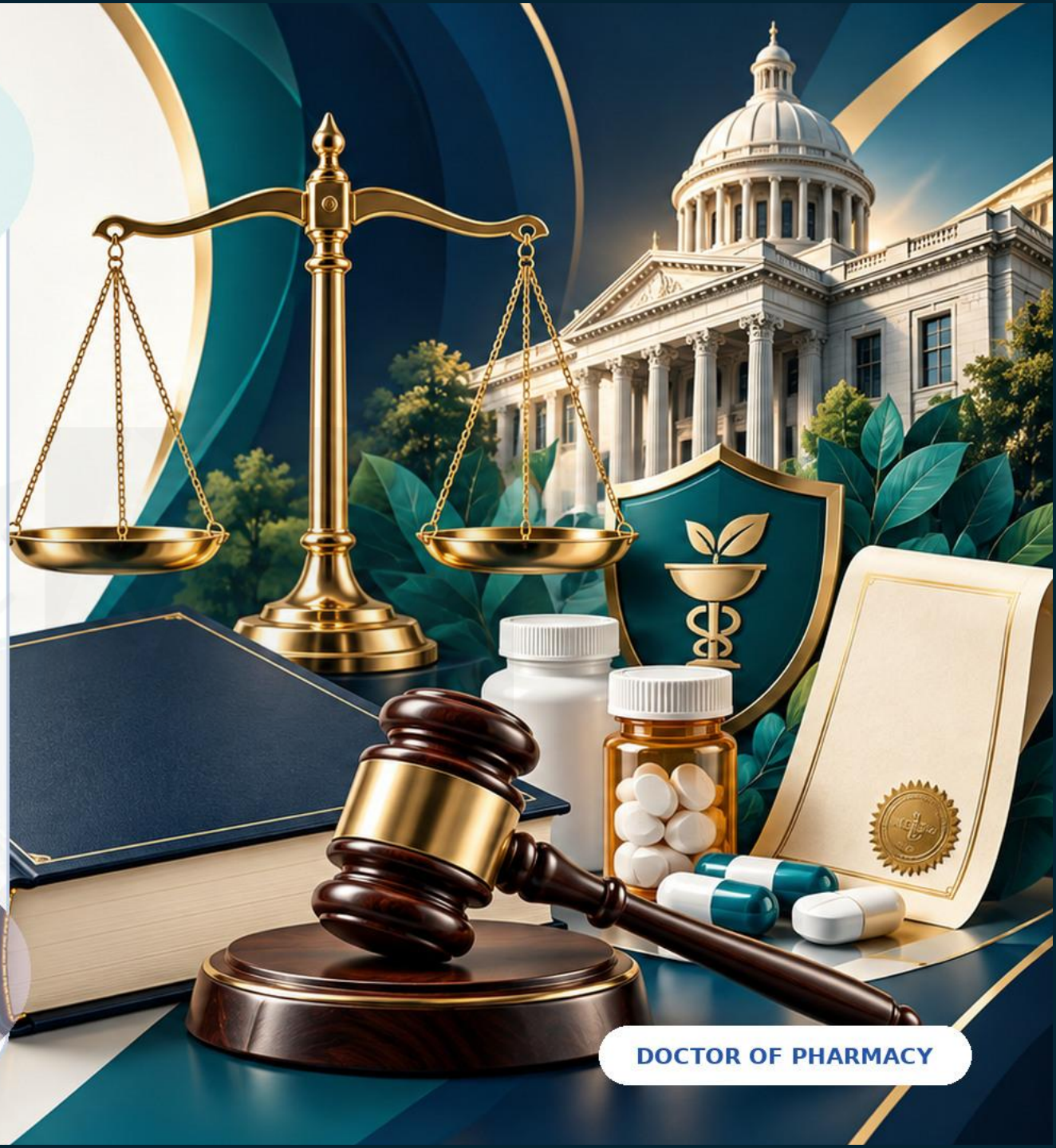
PHARM.D • YEAR 3

Pharmaceutical Analysis

CHAPTER 4.8

Mass Spectrometry

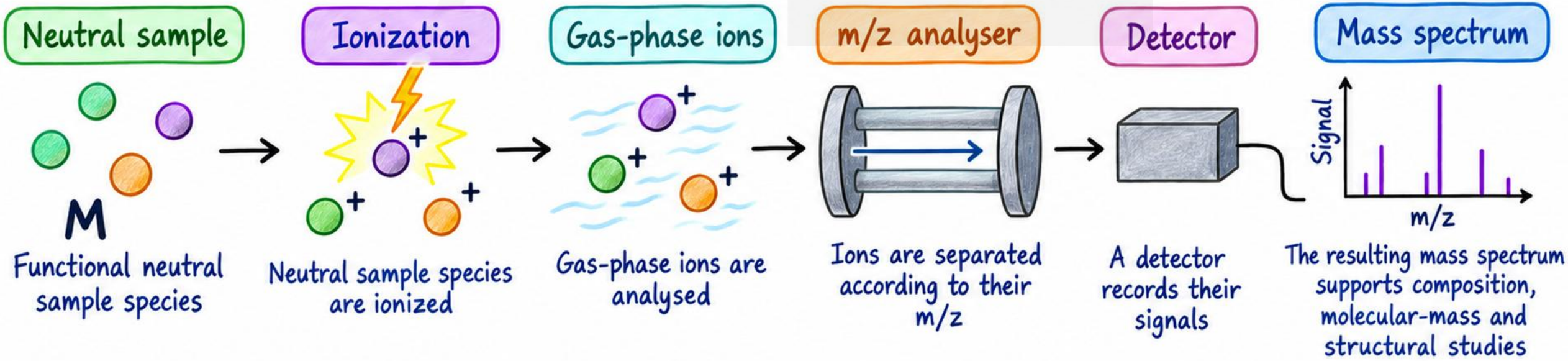
PPT CHAPTER COVER



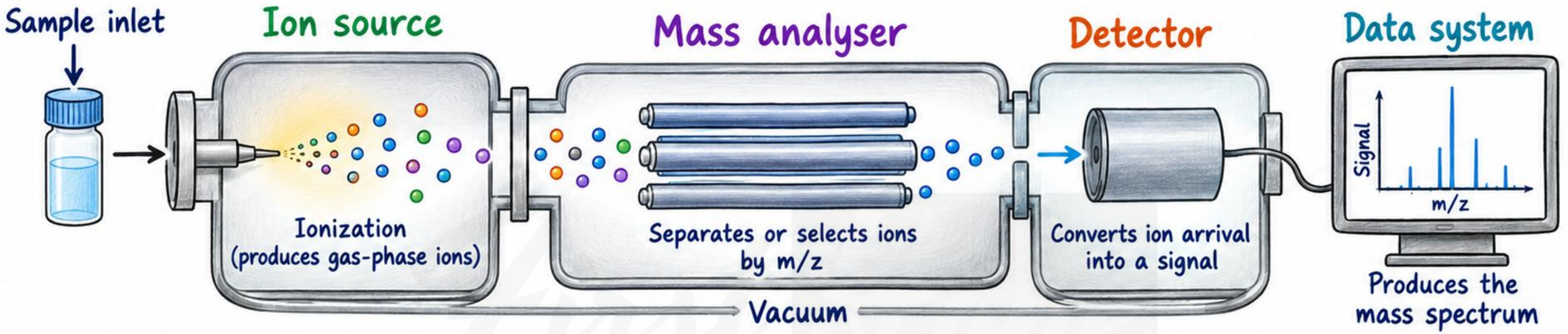
DOCTOR OF PHARMACY

MASS SPECTROMETRY: MEASURING IONS

- Mass spectrometry measures ions according to their mass-to-charge ratio, m/z.
- Neutral sample species are ionized, gas-phase ions are analysed and a detector records their signals.
- The resulting mass spectrum supports composition, molecular-mass and structural studies.
- MS does not directly detect neutral molecules.
- Although commonly grouped with spectroscopy in teaching, its core measurement is ion m/z rather than absorption or emission of optical radiation.



