

Combined use of Ion Mobility and Collision-Induced Dissociation to investigate the opening of disulfide bridges by Electron-Transfer Dissociation in peptides bearing two disulfide bonds

Philippe Massonnet(1), Gregory Upert(2), Nicolas Smargiasso(1), Nicolas Gilles(2), Loïc Quinton(1), Edwin De Pauw(1).*

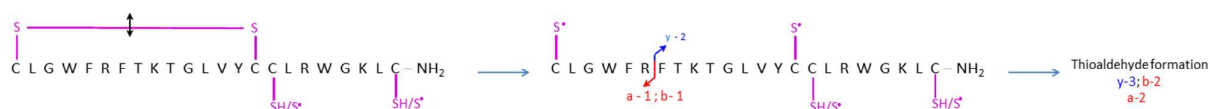
1. Laboratory of Mass Spectrometry-GIGA-R, University of Liege, Allée de la Chimie 3, B-4000 Liege, Belgium
2. Commissariat à l'Energie Atomique, DSV/iBiTec – S/SIMOPRO, F91191 Gif-sur-Yvette, France.

AUTHOR EMAIL ADDRESS: e.depauw@ulg.ac.be

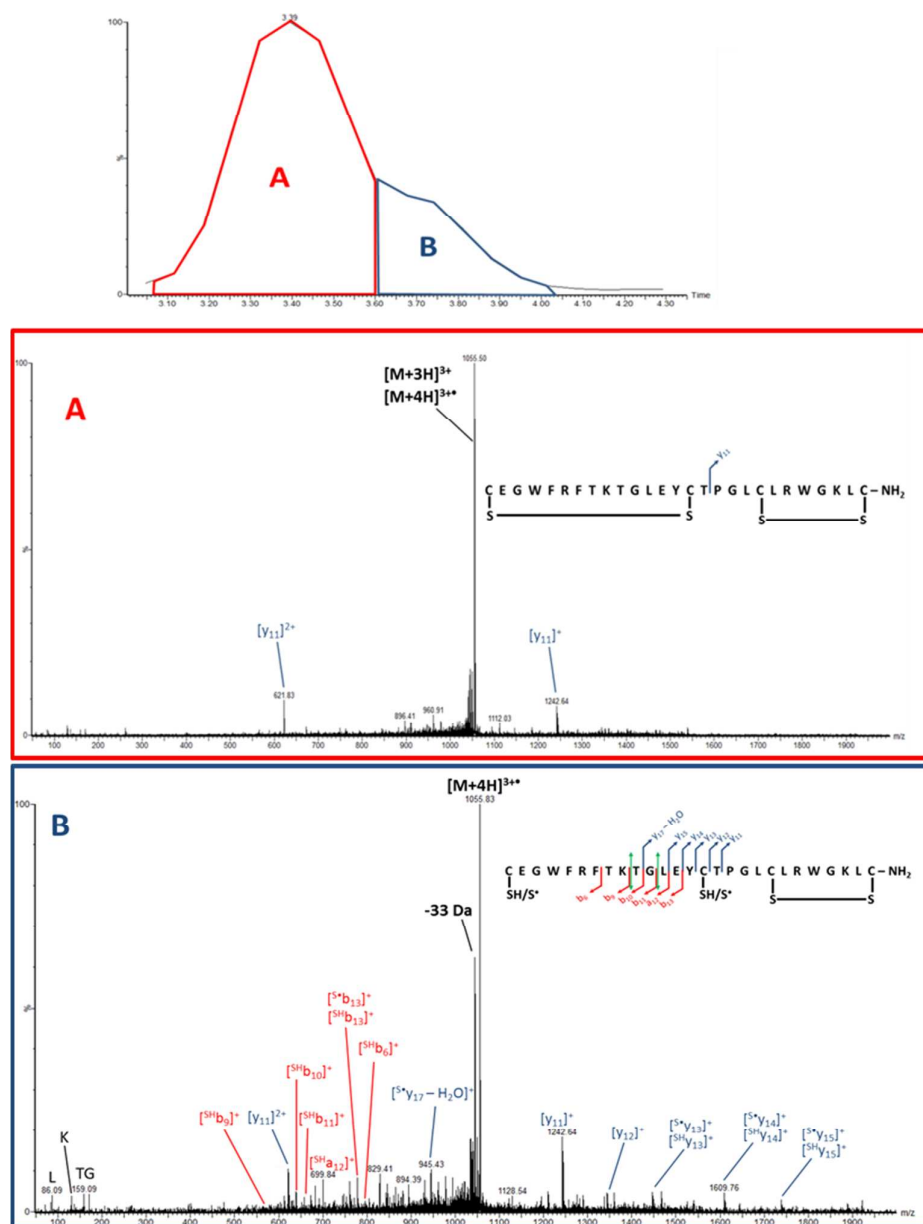
SUPPORTING INFORMATION

SI 1)	Fragmentation pathways involved when CID is performed on a disulfide bond
