Verdel Instruments: Two Dimensional Mass Spectrometry:
Fast, effective, true DIA

VERDEL

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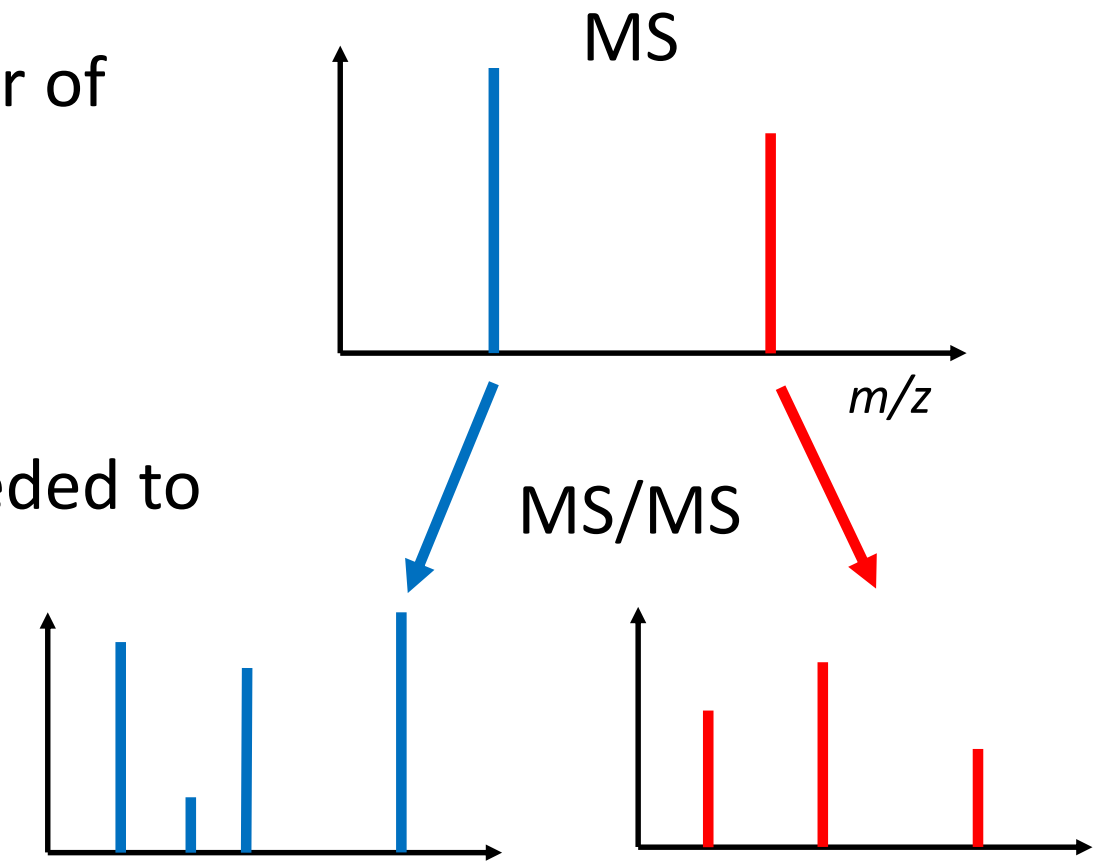
Innovate UK

Mass Spectrometry specializes in analysis of mixtures

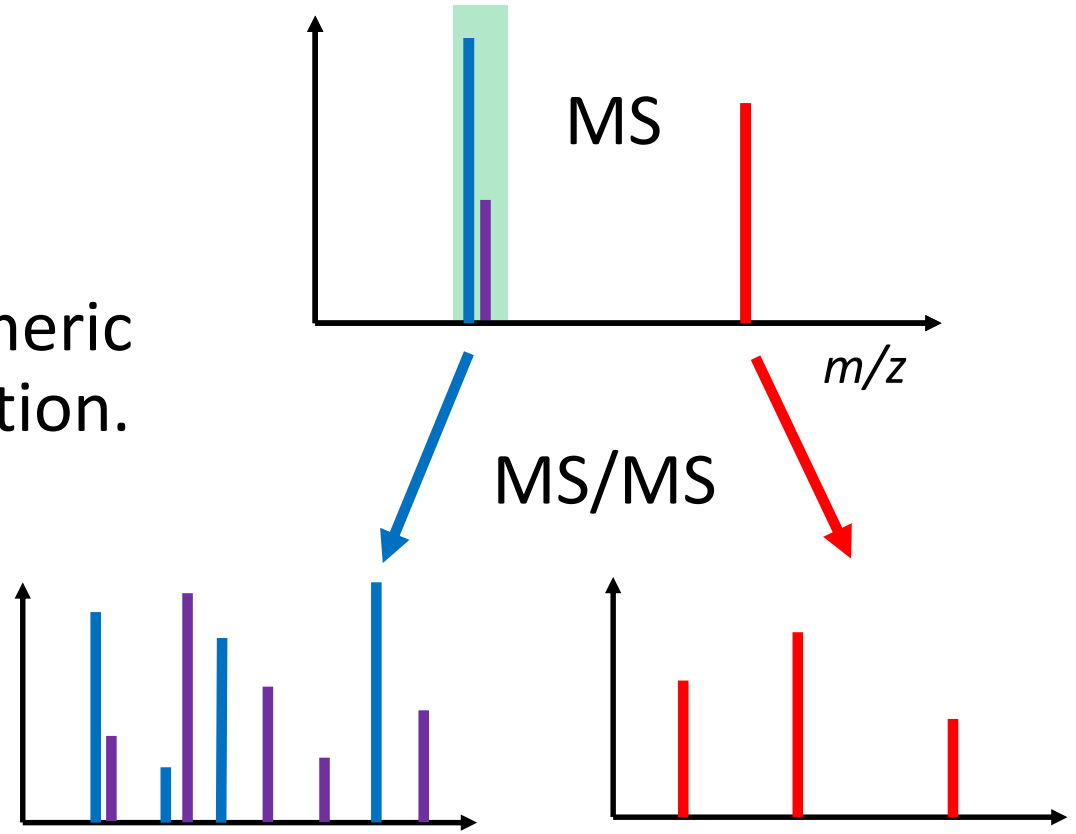
- Mass Spectrometry gives the total number of species and overall mass

