photosynthetic electron transport and early plant development, thereby providing a basis for further research in the context of sustainable weed management.

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O22: Nuclear Power Plants: For or Against? Analysis of Radiocarbon, Bioactivity, and Metabolic Profile in Crops Near Nuclear Power Plants

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Carbon-14 (^{14}C) is a naturally occurring radionuclide that enters the biosphere through atmospheric CO_2 fixation by plants. Nuclear power plants (NPPs) also release small amounts of ^{14}C during routine operations, raising concerns about its transfer through agricultural systems and potential implications for food safety [1]. Onion (*Allium cepa* L.) and tomato (*Solanum lycopersicum* L.), two economically important crops in Europe [2], were selected as bioindicators to investigate the influence of NPP proximity on radiocarbon accumulation.

This study evaluated the ^{14}C content of onion and tomato samples collected around the main NPPs in Spain, *i.e.* Almaraz, Ascó, and Trillo. Radiocarbon levels were determined by Accelerator Mass Spectrometry (AMS), while untargeted metabolomic profiling was performed using UPLC-QTof-MSE coupled with Progenesis QI software. In addition, phytotoxicity and cytotoxicity assays were conducted using etiolated wheat coleoptiles and HeLa cells, respectively [3].

Crops collected near the Almaraz NPP exhibited slightly elevated $F^{14}C$ values compared with contemporary atmospheric reference values ($P< 0.0001$), whereas samples from Ascó and Trillo showed $F^{14}C$ values consistent with current atmospheric background levels. Despite these localized variations, no significant differences in metabolomic profiles were associated with proximity to NPPs. Similarly, phytotoxic and cytotoxic activities were observed in several extracts but did not correlate with radiocarbon content. The estimated annual effective dose resulting from ^{14}C ingestion through onion and tomato consumption was negligible compared with internationally accepted radiation protection limits.

Metabolomic analyses revealed diverse classes of bioactive compounds in both crops; however, their variability appeared to be primarily influenced by intrinsic plant characteristics and environmental factors rather than by radiocarbon exposure. This study constitutes the first report on ^{14}C levels in crops cultivated near Spanish NPPs and indicates that, under the conditions evaluated, routine ^{14}C emissions would not pose a detectable radiological risk to crops or consumers.

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O23: Organ-Specific Lipophilic Metabolites In *Euphorbia peplis*: A Coastal Dune Species From Portugal

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Euphorbia peplis L. is a Near Threatened (NT) annual halophyte inhabiting embryonic coastal dunes, dynamic environments shaped by salinity, sand movement, high irradiance, wind exposure and nutrient limitation. Although *Euphorbia* is recognized for its terpenoid-rich phytochemistry, the organ-specific distribution of lipophilic metabolites in *E. peplis* remains poorly explored [1–3]. This study aimed to characterize the lipophilic fingerprints of leaves, stems and reproductive structures of wild *E. peplis* collected at Torrão do Lameiro beach, Portugal, during flowering and fruiting.

Dried organs were extracted with hexane, derivatized and analyzed by gas chromatography–mass spectrometry. The three organs showed distinct lipophilic signatures. Leaves were dominated by the long-chain fatty alcohol 1-octacosanol (~29%), followed by cycloartenyl, lanosterol, henicosanal, β-sitosterol and 24-methylenecycloartanol, suggesting a wax-related protective profile with relevant sterol/triterpenoid contribution. Stems displayed the strongest terpenoid/sterol-related signature, with cycloartenyl (~21%), 1-octacosanol (~13%), alkanes (~12%), 24-methylenecycloartanol (~11%), lanosterol (~10%) and β-sitosterol (~5%) as major constituents. This profile highlights stems as a key compartment of sterol/triterpenoid-related lipophilic specialization in *E. peplis* [3,4]. In contrast, reproductive structures were dominated by polyunsaturated fatty acids, especially α-linolenic (~42%) and linoleic acids (~15%), consistent with reproductive lipid demands, membrane dynamics and seed-associated reserves [5].

Overall, *E. peplis* showed clear organ-specific metabolic allocation [6]: leaves were characterized by wax-related protection, stems by terpenoid/sterol specialization, and reproductive structures by a PUFA-rich profile. These findings provide new insight into the phytochemical and ecological relevance of underexplored coastal *Euphorbia* species and support future comparative studies across dune habitats and targeted bioactivity assays.

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O24: Polyketides from *Trichoderma koningii* structural characterization by NMR and biological evaluatiom

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Endophytic fungi represent an important reservoir of specialized metabolites involved in plant–microbe interactions and are increasingly explored as sources of bioactive compounds for sustainable crop protection.[1] *Trichoderma spp*. are widely recognized as plant-associated fungi capable of establishing beneficial interactions with their host plants and the surrounding rhizosphere, thereby enhancing plant performance through a complex network of biological activities, including root colonization and competition with deleterious microorganisms.[2,3,4] These biological activities are largely mediated by the remarkable chemical diversity of specialized metabolites produced by *Trichoderma* species.

Within this context, the present study investigated the specialized metabolite profile of the endophytic fungus *Trichoderma koningii*, with particular emphasis on the phytotoxic activity of its metabolites and their potential relevance for weed management and sustainable agricultural applications.

To investigate its specialized metabolites, the hydroalcoholic extract obtained from the solid culture of *T. koningii* was sequentially partitioned with dichloromethane and ethyl acetate.

Following an initial phytotoxicity screening, using a coleoptile bioassay, which revealed promising activity in the dichloromethane fraction, a bioassay-guided fractionation approach using the same test, was undertaken. In this way three bioactive sub-fractions (D-F), were selected, and the most active one (-72% of inibition) was tested for further phytotoxic activity evaluation against cultivated (*Lactuca Sativa)* and weed plant species (*Portulaca oleracea*, *Lolium rigidum*, *Plantago lanceolata),* showing excellent growth inhibition agains*t Plantago lanceolata* (weed) and no inhibition against *Lactuca sativa* (cultivated).[5]

Based on the results the subfraction was purified by a combination of chromatographic techniques. The chemical structures of six metabolites have been elucidated by extensive spectroscopic analyses, including 1D and 2D NMR experiments (HSQC, H2BC, HMBC, and NOESY). Structural characterization revealed three polyketide derivatives bearing a tetrahydrobenzofuran-4(2H)-one scaffold, two koninginin-type polyketides, and one cyclonerale-type sesquiterpene. All isolated compounds will be evaluated for their phytotoxic activity against both weed and cultivated plant species.[5] These findings further expand the current knowledge of the chemical diversity of *T. koningii* and highlight its production of phytotoxic polyketides as a promising source of natural products for the development of sustainable weed management strategies.

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O25: Qualitative and quantitative characteristics of domesticated, commercial, and collected European *Gentiana* species

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Gentiana species, native to Europe, are deeply embedded as cultural and ecological symbol in the Alpine region. Some species are heavily utilized, not only for production of bitter beverages, but also for valuable medicinal purposes. Formally recognized in the European Pharmacopoeia, ESCOP, and HMPC monographs to treat dyspeptic complaints and stimulate appetite, *G. lutea* is currently the only permitted gentian species for official pharmaceutical use. To ensure quality of the root drug, the pharmacopoeia requires a bitterness value above 10,000, but does not specify tests to detect alterations. *G. lutea* root extracts are characterized by a complex metabolite pattern including a high carbohydrate content, xanthones, and bitter secoiridoids. To enable a quantitative comparison of secondary metabolite patterns across different species, an efficient and rapid UHPLC-method was developed. A total of 45 samples were analysed, encompassing five *Gentiana* species (*G. lutea*, *G. scabra*, *G. punctata*, *G. purpurea*, and a hybrid of the latter), samples of two cultivated *G. lutea* subspecies (ssp. *lutea* and ssp. *vardjanii*), as well as 15 commercial *G. lutea* samples. The optimized method successfully separated eight secondary metabolites within just six minutes and enabled the quantification of loganic acid, swertiamarin, gentiopicroside, sweroside, amarogentin gentioside, gentisin-7-glycoside, and two xanthones. A principal component analysis based on the quantification results revealed that commercial *G. lutea* samples formed a distinct group due to the content of loganic acid, sweroside, and the jointly quantified xanthones gentisin and isogentisin; but it could not be used as a tool for detecting adulteration. Therefore, the method was transferred to a UHPLC-HRMS/MS system, the samples were re-analysed, and the data obtained in positive ionization mode were visualized and evaluated using feature-based molecular networking. Through statistical analyses and bioinformatics-based annotation of detected compounds, markers were identified, with amaropanin emerging as a potential candidate to distinguish between gentian species.

O26: From Plant Biotechnology to Molecular Recognition: Papaveraceae Isoquinoline Alkaloids as Promising Bioactive Phytochemicals

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Papaveraceae plants are an important source of structurally diverse isoquinoline alkaloids (IQAs), responsible for many of the pharmacological properties. While several IQAs have attracted considerable attention due to their antimicrobial and therapeutic activities, their biosynthesis, biological functions, and interactions with molecular targets remain incompletely understood. Our research integrates plant biotechnology, phytochemistry, spectroscopy, and computational chemistry to investigate the production, biological activity, and molecular behavior of selected isoquinoline alkaloids. Using *in vitro* tissue and organ cultures together with cultivated plants, we monitored the biosynthesis and accumulation of isoquinoline alkaloids in *Chelidonium majus* and selected representatives of *Corydalis*, and *Fumaria* genera. Their antimicrobial activity was evaluated against clinically relevant *Candida* spp. and pathogenic bacteria, including biofilm-forming strains. In addition, a biohybrid culture system based on bacterial nanocellulose was developed to immobilize *C. majus* cells, providing a promising platform for stimulating secondary metabolite production and enhancing antimicrobial properties. To better understand the pharmacological potential of these metabolites, we investigated the interactions of less explored protopine and allocryptopine, with biological macromolecules using UV-Vis and fluorescence spectroscopy, circular dichroism, competitive binding assays, molecular docking, and quantum chemical calculations. Both compounds formed spontaneous and stable complexes with human serum albumin and α1-acid glycoprotein without altering protein secondary structure, suggesting favorable transport properties. Furthermore, they interacted selectively with duplex DNA through groove binding while preserving the native B-DNA conformation. DNA complex formation resulted in a pronounced fluorescence enhancement, indicating their potential as naturally derived fluorescent DNA probes. Our findings demonstrate that Papaveraceae alkaloids combine efficient biosynthetic accessibility, significant antimicrobial activity, favorable interactions with plasma proteins, and selective DNA recognition. These properties highlight their potential for future pharmaceutical, biotechnological, and bioimaging applications, while also emphasizing the contribution of other specialized metabolites, particularly polyphenols, to the overall biological activity of medicinal Papaveraceae species.

O27: Anti-inflammatory Activity-guided Isolation of Phenolic Compounds from *Hypericum salsugineum* N.Robson & Hub.-Mor.

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The genus *Hypericum* (Hypericaceae) comprises 521 species worldwide, many of which are traditionally used for their wound-healing, mild antidepressant, anti-diarrheal, analgesic, and febrifuge properties.[1,2] Bioactivity studies on this genus showed a wide variety of biological activities, such as antioxidant, antiviral, antibacterial, anti-inflammatory, cytotoxic, and analgesic effects, whereas phytochemical studies revealed a diverse array of secondary metabolites, including flavonoids, naphthodianthrones, phloroglucinols, benzophenones, xanthones, and phenolic acids.[3,4] *H. salsugineum*, a halophyte plant endemic to Türkiye, with a very limited number of studies based on LC-ESI-MS analysis of extracts, antioxidant activity, and enzyme inhibition assays.[5,6] However, these studies have failed to identify the specific secondary metabolites that may be responsible for its biological activities. As a part of our ongoing research on *Hypericum* species growing wild in Türkiye, this study focused on isolating metabolites with anti-inflammatory activity from *H. salsugineum*, via bioassay-guided fractionation. The aerial parts were extracted with EtOH, and then PE, EtOAc, *n*-BuOH, and H_2O subextracts were obtained through partition. The inhibitory effects of the EtOH extract, subextracts and their main fractions on nitric oxide production in RAW 264.7 cells were evaluated at 1 mg/mL using the Griess assay. Amongst, H_2O fractions exerted the most potent nitrite inhibitions (30-56 %), followed by *n*-butanol fractions (25-40 %). Chromatographic separations on H_2O and *n*-butanol fractions led to the isolation and identification of chlorogenic acid (**1**), cynarin (**2**), 1,5-dicaffeoylquinic acid (**3**), 3,5-dicaffeoylquinic acid (**4**), salidroside (**5**), 1,6-disinopylglucoside (**6**), 5-*p*-trans-coumaroylquinic acid (**7**), and myricetin 3-*O*-glucoside (**8**). Additionally, myricetin (**9**), I3,II8-biapigenin (**10**), quercetin (**11**) and toxyloxanthone B (**12**) were isolated from EtOAc subextract. Evaluation of the inhibitory effects of the isolates on NO, PGE_2, TNF-α, and IL-6 production is currently underway.

Keywords: *Hypericum*, anti-inflammatory activity, activity-guided isolation
Acknowledgment: This study was supported by TÜBİTAK (Project number: 225S382)

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O28: Activity-guided Isolation of Anti-inflammatory Secondary Metabolites from *Thliphthisa antalyensis* (Ehrend.) P.Caputo & Del Guacchio

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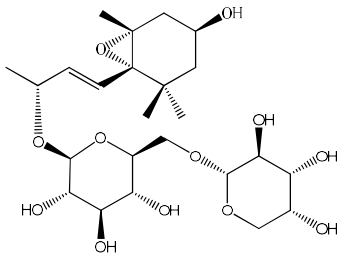
The genus *Thliphthisa* (Rubiaceae), comprising 23 species worldwide, was formerly placed in *Asperula* (sect. *Thliphthisa*) and subsequently reclassified as a separate genus based on phylogenetic evidence.[1] This study aims to isolate anti-inflammatory compounds from *T. antalyensis* through *in vitro* activity-guided fractionation. The whole plant of *T. antalyensis* was extracted with EtOH. The crude extract was dispersed in H_2O and then partitioned against *n*-hexane, $CHCl_3$, EtOAc, and *n*-BuOH, respectively, to yield solvent fractions. The crude extract, solvent fractions, and main fractions were tested for their *in vitro* nitric oxide (NO) inhibitory activities in LPS-induced RAW 264.7 cells. The *n*-hexane, EtOAc, and *n*-BuOH fractions exhibited remarkable inhibition of NO production, with rates of 67.8%, 80.5%, and 51.3%, respectively, at a concentration of 1 mg/mL. Among the main fractions, frs. I and III from *n*-hexane fraction, frs. 2 and 3 from EtOAc fraction, and frs. B and C from *n*-BuOH fraction displayed NO inhibition ranging from 53.1 to 70.3% at the same concentration. Chromatographic separations of the active fractions by MPLC (C_{18} and SiO_2) and Sephadex LH-20 CC afforded 11 secondary metabolites, namely (*E*)-10-(3,4-dihydroxycinnamoyloxy)loganin (**1**)**,** urolignoside (**2**), an inseparable 1:1 mixture of *rel*-(7*R*,8*S*)-3,3',5-trimethoxy-4',7-epoxy-8,5'-neolignan-4,9,9'-triol 4-*O*-*β*-D-glucopyranoside (**3**) and scorzonoside (**4**), hyperoside (**5**), quercetin 3-*O*-sophoroside (**6**), ursolic acid (**7**), chlorogenic acid (**8**), ferulic acid 4-*O*-*β*-D-glucopyranoside (**9**), hexacosyl-(*E*)-ferulate (**10**), and 1-hexacosanol (**11**). Additionally, nine compounds, including a new megastigmane glycoside (**12**), were isolated from the less-active fractions. Structures of isolates were elucidated by NMR and HR-MS analyses. Compounds **1**, **6**, **7**, and **10** exhibited NO inhibitory activity at 200 µM, with IC_{50} values in the range of 104.53–168.49 µM, without significant cytotoxicity to RAW 264.7 cells. Their effects on TNF-α, IL-6, PGE_2 release, and COX-2 expression were also evaluated. This is the first phytochemical and bioactivity study on *T. antalyensis*, an endemic species to Türkiye.