SI 2)	CID spectra of the ion mobility-separated species (45V CID) for the peptide 2. The ATD of the reduced species (3+ charge state) is presented in the upper . The corresponding CID-spectra are under.
SI 3)	ATD contributions of the peaks presented in the figure 6 (for the peptide 2).
SI 4)	CID spectra of the ion mobility-separated species (45V CID) for the peptide 3. The ATD of the reduced species (3+ charge state) is presented in the upper . The corresponding CID-spectra are under.
SI 5)	ATD contributions of some peaks of the figure 6 (for peptide 3). The -33 Da fragment corresponds to the dehydroalanine generation.
SI 6)	CID spectrum (CID 45V) of the ion mobility-isolated species for the peptide 4.

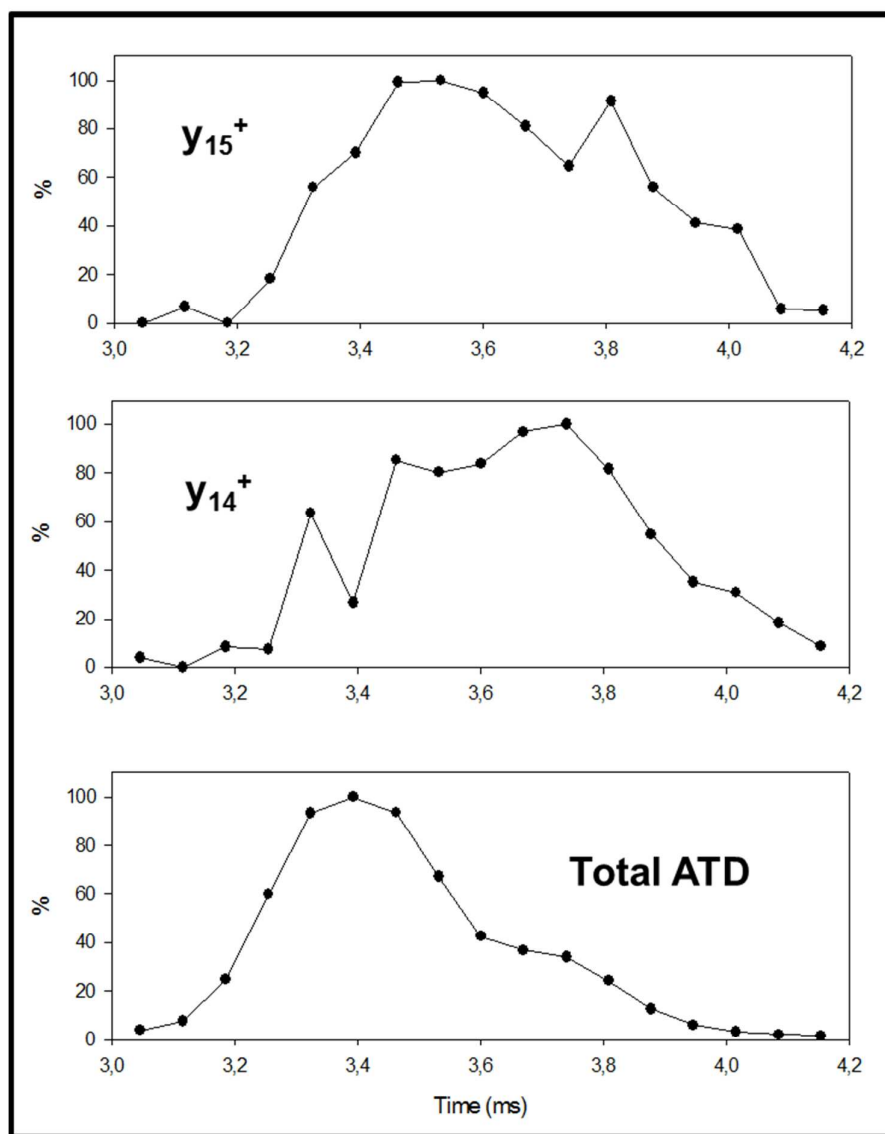
SI 1) : Fragmentation pathways involved when CID is performed on a disulfide bond



