

H/D Exchange Studies in Metabolite Identification

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Hydrogen/deuterium (H/D) exchange LC-MS experiments play an important role in identification and structure elucidation of metabolites. D₂O as sheath liquid and deuterated solvents are used as a mobile phase in deuterated LC-MS experiments for the analysis of metabolites. Deuterated experiments are useful in the structural characterization of metabolites by determining the numbers and positions of exchangeable protons present in different functional groups such as -NH-, -NH₂, -OH, -COOH and -SH in various metabolites [1,2]. The mass shift of the deuterated molecular ion from that of the protonated molecular ion gives information about the total number of exchangeable protons present in the structures of metabolites [3-6]. The structure elucidation of unknown metabolites can be effectively carried out by using deuterated precursor ions compared to protonated precursor ions where tandem MS spectra of deuterated metabolites help to determine the exact location of the exchanged protons [3,5]. It can be noted that the online deuterated experiments are useful to characterize the metabolites without the use of large scale preparation for other analytical characterizations. Further, the deuterated experiments allowed to distinguish the hydroxylated and glucuronide metabolites from other metabolites with the help of numbers of exchangeable hydrogens [3,5]. Moreover, deuterated experiments also allowed to distinguish the metabolites that have the same nominal mass and identical elemental compositions which may not be possible by normal LC-MS/MS [5]. In conclusion, deuterated studies can be used to further support the structural confirmation of metabolites irrespective of biological matrices.

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