Verdel Instruments: Total Correlation Mass Spectrometry™:
Fast, effective, true DIA

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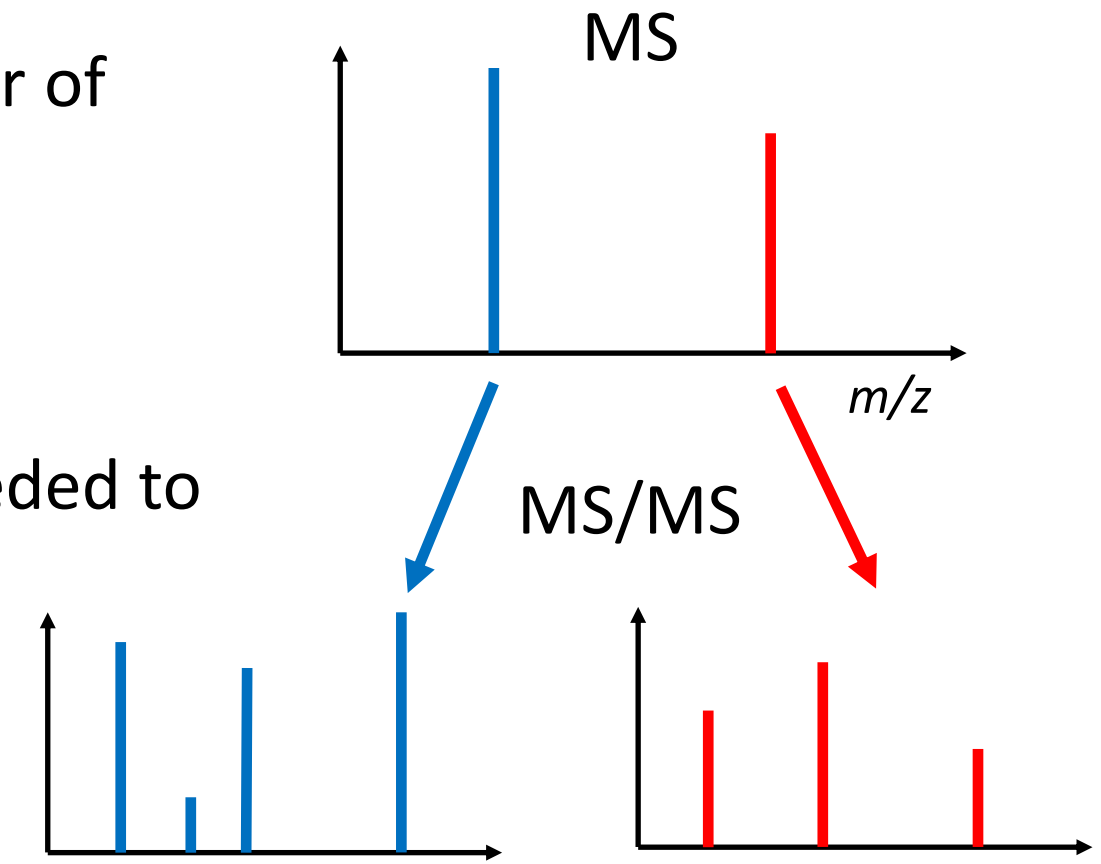
Innovate UK

Mass Spectrometry specialises in analysis of mixtures

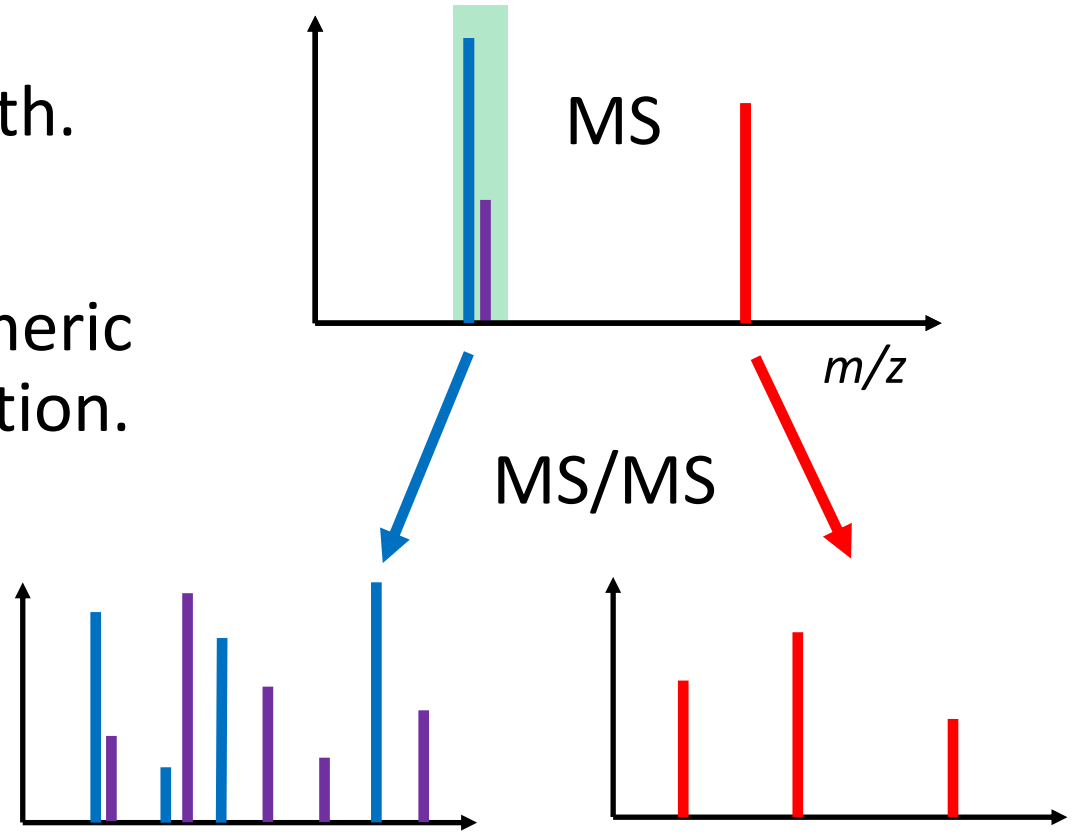
- Mass Spectrometry gives the total number of species and overall mass.

