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Charge transfer dissociation (CTD): a new activation method in Evry for probing the structure of natural or synthetic compounds



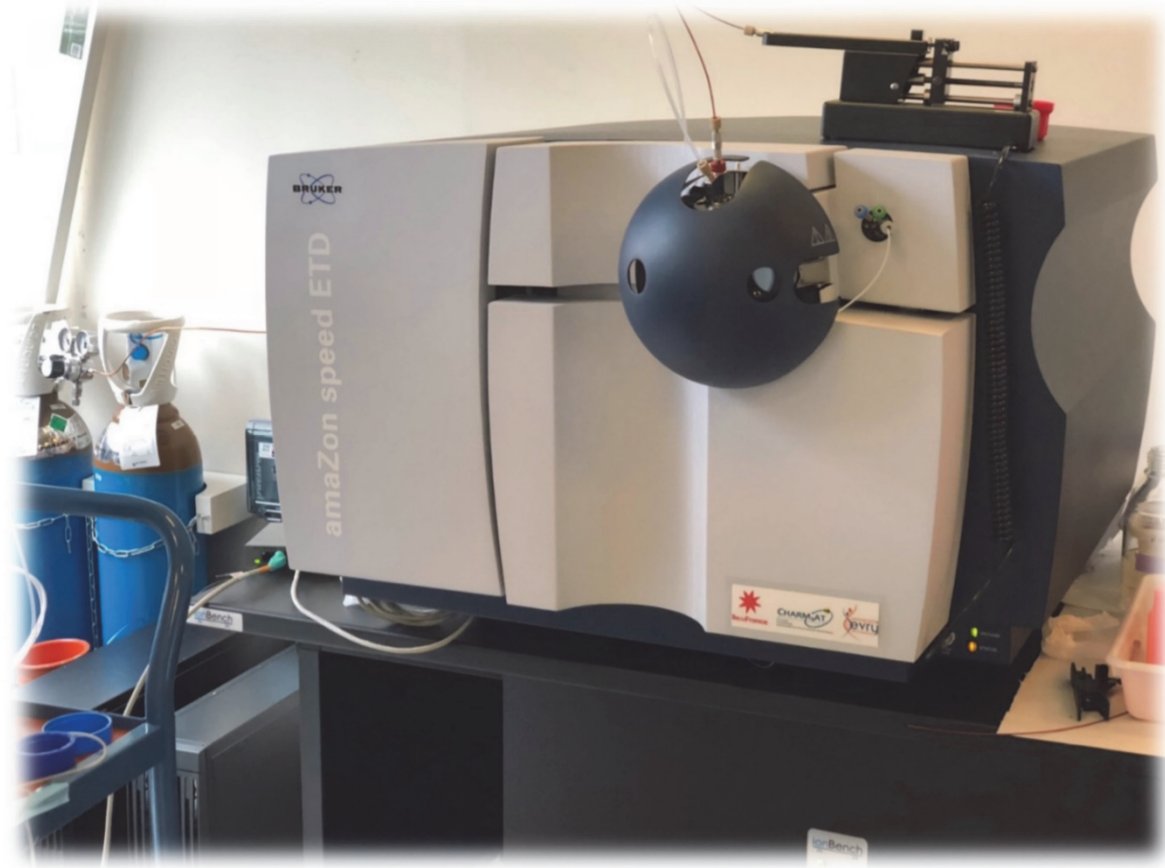
Jean-Yves Salpin¹, Salomé Poyer¹, William Buchmann¹, Riccardo Spezia^{1,2}, Régis Daniel¹, Glen P. Jackson³

1- LAMBE – Laboratoire Analyse, Modélisation, Matériaux pour la Biologie et l'Environnement – UMR 8587, Evry, France

2- Laboratoire de Chimie Théorique – UMR 7616, Paris, France

3- West Virginia University – Department of Forensic and Investigative Science, Morgantown, Etats-Unis

Introduction



The combination of soft ionization methods with tandem mass spectrometry (MS/MS or MSⁿ) has become an essential tool for the fine structural analysis of biomolecules. The most popular MS/MS method is based on collision-induced dissociation (CID) of the gas-phase analyte. However, this method suffers several limitations, such as incomplete fragmentation or the loss of labile chemical functional groups, leading to a loss of structural information. To reach a more complete characterization, especially for biomolecules with high isomerism, new activation methods have been developed for several years, including Charge Transfer Dissociation (CTD). We have implemented the CTD fragmentation method in 2022 on an ion trap of the LAMBE mass spectrometry platform.

