

Two is better than one: Deuterium in analytical mass spectrometry

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This review explores the diverse applications of deuterium in medicinal chemistry, particularly as an analytical tool in mass spectrometry. Deuterium applications extend beyond its traditional use as an analytical reference material to being integrated into drug structures and tagging reagents for quantitative proteomics. Hydrogen-deuterium exchange (HDX) of labile protons is applied for structural analysis and monitoring protein folding, interactions, and denaturation processes, whereas the metal-catalyzed HDX in C–H bonds provides site-specific deuterium labeling. Deuterated analytical reference materials and labeling reagents are used in the investigation of metabolic pathways, offering valuable insights into drug transformations. Deuterium has evolved into a powerful tool for mass spectrometry-based structural and quantitative analyses, however, challenges such as isotopic effects, chromatographic elution profile differences, and proton mixing in MS analysis still exist, necessitating ongoing technological advancements.

Słowa kluczowe

hydrogen deuterium exchange, isotope labeling, isobaric tags, high resolution mass spectrometry, proteomics

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