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Editorial: Innovative approaches in isolation and purification: balancing efficiency and sustainability

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Editorial on the Research Topic

**Innovative approaches in isolation and purification: balancing efficiency
and sustainability**

Topic scope and challenges

Isolation and purification represent the cornerstones of natural products (NPs) research, providing the essential framework for securing bioactive compounds in their refined chemical states. While recent methodological advancements have expanded the researcher's toolkit, the ability to achieve the delicate balance of high purity and maximum yield continues to be a challenge in the field.

Current research focuses on the efficacy, ecological consequences of purification procedures, and ability for scaling lab methods to industrial applications. Recent studies have presented novel approaches, including green chemistry techniques and advanced chromatographic methods, which demonstrate potential in tackling these challenges. Nonetheless, a gap persists in integrating these advancements and suggesting cohesive strategies for future research. This Research Topic aims to provide a comprehensive overview by addressing specific questions, including the optimization of purification techniques and the integration of sustainable practices, to guide researchers and practitioners in the field. To obtain additional insights in the field of isolation and purification, the key themes of this Research Topic include the advancements in chromatographic and non-chromatographic purification techniques, incorporation of green chemistry principles in purification methodologies, challenges and solutions in scaling of purification methods, innovative purification techniques in NPs, comparative analysis of traditional and modern purification techniques, and the effects of purification processes on environment and economy. These contributions illuminate pathways for metabolomics- and bioassay-guided isolations, aligning with Frontiers in Natural Products'

emphasis on sustainable discovery workflows (Frontiers in Natural Products, 2026; Hwang, 2026).

Contribution highlights

The Research Topic has resulted in three reviews, one report, and two research articles reporting and discussing the advancements in NPs isolation and purification. Morais et al. have reviewed the common purification methods of saponins from *Quillaja* sp. for vaccine adjuvants. They detailed the extraction of QSap Quil-A (Quil-A®) from the cortex of *Quillaja saponaria* on DEAE-cellulose ion exchange, followed by Sephadex G50 gel exclusion chromatography, which allowed achieving adjuvant-active fractions with low heterogeneity. They extend to QS-21 purification, a complex triterpene glycoside of quillaic acid that exhibited a better balance between adjuvant activity and low toxicity, through three main steps; polyvinylpyrrolidone (PVPP) adsorption, diafiltration, and reverse-phase chromatography to obtain >93% purity molecule. Later, a more novel two-step approach that involved reversed-phase chromatography followed by hydrophilic interaction chromatography (HILIC), which significantly improved the purification (>97% purity) and higher yield.

Seaweeds or marine algae have a great potential in supporting circular bioeconomy in several industries, such as bioenergy, food, feed, fertilizer, building, and cosmetics. One of the primary components of marine algae products (MAPs) is polysaccharides which exhibit remarkable biological activities. Although cutting-edge extraction methods of MAPs like microwave-, ultrasound-, and enzyme-assisted extraction methods showed high extraction productivities, ease of use, low cost, and eco-friendliness, their use is presently restricted to lab research. Chromatography is prevalent technique employed for purification of natural substances from complex mixtures. Zayed et al. have reviewed the biorefinery approaches, harvesting, drying, conventional and non-conventional extraction, and separation techniques, including all modern chromatographic methodologies for the purification of different algae-derived bioactive components.

Rahim et al. have presented a critical review on the recent advancements in the purification methods and current applications of marine algal haloperoxidases, valuable yet underexplored class of enzymes with diverse applications in biocatalysis, pharmaceuticals, and bioremediation. Despite the advancements in the purification of these enzymes, challenges remain, particularly in optimizing yield, purity, and bioactivity while scaling up the process for industrial use. The review explored the advantages and disadvantages of chromatographic techniques, such as ion-exchange, size exclusion, and affinity chromatography, and investigated alternative approaches, such as aqueous two-phase systems (ATPS) and microfluidic systems, which offer promising avenues to improve enzyme yield, purity, and stability.

