Resolving isomeric metabolites using high resolution IMS-MS

Michael Groessl
TOFWERK, Switzerland
ims-tof@tofwerk.com

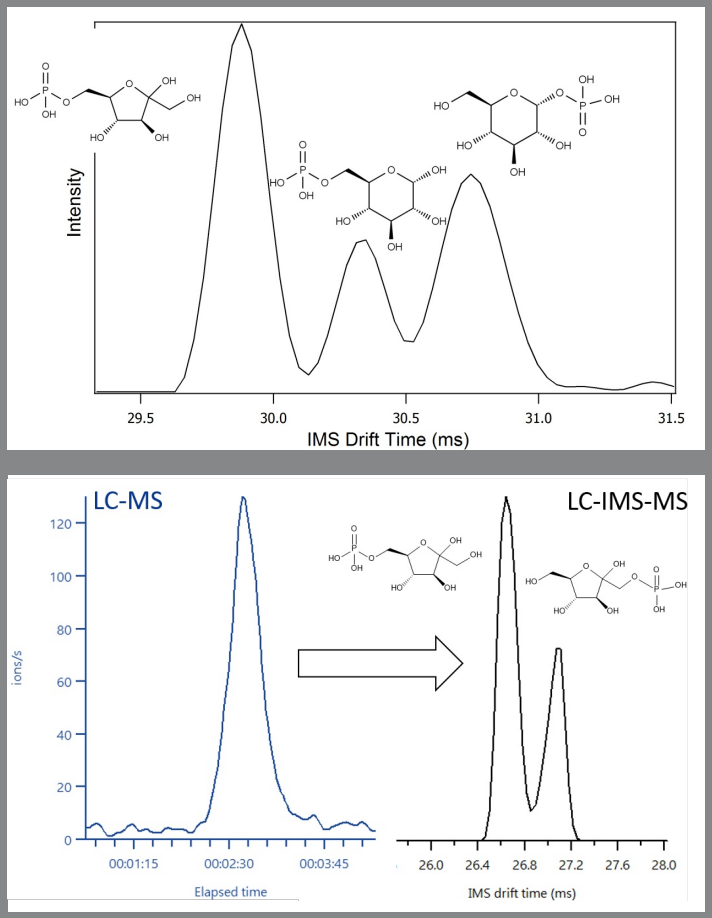
IMS-TOF

Metabolomics researchers frequently face extremely complex and challenging samples. The field is dominated by LC-MS based approaches; yet, chemical diversity of the samples makes the efficient separation and confident detection of a large number of metabolites extremely challenging. High resolution ion mobility spectrometry-mass spectrometry is especially powerful for the separation of isomers. IMS-MS can also be coupled to LC and is therefore an attractive technique to boost separation power and consequently increase the number of detected metabolites.

Sugar phosphates are critically involved in important metabolic pathways such as glycolysis or the pentose phosphate pathway. Due to their isomeric nature, many of them cannot be distinguished using LC or MS/MS. Nonetheless, the concentration of these sugar phosphates can provide crucial insights into a system's metabolic state.

Using the TOFWERK IMS-TOF, we show here that high resolution IMS-MS, either as a stand-alone technique or coupled to LC, improves the identification of isomeric sugar phosphates. IMS drift times are directly linked to collision cross sections and can therefore be used as molecular identifiers.

High-resolution IMS-MS can supplement or replace LC for the detection and identification of isomeric sugar phosphates.



Top: High resolution IMS-MS separation of the isomeric sugar phosphates fructose-6-phosphate, glucose-6-phosphate and glucose-1-phosphate. Bottom: UHPLC-MS trace of m/z 259.022 (corresponding to C6H12O9P-) using a HILIC column shows only a single peak. Right: Extracted IMS data for the LC-MS peak clearly shows the presence of two isomeric substances. Identification as fructose-1-phosphate and fructose-6-phosphate is based on comparison of the IMS drift times to standards.

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