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Keywords: *Thliphthisa antalyensis*, anti-inflammatory activity, secondary metabolites
Acknowledgement: This study was financially supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK, Project No: 125Z178).

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O29: From Waste to Bioactives: Metabolomics-Driven Valorization of *Cynara cardunculus scolymus* ('Carciofo di Paestum' PGI and 'Carciofo Bianco di Pertosa') leaf

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Globe artichoke (*Cynara cardunculus* subsp. *scolymus* L., Asteraceae) is a Mediterranean crop recognized as a functional food for its high content of minerals, bioactive phenolic compounds, and inulin.[1] Its cultivation and industrial processing generate substantial waste, with leaves accounting for 80–85% of the total biomass.[2] This study investigated the leaf of two cultivar of Campania region (Italy), 'Carciofo di Paestum' PGI and 'Carciofo Bianco di Pertosa', as sources of bioactive compounds.

Hydroalcoholic extracts (EtOH/H_2O 50:50 and 75:25) obtained by maceration from *C. cardunculus* 'Paestum' leaf were investigated for their phytochemical composition and antioxidant activity. The extracts exhibited high antioxidant capacity in TEAC, DPPH and FRAP assays and dose-dependent scavenging activity of reactive oxygen species in Caco-2 cells. To identify the metabolites responsible for these activities, LC-ESI/LTQ-Orbitrap/MS/MS analysis was performed, revealing metabolites belonging to the classes of sesquiterpenes, megastigmanes, quinic and hydroxycinnamic acid derivatives, flavonoids, lignans, triterpenoid saponins, and polar fatty acids), whose structures were confirmed by isolation and 1D- and 2D-NMR structure elucidation. To improve metabolite recovery, maceration was compared with ultrasound-assisted extraction (UAE) and Solid–Liquid Dynamic Extraction (SLDE-Naviglio). Principal Component Analysis (PCA) identified SLDE-Naviglio with EtOH/H_2O 75:25 as the most efficient extraction method, subsequently applied to *C. cardunculus* 'Bianco di Pertosa' leaf. LC-ESI/LTQ-Orbitrap/MS/MS and NMR analyses revealed, along with metabolites already characterized in *C. cardunculus* 'Paestum' leaf, several sesquiterpene lactones, including the previously undescribed chlorinated guaiane-type sesquiterpene lactone (pertosin A). Given the reported anti-photoaging activity of the sesquiterpene lactone cynaropicrin,[3] the extract and isolated sesquiterpenes were evaluated for tyrosinase inhibition. The extract showed IC_{50} = 55 µg/mL, among the isolated compounds, pertosin A (IC_{50} = 139 µM) exerted activity comparable to kojic acid (IC_{50} = 134 µM), commonly used as skin whitening. These findings support the sustainable use of *Cynara cardunculus* leaf for nutraceutical and cosmetic applications.

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O30: Chemical composition, oxidative stability and nutraceutical potential of cold-pressed pomegranate, blackcurrant and prickly pear seed oils

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Cold-pressed seed oils are promising nutraceutical ingredients owing to their unique fatty acid composition and diverse minor bioactive constituents. However, their biological properties depend not only on polyunsaturated fatty acid (PUFA) content but also on the balance between endogenous antioxidants and lipid unsaturation.[1] This study compared the chemical composition, oxidative stability and biological activity of cold-pressed pomegranate (*Punica granatum*), blackcurrant (*Ribes nigrum*) and prickly pear (*Opuntia ficus-indica*) seed oils together with phenolic-, tocopherol/carotenoid- and phytosterol-rich fractions isolated from the same oils.

Fatty acids, tocopherols, carotenoids, phytosterols and phenolic compounds were determined using GC-MS/MS, GC-MS, HPLC and UPLC-MS/MS. Oxidative stability was evaluated by differential scanning calorimetry (DSC), while biological activity was assessed in colon-derived cell models by determining cell viability, apoptosis, intracellular reactive oxygen species (ROS) generation and Rhodamine 123 accumulation.

Pomegranate seed oil contained the highest PUFA level (89.97%) and the greatest amount of quantified phenolic compounds (327 mg/kg), but also the lowest lipophilic antioxidant-to-PUFA ratio (5.92), resulting in the poorest oxidative stability. In contrast, blackcurrant seed oil contained the highest concentration of tocopherols (1650 mg/kg) and carotenoids (483 mg/kg), providing the greatest oxidative stability at elevated temperatures despite its high PUFA content. Prickly pear seed oil exhibited the highest oxidation induction time at 100°C and the highest activation energy (135 kJ/mol), indicating superior resistance to oxidation under moderate thermal conditions. Oils with greater oxidative susceptibility induced stronger ROS generation and apoptosis, whereas antioxidant-rich systems showed more moderate biological responses. Phenolic-rich fractions from pomegranate and blackcurrant oils exhibited the highest integrated biological activity.

These findings demonstrate that the nutraceutical value of cold-pressed seed oils is governed by the interaction between fatty acid composition, endogenous antioxidants and the native lipid matrix rather than by PUFA content alone, highlighting the importance of comprehensive compositional characterization when developing functional food ingredients.

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O31: Life Cycle Assessment of Cascade Grape Pomace Valorisation: Environmental Evaluation of Cellulose Acetate Biofilm Formulations

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Grape pomace (GP), one of the major by-products of the wine industry, is a promising renewable feedstock for circular bioeconomy applications [1]. Although several studies have demonstrated the technical feasibility of recovering phytochemicals and producing bio-based materials from GP [2-4], only a limited number of studies have assessed the environmental performance of integrated cascade valorisation pathways using Life Cycle Assessment (LCA) [5,6]. This study evaluates the environmental sustainability of a cascade biorefinery through LCA by considering the sequential recovery of phytochemicals followed by the production of cellulose acetate (CA)-based biofilms.

The proposed process includes hot water extraction of anthocyanin- and phenolic-rich fractions, followed by cellulose isolation from the exhausted biomass, chemical acetylation, and biofilm fabrication via solvent casting. Three biofilm formulations were assessed: neat cellulose acetate, cellulose acetate containing supercritical fluid extraction (SFE)-derived extracts, and cellulose acetate functionalised with anthocyanins recovered from the same biomass. The objective was to quantify the environmental impacts associated with each formulation. The LCA was performed in accordance with ISO 14040/44 standards to identify the main environmental hotspots and quantify the contribution of each processing stage to the overall impact profile. Comparison of the three scenarios enabled the evaluation of the influence of different functional additives on the environmental profile of the biofilms, highlighting the trade-offs between phytochemical valorisation and process sustainability.

The results demonstrate that cascade GP valorisation enhances biomass resource efficiency by generating multiple value-added products, reducing waste generation, and distributing environmental burdens across different product streams. The study demonstrates the value of LCA as a decision-support tool for the design and optimisation of sustainable biorefineries and the development of bio-based materials from agro-industrial residues.

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O32: Cascade Valorisation of Grape Pomace for Nutraceutical Development and Functional Food Applications

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Grape pomace (GP), the main by-product of winemaking, is a valuable source of health-promoting phytochemicals and structural polysaccharides that can be exploited for the development of functional foods and sustainable food packaging [1]. This study proposes a cascade biorefinery strategy in which anthocyanins are first recovered for nutraceutical applications, while the residual biomass is subsequently valorised for the production of biodegradable packaging materials. Cascade valorisation of Piedirosso grape pomace was achieved through a low-impact aqueous extraction process, enabling the sequential recovery of malvidin 3-*O*-hexoside and the subsequent isolation of cellulose from the exhausted biomass. The recovered compounds were characterized by spectroscopic and mass spectrometric analysis. Malvidin 3-*O*-hexoside (94% purity) was incorporated into a prototype nutraceutical jelly confectionery to evaluate colour stability, antioxidant capacity and gastrointestinal bioaccessibility [2]. The jelly formulation maintained a stable red colour, exhibited a sustained release profile and high radical scavenging activity. Simulated gastrointestinal digestion showed a progressive release of the anthocyanin (37% in the oral phase and 55% in the gastric phase), followed by complete degradation during the intestinal phase, highlighting the need for future strategies to improve intestinal bioaccessibility. Consumer evaluation (n = 116) demonstrated good acceptability, particularly among younger participants and regular users of nutraceutical products [2]. Following phytochemical recovery, the exhausted grape pomace was further processed to isolate cellulose, which was acetylated to produce cellulose acetate. The resulting biopolymer was used to prepare edible biodegradable films plasticized with triacetin. Physicochemical, mechanical and antioxidant characterization demonstrated the suitability of the recovered cellulose as a sustainable material for active food-packaging applications. This cascade biorefinery approach demonstrates how grape pomace can be transformed into high-value nutraceutical ingredients and functional food-packaging materials, providing an integrated strategy for sustainable food innovation and supporting the principles of the circular bioeconomy.

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S1: From Oxidative Distress to Oxidative Eustress: Ozoile® as a Novel Redox Signaling Technology

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Ozoile® is a patented formula composed of oxygen-rich lipid molecules, called stable ozonides[1], obtained through an exclusive green technology developed by Erbagil®.

For many years, oxidative stress was considered exclusively a harmful phenomenon. Today, it is known that the biological response depends not simply on the presence of oxidant molecules, but above all on the quality, intensity, and duration of the oxidative signal reaching cells.

When this signal is intense, uncontrolled, and persistent, a condition called oxidative *distress* occurs, characterized by an excess of reactive oxygen species (ROS) that exceeds the capacity of the body's antioxidant defenses. The result is an alteration in the redox balance that promotes inflammation, cellular damage, and loss of normal physiological function. On the contrary, when the oxidative signal is moderate, controlled, and transient, it represents a physiological stimulus capable of activating the cell's natural adaptive responses. This condition is called oxidative *eustress.* This is precisely the principle underlying Ozoile® technology. Stable ozonides do not act as simple oxidant molecules, but as lipid messengers of oxidation. Thanks to their stability, they release a controlled redox signal that modulates oxidative stress without causing the damage typical of distress. The mild and transient disruption of the redox balance thus becomes a physiological stimulus capable of activating the body's adaptive responses and its natural antioxidant defenses, in particular by activating the transcription factor NRF2[2], one of the main regulators of the cellular response to oxidative stress.

The eustress induced by stable ozonides represents the biological signal that triggers a cascade of adaptive responses. In response to this moderate oxidative stimulus, the body activates its physiological defense, adaptation, and repair mechanisms.

This mechanism results in:

• Activation of endogenous antioxidant defenses[3, 4]

• Anti-inflammatory activity[3,4]

• Antimicrobial activity

• Regenerative and repair activity[4]

• Support for tissue oxygenation[4]

• Antiproliferative activity[5]

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S2: Combextracoffee: The combined use of Supercritical fluid and Subcritical Water Extraction for Spent Coffee Grounds as Sustainable Process for Developing Personal Care Products

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The large amount of spent coffee grounds (SCG) generated by the increasing global consumption of coffee represents a significant environmental challenge while also offering valuable opportunities within the framework of the circular economy [1]. The project aims to develop an integrated strategy for the valorization of this by-product through the sustainable extraction of bioactive compounds and their application in the development of innovative and eco-friendly cosmetic formulations.
The project focuses on the optimization of green extraction processes based on the combined use of supercritical carbon dioxide extraction (SFE) [2] and subcritical water extraction (SWE) [3] to obtain extracts rich in polyphenols, fatty acids, alkaloids, and other high-value bioactive compounds [4], while preserving their functional properties and maximizing extraction yield and selectivity.
The obtained extracts will be chemically characterized using chromatographic techniques and quantification of bioactive compounds. Their biological properties will be evaluated through in vitro bioscreening using epidermal and dermal cell models to assess biocompatibility as well as antioxidant, anti-inflammatory, and regenerative activities. Selected extracts will then be incorporated into sustainable cosmetic formulations, whose stability, safety, and efficacy will be evaluated using appropriate analytical methods.
Throughout the project, all process and analytical data will be digitally recorded and archived to ensure transparency, traceability, and comprehensive documentation of the entire valorization pathway, from spent coffee grounds to the final cosmetic formulations.
The proposed approach represents an integrated framework for the valorization of agri-food by-products, with the potential to support the development of functional ingredients and sustainable cosmetic formulations in line with the principles of the circular bioeconomy.

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POSTER COMMUNICATIONS

P1: Isolation and Structure Elucidation of Key Intermediates in the Biosynthetic Pathway of Paclitaxel

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Paclitaxel is one of the most widely prescribed chemotherapeutic agents, used in the treatment of breast, ovarian, cervical, nasopharyngeal, and non-small cell lung cancers. Originally isolated from the inner bark of the Pacific yew (*Taxus brevifolia*), sourcing paclitaxel from natural material is unsustainable. While total chemical synthesis has been elegantly demonstrated, it remains commercially unviable owing to low yields and synthetic complexity. Industrial production relies on *Taxus* cell cultures or semi-synthesis from plant-derived precursors, methods that are costly and inefficient. Conversely, biotechnological production in heterologous systems could offer a cost-effective and sustainable alternative to current paclitaxel supply routes, but progress has been hindered by an incomplete understanding of its biosynthetic pathway.

In the framework of our investigations, we aimed to reconstruct paclitaxel biosynthesis in *Nicotiana benthamiana* (tobacco). A persistent challenge in prior studies has been the potential contribution of endogenous host enzymes, particularly in transient plant expression systems, leading to product assignments that may reflect background metabolic activity. Another limitation has been the absence of enzyme validation through isolation and structural characterization of pathway intermediates. To overcome these limitations, we systematically corroborated key steps in *Saccharomyces cerevisiae* (yeast) as an orthogonal host, distinguishing genuine pathway reactions from host-derived artifacts. Significant effort was paid to provide direct chemical validation of enzyme activities. The latter was achieved by the isolation of eight key pathway intermediates and one side-product through multiple steps of chromatographic separations and unambiguous structure elucidation of these previously undescribed taxanes on the basis of extensive analysis of their NMR spectroscopic data.

P2: Comparative Analysis of the Essential Oil of *Solidago virgaurea* L. from Greece and Bulgaria

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The genus *Solidago* (Asteraceae), commonly known as goldenrod, comprises *c.* 140 species distributed mainly in North America, while a limited number of species, including *Solidago virgaurea* L. (European goldenrod), are native to Europe and temperate Asia.[1,2]

Traditionally, *S. virgaurea* has been used against urinary tract infections, overactive bladder syndrome, prostate and kidney disorders. The aerial parts of the plant were also used for their antiseptic properties in allergies, diabetes, and gastrointestinal disorders.[3]

The genus is characterized by a wide spectrum of secondary metabolites, such as flavonoids, phenolic acids, terpenes and acetylenic derivatives, that contribute to the anti-inflammatory, diuretic, and antimicrobial properties attributed to the genus.[4]

Object of the present study was the comparative analysis of the essential oils obtained by hydrodistillation of the aerial parts of a Greek and a Bulgarian sample of *S. virgaurea*, analyzed by GC and GC-MS. Significant qualitative differences were observed between the two samples, the most notable being the presence of acetylenic derivatives (56.6%) in the sample of Bulgarian origin, with methyl lachnophyllate as the main representative, which was isolated and spectroscopically identified. This metabolite was isolated and identified for the first time from the genus *Solidago*.