- Further tandem mass spectrometry is needed to increase confidence of identification



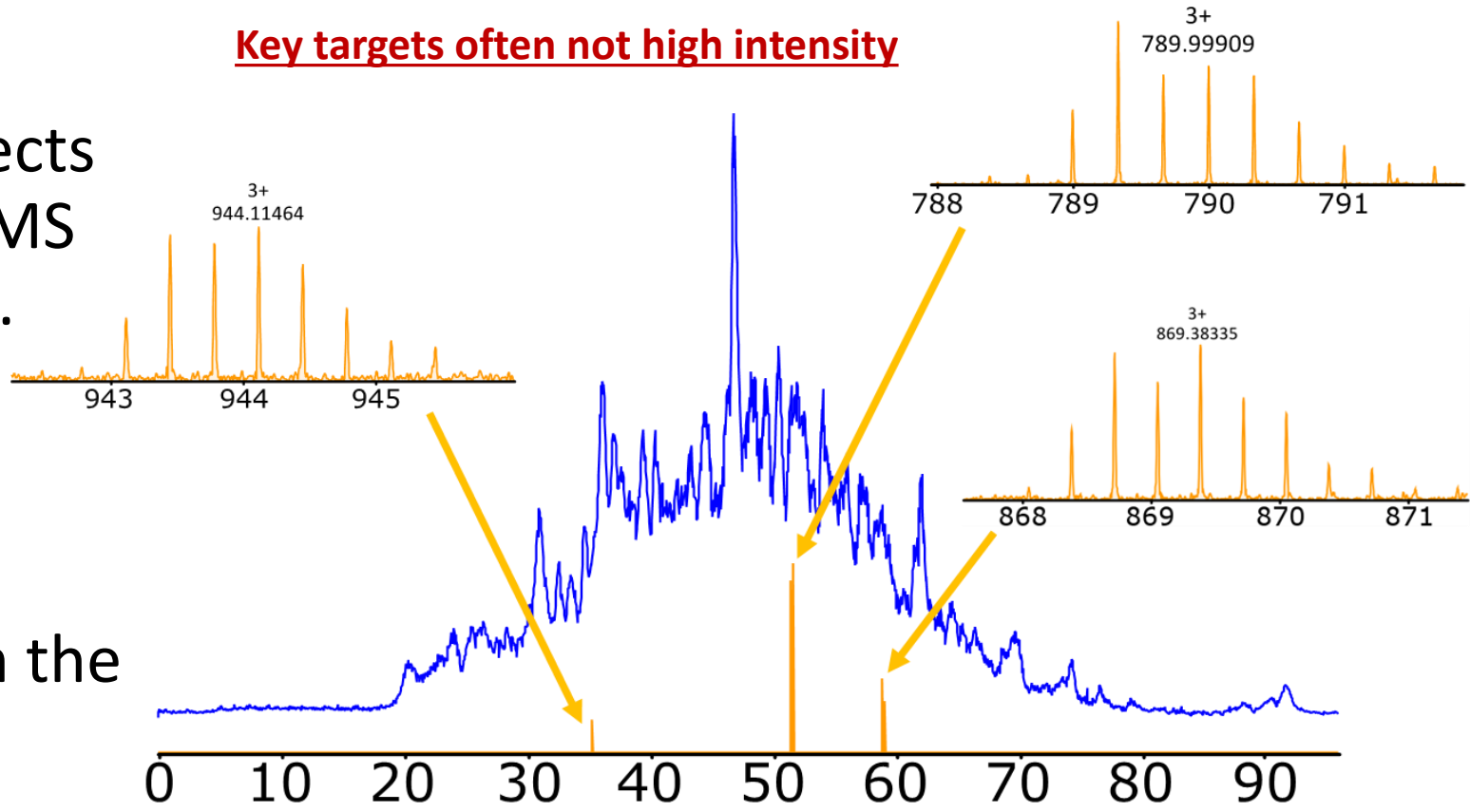
Mass Spectrometry specializes in analysis of mixtures

- Quadrupoles have limited isolation width.
- Possibility of overlap producing mixed/chimeric spectra decreasing confidence of identification.
- Practical isolation width > 1 *m/z* and loss of intensity



Liquid Chromatography is often added

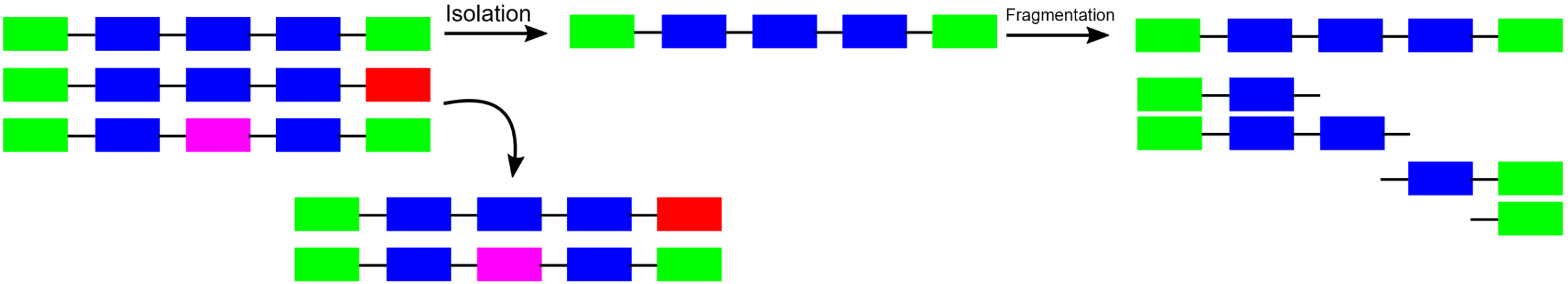
- DDA –LCMS systems operate on Top-X method.
- High resolution MS scan detects precursors, followed by MS/MS scans of precursors detected.
- Top-3, Top-5, and Top-10 strategies are common but precursors may be ignored in the interest of speed