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



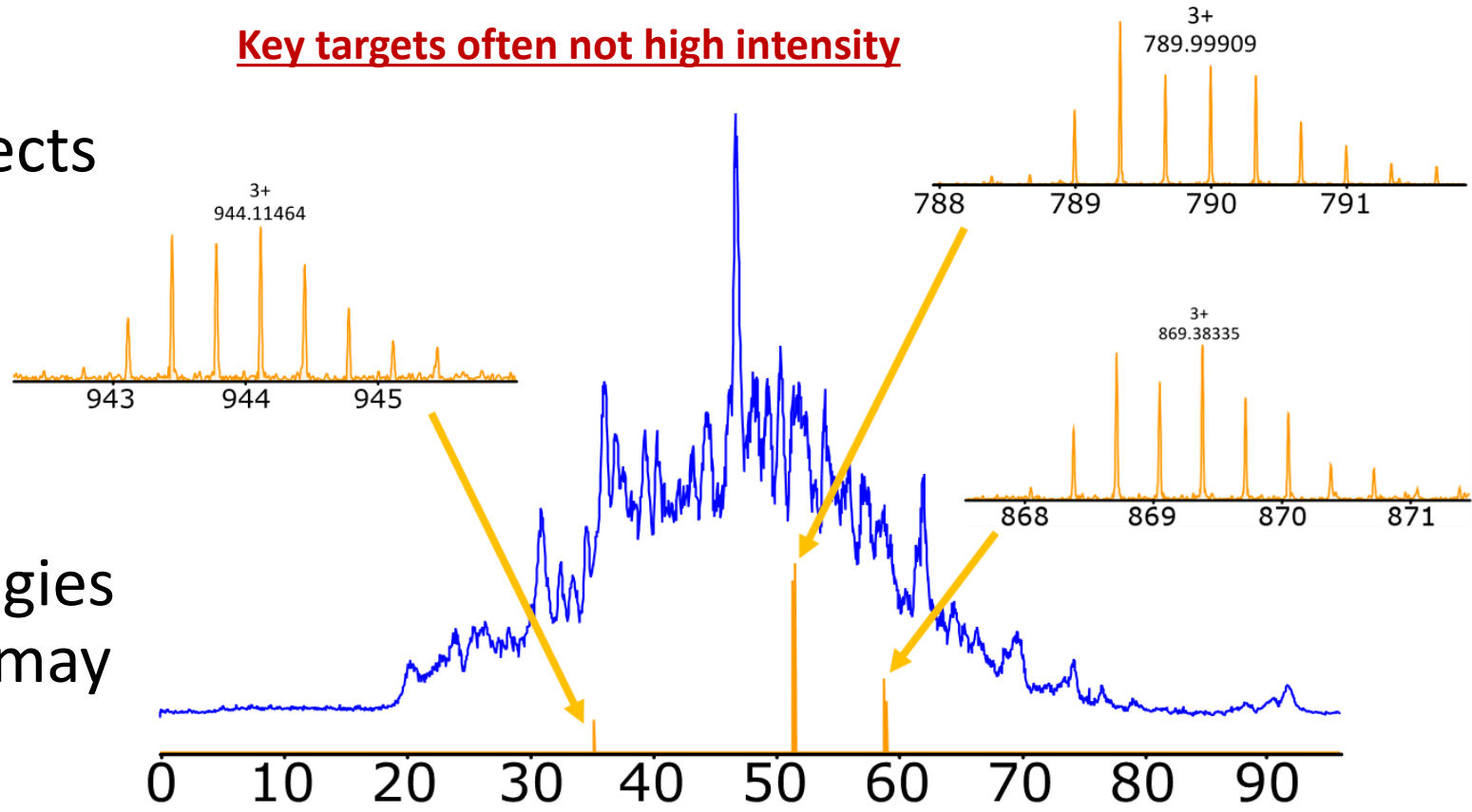
Mass Spectrometry specialises in analysis of mixtures

- Quadrupoles have a non-zero isolation width.
- Possibility of overlap producing mixed/chimeric spectra decreasing confidence of identification.
- Practical isolation wide > 1 *m/z*



Liquid Chromatography is often added

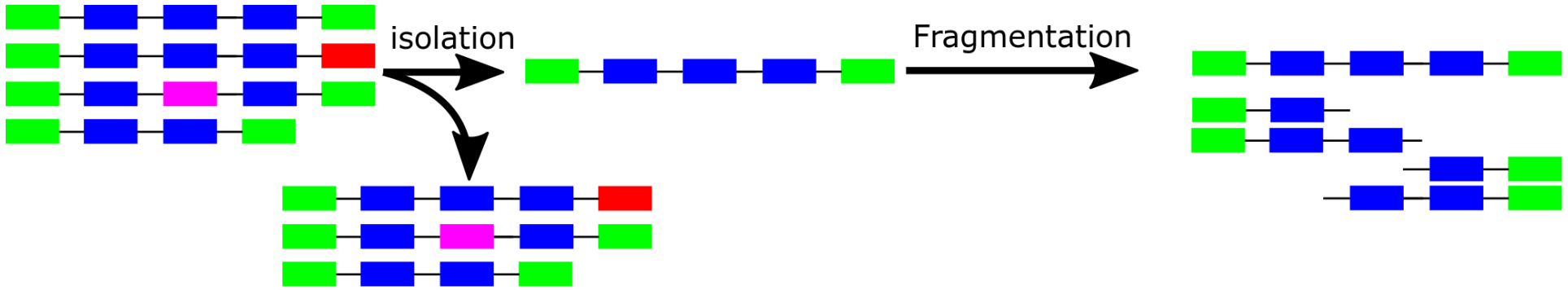
- DDA –LCMS systems operate on TopX structure.
- High resolution MS scan detects precursors and followed by MS/MS scans of precursors detected.
- Top3, Top5, and Top10 strategies are common but precursors may be ignored in the interest of speed.



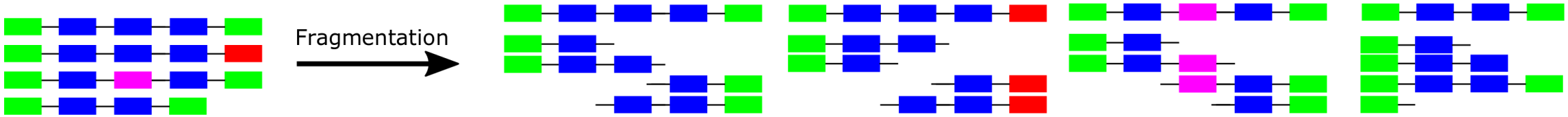
Is there another option?

- Isolation results in the loss of precursor information.

Tandem mass spectrometry

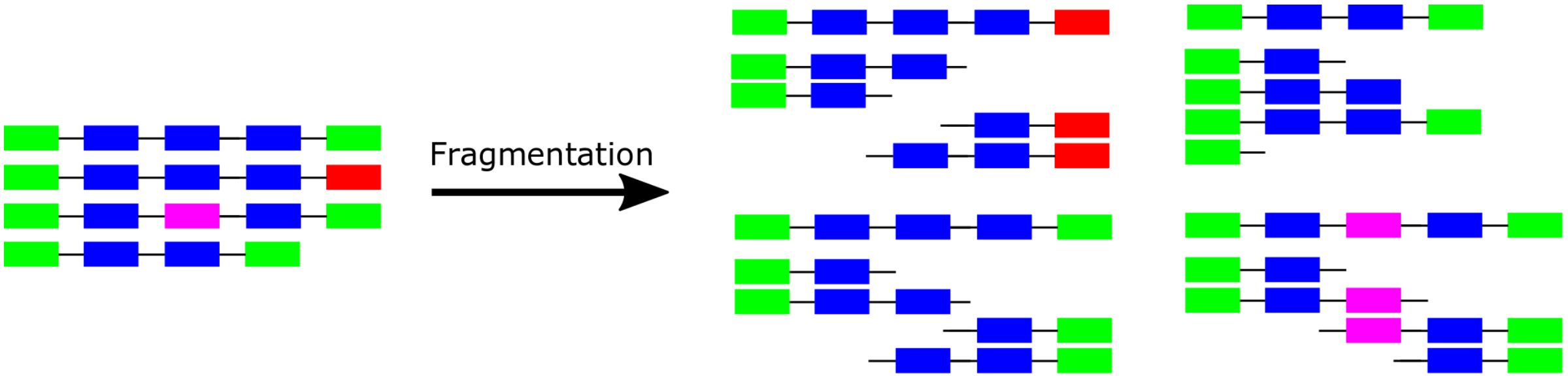


Total Correlation Mass Spectrometry™



Is there another option?

