Hyphenated MS in Pharmaceutical Applications: Data Independent Acquisition, Ion Mobility and Electron Based Dissociation

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Abstract:

The accurate and precise identification and quantification of pharmaceuticals and metabolites in biological samples relies mostly on the combination of separation sciences and mass spectrometric detection. One of the major challenges in is the chemical space and the dynamic range of the analytes of interest. Supercritical fluid chromatography (SFC) has experienced a renaissance in the last decade offering an additional separation dimension. In LC-MS the ionization conditions are predominantly controlled by the mobile phase composition, whereas in SFC-ESI/MS, the ionization can be tuned using the addition of a liquid make-up, which is independent of the chromatographic conditions. Significant improvement in MS response can be achieved when carefully selecting the make-up flow. Recent instrumental improvements in high resolution mass spectrometry (HRMS) have enabled data independent information acquisition (DIA) schemes, such as MSEverything or SWATH. With SWATH a collision induced MS/MS spectra can be generated for every precursor ion enabling simultaneous quantitative and qualitative analysis (QUAL/QUANT). Comparison with MS/MS database or the use of in-silico fragmentation tools can further improve compound and enables multianalytes quantification. However, improved selectivity, higher sample throughput or MS/MS structural information is needed. The implementing of mobility spectrometry (IMS) into the workflow as the use of electron based dissociation referred as ExD would significantly improve the performance of LC-MS analyses. In the present talk the benefits to apply multiple separation techniques (dual LC, SFC) with multiple MS and MS/MS techniques (DIA, IMS, ExD) will be presented for the analysis of pharmaceuticals and metabolites in biological samples.