Is there another option?

- Multiple isolation steps need to be carried out to characterize a whole mixture.
- Loss of precursor information if species cannot be easily separated via chromatography or isolated in the mass spectrometer.

Tandem mass spectrometry

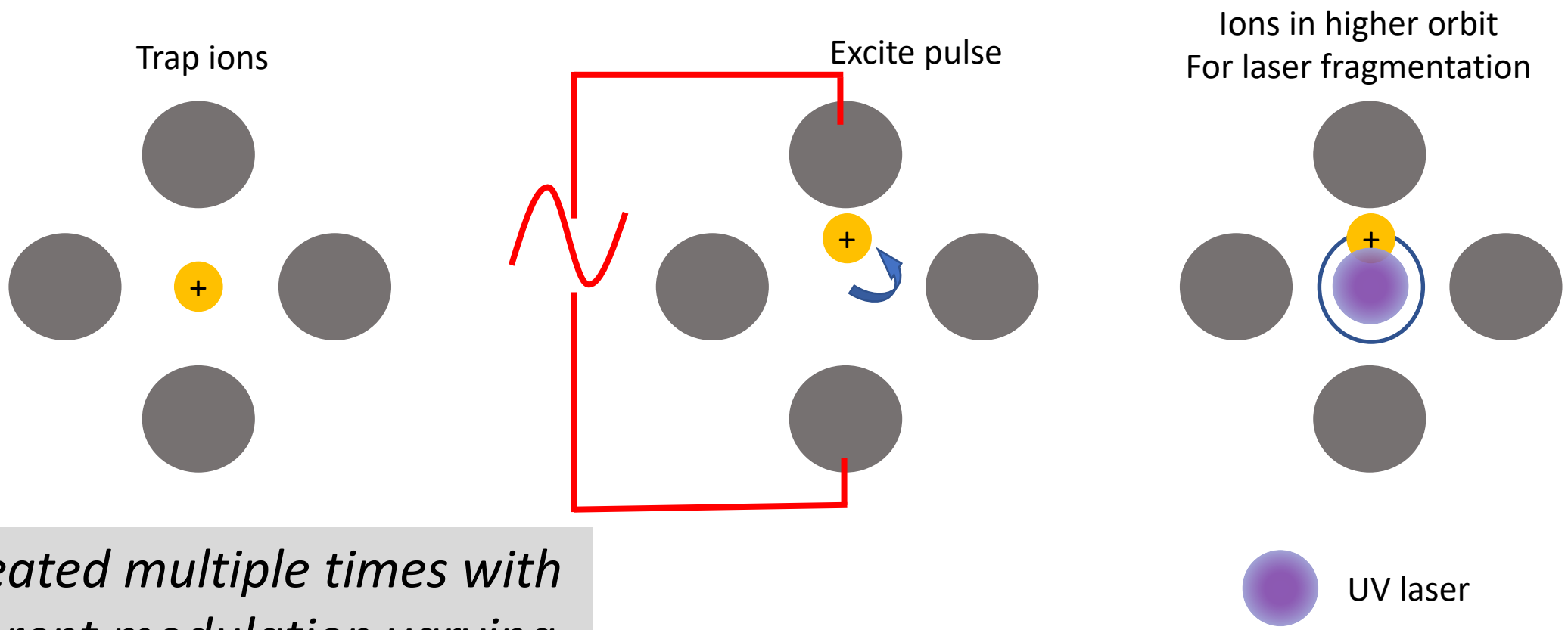


Is there another option?

- 2DMS – groups fragments and precursors together **without** prior isolation – no LC or quadrupole isolation needed and no loss in sensitivity
- True DIA – all precursors can be analysed
- Carried out on FT-ICR currently – Verdel is moving the technology to Q-TOF instruments from different manufacturers