- How can we correlate precursors and fragments without separation: Total Correlation Mass Spectrometry ™.



- Total Correlation Mass Spectrometry is the name for the FTICR 2DMS techqnique applies using a QTOF

Is there another option?

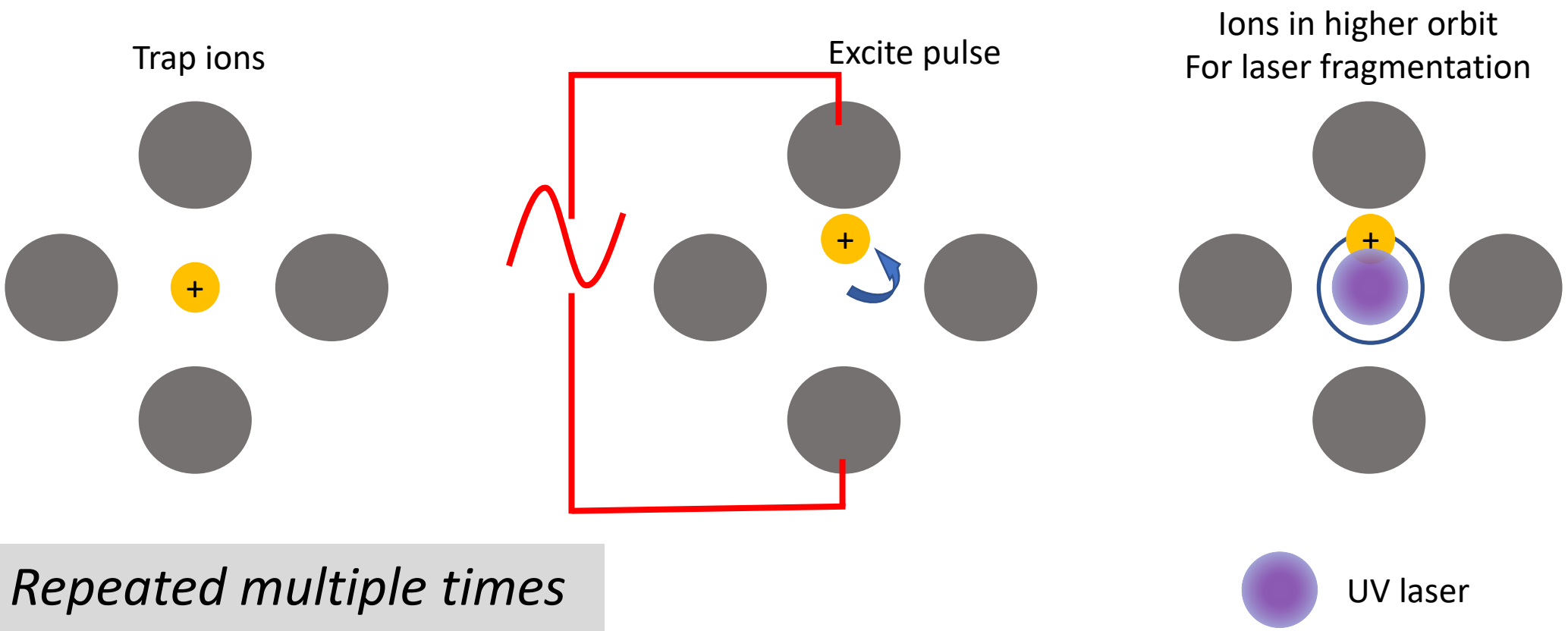
- TC-MS™ – groups fragments and precursors together **without** prior isolation – no LC or quadrupole isolation needed.

- True DIA – the number of precursors does not affect total acquisition time.

- Deveoloped on an FT-ICR– Verdel is moving the technology to a number of QTOF instruments from different manufacturers.

How does TC-MS™ outside of FT-ICR work?

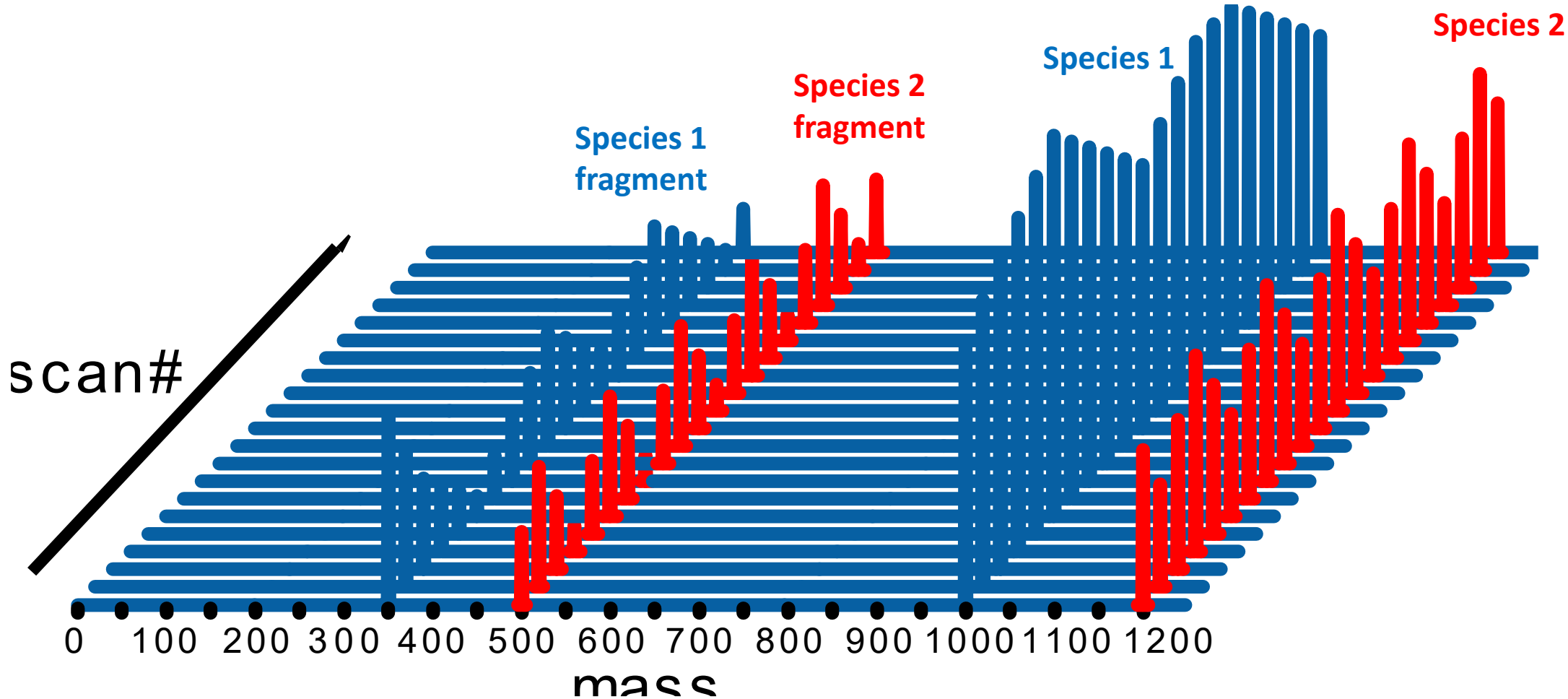
- Modified RF power supply for quadrupole modulates ions.