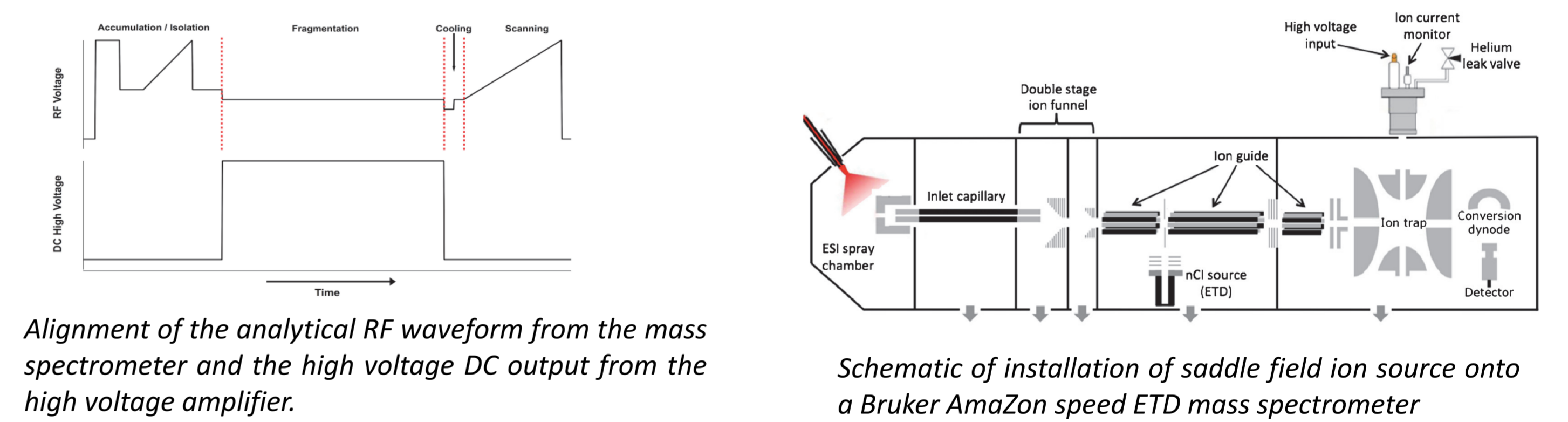
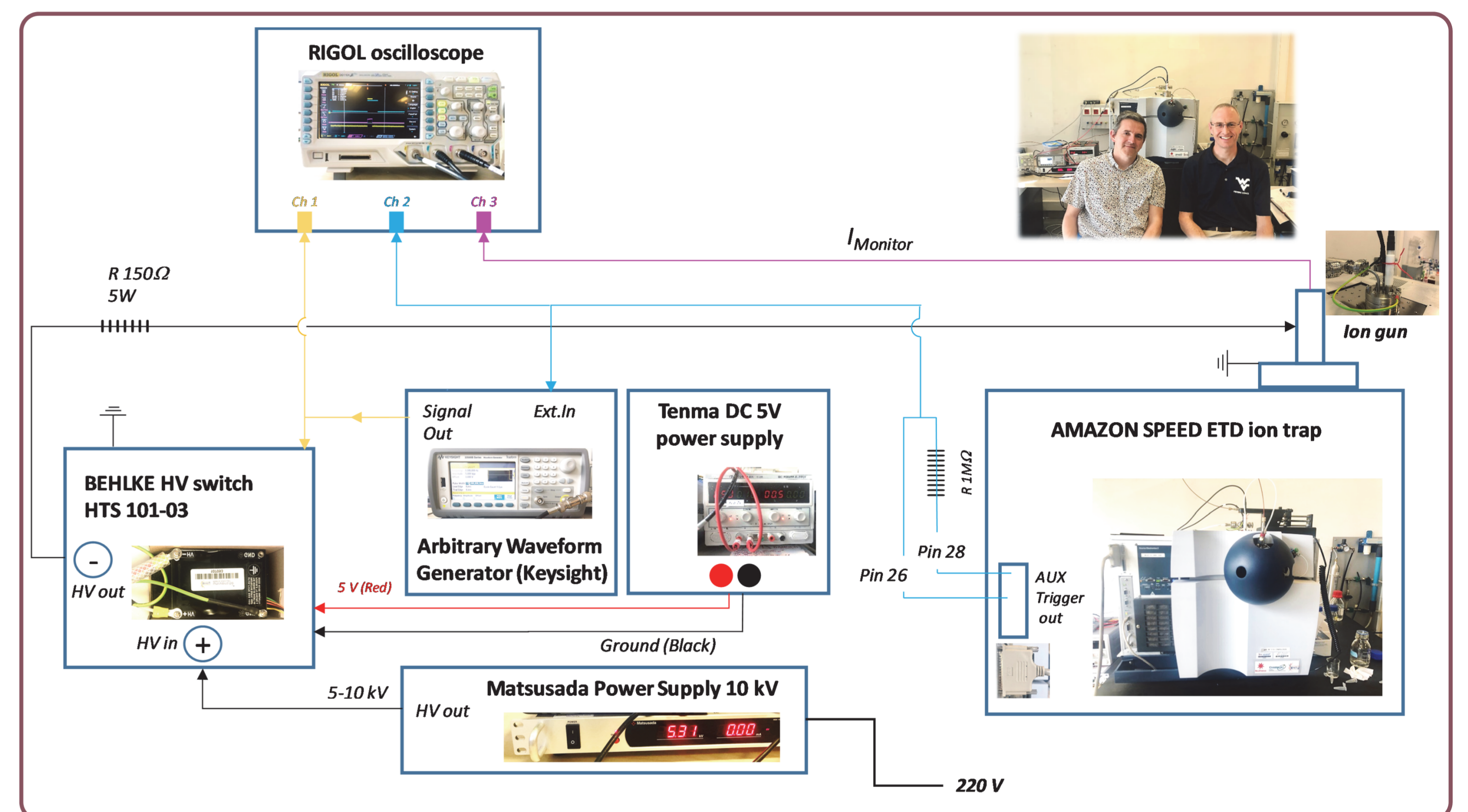
Principle of Charge Transfer Dissociation (CTD)

