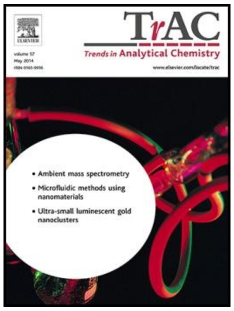

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Increasing selectivity and coverage in LC-MS based metabolome analysis

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HIGHLIGHTS

- Maximizing selectivity is crucial towards matching metabolome diversity.
- Structural isomers and in-source fragments challenge high-resolution mass spectrometry.
- The separation power of one-dimensional separations limits metabolome coverage.
- On-line combinations of orthogonal separations enhance coverage and throughput.
- Ion mobility separation can further supplement chromatographic selectivity.

ABSTRACT

The term non-targeted metabolomics implies a global and unbiased analysis. This involves the complex (and yet not routine) task of correct alignment and eventually annotation of statistically grouped ions as known metabolites according to accurate mass and chromatographic parameters. The comprehensiveness is practically compromised by the enormous chemical diversity of the metabolome. As solutions involving multiple methods are practically unfeasible for many extensive non-targeted metabolomics studies, increasing selectivity to yield a higher coverage of the metabolome considered (preferably within one analytical run) remains a crucial aspect for throughput, affordability and data processing considerations. This contribution presents an overview on proposed novel LC-MS-based workflows aiming to increase selectivity for maximizing metabolome coverage within a single analytical run. We suggest that analytical strategies involving on-line combinations of orthogonal liquid chromatographic separations with mass spectrometry or ion mobility-mass spectrometry are key to addressing this pursuit.

Keyword

non-targeted metabolomics; two dimensional liquid chromatography; heart-cut two dimensional liquid chromatography; comprehensive two dimensional liquid chromatography
high resolution mass spectrometry; ion mobility; collisional cross section