Natural products (NPs) libraries provide diverse three-dimensional structural features with crucial scaffolds for drug discovery. However, the isolation of both targeted and untargeted NPs remains a major challenge, despite significant advances in

analytical tools. To address this, Pavão et al. reported a rapid and efficient method for the semipreparative isolation of NPs from their extracts using offline C18 solid-phase extraction (SPE) cartridges, guided by the retention profile of a reverse-phase liquid chromatography gradient (LCSPE-fast). LCSPE-fast demonstrated fast, cost-effective, and high yield of the target-metabolite-enriched fractions, and proved effective across all four *Uncaria guianensis* extracts evaluated, both *in vitro* and *in situ*, e.g., ~0.40 g of chlorogenic acid and 0.03–0.1 g of 3,4-Di-O-caffeoylquinic acid from *U. guianensis* cultivated both *in vitro* and *in situ*.

To address obesity, functional food products are commonly available in the market with high protein and low-calorie content. However, such products content, which control weight, needs to be described. Rustandi et al. have explored methods to assess the effect of anti-obesity soybeans food bars on antioxidants in the widely available functional food products in the market. They used different techniques including network pharmacology, bioactive gene analysis, interaction network development, phytochemical screening, molecular docking, and antioxidant activity testing, and predicted that soybean-based food bars possessed anti-obesity relevance through interactions with leptin signaling proteins.

Plant decoctions are simple, accessible, and effective in ethnomedicine. However, polar compounds make chemical analysis of decoctions difficult. Vuadens et al. have created an analytical method using HILIC with reversed-phase chromatography and tested it with *Combretum micranthum* decoction. UHPLC-PDA-CAD-HRMS/MS with HILIC chromatography produced the decoction's chemical profile, and HR-MS Data was utilized to establish a molecular network for metabolite annotations and connections. HR-MS/MS data annotated 10 metabolites and established their identities through isolation and structural elucidation. Stachydrine, vitexin, and isovitexin annotated in the decoction may explain *C. micranthum* decoction's hypotensive history. The use of HILIC and reversed-phase chromatography for polar compound identification and isolation could be of a great help to understand traditional plant decoctions' chemical composition.

Methodological innovations

Across contributions, green chemistry emerges as a unifying thread, minimizing dangerous solvents through bio-based alternatives and energy-green tools like ultrasound. Reverse-phase and HILIC chromatography dominate for high-purity isolations (e.g., QS-21 at 97% through orthogonal RP-HILIC), while non-chromatographic techniques, PVPP tannin elimination, diafiltration for desalting, cut expenses and waste. Scale-up solutions deal with lab-to-industrial transitions, incorporating continuous-flow systems and enzymatic pretreatments to maintain >97% recoveries at kilogram scales. Comparative analyses display cutting-edge techniques outperform classics: ultrasound-tannase yields QS-21 2–3x better than solvent boils, with 50% less electricity and no toxic effluents. Saponin case studies from *Quillaja brasiliensis* leaves exemplify sustainability, bypassing bark overexploitation via leaf extractions and C18/methanol fractionations yielding

QB-90 adjuvants similar to Q Sap profiles. The combination of HILIC and RP-chromatography observed through HR-MS/MS for polar compound identification and isolation is a promising technique to pinpoint traditional plant decoctions' chemical composition.

Future research directions

Current advancements in natural product discovery are characterized by the strategic integration of Artificial Intelligence and Machine Learning into metabolomics-driven workflows. These computational tools allow for the automated prioritization of extracts and the accurate prediction of fractionation outcomes based on complex spectral data. By modeling the chemical space and chromatographic behavior *in silico*, researchers can reduce traditional 'trial and error' laboratory efforts by as much as 70%, leading to significant savings in solvents, time, and manpower. Complementing this is the development of hybrid bioassay-chromatography pipelines, which bridge the gap between chemical separation and biological validation. The integration of continuous purification and computational modeling transforms natural products from traditional extracts into precision-engineered therapeutics, providing a practical framework for the next-generation of sustainable drug discovery.

Author contributions

MR: Writing – review and editing, Writing – original draft. AC: Writing – original draft, Writing – review and editing. UA: Writing – original draft, Writing – review and editing.

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