- Charge Transfer Dissociation has been recently introduced.[1]
- CTD is based on the collision between strongly accelerated (keV) He⁺ ions and a precursor ion. This method allows a charge exchange process, leading to the formation of radical ions.

$$[M+H]^+ + He^+ \longrightarrow [M+H]^{2+} + He \longrightarrow \text{Fragments}$$

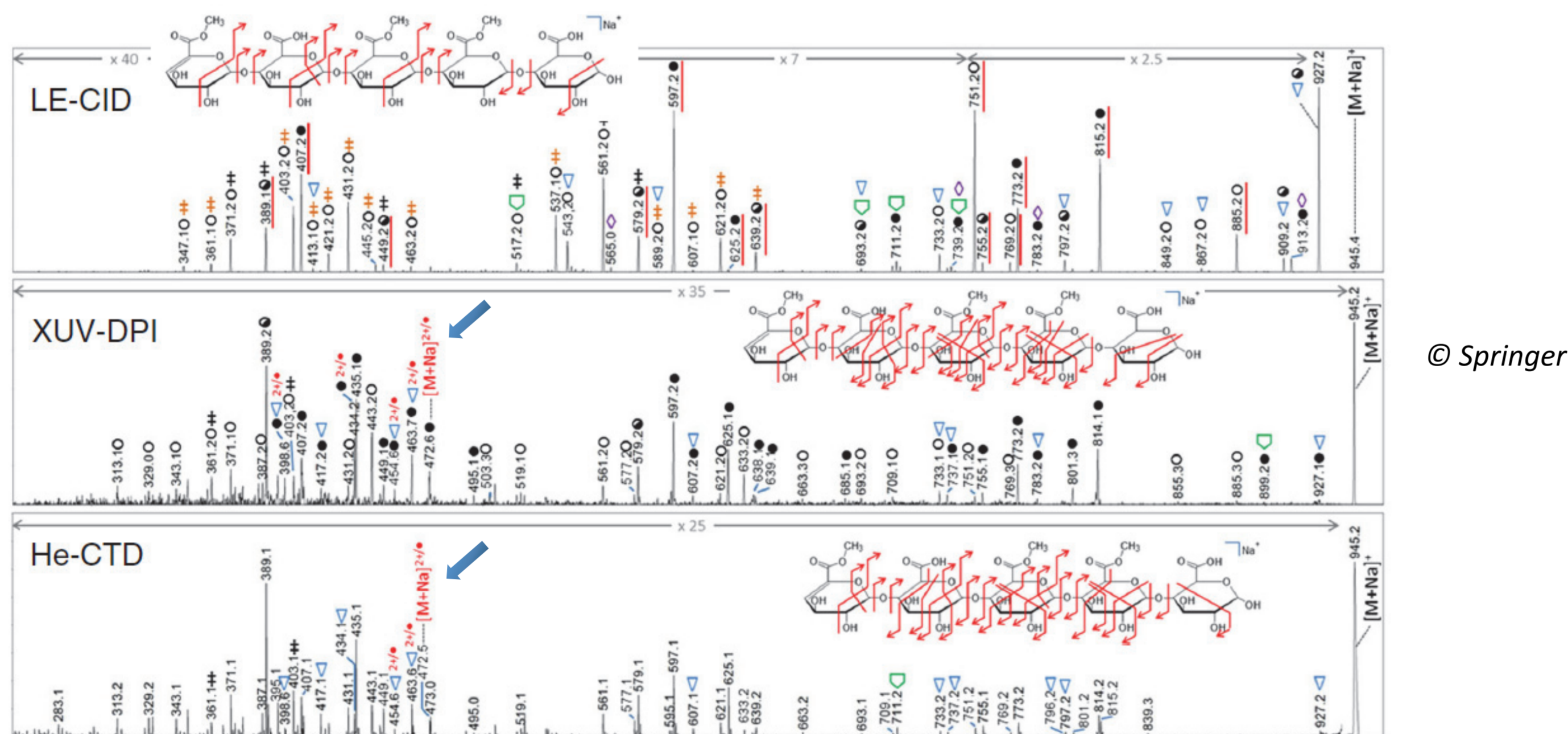
$$[M-nH]^{n-} + He^+ \longrightarrow [M+nH]^{(n-1)-} + He \longrightarrow \text{Fragments}$$
- CTD can be applied to both positive and negative ions, unlike commercial ETD setups limited to positive ions.
- Unlike ETD, no need to generate multiply-charged positive ions.
- The fragmentation of these radical ions lead to very informative spectra, and to structural information complementary to collision induced dissociation (CID), as shown for proteins [2] and polysaccharides [3].
- Generally, numerous fragment ions of low abundance.
- 2 CTD setups in France (see also BIBS platform, INRAE Nantes)

