Ion mobility as an added dimension for toxicology screening

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Several forensic laboratories have started to use UHPLC-HR-MS for drug screening because of its advantages compared to GC-MS, HPLC-DAD and immunoassays. But compared to GC-MS, these UHPLC-HR-MS methods lack the access to large libraries, inter laboratory reproducible spectra, and standardized gradients. Most laboratories using UHPLC-HR-MS build in-house libraries or get libraries with up to 2500 compounds from the manufacturer of the instruments. HR-MS instruments can in theory screen for an unlimited number of compounds, but in practice it gives a lot of false positive findings and is very time consuming regarding to data analysis.
We set out to develop a practical UPLC-IMS-QTOF-MS drug screening by processing HDMS^E acquired data from forensic blood samples against a >4000 compounds library (Targeted and Suspect Screening). Also we set out to find a practical way to identify unknown peaks (Non-Targeted Screening).