2DMS on an oTOF

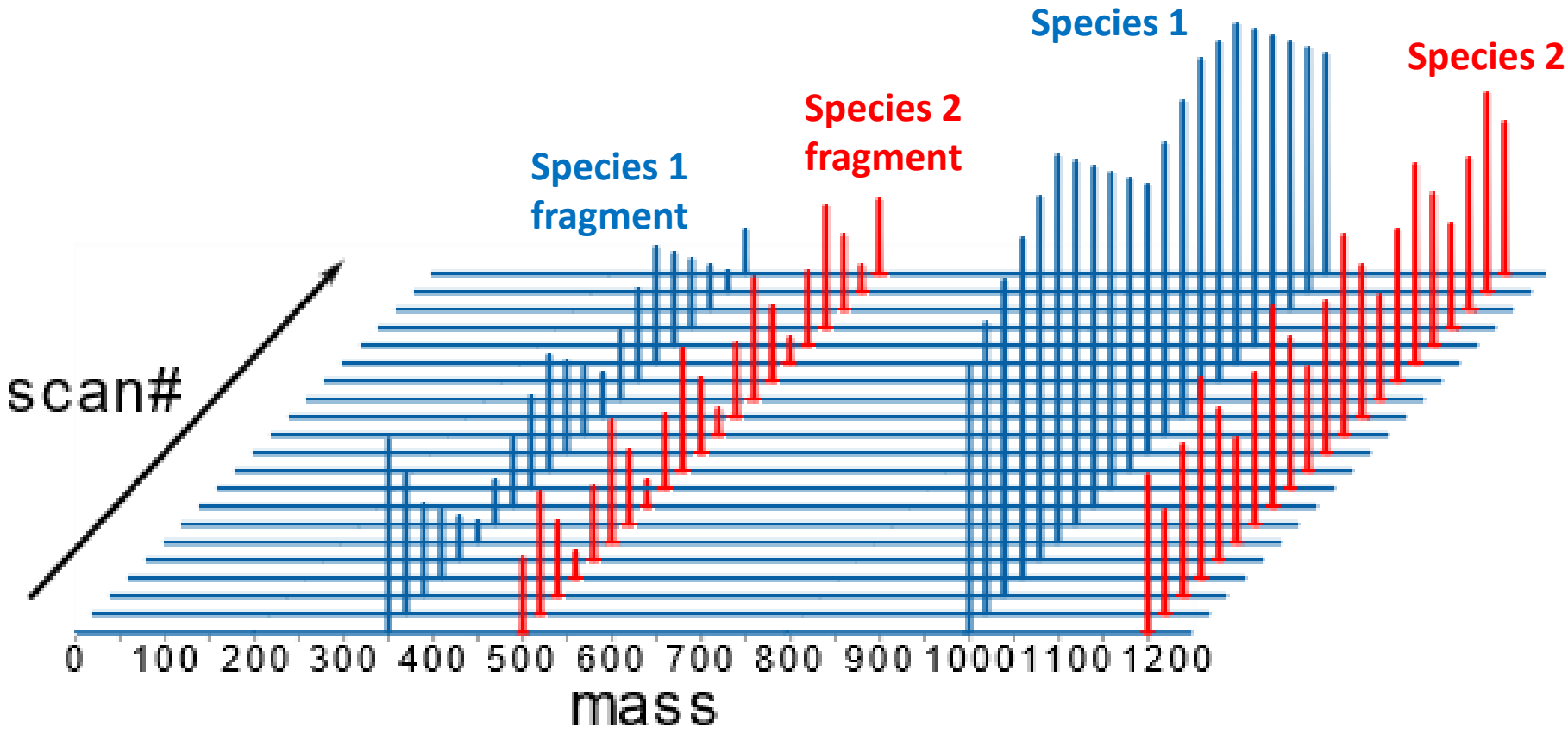
- Modified RF power supply for quadrupole modulates ions



Repeated multiple times with different modulation varying the degree of fragmentation

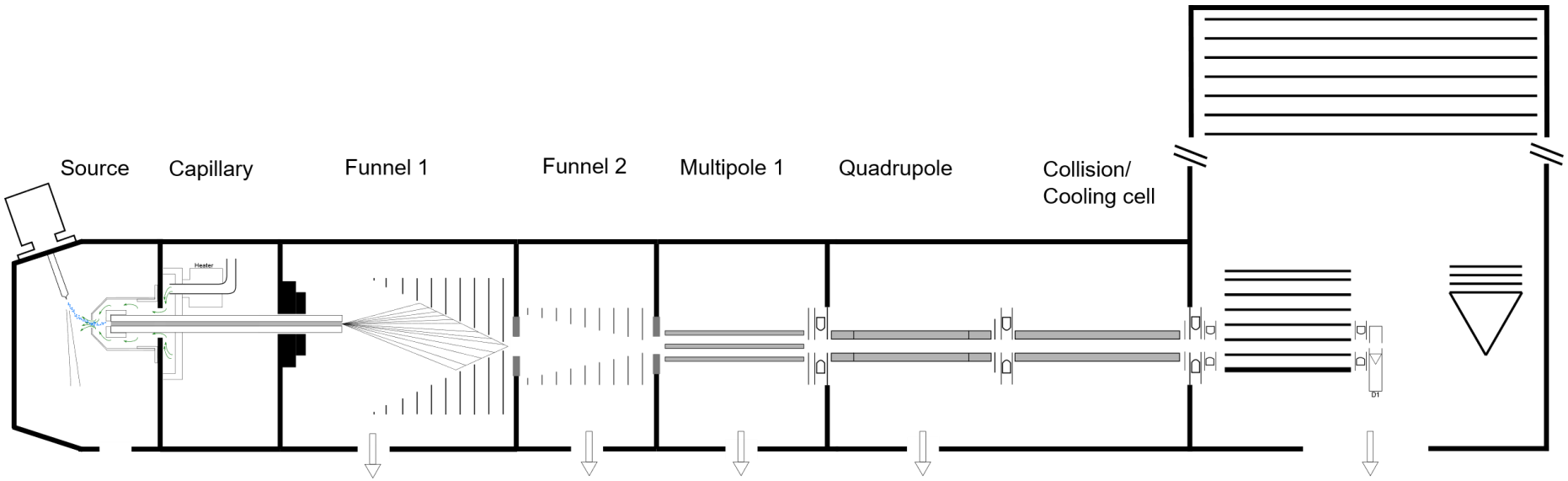
2DMS on an oTOF

- The radii of precursors are iterated multiple times producing an inverse relationship between precursors and their corresponding fragments:
- The data is Fourier transformed to generate the 2DMS spectrum