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P3: NMR-Based Metabolomics as a Starting Point for the Identification of Natural Products Targeting Colorectal Cancer Cells

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Colorectal cancer (CRC) remains a major global health challenge due to drug resistance and the limited efficacy of conventional therapies.[1] Among the signalling pathways involved in CRC progression, the MAPK cascade represents a central regulatory network controlling tumour growth and adaptation. Although ERK1/2 mutations are relatively uncommon in colorectal cancer, constitutive ERK activation frequently results from upstream oncogenic alterations involving *KRAS*, *NRAS*, *BRAF* and receptor-mediated signalling pathways such as *EGFR*. Multiple oncogenic inputs therefore converge toward persistent ERK1/2 activation, establishing ERK as a critical signalling bottleneck in colorectal tumorigenesis.[2]

Upon phosphorylation in the cytosol, ERK1/2 translocates into the nucleus, where it activates transcription factors regulating genes involved in cell-cycle progression, proliferation, survival, metabolic adaptation and stress responses. This cytosol-to-nucleus signalling axis converts oncogenic stimuli into stable transcriptional programs that sustain tumour maintenance and therapy resistance. Since inhibition of upstream targets often leads to compensatory pathway reactivation, direct ERK modulation may represent a more effective strategy to suppress tumour-promoting mechanisms.[3] In this context, Mediterranean flora represents an exceptional and underexplored source of structurally diverse specialized metabolites with potential anticancer activity and this work proposes an integrated platform to identify natural compounds capable of modulating ERK1/2 signalling and limiting its downstream effects in CRC.

Following untargeted NMR metabolomics profiling and preliminary extract fractionation, extracts and fractions will be screened through *in vitro* viability assays against CRC cell lines. The most active fractions will undergo *Western blot* analyses to evaluate their effects on ERK1/2 phosphorylation and downstream nuclear targets. Subsequently, active samples will be investigated through *ligand fishing* to isolate ERK1/2-interacting compounds.[4] Structural characterization will combine mass spectrometry and advanced NMR experiments (1D, 2D and in-solution NMR).[5,6]

Preliminary NMR metabolomics revealed a remarkable richness of secondary metabolites, including terpenoids, flavonoids and phenylpropanoids. The plant extracts will now undergo biological activity screening with the aim to identify sources of novel anticancer agents. Furthermore, this study will establish a target-oriented strategy overcoming the limitations of upstream MAPK pathway inhibition in CRC.

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P4: Structural Elucidation through NMR Analysis of Specialized Metabolites from *Myrtaceae* plants and Evaluation of their Antimicrobial Activities.

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Myrtaceae represents one of the most significant flowering plant families in the world, with numerous genera of considerable ecological and economic importance and a cosmopolitan distribution spanning multiple tropical and subtropical regions[1]. Among numerous plants belonging to this family there are species well known for their anti-inflammatory, antioxidant and antiseptic properties. At the base of their biological activities there is a wide range of bioactive specialized metabolites produced by these genera, just as terpenoid, phloroglucinols derivates and flavonoids[2,3]. Building on the promising biological activities reported for well-investigated *Myrtaceae* species, this study focuses on six unexplored plants: *Psidium cattleianum*, *Psidium myrtoides*, P*sidium guinensee, Myrrhinium atropurpureum*, *Hexachlamis edulis,* and *Psidium friedrichsthalianum*. Leaves crude extracts of all the selected species were tested for their antimicrobial activity against two strains of *Staphylococcus aureus*: ATCC 29213 and 43300 (a methicillin-resistant *Staphylococcus aureus* strain, MRSA). Among the tested extracts, *Psidium myrtoides*, *P. friedrichsthalianum*, and *Myrrhinium atropurpureum* exhibited the highest antimicrobial activity (with inhibition percentages relative to the control exceeding 85% at concentrations of 128, 64, and 8µg/mL, respectively) and were therefore selected for further phytochemical investigation. Preliminary structural characterization by 2D NMR spectroscopy (HSQC, HMBC, and HSQC-TOCSY) indicated terpenoid derivatives as the predominant class of metabolites. Ongoing chromatographic fractionation and purification of the bioactive extracts are aimed at isolating the compounds responsible for the observed antimicrobial activity, whose structures and biological properties will be further characterized.

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P5: The Influence of Biochar on Accumulation of Polyphenolic Compounds in *Paulownia Tomentosa* (Thunb). Steud. Leaves

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Paulownia is a perennial deciduous tree native to Southeast Asia and is now widely cultivated worldwide. *P. tomentosa* leaves are a rich source of various bioactive compounds, including flavonoids, lignans, and phenolic acids with anti-inflammatory, antibacterial, and neuroprotective properties[1]. Biochar is a stable carbon material produced by charring or pyrolysis, i.e., heating biomass under controlled oxygen and temperature conditions. Biochar has emerged as a versatile soil amendment with sustainable applications in agriculture, carbon sequestration, and plant growth[2]. The primary aim of this study was to investigate the influence of varying biochar amendment levels on the accumulation of polyphenolic compounds in *P. tomentosa* leaves compared with a control, and to characterize the phytochemical composition and antioxidant properties of the resulting leaf extracts.
Three biochar amendment rates (2, 4, and 6 L per plant) and a no-amendment control were tested, each with nine replicates and harvested across the 2025 vegetation season. Phytochemical analyses included total flavonoid content (TFC) and total phenolic content (TPC) by spectrophotometric methods. HPLC-PDA and LC-MS were used to identify and quantify individual compounds, and the ABTS assay was performed to determine antioxidant activity.
The highest TFC was determined in samples from trees amended with 4 L and 6 L throughout the growing season; these amounts were significantly higher than the control ($p < 0.005$). The highest yields were observed on 14th August 2025 for 4 L (0.904% ± 0.011) and 6 L (0.949% ± 0.014) amendments. The highest TPC was obtained in the 6 L treatment. HPLC-PDA and LC-MS identified three major phenolic compounds: verbascoside, luteolin-7-O-glucuronide, and diplacone. Antioxidant assays confirmed that biochar significantly increased radical scavenging activity.

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P6: Bioactivity-Guided Isolation of Secondary Metabolites from *Verbascum kurdicum* and Their Cytoprotective and Anti-Inflammatory Effects Against Cigarette Smoke Extract-Induced Bronchial Epithelial Cell Damage

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Verbascum species are traditionally used for the treatment of respiratory disorders and are known to contain biologically active iridoids, phenylethanoid glycosides and triterpenoid saponins.[1-2] However, the phytochemical composition and biological activities of *Verbascum kurdicum* have not previously been investigated. This study aimed to isolate bioactive constituents from *V. kurdicum* using bioassay-guided fractionation and evaluate their protective effects against cigarette smoke extract (CSE)-induced bronchial epithelial cell injury. The aerial parts of *V. kurdicum* were extracted with 50% methanol and fractionated following liquid-liquid partitioning. Based on cytoprotective and anti-inflammatory screening, the active *n*-butanol fraction was subjected to chromatographic purification and isolated compounds were identified by spectroscopic techniques (1D and 2D NMR). Cytotoxicity and cytoprotective activities against CSE-induced damage were determined in BEAS-2B cells using the MTT assay. Anti-inflammatory activity was assessed by ELISA analysis of IL-6 and IL-8 levels. In addition, intracellular glutathione (GSH), superoxide dismutase (SOD) activity and 8-hydroxy-2′-deoxyguanosine (8-OHdG) levels were determined to evaluate oxidative stress, while the expression of TLR4, MyD88, NF-κB and phosphorylated NF-κB proteins was analyzed by western blot to investigate the underlying molecular mechanisms. Bioactivity-guided isolation yielded ajugol, aucubin, ilwensisaponin A, ilwensisaponin C, sangarosaponin E, verbascoside, harpagoside and adenosine. Among the isolated compounds, ajugol and aucubin exhibited the highest cytoprotective activity against CSE-induced cell injury. Aucubin significantly suppressed IL-6 production, whereas ajugol showed the strongest inhibition of IL-8 release, indicating differential modulation of inflammatory pathways. These compounds also attenuated CSE-induced oxidative stress and were further investigated for their effects on the TLR4/MyD88/NF-κB signaling pathway. This study represents the first phytochemical and biological investigation of *V. kurdicum*. The isolated iridoids demonstrated promising cytoprotective, antioxidant and anti-inflammatory activities against cigarette smoke-induced bronchial epithelial damage, highlighting *V. kurdicum* as a potential source of lead compounds for inflammatory respiratory diseases.

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P7: Activity-Guided Isolation of Astragalin from *Erigeron annuus* (L.) Pers. Aerial Parts Reveals Tyrosinase Inhibitory, DNA-Protective, and Cosmeceutical Potential

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Natural products represent an important source of bioactive compounds for the development of cosmetic ingredients.[1] This study aimed to isolate secondary metabolites from the aerial parts of *Erigeron annuus* (L.) Pers. using an activity-guided approach based on tyrosinase inhibition and to evaluate their potential for skin-aging-related applications. According to previous reports, pyromeconic acid, identified as the major compound in E. annuus flower extracts, possesses a γ-pyrone structure similar to that of the well-established tyrosinase inhibitor kojic acid.[2] The active compound isolated from the most active fraction was identified as kaempferol 3-*O*-*β*-D-glucopyranoside (astragalin) by ^{1}H-NMR and ^{2}D-NMR analyses.[3] The crude methanol extract, *n*-butanol sub-extract, fraction G, and astragalin exhibited tyrosinase inhibitory activity with IC_{50} values of 95.38 ± 6.07, 77.62 ± 2.64, 73.77 ± 4.83, and 81.26 ± 4.65 µg/mL, respectively. The *n*-butanol sub-extract and fraction G also inhibited elastase, with IC_{50} values of 268.43 ± 33.10 and 124.22 ± 11.76 µg/mL, respectively. In addition, all tested samples demonstrated high radical scavenging activity. The crude methanol extract, *n*-butanol sub-extract, fraction G, and astragalin markedly protected pBR322 plasmid DNA against Fenton reagent-induced oxidative damage. HPLC quantification showed that astragalin is one of the major constituents of the crude methanol extract, accounting for 6.28% (w/w). Furthermore, DFT calculations and molecular docking indicated that deprotonation at the 7-OH group of astragalin is critical for its tyrosinase inhibitory activity. Consequently, our research suggests that the aerial parts of *E. annuus* constitute a promising natural source of bioactive compounds for cosmeceutical applications, with astragalin identified as the principal contributor to the observed biological activities.

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P8: Structural Elucidation of a New Kaurene Diterpene from Bioactive Leaf Extracts of *Atractylis gummifera* by Extensive 2D NMR Spectroscopy.

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Atractylis gummifera L. (Asteraceae) is a perennial species native to the Mediterranean region, where it grows in dry and rocky habitats. Although the roots of this plant are known to contain highly bioactive diterpene glycosides, including atractyloside and carboxyatractyloside, the phytochemical composition of its leaves has received comparatively little attention.[1,2]

In the present study, a phytochemical investigation of *A. gummifera* leaves was carried out. Dried leaf material was extracted using solvents of different polarity, and the resulting extracts were fractionated through chromatographic procedures to isolate their major secondary metabolites.

This investigation led to the identification of several known triterpenes and aromatic constituents together with a previously undescribed kaurene diterpene. The structure of the new metabolite was unambiguously established by mass spectrometry and extensive 2D NMR spectroscopy, including COSY, HSQC, H2BC, HMBC, HSQC-TOCSY, and NOESY experiments. The combined spectroscopic data allowed the complete assignment of both the molecular framework and its relative stereochemistry.

The isolated diterpene was also evaluated for its in vitro cytotoxic activity against human cancer cell lines, with the aim of assessing its potential biological relevance.

The discovery of a new kaurene diterpene expands the phytochemical knowledge of *A. gummifera* and further demonstrates that its aerial parts represent a valuable source of structurally diverse natural products with promising biological potential.

Keywords: *Atractylis gummifera*, Natural products, kaurene diterpene, *in-vitro* cytotoxicity, 2D NMR.

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P9: Sustainable Valorization by Foam Fractionation

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Industrial side streams constitute complex and underutilized sources of bioactive secondary metabolites. The valorization requires sustainable separation technologies combined with data-driven approaches capable of resolving relationships between process conditions, chemical composition, and biological activity. In this study, foam fractionation was investigated as a green separation technology for the selective enrichment of surface-active natural products through adsorption at the gas–liquid interface[1].

The separation process was systematically developed and optimized using design of experiment (DoE) approach. Process performance was assessed by integrating high-resolution chemical profiling (LC–PDA–HRESIMS) with antioxidant assays (DPPH, FRAP, and β-carotene bleaching) and a cell-based model of oxidative stress. Chemical fingerprints were evaluated in relation to the investigated process parameters and biological responses to identify characteristic compound classes and compositional patterns associated with enhanced activity. The data-driven analysis[2] revealed selective shifts in the chemical profiles of the generated fractions, particularly in features assigned to prenylated flavonoids and humulones and lupulones. DoE enabled the systematic assessment of pH, gas flow rate, feed concentration, temperature, and column length and identified feed concentration, pH, and column length as the principal factors governing chemical enrichment.

Fractions obtained under optimized conditions displayed enhanced antioxidant activity and improved cellular protection against tert-butylhydroperoxide-induced oxidative stress in HT1080 cells. Overall, the integration of experimental process design, high-resolution chemical profiling, and biological data provides a transferable strategy for understanding and optimizing the selective recovery of bioactive natural products from complex industrial side streams.

These findings support foam fractionation as a sustainable platform for generating functional fractions with potential applications in cosmetics, nutraceuticals, and functional ingredients.

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P10: Synergistic Antimicrobial Activity of Historical Herbal Recipes from a Seventeenth-Century Austrian Drug Book

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Antimicrobial resistance remains a major global health challenge and has renewed interest in complex plant-based formulations as potential sources of antimicrobial activity and synergistic interactions. This study investigated the antimicrobial and interaction profiles of historical herbal recipes from the Austrian *Koch- und Artzney-Buch* of 1688. Twenty-four recipes traditionally used for infectious diseases were selected, translated, reconstructed, and screened against methicillin-resistant *Staphylococcus aureus* (MRSA), an extended-spectrum beta-lactamase-producing strain (ESBL), and *Escherichia coli*. Antimicrobial effects were assessed by broth microdilution and IC_{50} calculation, while recipes with relevant activity were further evaluated using the Screening Method for Synergism (SMS) [1]. Twelve reconstructed recipes showed antimicrobial activity, and four were suitable for detailed interaction analysis. Recipe 1 displayed additive effects only, whereas recipe 9 showed fully synergistic activity against MRSA. Recipe 13 revealed a complex interaction pattern with synergistic, additive, and antagonistic contributions occurring simultaneously, while recipe 19 exhibited synergistic or additive effects depending on the pathogen tested. These findings highlight that selected historical multi-component herbal recipes can exert relevant antimicrobial effects and distinct interaction patterns. The observed activity appears to arise from formulation-dependent interactions, supporting the scientific relevance of historical recipe-based approaches for identifying synergistic antimicrobial combinations.

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P11: Oxygenated Diterpenes Isolated from Red Sea Soft Corals of the Genus *Sarcophyton*

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On a global scale, coral reefs are regarded as the most magnificent and diverse marine habitats, hosting a high number of species, including many which are currently undescribed. Among them, the coral reefs of the Red Sea, which is characterized by unique biotic and abiotic conditions, are considered the best-developed reefs in the western Indian Ocean. Nonetheless, its marine biota is underexplored, especially concerning its chemodiversity.

Octocorals are widely accepted as a rich source of biologically active compounds, featuring a wide range of chemical structures. Among them, soft corals of the genus *Sarcophyton* (Sarcophytidae) have been proven a prolific source of bioactive natural products, having afforded more than 1,000 metabolites until now, mainly sesquiterpenes, diterpenes, steroids and ceramides, exhibiting a broad range of biological activities.

In the framework of our research towards the isolation of bioactive metabolites from marine organisms, we investigated the chemical profiles of two populations of *Sarcophyton* sp. collected from the coastline of the Saudi Arabian Red Sea. Fresh specimens of the two populations were exhaustively extracted with mixtures of CH_2Cl_2/MeOH and the resulting organic extracts were subjected to a series of chromatographic separations that have so far led to the isolation of 10 new natural products, as well as 16 previously reported, all belonging to the class of cembrane diterpenes. The structure elucidation of the isolated metabolites was based on extensive analysis of their 1D and 2D NMR and MS data.

