Accurate Mass as a Bioinformatic Parameter in data-to-knowledge conversion: FT ICR for peptide de novo sequencing

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With the availability of ultra-precise mass spectrometric biomolecular data, the accurate mass is becoming a physical quantity of high interest for bioinformatics tools and strategies. Fourier transform ion cyclotron resonance mass spectrometry with electrospray ionization or matrix-assisted laser desorption/ionization sources now allows the easy determination of amino acid composition of medium size, unknown peptides when employing combinatorial calculation of hypothetical parent and fragment ion masses. This new method, which in a second step, allows the reliable de-novo sequencing of completely unknown peptides [“composition-based sequencing (CBS)”] appears to open a wide new field of bioanalytical investigation. It has been shown that even unspecifically cleaved proteins can be identified easily and reliably when accurate mass evaluation is combined with protein database search tools. It is quite clear that, while the nominal mass of a peptide has obviously no useful correlation to biomolecular structure, the accurate mass, instead, has a strong and direct correlation to structure that so far has not been exploited considerably by bioinformatic tools. It has already become obvious that accurate mass evaluation is going to become a central goal for bioinformatics strategies in the near future. Strategies for extracting structural, and even functional, information out of accurate mass values of biomolecules still have to be developed. Examples and prospects of accurate mass evaluation in bioinformatics for the field of proteomics are outlined in the following.

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