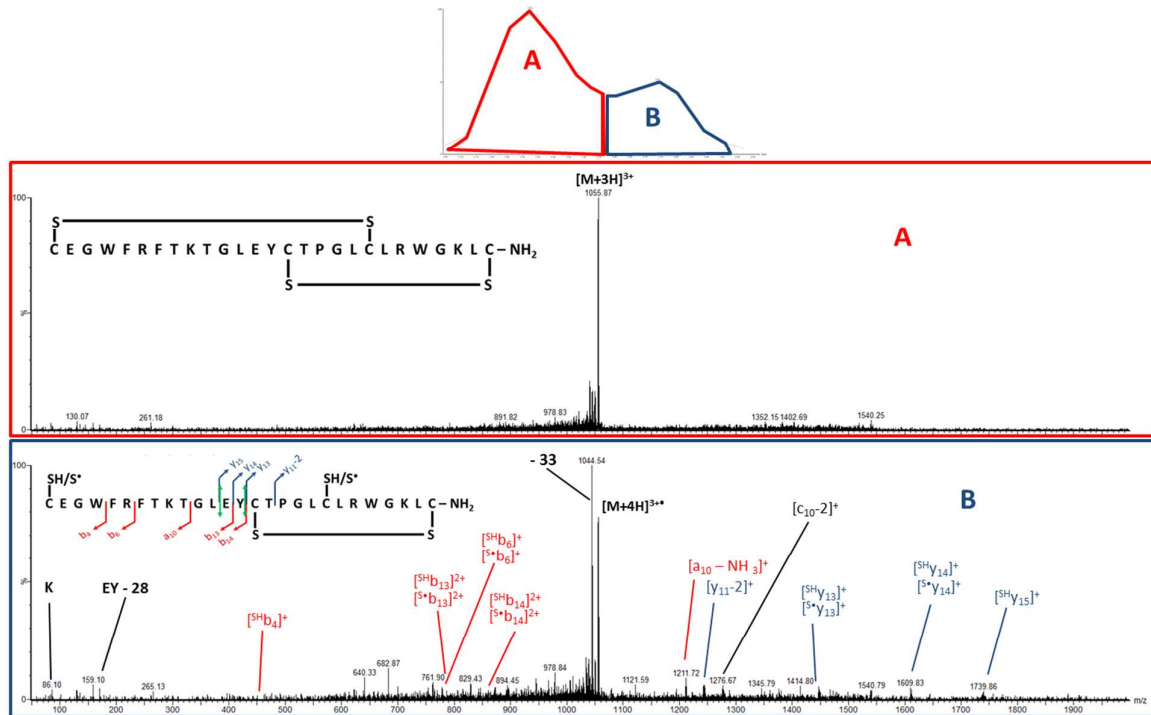
SI 2) : CID spectra of the ion mobility-separated species (45V CID) for the peptide 2. The ATD of the reduced species (3+ charge state) is presented in the upper . The corresponding CID-spectra are under.