P12: Antitrypanosomal Activity of Amaryllidaceae Alkaloids from *Crinum americanum*

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The Amaryllidaceae family is widely recognized for its diverse pharmacological potential, primarily attributed to the presence of unique isoquinoline alkaloids (AAs).[1] Among these, the genus *Crinum* has stood out as a prolific source of bioactive compounds with various therapeutic properties.[2–4] In particular, the search for new treatments against Neglected Tropical Diseases (NTDs) remains a priority, as current therapies for American Trypanosomiasis (Chagas disease) present significant limitations regarding toxicity and efficacy in the chronic phase.[5]

This study focuses on the evaluation of the anti-*Trypanosoma cruzi* activity of *Crinum americanum*. The hypothesis is centered on the synergistic or isolated effect of Amaryllidaceae alkaloids, which have historically demonstrated significant inhibitory action against protozoan parasites. The chemical investigation involved the extraction of alkaloids from the plant matrix, followed by preliminary profiling to ensure the presence of the target metabolites.

The biological evaluation aims to determine the half-maximal inhibitory concentration (IC_{50}) against the trypomastigotes and amastigote forms of *T. cruzi,* as well as assessing the cytotoxicity (CC_{50}) in mammalian cells to establish the selectivity index. Currently, the experimental tests are in development, with final biological screenings being conducted to consolidate the potency of the alkaloidal fractions. These results are expected to contribute to the discovery of new scaffolds for the development of alternative antitrypanosomal agents, reinforcing the importance of the Amaryllidaceae family in medicinal chemistry.

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P13: Neuroprotective Potential of *Myrtus communis* L. in Parkinson's Disease: Targeting Early-Stage *α*-Synuclein Oligomerization and Motor Deficits

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Parkinson's Disease (PD) is characterized by the pathological aggregation of *α*-synuclein (*α*-syn). *Myrtus communis* L. (Myrtaceae), a plant widely used in folk medicine for its diverse therapeutic properties, presents a promising source for neuroprotective agents. In this study, we investigated the effects of *M. communis* leaf extracts and their chromatographic fractions on *α*-syn fibrillization using both *in vitro* and *in vivo* models. To evaluate the therapeutic efficacy in a living system, *in vivo* animal experiments were conducted using a rat model where Parkinsonian pathology was induced via stereotactic injection of *α*-syn fibrils into the brain. The effects of these treatments on *α*-syn species were analyzed using Western Blot, and motor/cognitive functions were assessed through behavioral paradigms. Among the tested fractions, MCE-Fr.E was identified as the most potent candidate for reducing low-molecular-weight *α*-syn fibrils (0.36±0.10). This fraction was specifically selected for further investigation because it exhibited the highest inhibition of oligomer formation compared to other fractions. Phytochemical analysis revealed that MCE-Fr.E is particularly rich in triterpenoids. Chronic administration of MCE-Fr.E in the rat model significantly rescued motor function losses, as demonstrated by apomorphine-induced locomotor activity test results ($p<0.05$). Notably, no significant changes were observed in cognitive assessments, aligning with the early-stage nature of the pathology. Our findings suggest that MCE-Fr.E effectively modulates the early motor phase of PD by targeting low-molecular-weight *α*-syn oligomers and preserving striatal integrity. This study highlights the disease-modifying potential of *Myrtus communis* in the early stages of neurodegeneration, even before the onset of cognitive decline.

Keywords: *Myrtus communis*, Parkinson, *α*-synuclein, neurodegeneration, phytochemistry

P14: Bioactivity-Guided Discovery of Antidiabetic Agents from the Turkish Endemic *Onobrychis tournefortii* (Willd.) Desv.: From Folk Medicine to Bioactive Fractions

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Onobrychis tournefortii (Willd.) Desv. (Fabaceae), a species endemic to Türkiye locally known as "evliya otu," has long been utilized in traditional medicine for treating diabetes and respiratory disorders. Despite its ethnobotanical significance, its pharmacological potential remains scientifically unvalidated. This study aimed to investigate the antidiabetic and antioxidant efficacy of *O. tournefortii* using a bioactivity-guided fractionation approach. Aerial parts were extracted with 80% methanol and water to simulate traditional preparation methods. The aqueous extract, which demonstrated the most significant α-glucosidase inhibition (278,98 g/mL), was further fractionated using dichloromethane (DCM), ethyl acetate, and *n*-butanol. Antioxidant capacity (ABTS, CUPRAC, DPPH, FRAP) and antidiabetic activity (α-amylase and α-glucosidase inhibition) were evaluated at each stage. Fractionation markedly enhanced the biological potency, with the DCM fraction emerging as the most bioactive candidate. The DCM fraction exhibited superior enzyme inhibition against α-amylase (26,03 g/mL) and α-glucosidase (117,05 g/mL) compared to the crude extracts. Preliminary phytochemical screening and total content assays revealed that this high efficacy correlates with an exceptional phenolic concentration (373,01 mg GAE/g) and robust antioxidant activity (e.g., FRAP: 168,35 mg KE/g and ABTS: 83,16 mg TE/g). These findings suggest that the DCM fraction effectively concentrates the plant's bioactive secondary metabolites. Our results provide the first scientific validation for the traditional use of *O. tournefortii* in diabetes management. The identification of the DCM fraction as a potent source of dual-acting (antioxidant and antidiabetic) agents warrants further bioactivity-guided isolation and characterization of its specific molecular constituents.

Keywords: *Onobrychis tournefortii*, α-amylase, α-glucosidase, antidiabetic activity, bioactivity-guided fractionation

P15: Safety monitoring of tropane alkaloids in commercial herbal teas containing *Convolvulus* species

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Herbal teas are widely consumed and generally perceived as safe products with beneficial health properties. Nevertheless, ensuring their safety remains a critical challenge[1], particularly with respect to naturally occurring plant toxins. Tropane alkaloids (TAs) constitute a large and structurally diverse group of toxic secondary metabolites, including atropine and scopolamine, as well as other TAs reported in species belonging to the Convolvulaceae family[2,3]. These compounds can exert anticholinergic effects and, depending on exposure levels, may pose a risk to consumer health[2]. Commercial herbal teas containing *Convolvulus* species are available on the market; however, information on the occurrence and levels of TAs in these products remains scarce[3,4]. The lack of occurrence data limits the assessment of dietary exposure and hinders evidence-based evaluation of their safety. Therefore, monitoring studies are needed to determine the presence of both regulated and emerging TAs in products intended for human consumption. In this study, a collection of commercial herbal teas containing different proportions of *Convolvulus* spp. was investigated. Samples were analyzed using ultra-high-performance liquid chromatography tandem mass spectrometry (UHPLC-MS/MS) for targeted determination of 14 tropane alkaloids, including atropine, scopolamine, and other Convolvulaceae-associated TAs. This approach enabled a comprehensive characterization of their TA profiles. The resulting occurrence data provide valuable information on the prevalence and concentration of TAs in *Convolvulus*-containing herbal teas, contributing to consumer exposure assessment, food safety evaluation, and future regulatory monitoring of these emerging contaminants.

Acknowledgments
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P16: Antimicrobial potential of the hydroethanolic extract of *Massularia acuminata* leaves and characterization of its specialized metabolites

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Abstract

Antibiotics are a valuable resource and an essential tool in the fight against microbial infections in humans and animals. However, their effectiveness is declining globally due to the emergence of resistant strains[1]. According to the WHO, antimicrobial resistance could be responsible for up to 10 million deaths annually by 2050. To address these treatment failures, many researchers are increasingly turning to plants as potential sources of antimicrobial agents. *Massularia acuminata* (G. Don) Bullock ex Hoyle is a shrub reaching 9 meters in height, endemic to the dense forests of Africa. This plant is used in traditional medicine as an antimicrobial, antidiabetic, and anticancer agent, as well as an aphrodisiac. A leaf infusion is used to treat malaria and gastric disorders[2]. This study aimed to evaluate the antimicrobial potential of the plant and to isolate and characterize its specialized metabolites[3]. The hydroethanolic extract of *M. acuminata* leaves was fractionated and purified using various chromatographic techniques (open-column chromatography, CPC, and HPLC). Subsequently, the hydroethanolic extract and its fractions were tested against 36 microbial strains. The chemical structures of the isolated molecules were determined using NMR spectroscopy and UHPLC-MS analysis. The extract demonstrated activity against certain *Staphylococcus* species, as well as *Streptococcus agalactiae*, *Acinetobacter baumannii*, *Stenotrophomonas maltophilia*, and *Burkholderia cepacia*, with a minimum inhibitory concentration (MIC) of 1.2 mg/mL. Phytochemical analysis led to the characterization of chlorogenic acid, vicenin-2, massularosides B, H, and J, mussaendoside J, and ixoside. Based on these results, cytotoxicity tests will be performed on immortalized human keratinocyte (HaCaT) and U937 monocytic cell lines.

Keywords: Antimicrobial, *Massularia acuminata*, specialized metabolites, phytochemical

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P17: Exploring the Bioactive Profile of *Morus alba* and *Morus nigra* Extracts: Antioxidant, Anti-cholinesterase and Neuroprotective Properties

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Leaves of *Morus alba* and *Morus nigra* are recognized as rich sources of phenolic constituents with well-established pharmacological relevance. Here, we investigated the neuroprotective and antioxidant activities, and the cholinesterase inhibitory potential, of hydroalcoholic leaf extracts from *Morus alba (MAE)* and *Morus nigra (MNE)*. RP-UHPLC-PDA analysis revealed a higher accumulation of phenolic compounds in MNE than in MAE. Both extracts exhibited antioxidant properties, effectively scavenging hydroxyl radicals and inhibiting plasma lipid peroxidation, with MNE showing greater effects, as reflected by lower IC_{50} values. Furthermore, MNE demonstrated more potent inhibition of acetylcholinesterase (AChE) activity, with an IC_{50} value of 24.34 ± 0.86 μg/mL that approached the inhibitory efficacy of galantamine and exceeded that determined for MAE (IC_{50} = 46.87 ± 2.16 μg/mL). The *in vivo* neuroprotective efficacy of both extracts was evaluated using a zebrafish (*Danio rerio*) model of scopolamine-induced cognitive impairment. Administration of MAE and MNE at concentrations of 1 and 10 μg/L induced dose-dependent improvements in cognitive and behavioural performance, as shown by outcomes across the Y-maze, novel tank diving and novel object recognition paradigms NTT. Overall, these results indicate that *Morus* leaf extracts possess antioxidant, anticholinesterase, and *in vivo* neuroprotective effects, supporting their potential in mitigating neurodegenerative-associated cognitive dysfunction.

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P18: Phytochemical analysis and anti-inflammatory potential of *Echinacea angustifolia* extracts

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Echinacea (commonly known as purple coneflower) is a well-known medicinal plant traditionally used for the treatment of upper respiratory tract infections, including colds, coughs, and bronchitis, as well as inflammatory disorders[1]. In particular, the antioxidant and anti-inflammatory activities of *Echinacea* spp. have been attributed to their ability to reduce ROS (reactive oxygen species)/RNS (reactive nitrogen species) production and pro-inflammatory mediators, decrease the infiltration of inflammatory cells, and block the receptors of the immune cell[2]. In this study, the anti-inflammatory potential of *Echinacea angustifolia* roots was investigated highlighting the influence of the extraction technique on the observed anti-inflammatory activity. Ethanolic extracts were obtained by conventional maceration and non-conventional Solid–Liquid Dynamic Extraction (SLDE-Naviglio) technique. Their phytochemical profiles were characterized by liquid chromatography coupled with high-resolution mass spectrometry (LC–HRMS) in both negative and positive ion modes. LC-ESI/HRMS analysis enabled the identification of organic acids, quinic acid derivatives, hydroxycinnamic acids derivatives, flavonoids, phenylpropanoids, and oxylipins in negative ion mode, whereas alkylamides were identified in positive ion mode. Among these metabolites, alkylamides, polysaccharides, hydroxycinnamic acid derivatives, and the major phenylethanoid glycoside echinacoside have been widely associated with the anti-inflammatory activity of *Echinacea* spp., including modulation of the NF-κB signaling pathway and suppression of pro-inflammatory cytokine production[2,3]. The biological activity of *E. angustifolia* extracts was assessed through *in vitro* reporter gene assay. Both extracts inhibited TNF-α-induced NF-κB activation (in the range 50-100 μg/mL), supporting their ability to modulate a central regulator of inflammatory responses and highlighting their potential as a source of bioactive anti-inflammatory compounds.

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P19: From Botanicals to Nanocarriers: Inhibiting ocular glycation with Green coffee and Juniper fractions

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Ocular accumulation of advanced glycation end-products (AGEs), including Nε-(carboxymethyl)lysine (CML), may contribute to glaucoma-related trabecular meshwork dysfunction and retinal neurodegeneration through protein cross-linking, oxidative stress, inflammation, and cellular senescence. Glaucoma is a major cause of irreversible blindness and is projected to affect 111.8 million people aged 40–80 years worldwide by 2040. Because early glaucoma is frequently asymptomatic, a substantial proportion of cases remain undetected, limiting timely intervention. Current therapies primarily lower intraocular pressure but do not directly target AGE formation or AGE-induced tissue injury, supporting investigation of novel local anti-glycation strategies. To evaluate plant-derived inhibitors of glycation, we compared extracts from Juniperus communis pseudo-fruits and green coffee seeds (Coffea arabica L.). Both materials underwent identical fractionation, yielding ethanolic (F1), petroleum ether (F2), diethyl ether (F3), ethyl acetate (F4), n-butanol (F5), and aqueous (F6) fractions. Anti-glycation activity was assessed at 10, 100, and 1000 µg/mL using an in vitro human serum albumin model (HSA, 40 mg/mL) under hyperglycaemic (30 mM glucose) and ultra-hyperglycaemic (300 mM glucose) conditions. Glycation was quantified by fructosamine determination, fluorometric analysis of pentosidine and total fluorescent AGEs, and ELISA measurement of CML. Both botanical materials showed concentration-dependent activity. The ethyl acetate fractions from both sources most effectively reduced fructosamine formation, with approximately 8–12% inhibition at 100 µg/mL. Green coffee fractions inhibited fluorescent AGE formation by approximately 55–65% and reduced CML accumulation by 40–60% at 1000 µg/mL. However, the ethanolic extract and selected J. communis fractions produced the strongest overall inhibition of fluorescent AGEs and CML under ultra-hyperglycaemic conditions.These findings indicate that both materials are promising sources of anti-glycation compounds, while J. communis provides broader protection against advanced glycation. Further studies will focus on designing ophthalmic formulations containing the most active fractions for the prevention or adjunctive treatment of AGE-associated retinal and trabecular meshwork degeneration in glaucoma.

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P20: Sideritis raeseri Extracts for Multidirectional Protection Against UV-Induced Skin Damage

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Plants growing under challenging climatic conditions are often a valuable source of protective cosmetic ingredients.[1] *Sideritis raeseri* (Greek mountain tea, Lamiaceae) is one such plant, with well-documented antioxidant potential and favourable phytochemical profile rich in phenylethanoid glycosides (verbascoside), flavones (hypolaetin and isoscutellarein glycosides) and phenolic acids (chlorogenic acid).[2] However, in the CosIng database,[3] only one *S. raeseri* ingredient is currently registered (Flower/Leaf/Stem Extract; antioxidant function), limiting its cosmetic application. This study therefore aimed to systematically evaluate *S. raeseri* extracts across the multiple pathways involved in UV-induced skin damage.

S. raeseri flowers and leaves were extracted separately by ultrasound-assisted extraction (UAE) using 70% ethanol, water, 20% glycerol, and 20% propylene glycol. Extracts were characterized for total polyphenol content and radical scavenging capacity (IC_{50}, DPPH/ABTS), and *in vitro* SPF/UVA-PF. 70% ethanol extracts were selected for phytochemical profiling (LC-PDA-ESI-MS^n) and evaluation of tyrosinase, elastase, and collagenase inhibition, plus cytotoxicity in HaCaT keratinocytes.