Repeated multiple times with different modulation

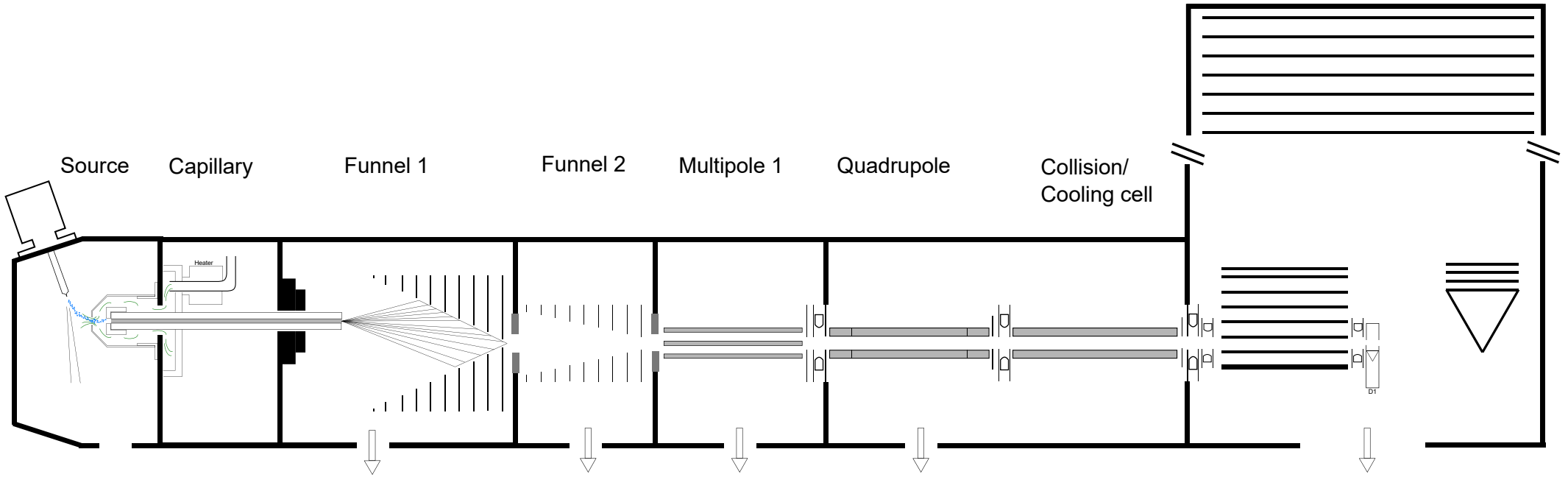
How does TC-MS™ outside of FT-ICR work?

- The radii of precursors are iterated multiple times producing an inverse relationship between precursors and their corresponding fragments:



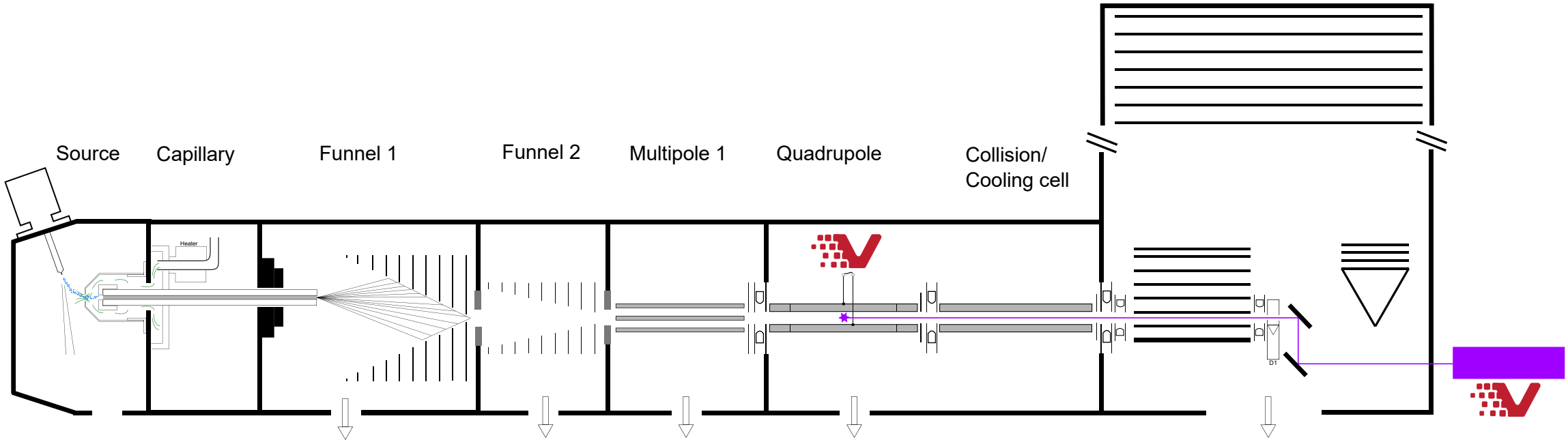
How does TC-MS™ outside of FT-ICR work?

- Small modification of standard TOF instrument (Bruker MaXis).



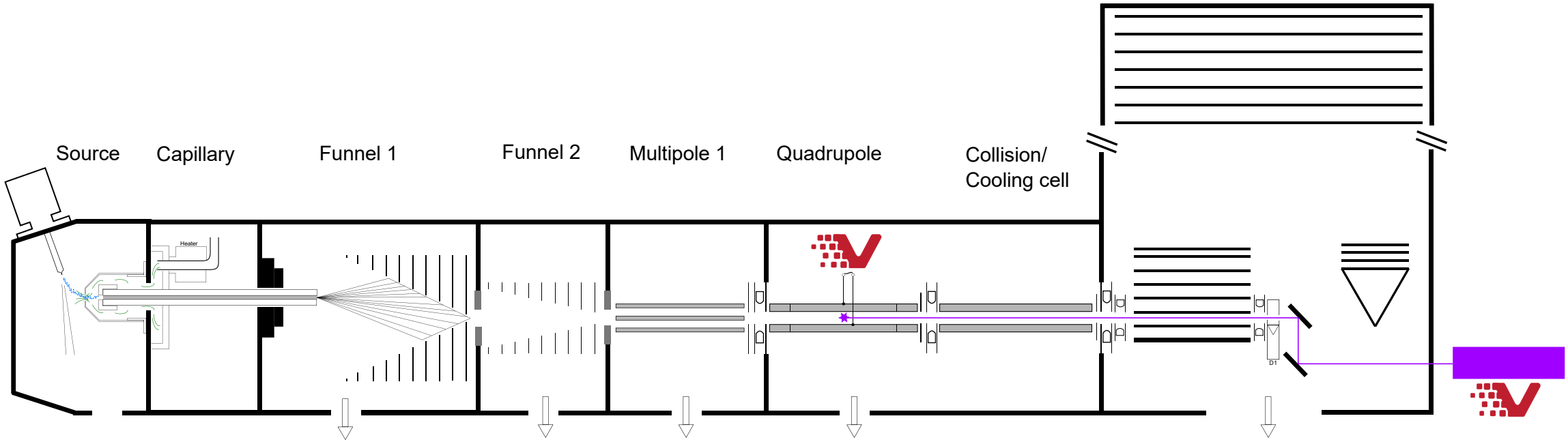
How does TC-MS™ outside of FT-ICR work?

