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Application of Current Approaches and Newer Trends in Identification of Drug Metabolites Using Liquid Chromatography- Mass Spectrometry

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Metabolite identification is amongst the important studies during early stages of drug development because metabolic products may be pharmacologically active or toxic in nature. In the last one decade, there have been revolutionary changes in the way metabolite identification is carried out. This has mainly become possible due to the advent of sophisticated analytical modalities, particularly, hyphenated liquid chromatography-mass spectrometry (LC-MS). There are varieties of LC-MS systems available with difference in their utility in metabolite identification. Particularly, HPLC coupled with high resolution-mass spectrometry (HR-MS) and multiple-stage MS (MS^n) plays a leading role in identification of metabolites (1-2). Sample preparation, mass fragmentation studies, *in silico* metabolite prediction and detection, chromatographic retention, UV spectra matching, determination of molecular formula, and establishment of possible site of metabolism are the important aspects in unequivocal identification of metabolites. In this same context, there have been several recent advancements in metabolite identification. These include approaches for detection of reactive metabolites, new generation LC systems and MS ion sources, isotopic pattern matching, hydrogen/deuterium exchange mass spectrometry, data dependent analyses, MS^E approach, mass defect filter, 2D and 3D approaches for elucidation of molecular formula, polarity switching, background subtraction-noise reduction algorithms (BgS-NoRA), etc. The same will be discussed with case examples, as appropriate.