

UPLC or DESI coupled to cyclic ion mobility spectrometry TOF-MS (LC-ESI-cIMS-TOF-MS or DESI-cIMS-TOF-MS)

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Brand

Waters Chromatography

Type

Acquity H-Class Plus Bio UHPLC or DESI XS source with Select Series Cyclic IMS MS



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Description

Intro to UPLC-ESI-cIM-TOF-MS and DESI

Ultra Performance Liquid Chromatography (UPLC) combined with ElectroSpray Ionization Time Of Flight Mass Spectrometry (ESI-TOF-MS) is a powerful technique to analyse and identify many different compounds like peptides, proteins, phytochemicals, and carbohydrates as present in complex mixtures. With cyclic Ion Mobility (cIM), the range of molecules that can be analysed is extended to the separation of isomeric compounds. The combination of the cIM-TOF-MS with Desorption ElectroSpray Ionization (DESI) enables the analysis of solid samples and surfaces, and offers possibilities for MS imaging of biological tissues.

The mass accuracy and resolution of the Select Series Cyclic IMS are highly dependent on the desired experimental setup and detection mode. The latest generation TOF has the possibility to operate in W-mode, enabling high resolution MS analysis at resolution > 100,000 FWHM, resulting in mass errors below 1 ppm. The m/z range of the TOF-MS is between 20 and 16000. The cIM offers high resolution and highly flexible ion mobility spectrometry (IMS) due to the ability to vary the number of passes in the cIM to fine-tune resolution (ranging from 100 to 750) and measurement time. The UPLC system is also equipped with photodiode array (PDA) and a fluorescence detector (FLR) to assist with identification and quantification.

Principles

Cyclic Ion Mobility (cIM)

The separation of isomeric compounds with ion mobility is based on the rotationally-averaged collision cross section (CCS) of the molecules in gas phase. CCS is an important characteristic of a molecule and is directly related to its chemical structure and three-dimensional conformation. The CCS of a molecule determines its mobility as it moves through a neutral gas under influence of an electric field and can thereby be directly related to its measured travelling time. Cyclic ion mobility (cIM) is the latest development in ion mobility spectrometry (IMS), in which ions can be cycled through the ion mobility module for consecutive passes, increasing resolution of the separation with each pass.

Desorption ElectroSpray Ionization (DESI) and MS imaging

Desorption ElectroSpray Ionization (DESI) is an ambient (soft) ionization technique that combines the principles of ESI and desorption ionization. In DESI, a spray of charged microdroplets is directed towards a dry sample at an angle, leading to desorption, ionization, and desolvation of the sample molecules. When coupled to MS, this technique can be used to analyse solid samples and surfaces, and to perform MS imaging of biological tissues. MS imaging can be used to visualize the localization of biomolecules in tissues by recombining MS spectra of spots in a grid over the sample. Each spot eventually represents a pixel in the visual overlay of the MS data and a microscopic picture of slice of the biological tissue.

Technical Details

Supplier Waters Corporation (Manchester, UK)

Specifications: Waters UPLC Acquity H-Class Plus Bio

- Titanium is used for the standard stainless steel parts

- Binary pumps (high pressure mixing system)
- Flow rate: 0.01 – 2.00 mL/min
- Max pressure: 15000 psi (at 1 mL/min)
- Injection type: Flow through injection
- Column oven: RT – 90°C
- Sample compartment: 4 – 40°C
- Detector 1: Acquity Photodiode array (PDA)
- Wavelength range: 190 – 500 nm
- Wavelength accuracy: ± 1.0 nm
- Detector 2: Acquity Fluorescence detector (FLR)
- Wavelength range: 200 – 890 nm (excitation), 210 – 900 nm (emission), Band width: 20 nm
- Wavelength accuracy: ± 3 nm

Specifications: Select Series Cyclic IMS

- Mass range: 20 – 16000 m/z
TOF
- Mass resolution: > 100,000 FWHM
- Mass accuracy: < 1 ppm
- Ion mobility: cyclic ion mobility (cIM)
- Ion mobility resolution: 100-750 (dependent on number of passes in cIM)

Specifications: DESI XS

Applications

- Proteomics(-like) approaches
- Profiling, identification, and quantification of diverse food(-related) molecules:
- Intact and modified proteins (e.g. glycoproteins)
- Protein hydrolysates or peptide mixtures
- Lipid mixtures from fats or oils
- Charged and neutral oligosaccharides
- Phytochemicals (e.g. from crude plant extracts)
- Separation and identification of isomeric molecules