- Addition of Verdel RF power supply for the Quadrupole.
- Addition of external UV laser and mirror setup within TOF section.



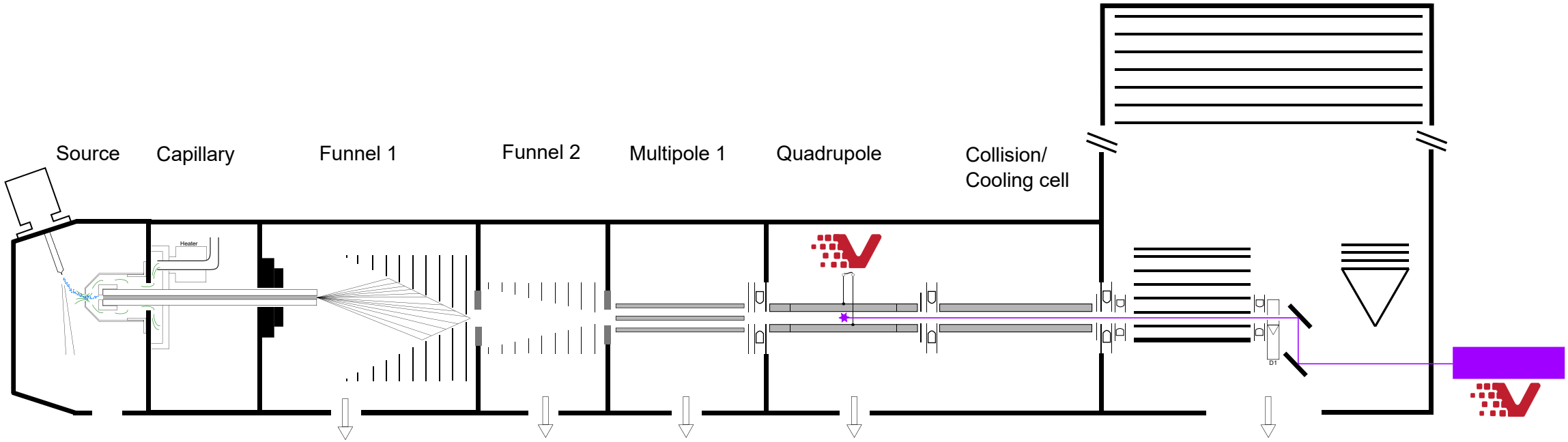
How does TC-MS™ outside of FT-ICR work?

- Quadrupole modification can be carried out without quadrupole replacement.



How does TC-MS™ outside of FT-ICR work?

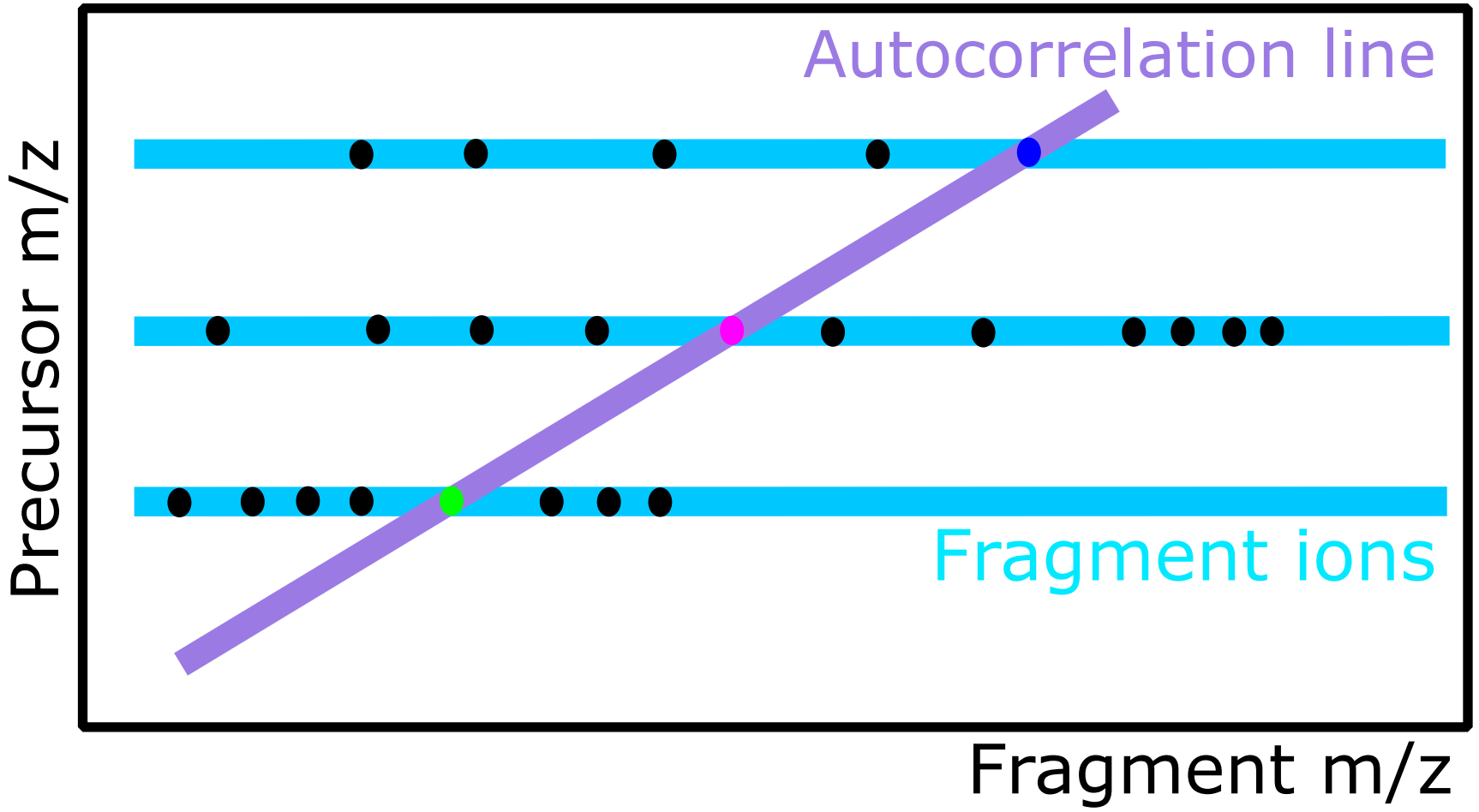
- Use of UVPD gives method with a wide array of applications, highly robust to sample type.