Among the tested solvents, 70% ethanol extracts showed the highest total polyphenol content (13.4-15.5 µg GAE/mL), lowest DPPH/ABTS IC_{50} values (0.07-0.10%), and highest SPF/UVA-PF, with leaf extracts outperforming flower extracts. LC-PDA-ESI-MS^n identified hydroxycinnamic acids, phenylethanoid glycosides (verbascoside as a major constituent in both organs) and flavone-7-O-glycosides, with a richer high-intensity profile in leaf extracts. Both flower and leaf extracts strongly and dose-dependently inhibited elastase (down to 3-5% residual activity at 100 µg/mL), while collagenase activity remained largely unaffected (85-105%). Tyrosinase inhibition was moderate and organ-dependent, with flower extracts more active than leaf extracts (residual activity ~50% vs ~65% at 100 µg/mL). No cytotoxicity was observed in HaCaT keratinocytes up to 200 µg/mL after 24 h treatment.

These results indicate that *S. raeseri* 70% ethanol extracts combine strong antioxidant and photoprotective properties with selective, elastase-targeted anti-aging activity and anti-melanogenic potential, without compromising keratinocyte viability, supporting their application as multidirectional, safe UV-protective cosmetic ingredients.

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P21: Enhancing the Antitumoral Potential of Scytonemin: Synthesis and Molecular Docking of a Novel Acetylated Derivative

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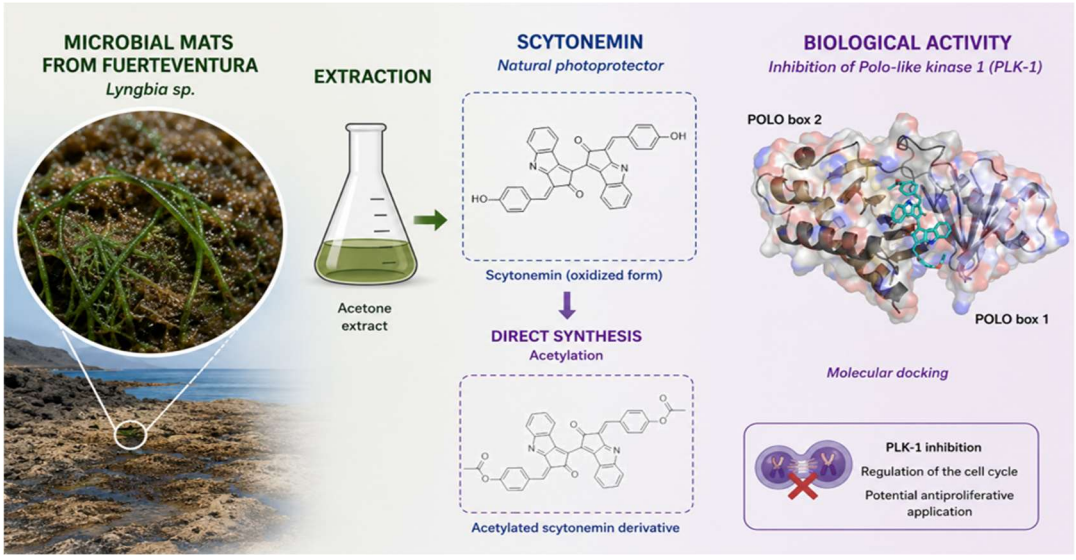
The search of novel anticancer therapies is increasingly important due to the emergence of drug resistance. Cyanobacterial secondary metabolites have gained attention as a source of bioactive compounds with therapeutic potential.[1] Scytonemin, an extracellular indole-alkaloid pigment produced by cyanobacteria, functions as a natural UV-A sunscreen and has demonstrated antiproliferative activity through inhibition of Polo-like kinase 1 (PLK-1), a key regulator of mitosis.[2] However, its limited stability restricts its pharmacological application.[3]

In this study, scytonemin was extracted from *Lyngbya sp.* microbial mats collected in Fuerteventura (Canary Islands, Spain). To enhance its properties, an acetylated derivative was synthesized through a direct one-pot reaction from the crude extract, providing a simple and efficient modification strategy.

Molecular docking studies were performed against PLK-1 (PDB ID: 9QMO) to evaluate binding affinity. The acetylated derivative showed a significantly higher predicted affinity compared to native scytonemin, suggesting improved interaction with the kinase active site.

These results indicate that acetylation may enhance the antitumoral potential of scytonemin and support its use as a promising scaffold for the development of new PLK-1 inhibitors.



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P22: Effect of Aqueous Fireweed (*Chamerion angustifolium* L.) Leaf Extract and its Main Component Oenothein B on Colon Cancer Cell Viability and Energy Metabolism

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Chamerion angustifolium L. (fireweed) is a medicinal plant recognized by the European Medicines Agency (EMA) for the relief of lower urinary tract symptoms associated with benign prostatic hyperplasia[1]. Rich in polyphenols, particularly Oenothein B, it exhibits anti-inflammatory, antioxidant, antiproliferative, and anticancer activities[2]. Due to high relevance of colorectal cancer, there is a need for novel bioactive compounds targeting cancer cell survival.

The aim of our study was to determine the effect of aqueous fireweed (*Chamerion angustifolium* L.) leaf extract and its main component Oenothein B on colon cancer (Caco-2) cell viability and energy metabolism.

Fireweed leaves were collected in Lithuania in July 2023. Caco-2 cells were treated with aqueous fireweed leaf extract (0.5–3 mg/mL) or Oenothein B (0.01–0.1 mg/mL) for 48 h. Cell viability was assessed by the MTT assay, while mitochondrial respiration and glycolysis was analyzed using high-resolution respirometry (Oxygraph-2k) at 37 °C with glutamate/malate and succinate as substrates.

IC50 values were detected 0.843 mg/mL (for fireweed) and 0.09 mg/mL (57 μM) (for Oenothein B). We revealed that fireweed leaf extract caused the decrease in mitochondrial respiration rate up 64% (glutamate/malate) and up to 56% (succinate), while Oenothein B caused the increase in leak respiration rate by 34–73% and reduced respiration rate by 24%. Moreover, fireweed leaf extract significantly reduced Caco-2 cell viability (by 84%), and maximal glycolysis rate (by 69%). Oenothein B on its own had an overall weaker effect on energy metabolism – maximal glycolysis decreased by 53%.

In conclusion, fireweed (*Chamerion angustifolium* L.) leaf extract and Oenothein B reduced Caco-2 cell viability and altered cellular energy metabolism. The stronger effects of the whole extract on mitochondrial respiration and glycolysis, compared with Oenothein B alone, suggest that its biological activity cannot be attributed solely to this major ellagitannin. Instead, synergistic interactions among multiple phytochemicals are likely to underlie the observed metabolic effects.

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P23: Natural Antioxidants as a Protective Strategy Against Environmental Pollutant-Induced Sperm Damage: Synergistic Effects of Ellagic Acid and Ascorbic Acid

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Natural products represent an important source of bioactive compounds with antioxidant and cytoprotective properties. Among these, ellagic acid (EA) and ascorbic acid (AA) have attracted increasing interest as potential agents against oxidative stress (OS), a key factor involved in male infertility[1-2]. On the other hand, exposure to environmental contaminants such as polystyrene microplastics (PS-MPs) and titanium dioxide nanoparticles (TiO_2-NPs) promotes reactive oxygen species (ROS) generation, leading to oxidative damage and impaired sperm function[3-4]. Therefore, the aim of this study was to evaluate the potential protective effect of EA and AA, against PS-MP- and TiO_2-NP-induced damage in human spermatozoa *in vitro*. Sperm were treated for 30, 60, and 90 minutes with EA (100 µM), AA (100 µM), PS-MP (210 µg/mL), and TiO_2-NP (10 µg/L), both individually and in combination. At the end of the exposure, seminal parameters and sperm viability, ROS production by NBT test and DNA fragmentation by TUNEL assay were assessed. The results showed that exposure to PS-MP and TiO_2-NP significantly compromised sperm quality, resulting in a reduction in sperm motility and viability, accompanied by an increase in ROS production and DNA fragmentation. Instead, EA and AA showed marked anti-genotoxic and cytoprotective effects, attenuating the harmful effects induced by contaminants. Specifically, EA was only able to partially reduce the damage, maintaining significant differences at longer exposure times, while AA showed protective efficacy at all experimental time points. However, the combination of EA and AA produced the most marked effect, suggesting a possible synergistic action between the two compounds. This synergism could enhance overall antioxidant capacity, improving the control of OS and limiting cytotoxic and genotoxic damage induced by environmental contaminants. Overall, these results support the potential combined use of EA and AA as a natural strategy to protect male fertility from the effects of environmental contaminants associated with OS.

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P24: Multi-Target Inhibition of the HIV-1 Replication Cycle by Withaferin A-Analogues

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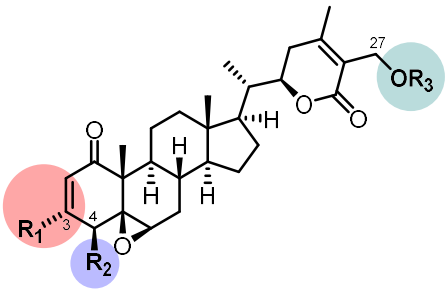
Despite advances in antiretroviral therapy, toxicity problems, emergence of drug-resistant strains to HIV-1 (human immunodeficiency virus 1) and viral reservoirs, emphasize the urgent need for new anti-HIV drugs.[1]

Based on previous studies highlighting the therapeutic potential of withaferin A, a natural steroidal lactone, and the emerging role of organosilicon motifs in drug design,[2] we explored the effects of this lead compound and a series of analogues on the HIV-1 replication cycle, including viral entry, reverse transcription, integration, and transcription. In addition, structure-activity relationship (SAR) studies were employed to understand the structural requirements of this series of analogues.

Studies on their HIV-1 mechanism of action revealed viral integration and transcription as main targets of these analogues, and structural modifications shift these primary targets towards viral entry and reverse transcription. Therefore, these analogues behave as multi-target compounds providing advantages to overcome HIV-1 multidrug resistance and long-life infection. Moreover, SAR analysis suggests that a 27-silyl ether with a short-chain aliphatic substituent, a 4-carboxylic acid or a heterocyclic moiety may enhance the antiretroviral profile of the lead compound.

The results herein underscore withaferin A as a robust and versatile structural platform to develop new antiretroviral drugs and might open new avenues for natural product-inspired molecules to contribute to the available therapeutic arsenal for emerging viral infections.



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P25: Antimicrobial activity and phytochemical profiling of selected medicinal plants of Côte d'Ivoire

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Abstract
Antimicrobial resistance is a major global issue, affecting human, animal, and environmental health alike. Medicinal plants play a key role in traditional medicine, particularly in Côte d'Ivoire. These natural resources offer a unique opportunity to develop new antimicrobials in line with the 'One Health' principles. The aim of this study is to investigate the antimicrobial potential of *Lecaniodiscus cupanioides*, *Terminalia superba*, *Uvaria ovata*, *Aucoumea klaineana, Millettia takou*, *Chaetachme aristata,* and *Leptoderris miegei*, medicinal plants from Côte d'Ivoire. Two different solvents, dichloromethane and methanol, were used to prepare the plant extracts. *In vitro* antibacterial activity[1] was assessed against a panel of 36 bacteria pathogenic to humans. Phytochemical screening was carried out using thin-layer chromatography. In addition, the phenolic compound content and the antioxidant potential of all the methanolic extracts were determined. Phytochemical analysis revealed the presence of flavonoids, alkaloids, tannins, and terpenoids in the extracts. The methanolic extracts of *Lecaniodiscius cupanioides*, *Terminalia superba*, *Uvaria ovata,* and *Leptoderris miegei* recorded the highest levels of phenolic compounds (200.61 to 405.31 mgEAG/g) and the strongest antioxidant activities, with IC_{50} values ranging from 0.066 to 0.389 mg/mL. The methanolic extracts of the plants were more active than the dichloromethanolic extracts, except in the case of *Aucoumea klaineana*. Of the seven methanolic extracts analysed, six showed an MIC of ≤ 0.3 mg/mL for one or more of the 36 microorganisms. This study would provide a scientific basis for the traditional use of these plants and offer valuable insights into the discovery of new antibacterial molecules.

Keywords: antimicrobial activity, phytochemistry, medicinal plant, antioxidant activity, phenolic compound, One Health

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P26: Evaluation of the Cytotoxic Effect of Extracts and Fractions of *Kalanchoe blossfeldiana* on Tumor Cell Lines

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Keywords: Kalanchoe; Plant Extracts; Prostatic Neoplasms; Breast Neoplasms; Cytotoxicity.

Abstract:
Cancer remains a leading cause of mortality worldwide, highlighting the need to identify novel antitumor agents from natural products. *Kalanchoe blossfeldiana* (Crassulaceae) is traditionally recognized for its anti-inflammatory properties; however, its cytotoxic potential remains poorly explored, particularly under neotropical cultivation conditions. This study evaluated the cytotoxic activity of ethanolic extracts and polarity-gradient fractions obtained from the leaves and flowers of *K. blossfeldiana* cultivated in Viotá (Cundinamarca, Colombia) against the human cancer cell lines MCF-7, MDA-MB-231, and PC-3.

Plant material was dried, pulverized, and extracted with ethanol using Soxhlet extraction. Crude extracts were fractionated by vacuum liquid chromatography using solvents of increasing polarity (hexane, dichloromethane, ethyl acetate, and ethanol). Cytotoxic activity was assessed by the MTT assay after 48 h of treatment, and IC_{50} values were determined by non-linear regression.

Leaf ethanolic extracts exhibited the highest cytotoxic activity, with IC_{50} values of 12.67, 75.75, and <1.6 µg/mL against MCF-7, MDA-MB-231, and PC-3 cells, respectively. Among the fractions, only the ethyl acetate and ethanol fractions showed significant activity, with the strongest effects against PC-3 cells (IC_{50} = 3.03 and <1.6 µg/mL, respectively). Flower extracts displayed moderate cytotoxicity while maintaining preferential activity against PC-3 cells.

These results are consistent with phytochemical findings in other *Kalanchoe* species, where metabolites from polar fractions, such as flavonoids and phenolic glycosides, have been associated with antitumor effects. This suggests their potential contribution to the observed biological activity and supports continuing this research line to identify the specific components responsible, whether acting individually or synergistically.
These findings highlight the remarkable selective antitumor potential of Colombian *K. blossfeldiana* polar fractions. This species provides a safe, valuable basis for bioguided fractionation targeting novel prostate cancer treatments.

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P27: Natural Antioxidants In The Fight Against Ovarian Cancer: *In Vitro* Effects Of Polyphenols

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Ovarian cancer is among the deadliest gynecological malignancies, mainly due to late diagnosis and the development of chemoresistance. The investigation for new therapeutic strategies has led to a growing interest in natural compounds with antioxidant and anticancer properties. Among these, ellagic acid (EA), a polyphenol present in pomegranates, and curcumin (CUR), the main component of turmeric, have gained attention for their anti-inflammatory, antioxidant, and antiproliferative effects. However, limited data are available on their activity in ovarian cancer cells. This study investigates the in vitro antiproliferative and cytotoxic effects of EA and CUR on IGROV-1 human ovarian cancer cells, as well as their ability to modulate cellular oxidative status. To assess the biological response to antioxidants, cells were exposed to CUR [8 μM; 16 μM], and EA [18 μM; 36 μM], for 24h, 48h, and 72h. Proliferation, viability, and NBT assays were initially performed. Based on preliminary results showing greater efficacy at higher concentrations, TUNEL, Wound Healing and Transwell assay were conducted to evaluate apoptosis and cell migration, limited to the highest concentrations. Both compounds inhibited proliferation and reduced viability, TUNEL results confirmed increased apoptosis, while Wound Healing and Transwell assay showed a marked reduction in migratory capacity. Therefore, treatment with CUR and EA modulated the cellular oxidative status, by a reduction in ROS levels compared to controls. This effect is associated with increased apoptosis, suggesting the involvement of redox regulation and related signaling pathways. This is also reflected in reduced viability, proliferation, and migratory capacity. Overall, the data confirm the antitumor potential of EA and CUR in IGROV-1 cells, highlighting differences in response between the two compounds, suggesting distinct but complementary mechanisms of action. Overall, these findings suggest that polyphenols may represent a promising supportive strategy, with potential benefits for the preservation of ovarian function and fertility in cancer patients.

