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Mass Spectrometry & Purification Techniques

Commentary

Advantages and Fragmentation in Tandem Mass Spectrometry

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DESCRIPTION

Tandem mass spectrometry sometimes referred to as MS/MS or MS2, includes a number of mass spectrometry selection steps with some sort of fragmentation taking place in between. Mass spectrometry is a potent tool for chemical analysis that can be used to pinpoint unknown substances, measure known substances, and analyize molecular structure. In order to comprehend how it works, it is established that a mass spectrometer is a "molecule smasher" that calculates the molecular and atomic masses of complete molecules, molecular fragments, and atoms through the production and detection of gas phase ions that are separated based on their mass-to-charge ratio (m/z). It measures masses that are in accordance with the atomic makeup and molecular structure of the parent molecule, enabling the determination and clarification of the molecular structure.

A biomolecule is extracted from a biological sample using tandem mass spectrometry, and its composition and sequence are identified by fragmenting it into various subunits. By connecting mass spectrometers in series, this is accomplished. In the first spectrometer, a sample is ionised and filtered for ions with a particular mass to charge ratio. Ions that have been filtered are then broken up and sent to a second mass spectrometer for analysis.

Structure

The triple quadrupole mass spectrometer (QqQ), multi-sector mass spectrometer, Quadrupole-Time Of Flight (Q-TOF), and hybrid mass spectrometer are all examples of tandem mass spectrometry.

Triple quadrupole mass spectrometer: The first and third quadrupoles are used as mass filters in triple quadrupole mass spectrometers. Analytes that pass the second quadrupole begin to fracture when they collide with gas.

Quadrupole-Time Of Flight (Q-TOF): Quadrupole-Time Of Flight (Q-TOF): Q-TOF mass spectrometer combines quadrupole and TOF instruments, resulting in excellent mass accuracy for product ions, accurate quantitation capability, and application for fragmentation experiments. This mass spectrometry technique uses a time-of-flight measurement to calculate the ion fragmentation (m/z) ratio.

Hybrid mass spectrometer: A hybrid mass spectrometer has several mass analyzers.

Advantages

The advantage of tandem MS over single stage mass analysis is the significantly higher level of analytical specificity. For instance, 25-hydroxy vitamin D3 undergoes ESI and generates a major M+H+ ion with a 400 m/z mass that loses water during collision-induced dissociation to generate a significant product ion with a 384 m/z mass. If the first and third quadrupoles are configured to transmit ions of just 400 and 384 m/z, respectively, 25-hydroxy vitamin D3 can be detected with high specificity. Single reaction monitoring is the method, and the fragmentation is identified as 400>384. Only those analytes that have this precursor/product ion pairing will be picked up. There may be more components in a complex biological sample that, when subjected to ESI, create a 400 m/z precursor ion, but there is a low likelihood that they will also fragment into a 384 m/z product ion.

Fragmentation in tandem mass spectrometry

In-source fragmentation: Metastable fragmentation is the process that occurs when the product ions remain in their non-equilibrium state for a reasonable amount of time prior to auto-dissociation. Nozzle-skimmer fragmentation is the deliberate induction of in-source fragmentation on typically electrospray based instruments by raising the nozzle-skimmer potential. Unless metastable ions are mass assessed or chosen prior to auto-dissociation and a second stage of analysis is carried out on the resultant fragment, it is not technically tandem mass spectrometry.

Post-source fragmentation: In addition to post-source collisions with neutral atoms or molecules, radiation absorption, or the transfer or capture of an electron by a multiply charged ion, energy can also be added to the ions, which are typically already vibrationally excited. The collision of an ion with a neutral atom

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or molecule in the gas phase, followed by the ion's subsequent dissociation, is known as Collision-Induced Dissociation (CID), also known as Collisionally Activated Dissociation (CAD).

Peptide fragmentation: A peptide can be located in a protein database using a tandem mass spectrometry-derived peptide sequence tag. For the purpose of identifying peptide fragments that result from a tandem mass spectrum, a notation has been created. If the charge is kept on the N-terminus, the peptide fragment ions are denoted by the letters a, b, or c; if it is kept on the C-terminus, the letters x, y, or z. The subscript gives the number of fragmented amino acid residues fragmentation of a peptide.