Verdel's TC-MS™ technology allows ***parallel analysis*** *of* ***all molecules*** *in a mixture* ***without prior separation,*** ***removing chromatography.***

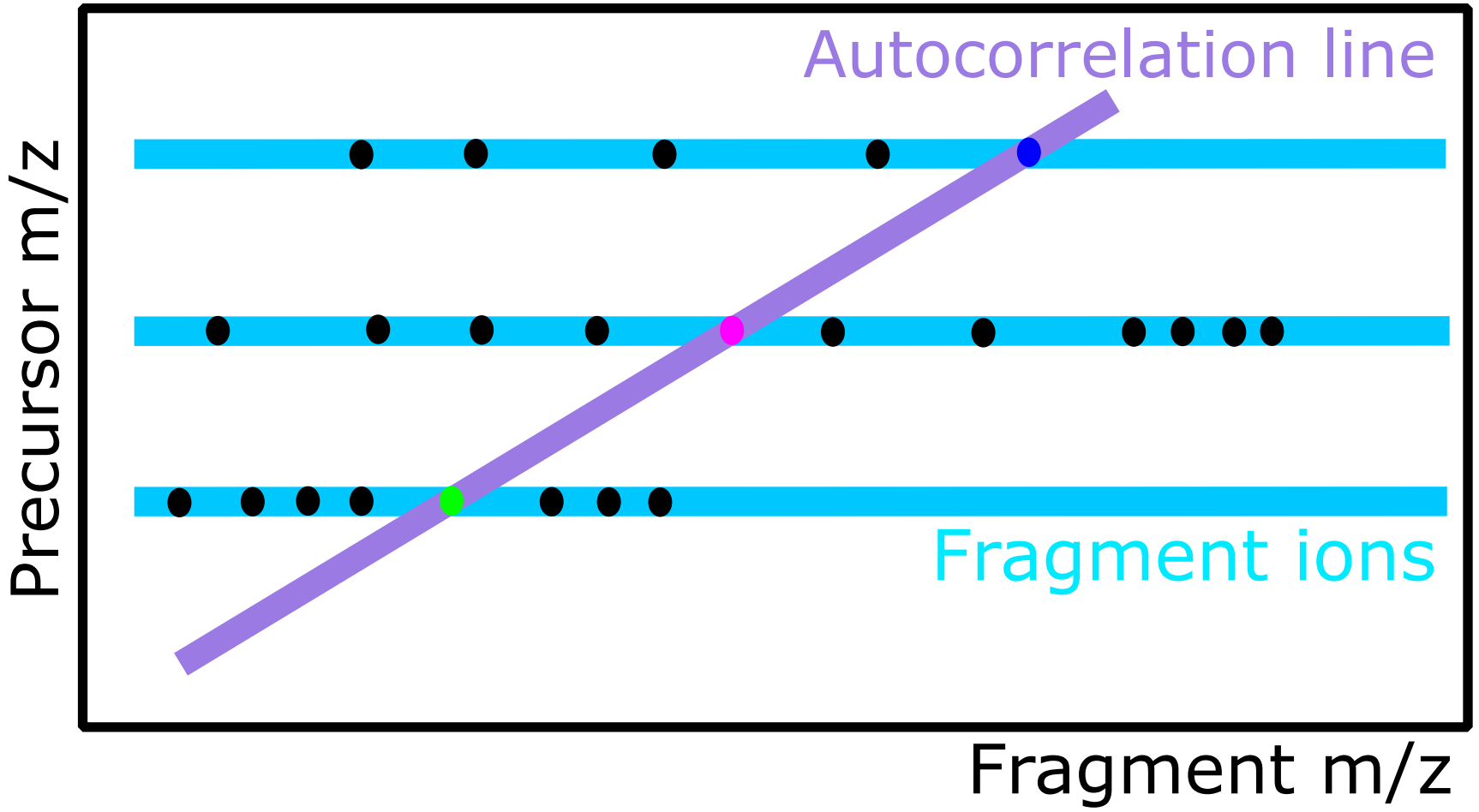
What results does TC-MS™ generate?

- TC-MS produces large TC spectra where fragments are correlated with their precursor ions within *m/z* space.



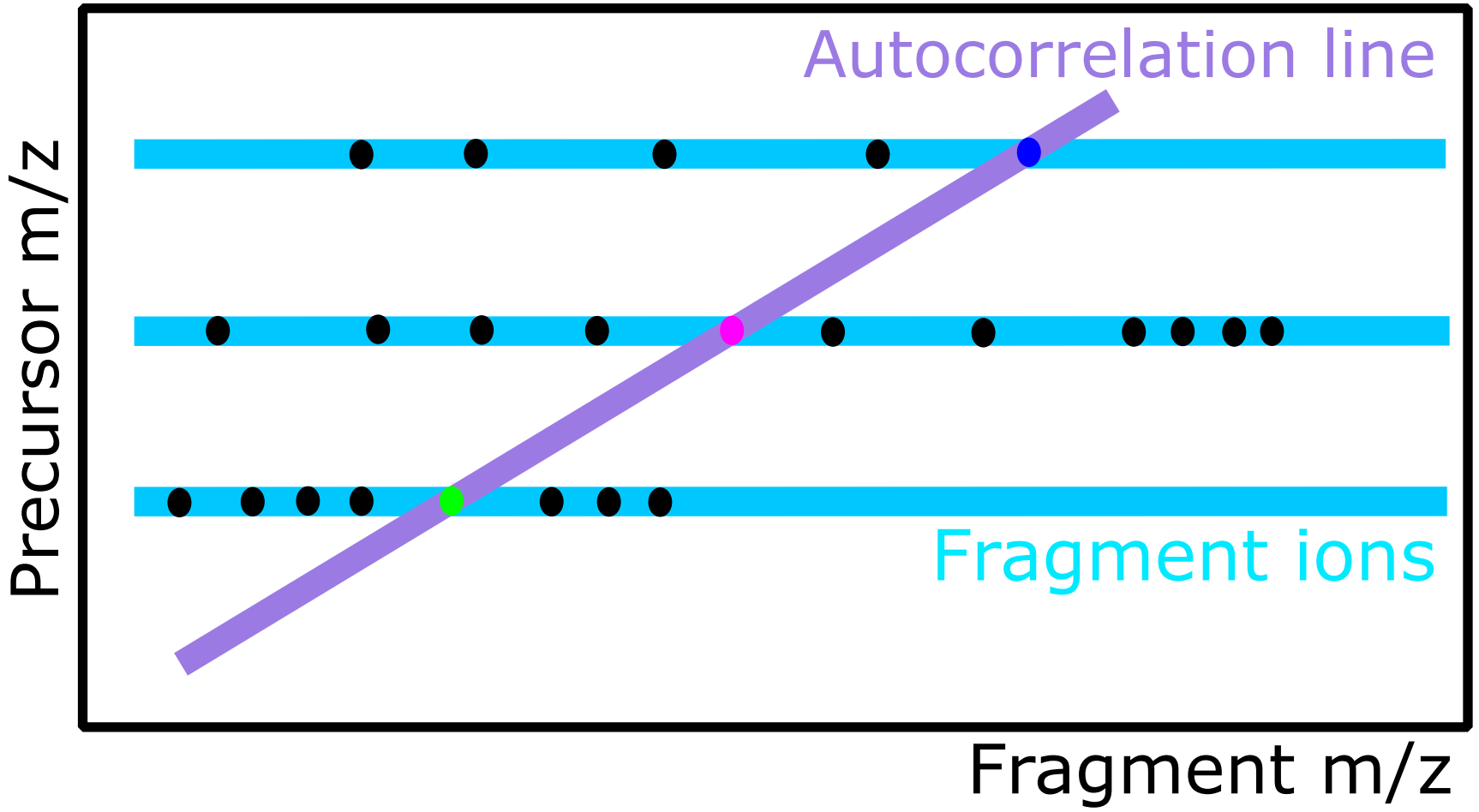
What results can TC-MS™ generate?

