ETD ON SMALL INTACT PROTEINS IN AN ULTRA HIGH RESOLUTION QUADRUPOLE TOF MASS SPECTROMETER

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The Bruker maXisTM is equipped with a nCI-source and a hexapolar ETD reaction cell. ETD Reagent anion and analyte ions were mass selectively transmitted through a mass resolving quadrupole. ETD reactions are performed in the reaction cell following the quadrupole, where the ions of different polarity are mutually stored. The ETD experiment (performed in trapping mode) consists of four steps: cation accumulation, anion accumulation, extension of the ETD reaction and finally the detection of the product ions in the orthogonal TOF. While ions are extracted, the next ETD experiment is performed in the reaction cell thus maximizing duty cycle.

During the ETD reaction already small intact proteins with a molecular weight below 10 kDa dissociate into more than 100 fragment ions. Taking into account that every ETD fragment ion occurs with its isotopic distribution, and most of them show up in several charge states, very complex ETD MS/MS spectra are obtained.

The algorithm SNAP II reduce the complexity of ETD MS/MS data taking full advantage from the resolution, high accuracy and dynamic range of the ESI Quadrupole TOF. The SNAP II algorithm is essential for separating overlapping isotope patterns and for unambiguous determination of the ^{12}C fragment masses needed for the DB search.