P28: Amazonian *Copaifera officinalis* Oleoresin Induces Apoptosis in Human Tumor Cells: Chemical Profiling and *In Silico* Target Validation

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Abstract:
Natural products are essential sources of novel anticancer agents, with *Copaifera* species recognized for their bioactive terpenoids. While copaiba oleoresins have been studied for their antimicrobial and anti-inflammatory properties, their specific cytotoxic mechanisms and molecular targets require further elucidation. This study aimed to evaluate the cytotoxic effects of *Copaifera officinalis* oleoresin and determine its cell death mechanisms and molecular interactions in human tumor models.

The cytotoxic activity of *C. officinalis* oleoresin (RE) was evaluated against MCF-7, MDA-MB-231, PC-3, HepG2, and A-375 human tumor cell lines using the MTT assay. Cell death mechanisms were assessed by Annexin V-FITC/7-AAD flow cytometry. Chemical profiling was performed by GC–MS. Additionally, computational studies were conducted for the major compounds (bergamotene, elemene, and caryophyllene) against p53, caspase-3, caspase-9, and Bcl-xL proteins. RE showed strong cytotoxicity, with IC_{50} values below 80 µg/mL across several cell lines. Morphological analysis revealed cell shrinkage, rounding, and detachment. Flow cytometry confirmed apoptosis as the predominant mode of cell death, with minimal necrosis. GC–MS analysis identified major sesquiterpenes, including β-caryophyllene, α-elemene, and bergamotene. *In silico* studies revealed that all three compounds interact with the target proteins, with caryophyllene demonstrating the highest binding affinity for p53, caspase-3, caspase-9, and Bcl-xL.

Copaifera officinalis oleoresin exerts cytotoxicity in breast, prostate, liver, and melanoma cell lines primarily through apoptosis induction. *In silico* analysis suggests that its major sesquiterpenes, particularly caryophyllene, trigger apoptosis by interacting with key apoptotic regulators. These findings highlight *C. officinalis* oleoresin as a promising source of anticancer compounds, underscoring the pharmacological potential of Amazonian biodiversity. *Copaifera officinalis* oleoresin exerts cytotoxicity in breast, prostate, liver, and melanoma cell lines primarily through apoptosis induction. *In silico* analysis suggests that its major sesquiterpenes, particularly caryophyllene, trigger apoptosis by interacting with key apoptotic regulators. These findings highlight *C. officinalis* oleoresin as a promising source of anticancer compounds, underscoring the pharmacological potential of Amazonian biodiversity.

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P29: Chemical profiling and anticancer activity of *Fomitopsis betulina* aqueous extract in A549 and CCRF-CEM cells

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Fomitopsis betulina is a medicinal polypore with potential anticancer activity, but the relationship between its chemical composition and cellular effects remains insufficiently characterized. We combined high-resolution LC–MS/MS profiling with in vitro evaluation in human A549 lung carcinoma and CCRF-CEM leukemia cells. The aqueous extract was analyzed by LC–MS/MS, and cells were exposed for 24 h to 1, 10, or 50 µg/mL extract, alone or combined with cisplatin (1 or 10 µM). Cellular responses were evaluated using DCF-DA and rhodamine 123 fluorescence, γH2AX activation, cell-cycle and apoptosis/cell-death analyses, and caspase assays. Statistical comparisons used Welch's t-test with Holm correction.

LC–MS/MS detected 2,290 molecular features and putatively annotated 729 metabolites. A curated set of 30 compounds comprised lanostane-type triterpenoids, betulin derivatives, sterols, sphingolipids, and lysophospholipids. Dehydroeburicoic acid predominated, followed by polyporenic acid-like compounds, pachymic acid, ergosterol, and phytosphingosine. In A549 cells, the extract increased γH2AX positivity and G0/G1 accumulation, while 50 µg/mL reduced the DCF-DA signal to 65.6% of control. Combinations with cisplatin enhanced late apoptosis/cell death and caspase-9-associated signaling, particularly with 10 µM cisplatin. CCRF-CEM cells showed greater pro-apoptotic responsiveness: 10 µg/mL extract increased total apoptosis, 50 µg/mL increased G0/G1 accumulation, and 50 µg/mL extract combined with 1 µM cisplatin increased total apoptosis to 14.9% versus 7.4% with cisplatin alone (adjusted $p = 0.009$), reducing live cells to 81.1%.

These findings identify *F. betulina* as a chemically rich source of bioactive triterpenoids and lipids and indicate cell-type-dependent anticancer activity, including enhancement of low-dose cisplatin effects in leukemia cells.

P30: A Strategy for the Discovery of Antikinetoplastid Lead Compounds: Bioassay-Guided Fractionation of *Argyranthemum frutescens*

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Chagas disease, caused by the protozoan *Trypanosoma cruzi*, and leishmaniasis, caused by different *Leishmania* species, remain major public health challenges, particularly in developing countries, due to their high prevalence and limitations of current treatments, including toxicity, drug resistance, and reduced efficacy.[1] Consequently, the discovery of new, safe, and effective antikinetoplastid agents remains a priority.

In this context, plant-derived natural products continue to represent an important source of structurally diverse bioactive molecules with therapeutic potential.[2]

The present work explores *Argyranthemum frutescens* as a potential source of plant-derived antiparasitic compounds. Bioassay-guided fractionation of its ethanolic root extract led to the isolation of four polyacetylenes. These compounds exhibited potent and selective activity against *Trypanosoma cruzi*, *Leishmania amazonensis*, and *Leishmania donovani*.

Subsequently, structure–activity relationship and mechanistic studies supported their potential as lead compounds for the development of novel antiparasitic agents.

Overall, these findings highlight *A. frutescens* as a valuable source of bioactive polyacetylenes and reinforce the potential of natural products for the development of new therapeutic strategies against kinetoplastid diseases.

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P31: Comparative Analysis of Phenolic and Capsaicinoid Profiles and *In Vitro* Biological Activities of Several *Capsicum chinense* Jacq. Cultivars

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The chili pepper belongs to the Solanaceae family and the *Capsicum* genus, comprising over 35 species. It is one of the crops exhibiting the greatest diversity in terms of shape and color. There are at least 2,000 varieties, each known locally by dialect names rooted in local culture—names that vary from town to town and region to region.
Capsicum chinense Jacq. is the most virus-resistant species and includes the world's hottest varieties. *C. chinense* is an important source of polyphenols, flavonoids, and capsaicinoids, compounds with antioxidant, anti-inflammatory, and metabolic properties[1]. The phytochemical composition varies considerably among cultivars and stages of ripeness, with direct effects on biological activity, including the hypoglycemic and enzyme-inhibitory potential already documented for related species[2]. To date, comparative studies on different *C. chinense* varieties regarding their metabolic and anti-inflammatory potential remain limited. The objective of this study was to characterize the polyphenol, flavonoid, and capsaicin content in different cultivars of Calabrian *C. chinense* and to evaluate their antioxidant activity (DPPH test), anti-obesity potential through the inhibition of pancreatic lipase and anti-inflammatory (NO inhibition in RAW 264.7 macrophages) properties *in vitro.* Among the cultivars analysed, Carolina Reaper Red had the highest total polyphenol content (14.00 ± 0.07 mg GAE/g), and the Carolina Reaper Chocolate had the highest capsaicin content. The Habanero Chocolate variety exhibited the best antioxidant activity in the DPPH assay (IC_{50} 121.2 ± 6.49 µg/mL). Regarding anti-obesity potential, the Carolina Reaper cultivars showed the greatest inhibition of pancreatic lipase, while some of the Habanero cultivars resulted in a more marked reduction in NO production in RAW 264.7 macrophages (IC_{50} (Habanero Chocolate) = 141.90 ± 11.10 µg/mL), followed by the Carolina Reaper varieties. These findings suggest a strong correlation between the specific phenolic profile of these cultivars and their potential health-promoting effects.

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P32: Covariance analysis of anticancer activity and marine natural products

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Cancer represents a significant worldwide health burden. Although antineoplastic therapies have improved, many cancer types, including vascularized solid tumors, exhibit resistance, highlighting the need for new treatment strategies. In this context, marine organisms are prolific producers of bioactive secondary metabolites with potential for the development of new antitumor agents[1]. This study aimed to investigate correlations between marine natural products and in vitro anticancer activity.

Crude extracts of *Phormidium laetevirens*, *Blennothrix lyngbyaceae*, *Dysidea avara*, *Laurencia dendroidea*, *Ulva* sp., *Dichotomaria marginata*, *Laurencia elata*, and *Anabaena* sp. were analyzed by GNPS MS/MS molecular networking, resulting in matches with analogs of emetine, transcinnamaldehyde, asiatic acid, emetine dihydrochloride, quercetin, kasianine, 5-chlorodivaricatinic acid, 3-epixestoaminol C, malingamide C, and curacin A. These extracts were further evaluated *in vitro* using the MTT assay on various immortalized cell lines, including HCT-116 (colorectal), MCF-7 (breast), A-549 (lung), and EA.hy926 (vascular endothelial) to evaluate cytotoxic and antiproliferative activities. For cytotoxicity, six concentrations were tested, while antiproliferative assays used subcytotoxic concentrations.

The results showed cytotoxic activity (IC_{50} µg/ml) in all tumor cell lines for *D. avara* (HCT116: 40.39; MCF7: 41.88; A549: 34.18), *L. dendroidea* (HCT116: 29.21; MCF7: 73.17; A549: 41.06), and *L. elata* (HCT116: 30.30; MCF7: 60.97; A549: 33.24), while *Anabaena* sp. was active only in HCT116 cells (49.14). Antiproliferative assays at 24, 48, and 72 h showed that only *Anabaena* sp., *D. avara*, *L. dendroidea*, and *L. elata* significantly inhibited endothelial cell growth.

Based on bioactivity and metabolic profiles, covariance analysis using the DAFDiscovery platform revealed a correlation coefficient of 0.4 between analogs of emetine dihydrochloride, asiatic acid, quercetin, malingamide C, and curacin A and the cytotoxic activity, as well as between asiatic acid and the antiproliferative activity. Overall, these findings highlight promising metabolites from *Anabaena* sp., *D. avara*, *L. dendroidea*, and *L. elata* for anticancer drug discovery.

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P33: Variation in solar intensity affect growth and essential oil content in *Kaempferia galanga* L.

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Ekangi (*Kaempferia galanga* L.), a member of Zingiberaceae, is an aromatic rhizomatous herb with potential medicinal properties. Earlier reports have shown that varying degree of shading significantly affected the quantity of tillers, number and rhizome biomass in *Zingiber officinale*. In this study, we attempted shade net cultivation of ekangi under different shading percentage (green coloured) to explore how variation in light intensity affect rhizome yield, morphological traits, biochemical constituents, mineral composition and essential oil profile. Shade net with 50% shading percentage turned out to be the most preferable cultivation condition for ekangi showing a higher rhizome yield with superior morphology viz. higher tiller number, rhizome diameter and length. Retention of highest concentrations of several macronutrients such as magnesium, phosphorus and potassium was also maintained under this condition. Total phenolic and flavonoid contents showed highest accumulation under 50% shade net attributing to the highest antioxidant capacities (ABTS and FRAP assays) in plants grown under this condition. The major phenolic compounds were identified to be ethyl *p*-methoxycinnamate (EPMC) and ethyl cinnamate (EC) which were also found out to be the major volatile compounds in the volatile profile of the ekangi rhizomes. When quantified by GC-MS, the content of EPMC in the internal pool of volatiles was found to be higher in ekangi rhizomes when cultivated under 35% and 50% shading conditions. Under 50% shading, both the essential oil content and essential oil yield of ekangi rhizome significantly elevated compared to the other growing conditions. Quantitative analysis using GC-FID demonstrated that both EPMC and EC concentrations in the rhizome essential oil were highest under 50% shading condition when open field grown plants showed the lowest concentrations of the same. Overall, these findings in ekangi suggest that optimizing incident light by adjusting shade-net percentage can boost aromatic and bioactive compound production.

Keywords: *Kaempferia galanga*, Shade nets, Antioxidant, Nutrients, Ethyl p-methoxycinnamate, GC-FID.

P34: Edible feijoa flowers: chemical characterization, edible coating and *in vitro* bioaccessibility

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Edible flowers are increasingly recognized for their aesthetic appeal and nutraceutical potential due to their high content of bioactive compounds.[1] Among them, feijoa flowers (*Acca sellowiana* (O. Berg) Burret, Myrtaceae) represent a promising source of polyphenols, although their phytochemical composition remains poorly characterized and their high perishability limits commercial exploitation.[2,3] This study aimed to investigate the phytochemical profile and biological potential of different floral tissues, while developing an edible coating to improve postharvest preservation.[4]
Petals, pistils, and bracts were freeze-dried, extracted with acidified ethanol, purified by XAD-4 resin chromatography, and characterized by UV-Vis spectroscopy, ATR-FTIR spectroscopy, and HPLC-ESI-TQ-MS/MS, revealing a rich and diverse polyphenolic profile. The antioxidant capacity of the extracts was evaluated using DPPH and ABTS radical scavenging assays, while cytocompatibility and protection against oxidative stress were assessed in immortalized human cell lines.
Fresh whole flowers were coated by immersion in a chitosan-based film-forming solution containing citric acid, glycerol, and ascorbic acid, resulting in a homogeneous protective layer over all floral tissues. The coating effectively delayed flower senescence, as evidenced by ATR-FTIR analysis, and contributed to preserving tissue structural integrity during storage.
Polyphenol bioaccessibility was assessed using a kinetic release assay in simulated intestinal fluid and the standardized INFOGEST *in vitro* digestion protocol. The digested fractions were analyzed by HPLC-ESI-TQ-MS/MS to evaluate changes in the polyphenolic profile and identify the compounds remaining bioaccessible after simulated gastrointestinal digestion.
The proposed strategy integrates phytochemical characterization, postharvest preservation, and *in vitro* bioaccessibility assessment, providing a comprehensive approach for the valorization of feijoa flowers as an underutilized edible resource and supporting their potential application as a sustainable functional food.

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P35: From North to South: Metabolic Profiling and Bioactivity of Extracellular Vesicles Derived from Finnish Cloudberry and Italian Apple

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Extracellular vesicles (EVs) are naturally occurring, membrane-enclosed nanoparticles that facilitate cell-to-cell communication by carrying lipids, proteins, metabolites, and nucleic acids[1]. Historically, EVs have been mainly isolated and analysed from human cells. Recently, plant-derived EVs have gained significant attention due to their ability to carry a wide array of natural bioactive compounds with therapeutic potential for human health[2]. For instance, fruit-derived EVs are enriched in phenolic acids that inhibited cancer cell proliferation without affecting healthy cells[3]. In collaboration with the University of Oulu (Finland), we isolated and characterized EVs from two distinct species: Annurca apple (native to Southern Italy) and Cloudberry (native to Nordic forests). This selection highlights the rich diversity of European fruit species possessing health-promoting properties. EV morphology and concentration were evaluated using Nanoparticle Tracking Analysis (NTA) and Transmission Electron Microscopy (TEM). Their metabolomic profiles were analysed via UHPLC-MS/MS to identify accumulated bioactive metabolites. Finally, cytotoxicity and antioxidant activity were assessed on human cells using MTT and ABTS assays, respectively. We obtained a high yield of EVs, reaching 4.69×10^{11} particles mL^{-1} for apple and 6.20×10^{12} particles mL^{-1} for cloudberry. At a dose of 5 µg, cell viability reached 120% with apple EVs and 80% with cloudberry EVs. Both EV types exhibited a rich polyphenolic profile, with total polyphenol contents of 17.63 µg GAE mL^{-1} (apple) and 33.74 µg GAE mL^{-1} (cloudberry), and antioxidant activities of 69.98% and 65.60%, respectively. Metabolomic characterization revealed an enrichment in both polyphenols (ellagic acid, quercetin, rutin) and triterpenic acids (6α-hydroxybetulinic acid, madecassic acid). Altogether, these findings highlight the beneficial potential of plant-derived EVs on human cells, establishing a strong correlation between their bioactivity and metabolic cargo. Future studies will help investigate their specific intracellular delivery mechanisms.