- The Autocorrelation line contains all the precursors.



TC-MS™ data

- The fragments corresponding to each precursors are present on horizontal fragment lines.



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*

- TC-MS™ of a phosphopeptide mixture.
- Autocorrelation and fragment lines show high species characterisation.

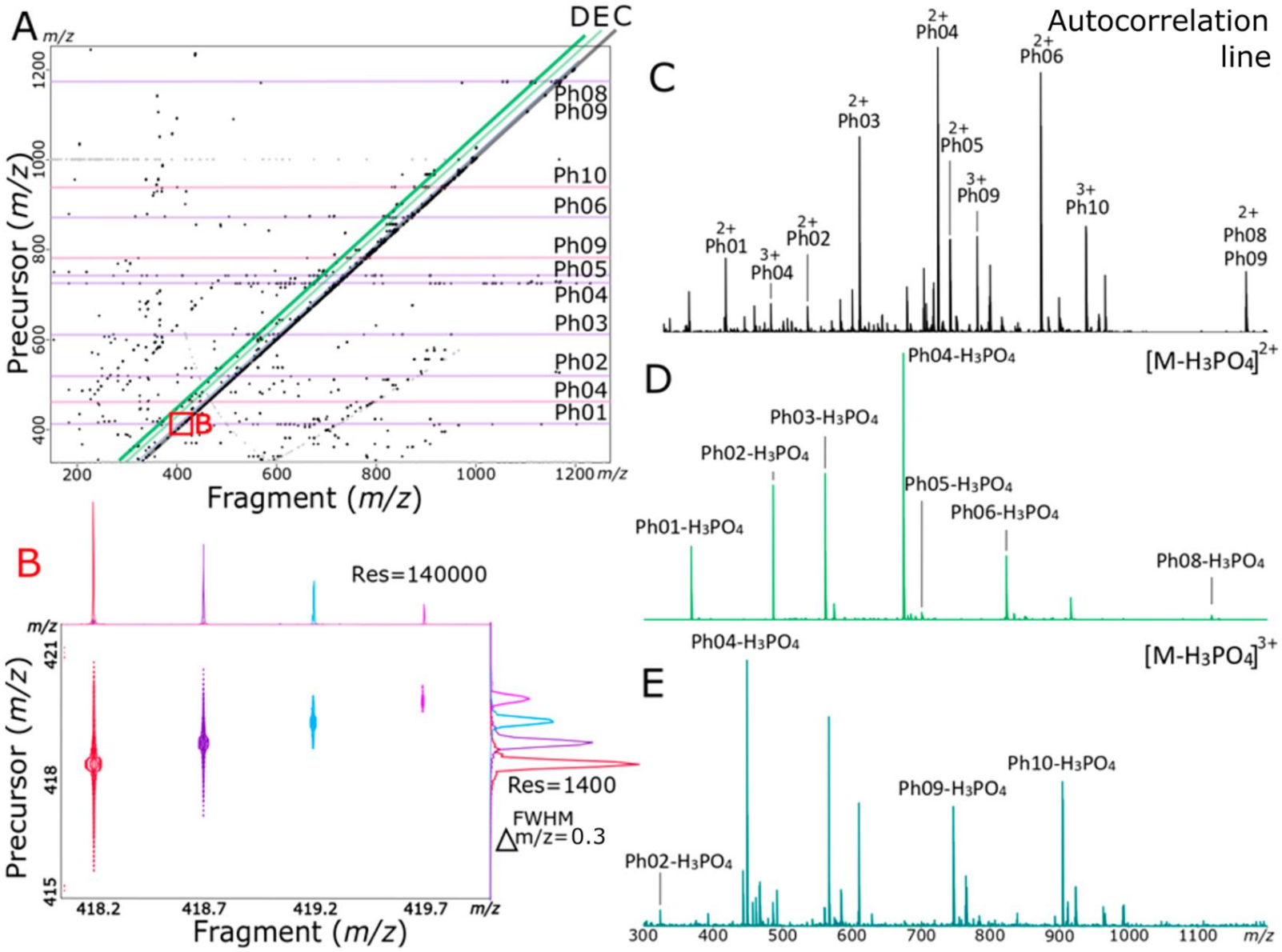


Figure 1. (A) Full 2DMS spectrum of phosphopeptide mixture; color code in Figure 1A: purple, 2+ species; pink, 3+ species. (B) Zoom of $[Ph01 + 2H]^{2+}$. Resolution in the vertical and the horizontal axes. (C) Autocorrelation line reveals all the fragmented precursors (similar to a 1D MS spectrum).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

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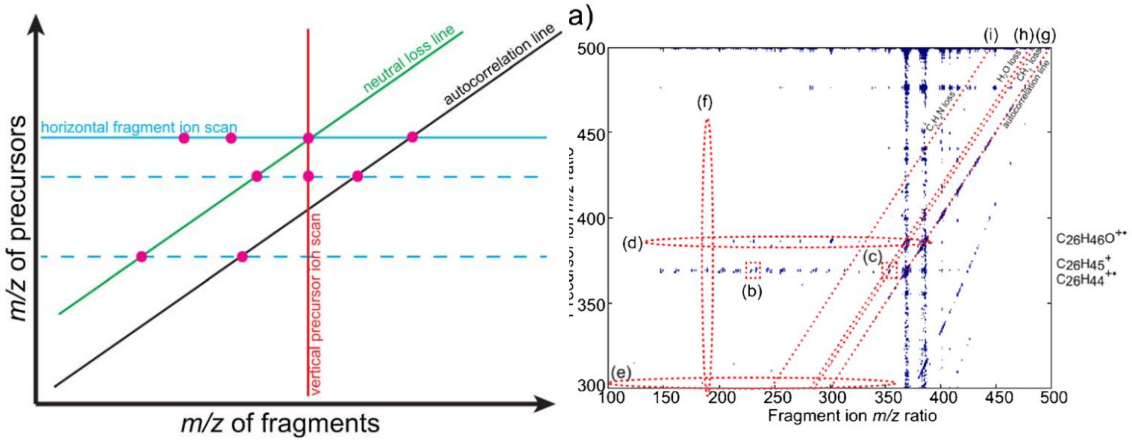
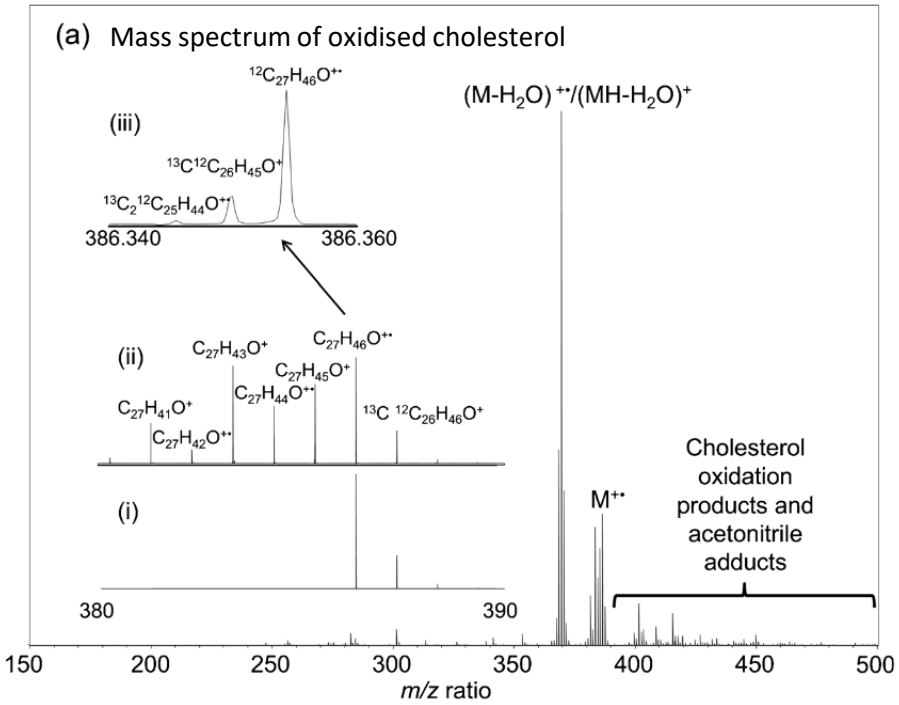
DOI: 10.1007/s13361-015-1226-7