2DMS on an oTOF

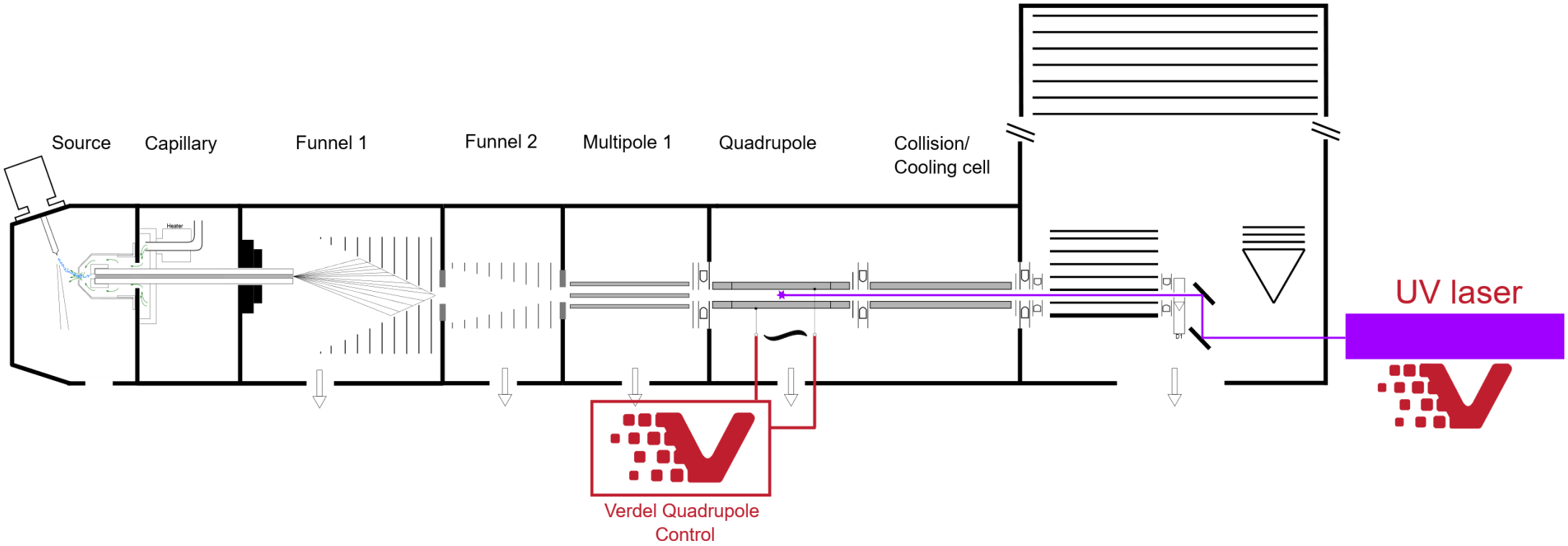
- Standard oTOF instrument setup



Bruker Maxis oTOF

2DMS on an oTOF

- Addition of Verdel RF power supply for the Quadrupole
- Addition of external UV laser and mirror setup within TOF section
- Quadrupole modified without replacement

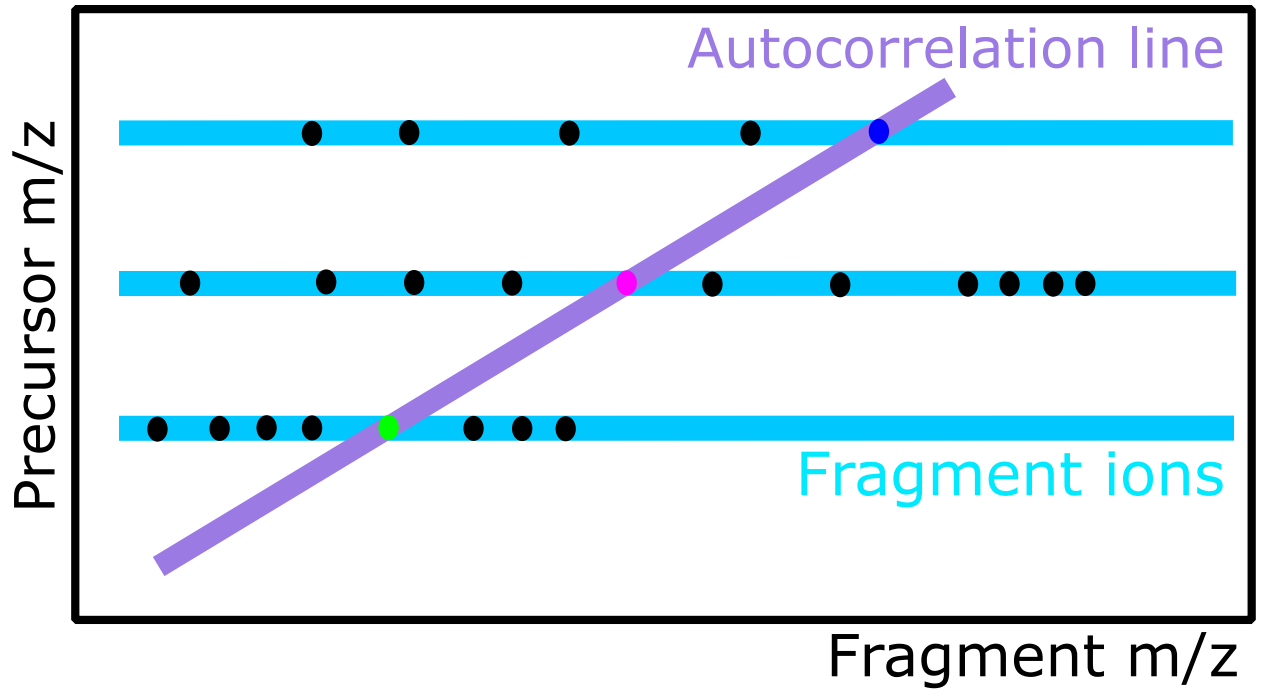


- UVPD gives method with a wide array of applications, robust to sample type

Verdel's 2DMS technology allows ***parallel analysis*** *of* ***all molecules*** *in a mixture* ***without prior isolation***

What results can 2DMS generate?