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P36: Natural Deep Eutectic Solvents vs. Conventional Solvents for the Extraction of Bioactive Compounds from *Aronia melanocarpa*

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Aronia melanocarpa (black chokeberry) is among the richest dietary sources of anthocyanins in the temperate flora, positioning it as an attractive raw material for cosmetic and nutraceutical applications.[1] Extract standardization strongly depends on the extraction solvent. This study compared six Natural Deep Eutectic Solvents (NaDES; four choline chloride- and two betaine-based systems) against four conventional/semi-conventional solvents (water, 70% ethanol (EtOH), 20% glycerol (G), 20% propylene glycol (PG)) for the recovery of bioactive compounds from aronia fruits.

Total polyphenol and anthocyanin content were determined spectrophotometrically, while LC-MS enabled quantification of the major anthocyanins, phenolic acids and flavonoids in each extract. Antioxidant activity was assessed by DPPH and ABTS assays. Extract safety and functional potential for cosmetic use were evaluated in HaCaT keratinocytes by neutral red and resazurin cytotoxicity assays, and anti-inflammatory activity was assessed using a stable NF-κB-luciferase reporter HaCaT cell line following TNF-α stimulation.[2]

Polyphenol and anthocyanin content in most NaDES extracts were comparable to G and PG extracts, whereas one choline chloride-based NaDES (NaDES3) contained markedly higher levels of bioactive compounds. LC-MS confirmed NaDES3 had the highest content of neochlorogenic acid, chlorogenic acid, procyanidin B, quercetin hexoside, quercetin vicianoside, and three anthocyanins (cyanidin hexoside, -arabinoside, -xyloside). Due to their low pH, most NaDES extracts required neutralization before testing to reduce HaCaT cytotoxicity. Among ten neutralized extracts tested (0.25-1%), two NaDES-based extracts significantly inhibited NF-κB activity in TNF-α-stimulated HaCaT cells; a comparable effect was observed for the solvent controls alone, suggesting an intrinsic solvent contribution to the anti-inflammatory response.

These results demonstrate that NaDES represent an efficient, tunable alternative to conventional solvents for recovering bioactive, safe, and functionally active compounds from *Aronia melanocarpa*, supporting their application in cosmetic formulations targeting skin antioxidant protection and inflammation; the solvent's contribution to the anti-inflammatory effect warrants further mechanistic study.

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P37: Isoflavonoid-Rich Extracts from *Trifolium rubens* L. Parent Plant and Callus Cultures: Phytochemical Characterization and Anti-Aging Potential

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Trifolium rubens L. (ruddy clover) is a rare and underexplored perennial species native to Central and Southern Europe. Owing to its limited distribution and endangered status in several European countries, including Poland, its phytochemical composition and biological activity remain poorly investigated [1]. The present study compared the polyphenolic profile, with particular emphasis on isoflavonoids, and the elastase- and tyrosinase-inhibitory activities of extracts obtained from the leaves, flowers, and *in vitro* callus cultures of *T. rubens*.

Leaves and flowers of *T. rubens* were collected from the Botanical Garden in Kielce (Poland), whereas seeds were used as explants for callus induction. The callus cultures were maintained on Murashige and Skoog (MS) [2] medium supplemented with 1 mg/L BA (6-benzyladenine), 0.5 mg/L NAA (1-naphthaleneacetic acid), and 0.25 mg/L GA_3 under controlled conditions (25±2°C, continuous lighting). The biomass was harvested after 20 days of culture. The polyphenolic composition of 70% ethanol extracts was characterized by HPLC-DAD [3], while elastase and tyrosinase inhibitory activities (mushroom tyrosinase and murine B16F10 melanoma cell lysates) were determined using spectrophotometric assays [4,5].

HPLC-DAD analysis identified three major groups of polyphenols: flavonoids, isoflavonoids, and phenolic acids. The leaves contained the highest levels of polyphenols, particularly trifolin (1257.13 mg/100gDW) and myricetin (1068.20 mg/100gDW), whereas callus cultures exhibited a distinct isoflavonoid profile dominated by calycosin-7-*O*-glucoside (516.01 mg/100gDW) and formononetin (103.26 mg/100 g DW). Flower extracts showed the strongest elastase inhibitory activity (25–35% inhibition at 0.025–0.1 mg/mL), while callus and leaf extracts showed the strongest murine tyrosinase inhibition among the tested extracts (15–20% at 0.1 mg/mL). Inhibition of mushroom tyrosinase was observed only for flower extracts (approximately 25% at 0.1 mg/mL).

T. rubens represents a promising source of bioactive polyphenols with anti-aging potential. Moreover, callus cultures provide a sustainable source of valuable phytochemicals.

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P38: Phytochemical Characterization and Anti-Aging Potential of *Lathyrus latifolius* L. Parent Plants and *In Vitro* Shoot Cultures

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Lathyrus latifolius L. (broadleaf pea) is a rare and underexplored species with limited information available on its phytochemical composition and biological activity. Although preliminary studies suggest that it may be a rich source of secondary metabolites. Moreover the phytochemical potential and biological properties of its in vitro cultures have not yet been investigated. Therefore, the aim of this study was to compare the polyphenolic composition and anti-aging potential of extracts obtained from the aerial parts and *in vitro* shoot cultures of *L. latifolius*.

Leaves, flowers, herbs, and seeds of *L. latifolius* were collected from the Botanical Garden in Kielce (Poland). *In vitro* shoot cultures were established from surface-sterilized seeds and maintained on Murashige and Skoog (MS) [1] medium supplemented with 1 mg/L BA (6-benzyladenine), 0.5 mg/L NAA (1-naphthaleneacetic acid), and 0.25 mg/L GA_3 (gibberellic acid) under controlled conditions (25±2°C, continuous light). The shoot biomass was harvested after 20 days of culture. The polyphenolic composition of 70% ethanol extracts was characterized by HPLC-DAD analysis [2], while elastase- and tyrosinase-inhibitory activities (mushroom tyrosinase and murine B16F10 melanoma cell lysates) were determined using by spectrophotometric method [3,4].

HPLC-DAD analysis identified six phenolic acids, two phenylpropanoid glycosides, and catechin. The leaf extract contained the highest level of polyphenols, with verbascoside (514.67 mg/100 g DW) and catechin (407.82 mg/100 g DW) as the predominant compounds. None of the extracts inhibited mushroom tyrosinase. In contrast, herb and shoot culture extracts showed the strongest inhibition of murine tyrosinase (23–30%), while the leaf extract showed the highest elastase inhibitory activity (27–39%). Notably, shoot culture extracts also demonstrated considerable elastase inhibition, indicating their potential as a source of anti-aging phytochemicals.

These findings highlight *L. latifolius* as a promising source of bioactive polyphenols with potential cosmetic and anti-aging applications and highlight *in vitro* cultures as a sustainable alternative to natural plant material. Furthermore, shoot cultures may represent a sustainable alternative source of valuable phytochemicals, reducing dependence on natural plant populations.

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P39: Antioxidant potential and modulation of oxidative stress by a polyphenol-rich onion peel extract

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The growth of the world's population has led to an increase in food production and, consequently, the amount of waste produced by the food industry [1]. This situation challenges sustainability, but offers opportunities for circular economy valorization. Onion peels are a rich source of phenolic compounds, and several studies have reported the significant antioxidant potential of their derived extracts [2]. However, evidence of the antioxidant capacity of onion extracts at the cellular level remains limited. This study investigated the antioxidant potential of an onion peel extract, previously optimized in terms of phenolic compounds using *in vitro* assays and Caco-2 cell model. The in vitro antioxidant capacity was characterized using DPPH, ABTS, and FRAP assays. Furthermore, cytocompatibility and protective effect against H_2O_2-induced acute oxidative stress were evaluated in Caco-2 cell line, using the Alamar Blue method and the DCFH-DA fluorescent probe, respectively.

In the spectrophotometric assays, the extract demonstrated an excellent capacity to neutralize free radicals and a remarkable reducing power, achieving 160.67±29.16; 9.72±2.86 and 9.09±4.53 mg Trolox equivalents/g dw in the FRAP, ABTS and DPPH assays, respectively. Alamar Blue assay on Caco-2 confirmed the safety of the bioactive extract across the 1–500 µg/mL range, with no alterations in their typical morphology or decreases in viability. Intracellular monitoring using the DCFH-DA probe demonstrated that the extract exerts a potent, dose-dependent protective effect against oxidative stress induced H_2O_2. Concentrations ≥ 150 µg/mL significantly mitigated ROS accumulation, with the 500 µg/mL dose significantly restoring cellular levels to those of the physiological control.

These findings demonstrate that the onion peel extract is both safe and biologically active at the cellular level. Therefore, this extract is a promising candidate for developing high-value antioxidant ingredients, offering the nutraceutical and food industries a sustainable, clean-label alternative to synthetic additives.

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P40: Extruded Snacks Fortified with Schisandra chinensis: Phenolic Profile and Antioxidant Capacity

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A balanced diet is a key determinant of human health and well-being[1]. It represents an essential component in both the prevention and management of numerous lifestyle-related diseases, such as type 2 diabetes, obesity, hypertension, neurodegenerative disorders and cancer. These functions are fulfilled by functional foods. One of the strategies for their production is fortification with plant-based ingredients exhibiting health-promoting potential, for example those rich in polyphenolic compounds[2].

The aim of the study was to analyse a novel assortment of health-promoting fortified foods that could potentially be manufactured on a large scale in the future. The fortified food products were produced using Chinese magnolia vine (*Schisandra chinensis* (Turcz.) Baill.), a plant cultivated in the Lublin region of Poland.

Snacks enriched with 5, 10, 15, and 20% addition of Chinese magnolia vine fruit were produced at different screw speeds of a single-screw extruder (80, 100, and 120 rpm), subjected to extraction, and then analysed for their antioxidant properties using complementary assays (TPC, FRAP, CUPRAC, and DPPH). Selected phenolic acids were quantified using ultra-high-performance liquid chromatography[3].

The results demonstrated that Chinese magnolia vine fruit and the fortified snacks produced therefrom are rich sources of antioxidant compounds. Snacks enriched with Schisandra fruit exhibited markedly higher antioxidant activity compared with the non-fortified control. Strong positive correlations were observed between the level of Schisandra addition and the antioxidant properties of the samples. The highest antioxidant activity was found for the snack containing 20% Schisandra fruit produced at a screw speed of 120 rpm. In extracts enriched with this plant, the following phenolic acids were identified and quantified: protocatechuic, p-hydroxybenzoic, vanillic, caffeic, syringic, p-coumaric, ferulic, and synaptic acids.

These findings indicate a high potential of Chinese magnolia vine as a health-promoting fortifying ingredient for functional foods and represent the first comprehensive experimental study on Schisandra-enriched extruded snacks.

Keywords: *Schisandra chinensis*; extruded snacks; phenolic acids; antioxidant activity

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P41: From Extruder to Gut: Bioactive Phenolics and Antioxidant Properties of Ginseng-Enriched Snacks after Simulated Digestion

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In recent years, an increasing number of individuals have adopted a healthy lifestyle. Consumers increasingly recognize the need to include health-promoting components in their diet, such as antioxidants, among which polyphenols[1] are of particular importance.
It is well established that the biological activity of such compounds may differ substantially under in vitro and in vivo conditions. Simulated gastrointestinal digestion is a laboratory technique used to mimic the digestive processes occurring in the human gastrointestinal tract. During in vitro digestion, polyphenolic compounds may undergo various transformations (induced by digestive enzymes, pH changes, and interactions with other food constituents)[2], which markedly affect their bioaccessibility and, consequently, their potential impact on human health. Therefore, the aim of the present study was to evaluate the content of selected bioactive compounds and the antioxidant properties of a new range of food products - snacks enriched with ginseng root, before and after a two-step in vitro digestion process.
Snacks fortified with 15% ginseng root[3] were produced using extrusion method at screw speeds 80, 100, and 120 rpm, and subsequently subjected to extraction. In the resulting extracts, the total polyphenol content (TPC), total flavonoids, and total phenolic acids were determined. In addition, selected phenolic acids were quantified using ultra-high-performance liquid chromatography.
Strong, positive correlations were observed between the contents of polyphenols, flavonoids, and phenolic acids and the level of the functional ginseng addition. The use of a screw speed of 80 rpm resulted in the highest contents of phenolic acids, total polyphenols, and flavonoids in the extracts. For this reason, snacks enriched and processed at 80 rpm were selected for in vitro digestion. A decrease in TPC, total phenolic acids, and total flavonoids was observed after both stages of digestion in comparison with the undigested samples.
The present work provides the first comprehensive experimental assessment of the impact of simulated gastrointestinal digestion on the antioxidant properties of ginseng-enriched extruded snacks

Keywords: ginseng root; extruded snacks; simulated gastrointestinal digestion; antioxidant activity

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P42: Carbohydrate modulation through solar drying: Enhanced functional value of figs

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Plant-derived oligosaccharides and pectic polysaccharides are increasingly recognized as promising functional food ingredients due to their prebiotic potential and contribution to plant-based nutrition [1]. Drying alters the nutritional composition of plant foods [2]; however, its effects on less-studied molecules such as carbohydrate, particularly oligosaccharides and polysaccharides, remain insufficiently explored. In figs, drying may enhance the concentration, availability, and functional potential of these components, highlighting dried fruits as a valuable source of prebiotic compounds and functional dietary fibers.

The fig cultivar Pingo de Mel was evaluated at three processing stages: ripe fresh, overripe fresh, and overripe solar-dried at 50 °C. Carbohydrates were sequentially fractionated into alcohol-soluble extract (ASE), cold-water extract (CWE), hot-water extract (HWE), and water-insoluble residue (WIR). Monosaccharide composition was determined by gas chromatography with flame ionization detection (GC-FID), uronic acids were quantified spectrophotometrically, and soluble oligosaccharides were characterized by gas chromatography coupled with mass spectrometry (GC-MS).

Solar drying increased soluble sugars from 19-26% in fresh fruits to 45% in dried samples while maintaining a structurally diverse carbohydrate matrix. The soluble fractions (CWE and HWE) were enriched in uronic acids (34-77 mol%) and arabinose (7-11 mol%), indicating the presence of arabinan-rich pectic polysaccharides. In contrast, the WIR fraction was mainly composed of glucose (27-43 mol%) and xylose (9-13 mol%), suggesting the presence of xyloglucan structures. Solar drying also increased the abundance and structural diversity of soluble oligosaccharides, expanding the pool of potentially bioaccessible glycans with prebiotic potential.

These findings demonstrate that solar-dried overripe figs represent a valuable source of structurally diverse carbohydrates. The preservation and enrichment of pectic polysaccharides and oligosaccharides, combined with the sustainable valorization of overripe fruits, support solar drying as an environmentally friendly strategy for producing nutraceutical and functional food ingredients, warranting further investigation of their biological functionality.

Keywords: Fig, functional dietary fiber, polysaccharides, oligosaccharides, drying.