THE MASS-SPECTROMETER WORKFLOW

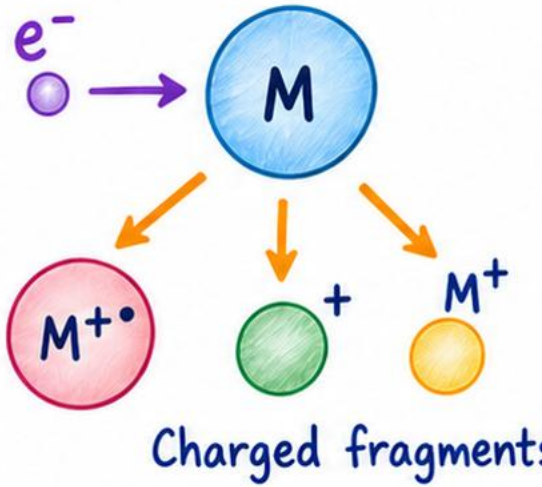


- Ionization creates gas-phase ions from a suitable introduced sample.
- The mass analyser separates or selects ions by m/z, and the detector converts ion arrival into a signal. A data system produces the mass spectrum.
- Ionization method, analyser performance and sample preparation determine what ions are observed.
- Mixtures may require chromatographic separation before MS.
- Detector response is not automatically identical for different compounds or all ionization conditions.

HARD AND SOFT IONIZATION

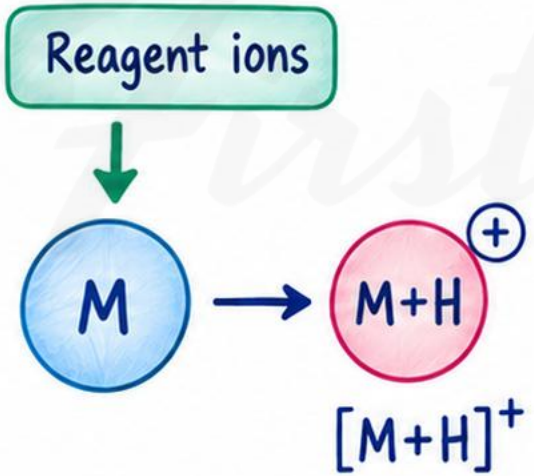
Electron ionization (EI)

commonly produces a radical cation $M^{+\bullet}$ and often extensive fragmentation.