- 2DMS Produces large 2D spectra where fragments are correlated with their precursor ions within *m/z* space
- The autocorrelation line contains the precursor information
- The fragment lines contain the fragment information



analytical chemistry

pubs.acs.org/ac Letter

Facile Determination of Phosphorylation Sites in Peptides Using Two-Dimensional Mass Spectrometry

Johanna Paris, Tomos E. Morgan, Christopher A. Wootton, Mark P. Barrow, John O'Hara, and Peter B. O'Connor*

- 2DMS of a phosphopeptide mixture

https://pubs.acs.org/doi/abs/10.1021/acs.analchem.0c00884

- Autocorrelation and fragment lines show high species characterization

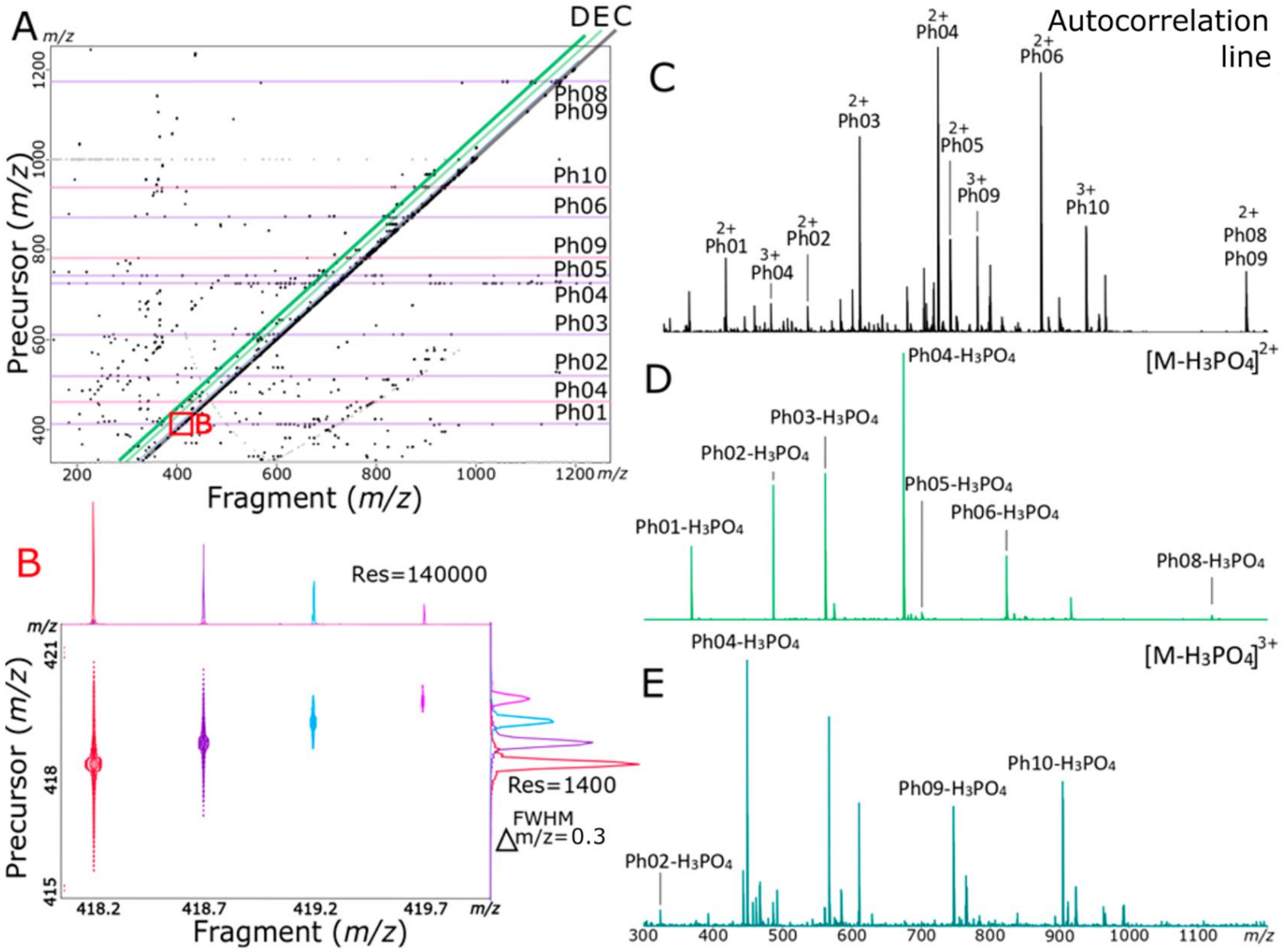


Figure 1. (A) Full 2DMS spectrum of phosphopeptide mixture; color code in Figure 1A: purple, 2+ species; pink, 3+ species. (B) Zoom of $[Ph01 + 2H]^{2+}$. Resolution in the vertical and the horizontal axes. (C) Autocorrelation line reveals all the fragmented precursors (similar to a 1D MS spectrum). (D) Extracted 2+ phosphate neutral (H_3PO_4) loss line. (E) Extracted 3+ phosphate neutral (H_3PO_4) loss line.