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P43: Phytochemical investigation of the edible wild plant 'Aspraggine' (*Helminthotheca echioides*): extraction, LC-MS metabolomics, isolation of compounds and evaluation of antioxidant activity

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Helminthotheca echioides belongs to the Asteraceae family, which includes numerous wild edible species native to the Mediterranean basin. Many of these species are traditionally consumed for their fresh, tender leaves as salad vegetables. Their consumption represents an integral component of the Mediterranean diet and has been associated with several health benefits[1]. In addition to essential nutrients and minerals, these plants are rich sources of bioactive compounds[2]. This study aims to investigate the phytochemical profile of *H. echioides* ("Aspraggine") using different extraction techniques and solvent systems, and to evaluate the antioxidant activity of the resulting extracts.
Leaves of *H. echioides* were extracted using conventional maceration and the unconventional techniques ultrasound-assisted extraction (UAE) and microwave-assisted extraction (MAE), employing three EtOH:H_2O mixtures (100:0, 70:30, and 50:50, v/v). The extracts were analysed by ultra-high-performance liquid chromatography coupled with high-resolution tandem mass spectrometry (UPLC-HRMS/MS, Q-Exactive Orbitrap) operating in negative ionization mode, which allowed the putative identification of metabolites belonging to the classes of phenolic acid derivatives, flavonoids, iridoids, sesquiterpenes, and oxylipins. LC-MS data were further processed using multivariate statistical analysis with MetaboAnalyst. Principal component analysis (PCA) revealed a clear clustering pattern primarily driven by solvent composition rather than extraction technique. To isolate the metabolites putatively identified by LC-MS analysis, the extract obtained by maceration using 50% EtOH was fractionated on Sephadex LH-20. The resulting fractions were further purified by HPLC-UV, and the structures of the isolated compounds were elucidated by one- and two-dimensional NMR spectroscopy together with mass spectrometry analyses. Antioxidant activity was evaluated using the DPPH and TEAC in vitro spectrophotometric assays. Extracts obtained with 50% and 70% EtOH:H_2O mixtures exhibited the highest antioxidant activity, suggesting that aqueous ethanol provides the most effective extraction of antioxidant constituents from *H. echioides*.

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P44: Acclimation of *Galdieria daedala* to a Grape-Pomace- derived Aqueous Matrix for Biomass and Phycobiliprotein Production

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Grape pomace is an abundant winery by-product and a promising feedstock for circular bioprocesses[1]. Owing to its metabolic flexibility, the thermoacidophilic red microalga *Galdieria* spp. can grow on organic-rich food-processing streams while generating biomass and phycobiliproteins[2–4]. Among these pigments, C-phycocyanin (C-PC) is of particular biotechnological interest as a natural blue colorant and fluorescent biomolecule[5]. This study evaluated *Galdieria daedala* ACUF 427 cultivated on a grape-pomace-derived aqueous matrix. Dried pomace was extracted in water (1:3, w/v; 65 °C, 1 h), clarified, filtered, and sterilized. Cultures were progressively acclimated through four consecutive 14-day stages containing 25%, 33%, 50%, and 100% grape extract; algae growth on standard Allen medium served as the control. All the biological replicates were maintained at 38 °C under continuous illumination and orbital shaking. Growth, dry biomass, chlorophyll a, C-PC, allophycocyanin, and phycoerythrin were monitored. Statistical analysis ANOVA revealed significant effects of cultivation condition, time, and their interaction on biomass accumulation (all $p \leq 0.0012$). After the final 14-day stage in undiluted grape extract, biomass accumulation was 57% higher than in Allen medium. Chlorophyll a reached 0.161 ± 0.018 g L^{-1} versus 0.093 ± 0.003 g L^{-1}, and biomass-normalized chlorophyll differed significantly between treatments ($p < 0.005$). Crude-extract concentrations of C-PC, allophycocyanin, and phycoerythrin reached 1.77 ± 0.28, 2.15 ± 0.05, and 12.80 ± 0.10 mg mL^{-1}, corresponding to increases of 79%, 36%, and 38% over the control, respectively. These findings demonstrate that stepwise acclimation enables *G. daedala* to grow in an undiluted grape-pomace-derived matrix while enhancing biomass production and crude-extract pigment concentrations. This approach integrates winery-residue valorization with the generation of high-value algal bioproducts within circular green technologies.

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P45: Cold-pressed *Cannabis sativa* and *Silybum marianum* seed oils: physicochemical characterization and selective biological activity in hepatic cell lines

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Seed oils from medicinal plants are increasingly recognized as functional foods due to their rich profile of fatty acids and bioactive minor constituents; however, their specific bioactivities remain insufficiently characterized. This study provides a comparative physicochemical and biological evaluation of cold-pressed seed oils from *Cannabis sativa* (hemp oil, HO) and *Silybum marianum* (milk thistle oil, MTO), assessing their effects on hepatic cell lines.

Gas chromatography-mass spectrometry (GC-MS) analysis revealed distinct fatty acid profiles: HO exhibited higher linoleic acid (56.21 ± 1.08% vs. 52.34 ± 1.32%) and lower oleic (16.23 ± 0.62% vs. 29.79 ± 1.25%) than MTO, while α-linolenic acid was detected at appreciable levels only in HO (10.80 ± 1.95%). Conversely, MTO displayed a higher total phenolic content (13.72 ± 2.13 vs. 9.93 ± 1.35 mg GAE/100 g oil) alongside greater ferric reducing antioxidant power (FRAP).

Cell viability and lactate dehydrogenase (LDH) release assays demonstrated that HO was more cytotoxic than MTO toward hepatocellular carcinoma cells (HepG2). Real-time cell analysis (xCELLigence system) confirmed a time and concentration-dependent anti-proliferative effect for both oils (0.02–0.2 mg/mL) with HO being more potent. In non-tumoral hepatic cells (THLE-2), neither oil significantly impaired viability across the tested range; however, MTO actively supported cell proliferation. Furthermore, pre-treatment with MTO conferred a stronger cytoprotective effect against tert-butyl hydroperoxide -induced oxidative stress, significantly inhibiting intracellular reactive oxygen species (ROS) production and reducing lipid peroxidation.

These preliminary findings indicate that both cold-pressed oils act selectively on hepatocellular carcinoma cells by reducing viability and proliferation without significantly affecting non-tumoral hepatocytes. Notably, milk thistle oil protects liver cells against oxidative damage, supporting its further investigation for targeted hepatoprotective applications.

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P46: Differential Red-Blue Combinations of LED Lights Influence Physiology and Metabolic Efficiency in Celery (*Apium graveolens* L.)

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In addition to providing energy for photosynthesis, light dictates specific signals which regulate the biosynthesis of phytochemicals. The three light parameters viz. quantity (intensity and photoperiod), quality (spectral composition) and distribution affect physiological responses in plants among which, the spectral composition of light is known to play a crucial role in plant specialized metabolism. Modulating the light spectra with the help of light emitting diode (LED) can augment the plant development, growth, and nutritional quality. In the present study, we have explored the consequences of growing an aromatic culinary herb, *Apium graveolens* L. (celery) under different combinations of red and blue LED spectral lights viz. 100% red (100R), 50% red: 50% blue (50R:50B), 75% red: 25% blue (75R:25B), 25% red: 75% blue (25R:75B), 100% blue (100B), and warm white (WW, served as control) to see their impact on growth and specialized metabolism. Celery, belonging to the Apiaceae family, has several medicinal properties due to the presence of terpenes, phthalides, phenolics, flavonoids and vitamins. Maximum contents of phthalides were detected in celery grown under 50R:50B. Our research demonstrated that light spectra can enhance the accumulation of vital antioxidants including ascorbic acid, chlorogenic acid, apigenin and thus potentially improve the nutritional profile of celery. Metabolite analysis of plant tissues also revealed the presence of three main sugars viz. glucose, fructose, sucrose and a major sugar alcohol, D-Glucitol along with substantial amounts of organic acids and fatty acids. Expression of key genes in ascorbic acid (AsA) pathway such as phosphomannose mutase (PMM), GDP-D-mannose-3′,5′-epimerase (GME), GDP-L-galactose phosphorylase (GGP1) and L-Galactono-1,4-lactone dehydrogenase (GalLDH) supported enhancement of AsA under 25R:75B and 100B. These studies suggest that proper combinations of blue and red spectra of light could play an important role to supplement the growth and nutritional characteristics of celery under indoor cultivation.

Keywords: antioxidants, specialized metabolites, culinary herb, phytonutrients.

P47: Artificial induction of tetraploidy enhances essential oil biosynthesis and accumulation in patchouli

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Induction of artificial tetraploidy in aromatic plants is an effective technique to improve phytochemical components. *Pogostemon cablin* (Blanco) Benth. known as patchouli, is an aromatic (Lamiaceae) herb popular for its high essential oil content[1]. This study aimed to generate autotetraploid patchouli plants (2n=4x=128) from diploid stock (2n=2x=64) via *in vitro* exposure to colchicine at concentrations of 0, 0.02, 0.04, or 0.06% (w/v) for 4, 8 and 12 h, respectively. The most effective treatment was shown to be 0.04% colchicine for 8 h. The ploidy level of the plants was confirmed by chromosome counting. After hardening, when the plants were cultivated in open fields, the tetraploid plants showed enhancement in key morphological features including stem height, axillary branch number, leaf count, leaf area, and overall biomass. The tetraploid plants showed significant increase in the leaf internal volatile profile when analysed in GC-MS. Concentrations of major sesquiterpenoids such as patchouli alcohol and γ-curcumene showed nearly two fold increase. Moreover, a huge increase (~14 times) in both the essential oil content (%) and yield (g/ plant) was observed in tetraploid plants in comparison to earlier reports[2]. Concentrations of both major and minor compounds were found to be significantly higher in essential oil of tetraploid plants which correlated with the concentrations in leaf internal volatiles. RT-qPCR analyses validated the biosynthetic boost by showing upregulated expression of mevalonate (MVA) pathway genes (*PcAACT, PcHMGS, PcMVK, PcMVD, PcPTS*) central to patchouli-specific terpene synthesis. Histological studies further revealed significantly higher densities of glandular trichomes and mesophyll glands which act as the reservoirs of essential oil. They were further substantiated by the increased relative expression of the trichome differentiating transcription factors (*PcHD8, PcGL2, PcCD2*)[3]. Collectively, these attributes to the potential vigour of the artificially induced tetraploid plants as a superior higher essential oil yielding variety of patchouli.

Keywords: *Pogostemon cablin*, colchicine, patchouli alcohol, γ-curcumene, glandular trichome, mesophyll gland

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P48: Effects of the invasive ornamental species *Solanum elaeagnifolium* (Solanaceae) on soil biological activity in Mediterranean environment

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Key words: invasive plant, microbial biomass, enzyme activities

Solanum elaeagnifolium Cav., (Solanaceae), native to southern parts of North America, turned to be one of the most invasive and noxious plants in several Mediterranean habitat, from urban area to cultivated land, and negatively affecting a broad spectrum of ecosystem services, and environmental parameters [1]. Plant tissues contain bioactive compounds such as flavonoids, alkaloids, and characteristic toxic substances such as glycoalkaloids (e.g., solasodine, solanine) with pesticidal activity [2].
In Mediterranean ecosystems, characterized by high climatic variability and often nutrient-poor soils, the spread of invasive plant species can significantly affect the structure and functioning of soil-plant systems influencing carbon cycling, nutrient mineralization, and soil enzymatic activity [3]. According to [1], *S. elaeagnifolium* occurs in a wide range of soil types, but very few studies analyze its impact on soil properties [4] and, to the current state of our knowledge, no studies evaluate its effect on metabolism.
The aim of our study was to analyze how invasive species alter soil biological functionality in native vegetation. In a coastal area of Apulia (Southern Italy), we compared soils metabolism associated with the invasive *S. elaeagnifolium* and the native *Cistus creticus* subsp. *eriocephalus*. Soil was sampled in May over two consecutive years under comparable climatic conditions. Nine sites per species were selected and surface soil samples (0–20 cm) collected for analysis of the following parameters: microbial carbon biomass, basal respiration, fungal biomass, and enzymatic activities such as dehydrogenase, phosphatase, cellulase, arylsulfatase, urease, and β-glucosidase. Data was analyzed using two-way ANOVA.
Despite homogeneous soil properties, soils under native vegetation showed significantly higher microbial biomass, basal respiration, and enzyme activities than those under *S. elaeagnifolium*, highlighting that it negatively affects biogeochemical cycles and soil functionality. Soil enzymatic activity emerges as a biochemical indicator for assessing plant ability to sustain microbial communities and soil regeneration.

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P49: Linking Phenolic Composition with Epiphytic Microbial Communities in Edible Snapdragon and Viola Flowers

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Edible flowers have gained increasing attention as functional foods owing to their attractive appearance and high content of bioactive phytochemicals [1]. Besides their nutritional value, the naturally occurring microbial community on flower surfaces plays an important role in food quality, shelf life, and consumer safety [2]. However, little is known about the relationship between phenolic composition and microbial abundance in edible flowers.

In this study, flowers of *Antirrhinum majus* (snapdragon) and *Viola* × *wittrockiana* (garden pansy), representing different flower colours, were analysed for a broad spectrum of phenolic compounds occurring in free, esterified, glycosylated, and bound forms [3] using targeted UHPLC–MS/MS [4]. The same flower samples were subjected to microbiological analyses, including total aerobic bacteria, psychrotrophic bacteria, lactic acid bacteria, Enterobacteriaceae, yeasts, moulds, and members of the Bacillus cereus group. Multivariate statistics, including principal component analysis (PCA) and Pearson correlation analysis, were used to investigate relationships between phytochemical composition and microbial communities.

PCA clearly separated snapdragon and viola samples, demonstrating species-specific phenolic fingerprints that exceeded differences associated with flower colour. Phenolic acids, particularly esterified derivatives of 4-hydroxybenzoic, ferulic, caffeic, vanillic, and *p*-coumaric acids, were among the major contributors to sample discrimination. Correlation analysis revealed distinct associations between individual phenolic compounds and microbial groups. Salicylic acid derivatives and several *p*-coumaric acid conjugates were negatively correlated with selected microbial populations. In contrast, esterified phenolic acids showed positive associations with total aerobic bacteria and other microbial groups.

These findings demonstrate that the phenolic composition of edible flowers is closely associated with the structure of their naturally occurring microbiota. Understanding these relationships may contribute to the selection of flower cultivars with improved microbiological quality and enhanced functional properties, providing new insights into the ecological role of specialized metabolites in edible horticultural crops.

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P50: Bioactive Polyphenolic Phytocomplexes from Leaves of *Thymus vulgaris* Cultivated in Former Tobacco-Growing Areas of the Sannio Region

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Thymus vulgaris L. (Lamiaceae) is an aromatic plant rich in phenolic compounds with relevant biological activities. In this study, a polyphenol-enriched extract was obtained from dried *T. vulgaris* leaves cultivated within the RIPOT project, aimed at converting former tobacco-growing areas in the Sannio region into land for medicinal and officinal plants.

Dried leaves were sequentially extracted with chloroform and methanol, and the latter extract was partitioned by liquid–liquid extraction. The ethyl acetate fraction was found to be enriched in polyphenolic constituents. LC/MS and LC/MS/MS analyses allowed the identification of 16 metabolites, whose levels were subsequently determined by Multiple Reaction Monitoring (MRM) using quercetin as an external standard.[1]

The polyphenol-enriched extract was evaluated against human neuroblastoma SK-N-BE(2)-C and SH-SY5Y cells.[2] MTT and SRB assays showed a dose- and time-dependent cytotoxic effect, with pronounced activity after 72 h at 125 μg/mL, exceeding that of vinblastine. At the highest concentration tested, the extract increased intracellular ROS levels and induced apoptosis in SH-SY5Y cells, associated with activation of caspases 3 and 8.

Overall, these findings highlight the biological potential of *T. vulgaris* polyphenol-enriched extracts and support further investigation of their mechanisms of action, while contributing to the valorization of medicinal plants cultivated in former tobacco-growing areas.

Keywords: *Thymus vulgaris*, polyphenols, LC/MS, MRM, cytotoxicity, neuroblastoma, apoptosis, ROS, medicinal plants

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