

Mass Spectrometry Instruments and Methods offered in the MS-Plattform of the Department of Chemistry

PD Dr. M. Schäfer

Operators: CTA Astrid Baum, CTA Michael Neihns

Instruments	Location
LTQ-Orbitrap XL	Institute of OC in Lab 318
Finnigan MAT 95	Institute of AC in Lab 212b
Thermo ISQ GC-MS	Institute of OC in Lab 317

Electron (Impact) Ionization MS (EI-MS): appropriate for small, unpolar and hence volatile compounds with low boiling points ($M < 900 \text{ g mol}^{-1}$)

Finnigan MAT 95: operated by CTA Astrid Baum

→ Direct Inlet EI-MS with variable ionization energy (70 – 15eV) – exclusively suited for clean single component samples!

→ Determination of exact ion masses with EI-MS at elevated resolution ($R < 10000$)

ISQ GC-MS with Direct Inlet Probe Option: operated by CTA Michael Neihns

→ Sample inlet via direct Inlet Probe EI-MS with fixed ionization energy (70 eV) – exclusively suited for clean single component samples!

→ Mixture analysis with GC-EI-MS; GC-Temperature programming possible up to 350°C; EI-MS spectra library NIST.

Important for the successful use of GC-MS:

→ Only compounds of low polarity and low molecular mass ($M < 900 \text{ g mol}^{-1}$) are amenable for GC-EI-MS as they are thermally vaporized.

→ Only analyte solutions of volatile organic solvents can be injected in the GC (CH_3CN , CH_2Cl_2 , CH_3OH , Hexane etc.) → No DMSO, H_2O , DMF etc.!

→ In case of dissolved samples: Specify the solvent used and pay close attention to the concentration of the solution! The sample solution supplied **must not** exceed 10^{-3} mol/l to avoid column overload and detector saturation/damage.

Electrospray-MS (ESI-MS): ESI-MS is in principle appropriate for the analysis of small and unpolar as well as for the analysis of large and polar compounds; however, the more polar the analyte is, the better. Analyte solutions are introduced into the MS instrument → Insoluble compounds can not be measured! Please submit dry samples and do not forget to name appropriate solvents for your analyte.

LTQ-Orbitrap XL: operated by CTA Michael Neihns, (M. Schäfer)

→ Single step electrospray-MS (ESI-MS) at routine (low) resolution in the linear ion trap LTQ or determination of exact ion masses in the orbitrap at elevated resolution ($R \geq 30000$).

→ Tandem-MS Experiments: Electrospray-MSⁿ in the linear ion trap LTQ; exact ion masses of precursor- and product ions can be determined in the orbitrap.

Matrix Assisted Laser Desorption-MS (MALDI-MS)

MALDI-MS measurements are possible at an **AB Voyager STR MALDI-MS** (Institute of OC); the instrument is operated by co-workers of Professor Reinhard Predel (Institute of Zoology).

Please pick up a MS-analysis form and provide all pieces of information on the compounds you want to analyze:

- Structural and elemental formula, appropriate solvent, demanded measurements, etc.
- Please provide only weighted samples in range of 1-3 mg!

In case you are not sure how to process the analysis or which ionization technique to choose: Please ask! We are happy to assist you!

You find us in the Institute of Organic Chemistry, Labs 316-318, green floor

PD Dr. Mathias Schäfer