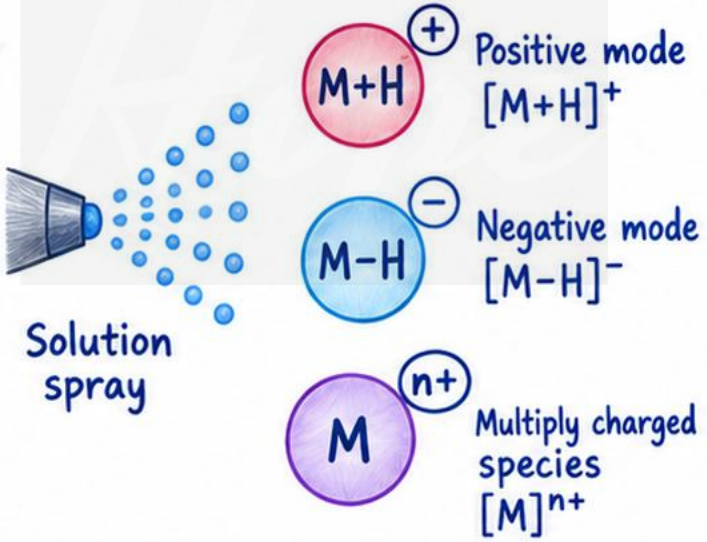
Chemical ionization (CI)

can give gentler ion formation through reagent-ion chemistry.



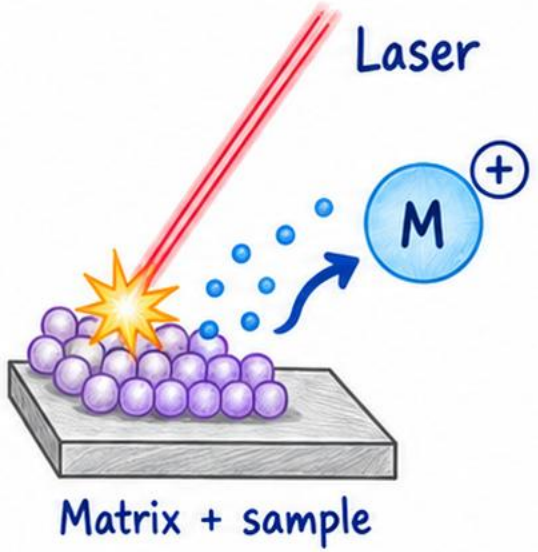
Electrospray ionization (ESI)

generates ions from solution and often produces protonated, deprotonated or multiply charged species.



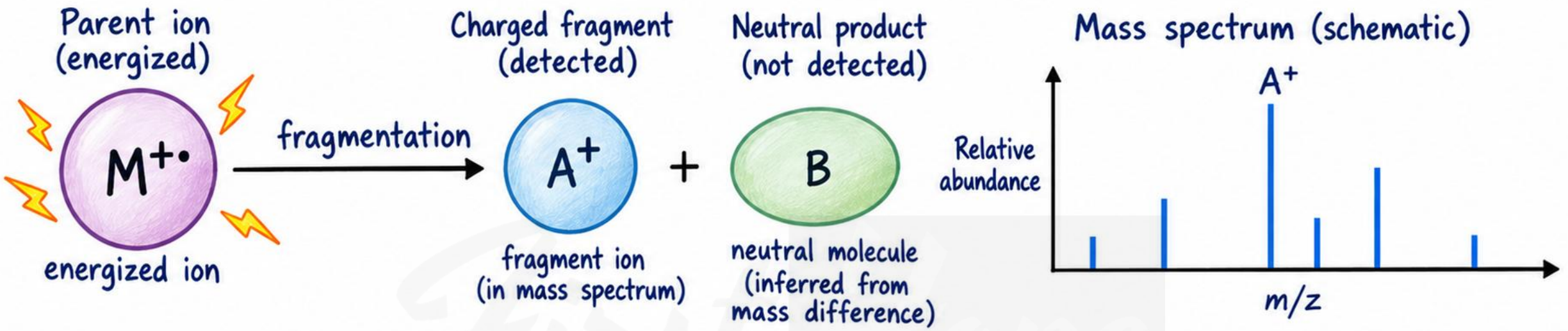
MALDI

uses a matrix and laser to generate ions from a prepared sample.



Choose the method for sample properties and required information; soft ionization does not mean absolutely no fragmentation.

WHY FRAGMENT IONS ARE USEFUL



1. Structural clues

- An energized ion can break into charged fragments and neutral products.
- Fragment-ion masses and abundance patterns provide structural clues and support library comparison.

2. Neutral products

- Neutral products are usually inferred from mass differences, not directly detected in an ordinary mass spectrum.

3. Important considerations

- The pattern depends on ionization and conditions; it is not guaranteed to be unique for every isomer.
- Combine fragmentation with precursor information and complementary evidence.

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