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A prototype TIMS-FT-ICR MS instrument capable of deep characterisation of complex samples and biomolecules

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Trapped ion mobility spectrometry (TIMS) spatially separates ions when suspended in a high-pressure region between a retarding electric field gradient and constant gas flow from the atmospheric pressure inlet of the mass spectrometer. TIMS allows high resolution separation of ions/isomers/conformers with varying duty cycles in a relatively small device (<10cm). TIMS is also particularly well suited to slower scan speed instruments such as FT-ICR MS via the use of gated-TIMS. Herein we show initial data from a novel, fully integrated gTIMS-FT-ICR MS instrument, optimisation of this marriage, and its application to key areas such protein conformer-selective ExD MSMS.

The new gTIMS-MRMS system codenamed MATCH was built by combining commercial SolariX MRMS and TIMS-ToF Flex (Bruker Daltonics, Germany) instruments into a prototype. The front of the TIMS Tof Flex , including dual ESI+MALDI source, accumulation during separation dual-TIMS cartridge, mass-resolving quadrupole, and collision cell were combined via a custom transfer region with the back-end elements of the SolariX MRMS system; UHV-isolating beam valve, ~1m transfer hexapole to inject ions through the fringe field of the 7T superconducting maxwell magnet, Paracell detector with electron dissociation (ExD) cathode, and 2-omega detection.

Native MS analysis of proteins was conducted on model isolated proteins to investigate the ability of gTIMS to separate and analyse proteins of interest without significantly affecting structure. Match was developed to use an ultra-low energy transfer and storage energy gradient throughout the TIMS separation, storage, and transfer processes, enabling batch-accumulation of conformer ensembles selected for enhanced dynamic range of downstream MS/MS. Collision-induced unfolding (CIU) was achieved using gradient potentials between the accumulation and analysis portions of the TIMS funnel. Subsequent IMS and quad selections of conformers of interest along the CIU profile followed by ECD MS/MS in the ICR cell revealed changes in fragmentation patterns depending on the conformer selected.

User consent

yes

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