Measurement of Protein Molecular Weight using MALDI MS

In MALDI MS measurements, the dominant ion signal corresponds to the protonated molecule, denoted $[M + H]^+$. In spectra taken from larger proteins, higher charge states and cluster ions may also be observed, e.g., $[M + 2H]^{2+}$, $[M + 3H]^{3+}$, or $[2M + H]^+$ (the protein dimer).

To calculate the molecular weight, the mass of a proton (1.0079 Da) is subtracted from the measured m/z value. The other ion signals can be used to verify this measurement.

Measurement of Protein Molecular Weight using ESI MS

In ESI MS measurements, a large number of ion signals are observed which correspond to different charge states of the intact protein molecule; these are denoted [M + nH]n+ where n is the net charge. The total charge on the protein is determined by the number of ionizable residues (basic residues such as arginine, lysine, and histidine in positive ion mode or acidic residues such as aspartic and glutamic acid in negative ion mode). For most proteins, the predominant ion signals are observed between m/z 500 and m/z 2000, independent of the molecular weight of the protein.

To calculate the molecular weight of the protein, the measured m/z value of charge state, n, is multiplied by n and then n protons (n * 1.0079) are subtracted to give the measured molecular weight.

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