Instrumental modification

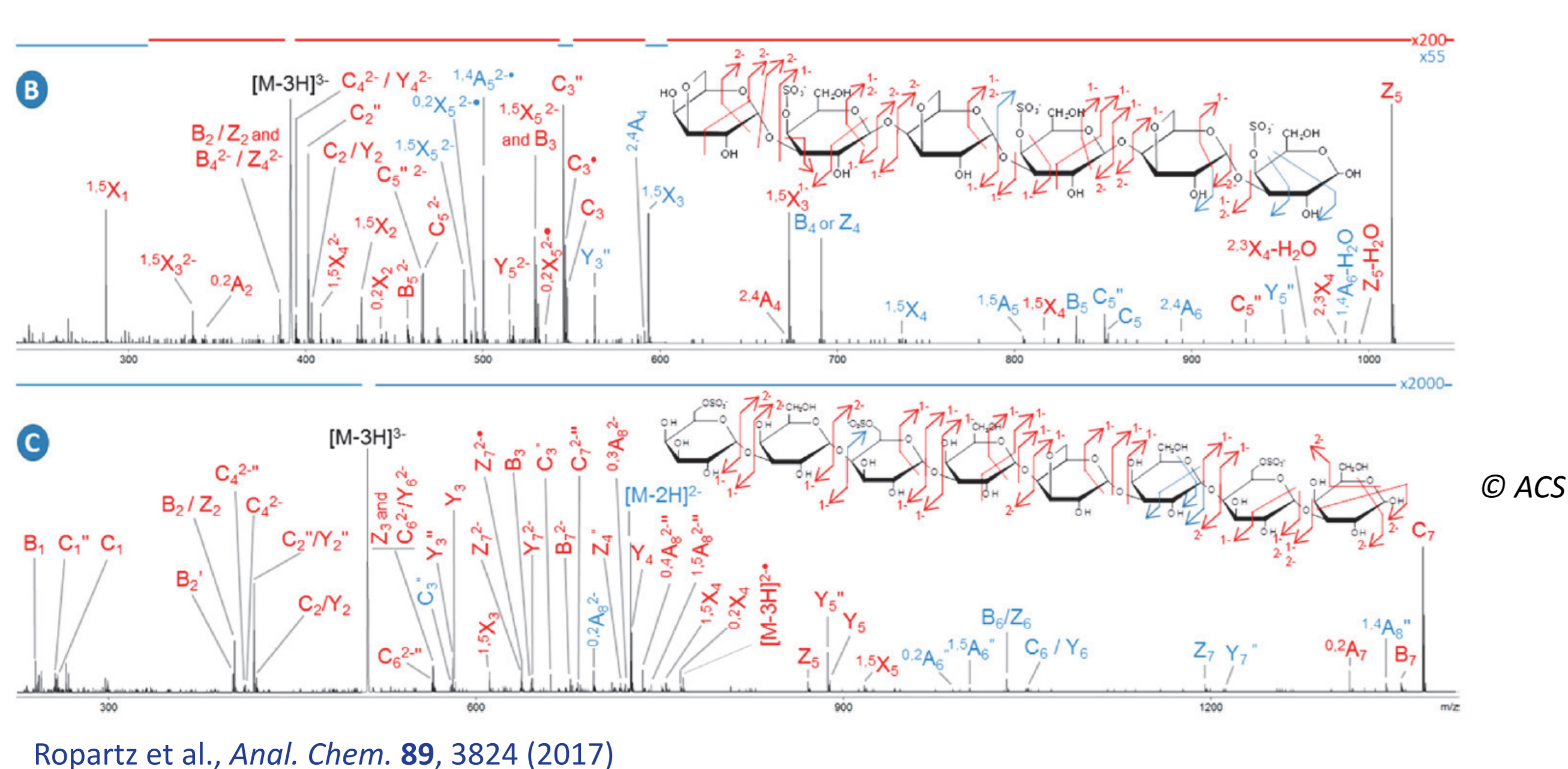


Examples

- CTD of sodiated saccharides : precursor ion : $[M+Na]^+ \rightarrow [M+Na]^{2+}$.

