Massenspektrometrie

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Genral Notes

- Masse zu Ladung verhältnis wird gemessen und ein Massenspektrum erstellt
- Die zu analysierende Substanz wird ionisiert
- Verschiedene Ionisierungsmethoden (ESI, MALDI, EI, CI)
- Diese Ionen werden in einem Massenspektrometer nach ihrem m/z getrennt
- Nur die positiven Ionen werden zum Detektor geleitet, also die Kationen
- Die Anzahl an zu analysierenden Molekülen wird von den Analysator begrenzt, wegen verschiedenen Ionisierungsmethoden (https://userpage.fu-berlin.de/~springer/guide_eng.html)

Quick outline

- Motivation: why MS (sensitivity, specificity, molecular weight, structural info)
- Sample preparation (matrix effects, ion suppression, cleanup)
- Ionization methods (ESI, MALDI, EI, CI)
- Mass analyzers (TOF, Quadrupole, Orbitrap, FT-ICR)
- Tandem MS and fragmentation (MS/MS strategies)
- Data interpretation and reporting (m/z, isotopic patterns, mass accuracy)
- Common pitfalls and troubleshooting
- Take-home messages

Key concepts (short)

- m/z: mass-to-charge ratio; observed peaks indexed by charge state.
- Mass accuracy: difference between measured and theoretical mass (ppm).
- Resolving power: $R = \frac{m}{\Delta m}$ (often defined at FWHM).
- Isotopic distributions reveal elemental composition clues.

- Tandem MS provides structural information via controlled fragmentation.
- Calibration and internal standards improve quantitation and accuracy.

Ionization methods (one-line reminders)

- ESI: soft ionization, good for polar/large biomolecules, generates multiply charged ions.
- MALDI: pulsed laser, solid matrix, often singly charged, good for peptides/proteins.
- EI/CI: gas-phase small molecules, good library matching (GC-MS).

Mass analyzers (strengths / when to mention)

- TOF: high mass range, fast acquisition.
- Quadrupole: robust, good for targeted quantitation (SRM/MRM).
- Orbitrap / FT-ICR: very high resolving power and accuracy.
- Ion traps: MSn capability but limited mass range/resolution.

Tandem MS notes

- Collision-induced dissociation (CID) basics: b/y ions for peptides.
- Use MS/MS to confirm identity and reduce false positives.
- Design experiments: targeted (SRM) vs discovery (DDA/DIA).

Common pitfalls / troubleshooting

- Contamination: plasticizers, salts, detergents – degrade spectra.
- Ion suppression: co-eluting species reduce sensitivity.
- Incorrect charge assignment: check isotopic spacing.
- Over-interpretation of low S/N peaks.

Presentation tips (for slides)

- Show one clear spectrum and annotate peaks (m/z, charge, assignment).
- Use schematic diagrams for ionization and analyzer operation.
- Keep equations minimal: show m/z and resolving power only.
- Include a short example workflow (sample $\rightarrow$ prep $\rightarrow$ run $\rightarrow$ analyze).

Take-home messages

- MS answers both identity and quantity questions when used correctly.
- Instrument choice depends on the question: high resolution vs robustness.
- Good sample prep and controls often matter more than marginal instrument upgrades.