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LC-MS based metabolomics in pharmaceutical research and its significance

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As metabolism significantly affects safety and efficacy of drug, determination of the metabolic profile of a drug is a complicated part of drug development. The application of an LC–MS based metabolomic approach has gained popularity in identifying drug metabolites, developing metabolic maps and lending clues to mechanisms of bioactivation. Therefore, the LC–MS based metabolomic approach is a powerful technique for profiling of drug metabolism and bioactivation. Although, NMR based metabolomics has been widely used in metabolomic studies, MS based metabolomics is increasingly employed because of its high resolution and sensitivity as well as the more wide availability of instruments. Gas chromatography mass spectrometry (GC–MS) and LC–MS are the prevailing analytic instruments in MS based metabolomic studies. Compared with GC–MS, the advantage of LC–MS is that no chemical derivatization is required and the run times are faster resulting in high throughput capabilities. With the advent of ultra-performance liquid chromatography (UPLC) and highly accurate MS, the application of UPLC–MS has dramatically increased in metabolomic studies. Metabolomics is a nun biased approach for metabolite identification. For *in vivo* studies, biological samples (urine and/or feces) are required from both the vehicle-treated and drug-treated groups. These samples can be analyzed using LC–MS. Subsequently, chromatographic and spectral data are collected and processed using methods such as centroiding, de isotoping, filtering and peak recognition to generate a data matrix including sample identity, ion identity and ion abundance. The data matrix is then subjected to PCA and OPLS-DA analyses. Because the target drug and its metabolites only exist in the drug treated group, they will highly contribute to the separation of the vehicle and drug treated groups in the S-plot generated from OPLS-DA analysis. Therefore, the metabolites can be readily identified from a large data set.

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