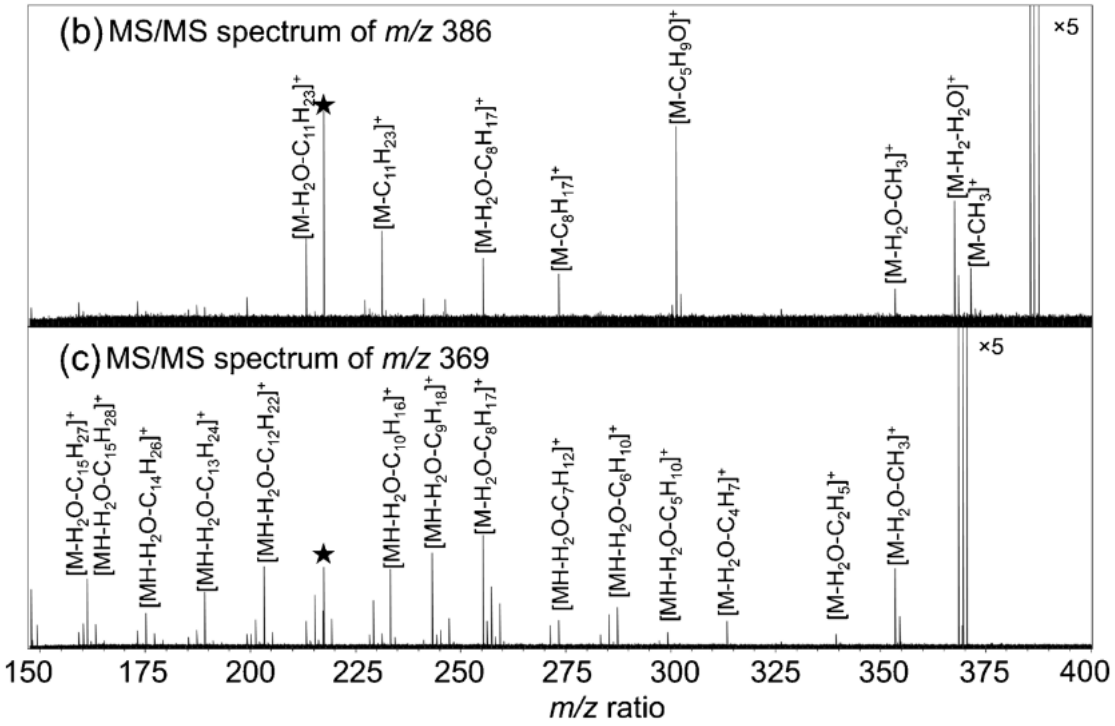
RESEARCH ARTICLE

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]







Publications describing TC-MS™

analytical chemistry

Article

pubs.acs.org/ac

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]

AS MS

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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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RESEARCH ARTICLE

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

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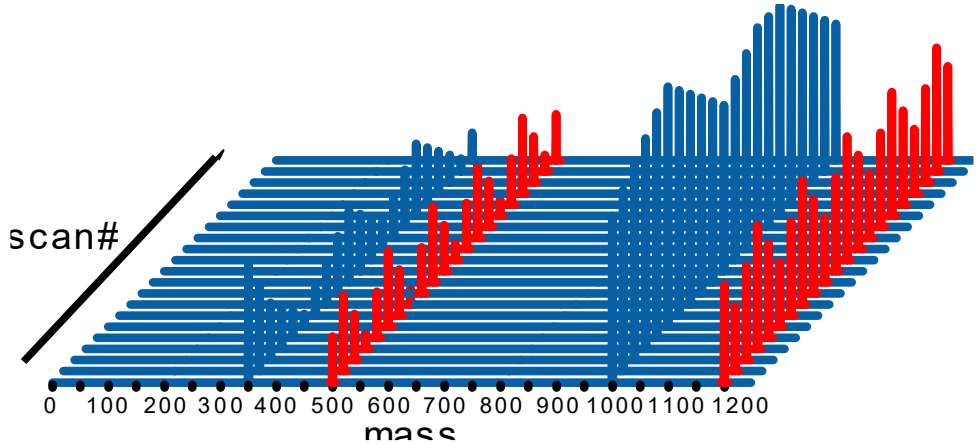
Huge array of applications

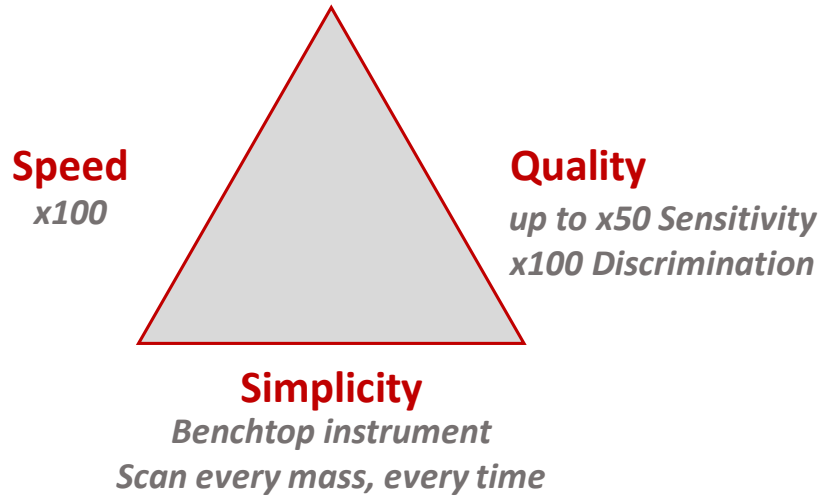
- Any analyte present within a complex mixture and fragmented by UVPD
- Proteins/peptides
  - Large *m/z* range accessible making top-down and bottom-up possible
- Polymers
- Lipids
- Agrochemicals
  - Present within complex matrices
- Small molecule pharmaceuticals

- Plus many more

One fast, parallel, and detailed experiment

- Removes the need for separation techniques.
  - Eliminates column bias or variation
- Analyses all the ions in a sample, every time; offers true DIA.
- No prior 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.





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