Omic-Scale High-Throughput Quantitative LC-MS/MS Approach for Circulatory Lipid Phenotyping in Clinical Research.

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Lipid analysis at the molecular species level represents a valuable opportunity for clinical applications due to the essential roles that lipids play in metabolic health. However, a comprehensive and high-throughput lipid profiling remains challenging given the lipid structural complexity and exceptional diversity. Herein, we present an 'omic-scale targeted LC-MS/MS approach for the straightforward and high-throughput quantification of a broad panel of complex lipid species across 26 lipid (sub)classes. The workflow involves an automated single-step extraction with 2-propanol, followed by lipid analysis using hydrophilic interaction liquid chromatography in a dual-column setup coupled to tandem mass spectrometry with data acquisition in the timed-selective reaction monitoring mode (12 min total run time). The analysis pipeline consists of an initial screen of 1903 lipid species, followed by high-throughput quantification of robustly detected species. Lipid quantification is achieved by a single-point calibration with 75 isotopically labeled standards representative of different lipid classes, covering lipid species with diverse acyl/alkyl chain lengths and unsaturation degrees. When applied to human plasma, 795 lipid species were measured with median intra- and inter-day precisions of 8.5 and 10.9%, respectively, evaluated within a single and across multiple batches. The concentration ranges measured in NIST plasma were in accordance with the consensus intervals determined in previous ring-trials. Finally, to benchmark our workflow, we characterized NIST plasma materials with different clinical and ethnic backgrounds and analyzed a sub-set of sera (; n; = 81) from a clinically healthy elderly population. Our quantitative lipidomic platform allowed for a clear distinction between different NIST materials and revealed the sex-specificity of the serum lipidome, highlighting numerous statistically significant sex differences.

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