Development of timsMRMS: A Gated-TIMS FT-ICR MS instrument to decipher isomeric content of complex organic mixtures

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Conflict of Interest (CoI) statement:

Christopher A. Wootton, Alina Theisen, Jochen Friedrich, Susanne Alfken, Greg Brabeck, and Roland Jertz are currently employees of Bruker Daltonics, manufacturer and provider of FT-ICR MS (commercialised as MRMS) and TIMS based systems.

Introduction:

FT-ICR MS (commercially sold as MRMS) is known as not only the highest performance mass spectrometry technique in terms of raw metrics for resolving power and mass accuracy, but also as the most flexible platform in terms of MS/MS, isolation, and ion manipulation techniques.

However, conspicuously missing from current MRMS systems is the ability to natively and effectively conduct ion mobility (IMS) separations.

Thus a new MRMS platform was created as a successor to the solariX and scimaX systems, codenamed MATCH, which was designed to effectively incorporate state of the art dual accumulation+analysis TIMS hardware, updated ion optics, improved SB3D MALDI laser, and micro grid MALDI stage hardware.

The new platform was then energy and transmission optimised for wide m/z range, sensitivity, and high flux limits for large ion ensemble analysis to feed the high dynamic range ParaCell analyser – with up to 15,000,000 ions per scan possible to date.

Application areas for this system include complex mixture analysis such as environmental extracts, green fuel analysis (bio-oils etc), conformer selective MS/MS using ExD techniques and MALDI imaging (shown separately).

The work presented herein was recently published in Analytical Chemistry, please see full details here:

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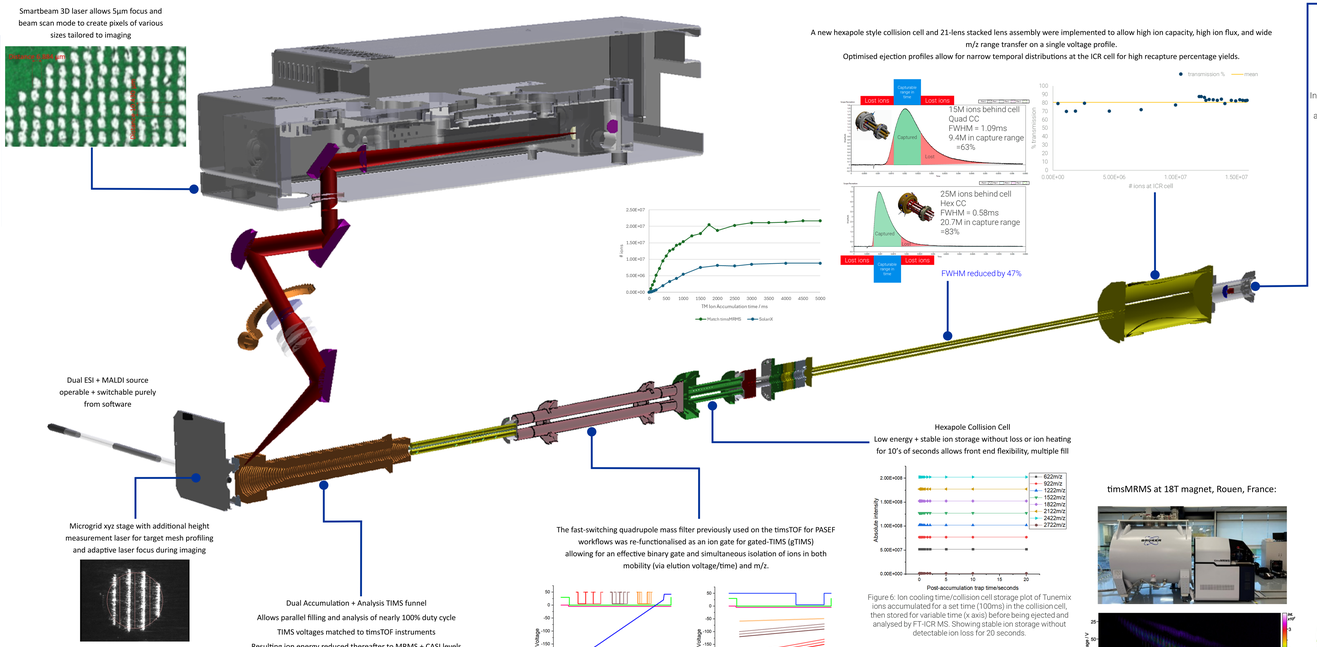
Smartbeam 3D laser allows 5µm focus and beam scan mode to create pixels of various sizes tailored to imaging
Dual ESI + MALDI source operable + switchable purely from software
Microgrid xyz stage with additional height measurement laser for target mesh profiling and adaptive laser focus during imaging
Dual Accumulation + Analysis TIMS funnel
Allows parallel filling and analysis of nearly 100% duty cycle
TIMS voltages matched to timsTOF instruments
Resulting ion energy reduced thereafter to MRMS + CASI levels
Allows compatibility without activation
TIMS IN pressure adjusted to mobility range and resolution requirements
The fast-switching quadrupole mass filter previously used on the timsTOF for PASEF workflows was re-functionalised as an ion gate for gated-TIMS (gTIMS) allowing for an effective binary gate and simultaneous isolation of ions in both mobility (via elution voltage/time) and m/z.
Hexapole Collision Cell
Low energy + stable ion storage without loss or ion heating for 10's of seconds allows front end flexibility, multiple fill
A new hexapole style collision cell and 21-lens stacked lens assembly were implemented to allow high ion capacity, high ion flux, and wide m/z range transfer on a single voltage profile.
Optimised ejection profiles allow for narrow temporal distributions at the ICR cell for high recapture percentage yields.
Lost ions
Capture range - lens
Capture
1.5M ions behind cell
Quad CC
FWHM = 1.09ms
9.4M in capture range
=63%
25M ions behind cell
Hex CC
FWHM = 0.58ms
20.7M in capture range
=83%
Ejection range - lens
Eject
FWHM reduced by 47%
Lost ions
Lost ions
Lost ions