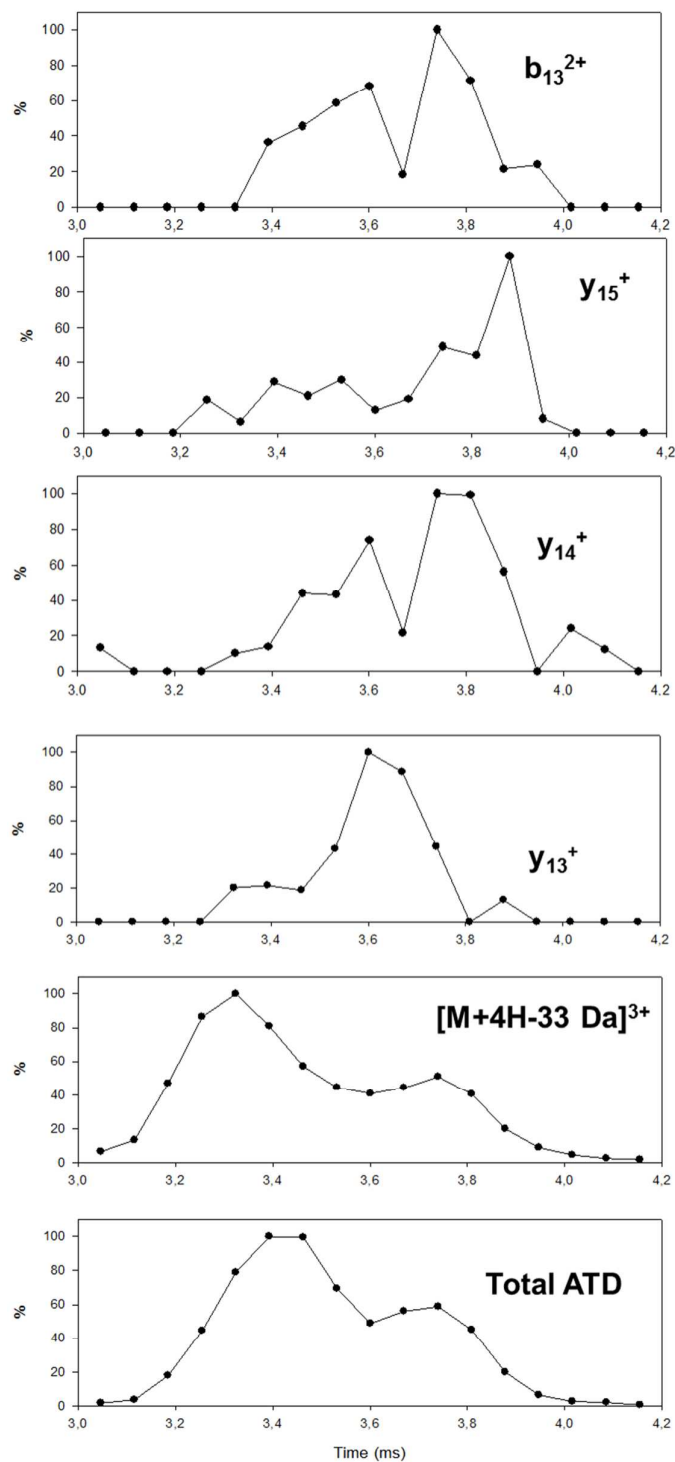
SI 3) : ATD contributions of the peaks presented in the figure 7 (for the peptide 2).



SI 4) : CID spectra of the ion mobility-separated species (45V CID) for the peptide 3. The ATD of the reduced species (3+ charge state) is presented in the upper . The corresponding CID-spectra are under.



SI 5) : ATD contributions of some peaks of the figure 7 (for peptide 3). The -33 Da fragment corresponds to the dehydroalanine generation.



SI 6) : CID spectrum (CID 45V) of the ion mobility-isolated species for the peptide 4.