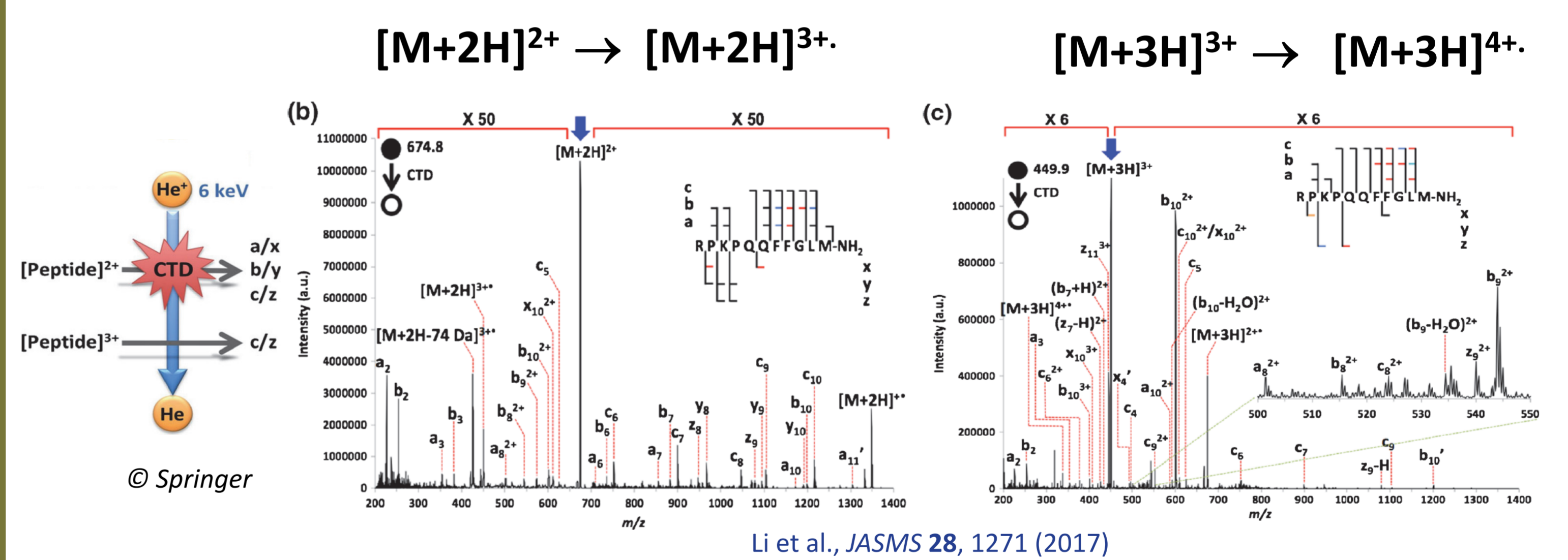


- CTD of sulfated polysaccharides : precursor ion : $[M-3H]^{3-} \rightarrow [M-3H]^{2-}$.

