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Editorial: NMR insights into natural product chemistry

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Editorial on the Research Topic
NMR insights into Natural Product Chemistry

The 19th NMR Users Meeting, held in Rio de Janeiro, Brazil, from September 25 to 29, 2023, brought together approximately 160 researchers from various regions of Brazil and Latin America. The attendees included seasoned and junior scientists from both industry and academia, as well as postdoctoral fellows, graduate, and undergraduate students, creating a unique integrative environment for networking. Its scientific program featured significant international participation and covered a broad spectrum of state-of-the-art interdisciplinary research in various fields of NMR spectroscopy, including organic chemistry, inorganic chemistry, theoretical chemistry, analytical chemistry, environmental chemistry, biochemistry, physics, materials science, geology, physiology, and medicine. The meeting highlighted new advancements in theoretical and experimental aspects of diverse NMR applications, encompassing the study of natural products, pharmaceuticals, foods, biomolecules, polymers, catalysts, petroleum, and biofuels. This inspired a group of expert researchers in NMR and its applications in natural products to propose the Research Topic "NMR Insights into Natural Products Chemistry," aiming to explore the most recent advances and applications of NMR in the field of natural products.

This Research Topic features five papers, comprising one review, two mini-reviews, and two original research articles. These contributions explore important aspects of current research in natural products, highlighting the significant role of NMR spectroscopy in advancing the field.

In their mini-review, Borges and Teixeira emphasize the combination of NMR spectroscopy with mass spectrometry (MS) to overcome MS's limitations in metabolomics, particularly in natural product investigations. While MS excels in metabolite detection due to its high sensitivity, it falls short in detailed structural elucidation. Thus, NMR can act as a valuable complement to MS by addressing specific challenges, such as isomer differentiation and misidentification, which MS alone may struggle with, ultimately contributing to more accurate compound identification. The authors highlight the significance of quality control (QC) samples for enhancing compound annotation, while presenting tools like COLMAR, NMRfilter, and DBsimilarity, which assist in integrating NMR and MS data for more robust analysis. By harnessing the strengths of both NMR and MS, researchers can unlock new levels of precision and depth in metabolomics studies, pushing further the boundaries of natural product research.

In the subsequent original research article, Novais et al. investigated whether creatine, a metabolite synthesized in the liver, pancreas, and kidneys from the transamination of amino acids such as arginine, glycine, and methionine, is truly present in plants as previously reported in the literature. To address this question, the authors employed HR-MAS NMR spectroscopy to investigate the chemical composition of leaves and cherries of *Eugenia uniflora* in their natural swollen state, a noteworthy approach for studying unprocessed plant matrices. An exhaustive NMR investigation, including two-dimensional methods, revealed that the signal at 3.05 ppm, previously assigned to creatine, was due to the amino acid 4-hydroxy-N-methyl proline, indeed. Thus, Novais et al. provide another excellent example of how NMR, through non-invasive methodologies, can significantly contribute to reassessing previously misinterpreted spectroscopic data in natural products.

The mini-review paper from Ravaglia et al. provides an exploration of practical considerations for using quantitative NMR (qNMR) in natural product research. The authors highlight the common challenges in the process, including plant sampling, extraction procedures, and key qNMR parameter settings necessary for reliable data. They highlight the importance of validation steps, such as ensuring adequate relaxation times, acquiring accurate data, and selecting appropriate quantifiable signals in the complex matrices of natural products. The paper also presents a clear protocol for researchers, covering experimental design and method optimization, which are often underreported in existing literature. With tools and tips to ensure reliable results in complex natural matrices, this mini-review is essential reading for anyone aiming to quantify metabolites in natural products.

The review by Ocampos et al. presents a detailed guide to NMR-based plant metabolomics, offering researchers a step-by-step protocol for high-quality data acquisition and analysis. With detailed insights into sample preparation, pulse sequences, and advanced data processing techniques, this review highlights how NMR can unlock a deeper understanding of plant metabolites. It also explores essential tools such as chemometric tools and metabolite databases that facilitate metabolite identification. This guide provides indispensable insights for advancing plant metabolomics research especially for researchers who are new to applying NMR in metabolomics studies of natural products.

Last but not least, the original research paper by Thirion et al. employs NMR spectroscopy in conjunction with univariate and multivariate statistical analyses to investigate metabolic alterations in the neurometabolic profile resulting from HIV infection. Although this study is situated within clinical metabolomics, a consolidated area for the use of NMR techniques, it also draws attention to the application of NMR in metabolomic studies of natural product matrices. This study examines cerebrospinal fluid samples from pediatric patients in South Africa, both HIV-positive and HIV-negative. Thirion et al. propose that neuroinflammation, as indicated by a model based on ^{1}H NMR data from nine key cerebrospinal fluid biomarkers - glucose, lactate, glutamine, 1,2-propanediol, acetone, 3-hydroxybutyrate, acetoacetate, 2-hydroxybutyrate, and myo-inositol—disrupts astrocyte-neuron communication, resulting in diminished neuronal activity among HIV-affected children. The authors suggest that these findings may contribute to the neurodevelopmental delays observed in this cohort. Furthermore, this study highlights significant metabolic dysregulation, including increased glycolysis and impaired ketone body metabolism, both of which are associated with persistent immune activation. This paper exemplifies the powerful application of NMR in metabolomic studies of complex biological matrices within the medical field.

Together, the papers in this Research Topic offer valuable insights to the researchers aiming to improve their NMR methodologies and deepen their investigation of natural products. Featuring practical protocols and key findings, this Research Topic serves as a valuable resource for both seasoned scientists and newcomers to NMR-based research, providing them with useful tools and perspectives to improve their analytical techniques and foster future progress in the field of Natural Products.

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