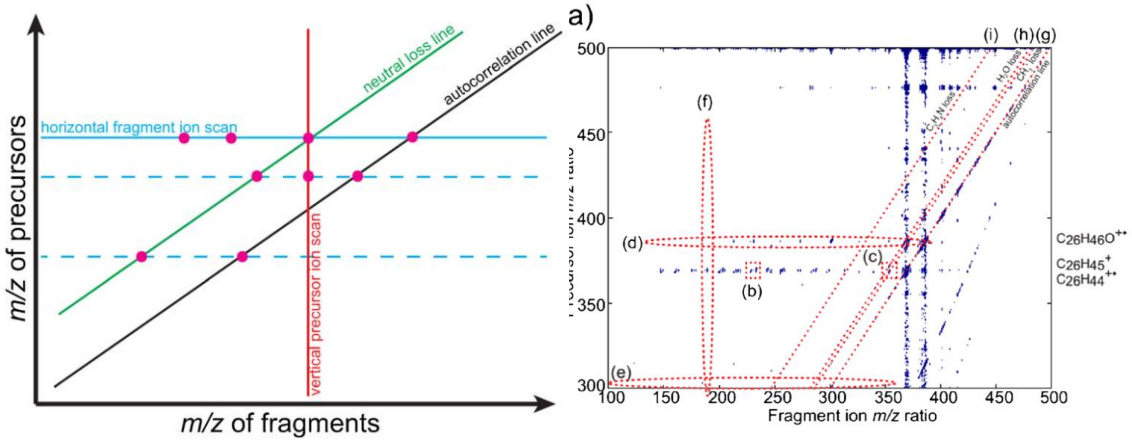
J. Am. Soc. Mass Spectrom. (2015) 26:2105–2114
DOI: 10.1007/s13361-015-1226-7

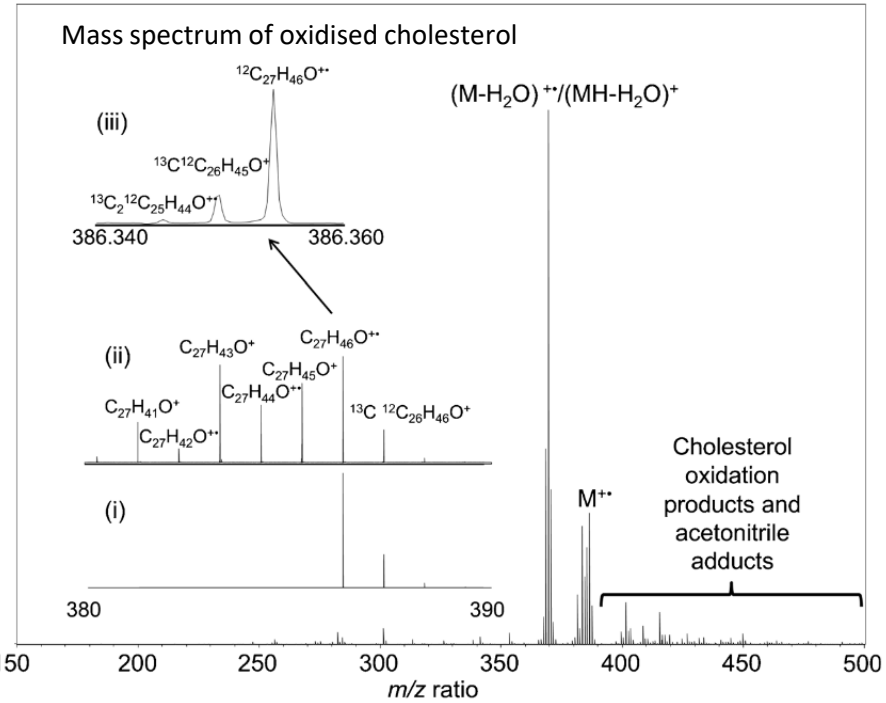
RESEARCH ARTICLE

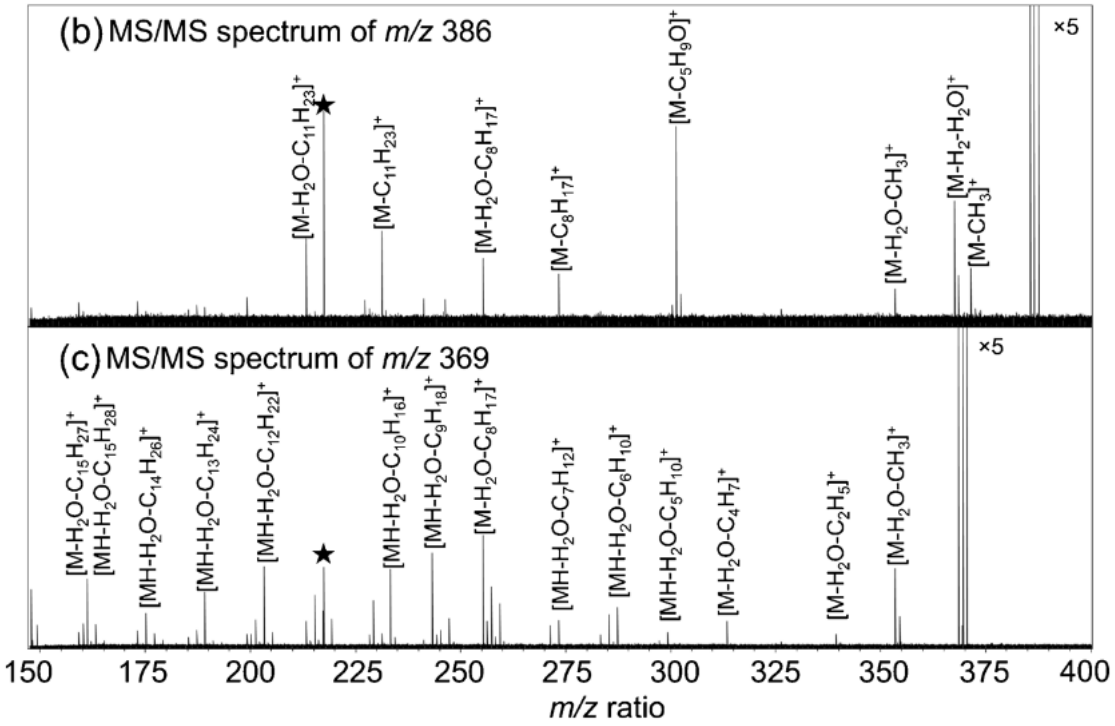
Differentiating Fragmentation Pathways of Cholesterol by Two-Dimensional Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

