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Integrating Medicinal Chemistry and Mass Spectrometry: New Opportunities and Challenges

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Message from the Guest Editor

Dear Colleagues,

Mass spectrometry (MS) is an indispensable tool in medicinal chemistry due to its ability to provide precise and detailed information about different aspects of potential therapeutics. These include structural elucidation, drug metabolism and pharmacokinetics evaluation, and analysis of drug modes of action, thereby supporting various stages of drug development, from discovery through production and quality control, enhancing our understanding of drug behavior, and improving the safety and efficacy of pharmaceuticals. Beyond this, structural MS approaches such as native MS and hydrogen–deuterium exchange MS (HDX-MS) are emerging as powerful technologies for analyzing the interactions between drugs and their targets as well as the influence of small molecules on protein–protein interactions.

These techniques bear great potential for guiding the design of novel pharmaceuticals, this Special Issue aims to showcase the latest advancements in combining mass spectrometry with medicinal chemistry.

Dr. Francesco Fiorentino

Guest Editor



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Special Issue



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