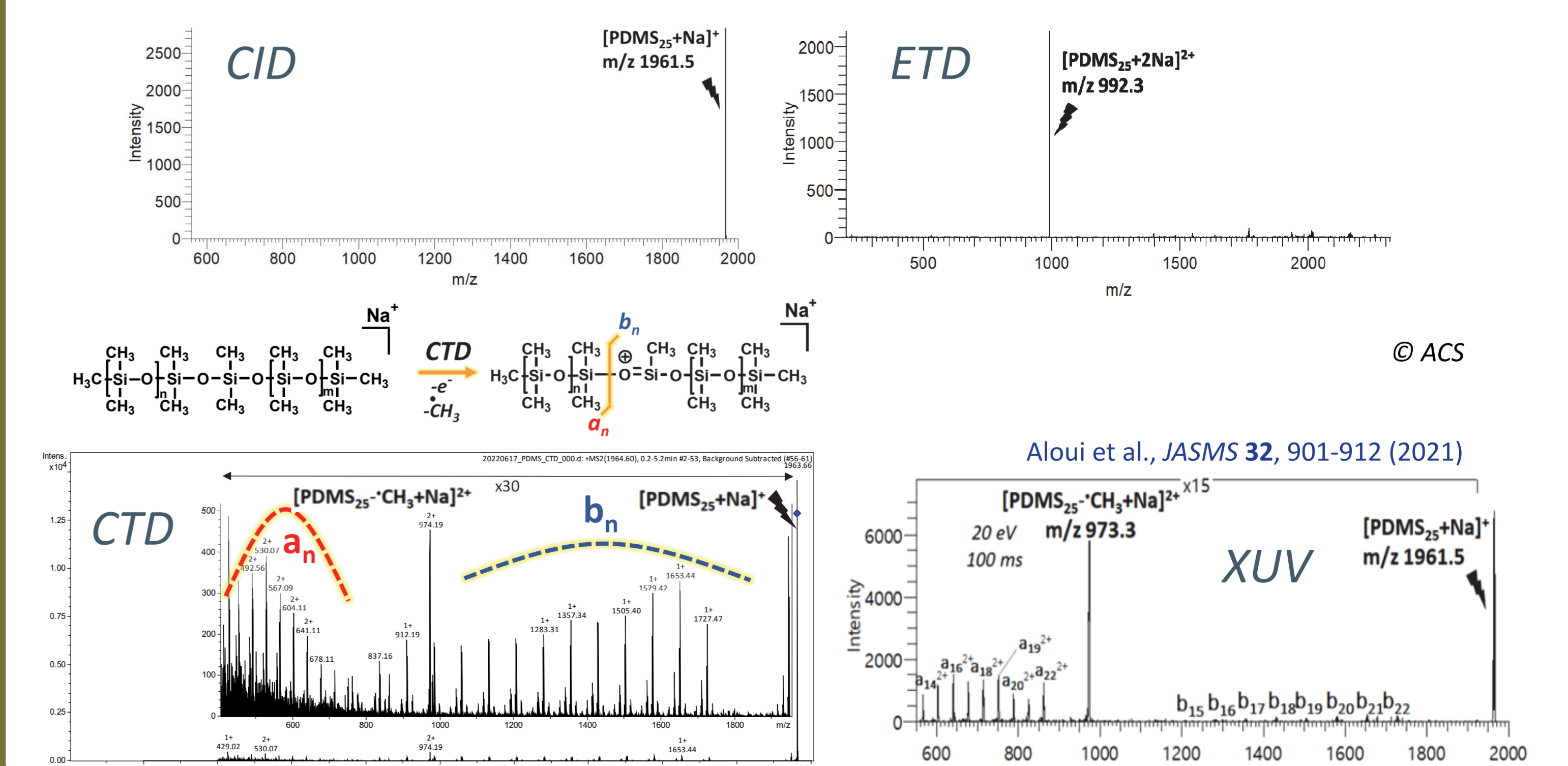


Examples

- CTD of peptides (substance P)



- CTD of synthetic polymers



References

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- Ropartz D., Li P., Jackson GP., Rogniaux H. *Anal. Chem.* 89, 3824-3828 (2017).



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