Poster T09

CRAM ALGORITHM FOR HIGH RESOLUTION ESI FT-MS ANALYSIS OF BIOPOLYMERS

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Electrospray ionisation (ESI) in combination with Fourier transform mass spectrometry (FT-MS) is routinely applied for accurate mass determination of biopolymers. The high mass resolution capability of ion cyclotron resonance (ICR) mass spectrometers resolves multiply charged ions according to their isotopic composition. In order to obtain a mass accuracy in the part-per-million (ppm) range, both the accurate determination of the ion charge (z) and the correct assignment of an ion's isotopic composition are required. We have developed the charge ratio analysis method (CRAM) for high resolution ESI FT-MS analysis of biopolymers [1, 2]. The unique feature of the CRAM in processing the FT-MS data is that the charge states of ions are identified from analysis of the ratios of *m/z* values of isotopic peaks of different multiply charged ions. The CRAM process also correlates the isotopic peaks of different multiply charged ions that share the same isotopic compositions.

The CRAM algorithm has been implemented using the perl programming language for flexibility, in combination with unix command line utilities for efficient sorting and stream editing. The program accepts as input a comma separated file containing the *m/z* and peak intensities. The program approaches the analysis by first populating the space of all possible solutions and to then efficiently identify physically realistic solutions within that space. The solution space is four-dimensional since each pair of spectral peaks (i and j) is combined with candidate charge values (k and l). CRAM analysis dictates that the value for Δi/j-k/l will be zero when the charges for i and j are assigned the correct values k and l. The peak sets are correlated by additional adjacency conditions and displayed in increasing Δi/j-k/l values. Here we present the CRAM algorithm for processing of high resolution ESI FT-MS data of several proteins as well as protein mixtures.

References:

1. Maleknia SD, Downard KM (2005) Charge ratio analysis method: approach for the deconvolution of electrospary mass spectra. *Anal. Chem.* 77, 111 – 119.

2. Maleknia SD, Downard KM (2005) Charge ratio analysis method to interpret high resolution electrospray Fourier transform ion cyclotron resonance mass spectra. *Int. J. Mass Spectrom.* 246, 1 - 9.