

SP 01

High-resolution mass spectrometry in drug discovery and design – trends and perspectives

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Mass spectrometry has for decades been the analytical workhorse in research and development of novel pharmaceutical substances. An inherent property of mass spectrometry is that it allows detection and quantification of almost all compounds one could encounter in a sample mixture. With the development of high-resolution mass spectrometry and a wide adoption of Orbitrap-type instruments, many novel approaches to different analytical questions have been developed. These instruments give valuable molecular information for pharmaceutical analysis and have matured to a point where they are beginning to enter QC laboratories in pharmaceutical industry. This lecture aims to highlight applications, new approaches, and future perspectives in drug discovery and design. Label-free in vitro assays, multiplexed cellular phenotypic tools and various high-throughput applications will be discussed, as well as the most widely used instrumental setups. Finally, an overview of the future developments in the field of drug discovery and design will be presented.