

CHARGE RATIO ANALYSIS METHOD (CRAM): A NEW APPROACH TO INTERPRET ESI MASS SPECTRA

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Electrospray ionization mass spectrometry (ESI-MS) has revolutionized the analysis of biopolymers directly from solution and is easily coupled to chromatographic separation techniques. A unique feature of the ionization process is the production of a distribution of multiply charged ions over a limited m/z range. A fundamental step in the interpretation of ESI mass spectra involves a deconvolution process to calculate molecular weights from the m/z values of multiply charged ions. For mass spectra recorded on instruments at relatively low to moderate mass resolution, deconvolution algorithms first calculate the charge states of the ions and subsequently the molecular weight of the compound. These algorithms work by assuming that adjacent ions of a distribution differ by one charge integer and that all ions of the distribution support the same charge carrying species.

A new method to interpret electrospray mass spectral data known as the charge ratio analysis method (CRAM) is described based on calculating the ratio of mass-to-charge (m/z) values of multiply charged ions. In contrast to existing deconvolution processes, the charge ratio analysis method (CRAM), identifies the charge states of multiply charged ions without any prior knowledge of the nature of the charge carrying species. In the case of high resolution electrospray mass spectral data, where multiply charged ions are resolved to their isotopic components, the CRAM is capable of measuring the charge of the ions with high precision and can identify the peaks of different multiply charged ion clusters that share a common isotopic composition.

The basis and application of the charge ratio analysis method will be illustrated for electrospray mass spectral data of a series of proteins recorded at modest to high mass resolution on quadrupole ion-trap and Fourier transform ion cyclotron resonance mass spectrometers.

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