Maria A. van Agthoven,[1] Mark P. Barrow,[1] Lionel Chiron,[2] Marie-Aude Coutouly,[2] David Kilgour,[3] Christopher A. Wootton,[1] Juan Wei,[1] Andrew Soulby,[1] Marc-André Delsuc,[2,4] Christian Rolando,[5] Peter B. O'Connor[1]

https://link.springer.com/article/10.1007/s13361-015-1226-7







Further Publications describing 2DMS

analytical chemistry

Article

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Two-Dimensional Mass Spectrometry for Proteomics, a Comparative Study with Cytochrome *c*

Maria A. van Agthoven,[‖] Christopher A. Wootton,[‖] Lionel Chiron,[⊥] Marie-Aude Coutouly,[§,¶] Andrew Soulby,[‖] Juan Wei,[‖] Mark P. Barrow,[‖] Marc-André Delsuc,[‡,⊥] Christian Rolando,[†] and Peter B. O'Connor*[,‖]

European Biophysics Journal (2019) 48:213–229
https://doi.org/10.1007/s00249-019-01348-5

EBSA

TECHNICAL PRIMER

Check for updates

Two-dimensional mass spectrometry: new perspectives for tandem mass spectrometry

Maria A. van Agthoven[1] · Yuko P. Y. Lam[1] · Peter B. O'Connor[1] · Christian Rolando[2] · Marc-André Delsuc[3,4]

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J. Am. Soc. Mass Spectrom. (2016) 27:1531–1538
DOI: 10.1007/s13361-016-1431-z

RESEARCH ARTICLE

2D FT-ICR MS of Calmodulin: A Top-Down and Bottom-Up Approach

Federico Floris,[1] Maria van Agthoven,[1] Lionel Chiron,[2] Andrew J. Soulby,[1] Christopher A. Wootton,[1] Yuko P. Y. Lam,[1] Mark P. Barrow,[1] Marc-André Delsuc,[2,3] Peter B. O'Connor[1]

analytical chemistry

Article

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Polymer Analysis in the Second Dimension: Preliminary Studies for the Characterization of Polymers with 2D MS

Federico Floris,[†] Claudio Vallotto,[†] Lionel Chiron,[‡] Alice M. Lynch,[†] Mark P. Barrow,[†] Marc-André Delsuc,[‡,§] and Peter B. O'Connor*[,†]

Analyst

ROYAL SOCIETY OF CHEMISTRY

ARTICLE

Uncoiling Collagen: A Multidimensional Mass Spectrometry Study

H. J. Simon,[a] M. A. van Agthoven,[a] P. Y. Lam,[a] F. Floris,[a] L. Chiron,[b] M.-A. Delsuc,[b,c] C. Rolando,[d] M. P. Barrow,[a] and P. B. O'Connor[a]

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Differentiating Fragmentation Pathways of Cholesterol by Two-Dimensional Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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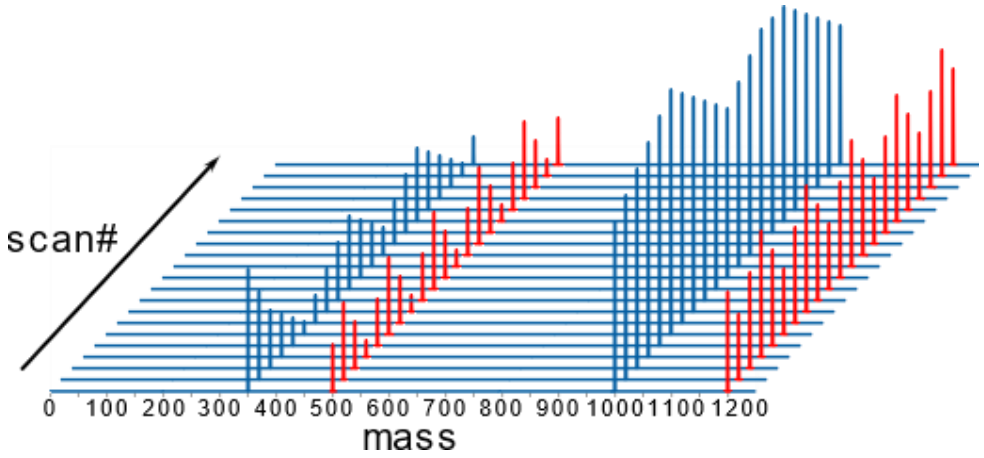
Huge array of applications

- Any analyte present within a complex mixture and fragmented by UVPD!
- Proteins/peptides
  - Large *m/z* range accessible making top-down and bottom-up possible
- Polymers
- Lipids
- Agrochemicals
  - Present within complex matrices
- Small molecule pharmaceuticals

- Plus many more

One fast, parallel, and detailed experiment

- Removes the need for separation techniques
  - Eliminates column bias or variation
- Analyses all the ions, every time; offering true DIA
- No sample knowledge needed prior to analysis
- Offers both high quality data and rapid analysis
- Can be supplied as an upgrade to a range of QTOF instruments from different suppliers
- No specialist training needed



Please contact us with any further questions!

www.verdelinstruments.co.uk