Separation of isomers in lipidomics and metabolomics experiments by high resolution ion mobility spectrometry-mass spectrometry (IMS-MS)

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Overview
► Current separation and identification techniques for isomeric substances are often insufficiently powerful, slow or ambiguous.
► High resolution ion mobility spectrometry-mass spectrometry (IMS-MS) can be used for separation of isomers without adding experimental complexity across many substance classes.
► Isomers are separated based on differences in their ion-neutral collision cross sections which define their hydrodynamic “shape”.
► IMS resolving power R > 150 is usually needed for separation of isomers - the TOFWERK IMS-TOF with multiplexing and post-processing reaches R > 250.
► IMS-MS can be used as a stand-alone technique for direct infusion measurements or coupled online to liquid chromatography.

Methods and Instrumentation
► All measurements were carried out on a TOFWERK IMS-TOF. The system comprises an ESI source, a 10 cm desolvation tube, a 20 cm drift tube (both made from resistive glass) and a TOFWERK HTOF TOFMS.
► Desolvation and drift tube were thermostated between 60-100°C with nitrogen as the buffer gas.
► Ion mobilityseparator was carried out at reduced field strengths of ca. 2 Td. Drift-tube pressure was set between atmospheric and 1.4 atm (nitrogen).
► Measurements were carried out in both positive and negative ion mode (applied potential approx. 2 kV). Raw IMS-TOF data was post-processed using Tofware (TOFWERK, Switzerland).
► Lipids were obtained from Avanti Polar Lipids (USA) or extracted from natural sources using Bligh-Dyer extraction. All other chemicals were obtained from Sigma-Aldrich (Switzerland).
► Schematic and picture of the TOFWERK IMS-TOF.

Results
► Complex Lipid Samples
   ► Metabolite extracts
   ► Fatty acids
   ► Disaccharides
   ► Amino Acids
   ► Naphthoic Acids

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