General aspects of mass spectrometry

Overview of the basic theory and main features of mass spectrometry

Assoc. prof. Koit Herodes

Mass spectrometry

Mass spectrometry (MS) is an analytical technique for qualitative and quantitative analysis of compounds.

It is based on the separation of the components according to their **mass-to-charge (*m/z*) ratio**.

MS can be used

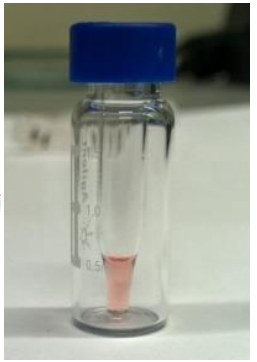
- for the analysis of gaseous, liquid, and solid samples.
- as an individual method (direct MS);
- as a detector for other methods (GC, LC, etc.);
- for isotope ratio analysis (GC-C-IRMS, EA-IRMS);

Mass spectrometry

MS is suitable for the analysis of:

- pesticides
- drugs
- doping

- proteins/peptides
- lipids
- resins
- dyes
- carbohydrates/sugars
- polymers

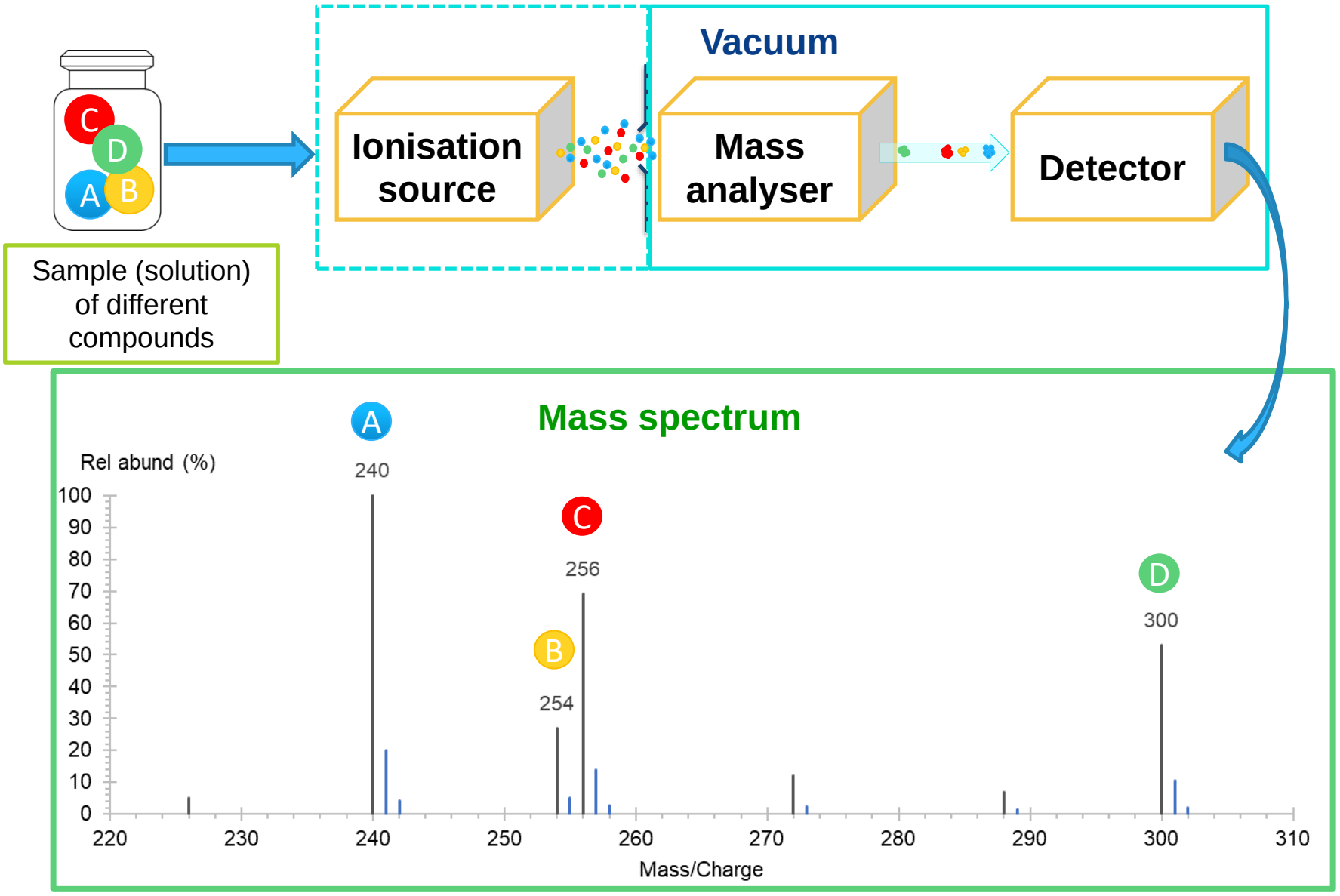


Sample solution:
LC-MS,
ESI/APCI/MALDI-FT-ICR-MS

Horse blanket
Estonian National Museum
(end of the 19th century)

Sample for MALDI-FT-ICR-MS analysis

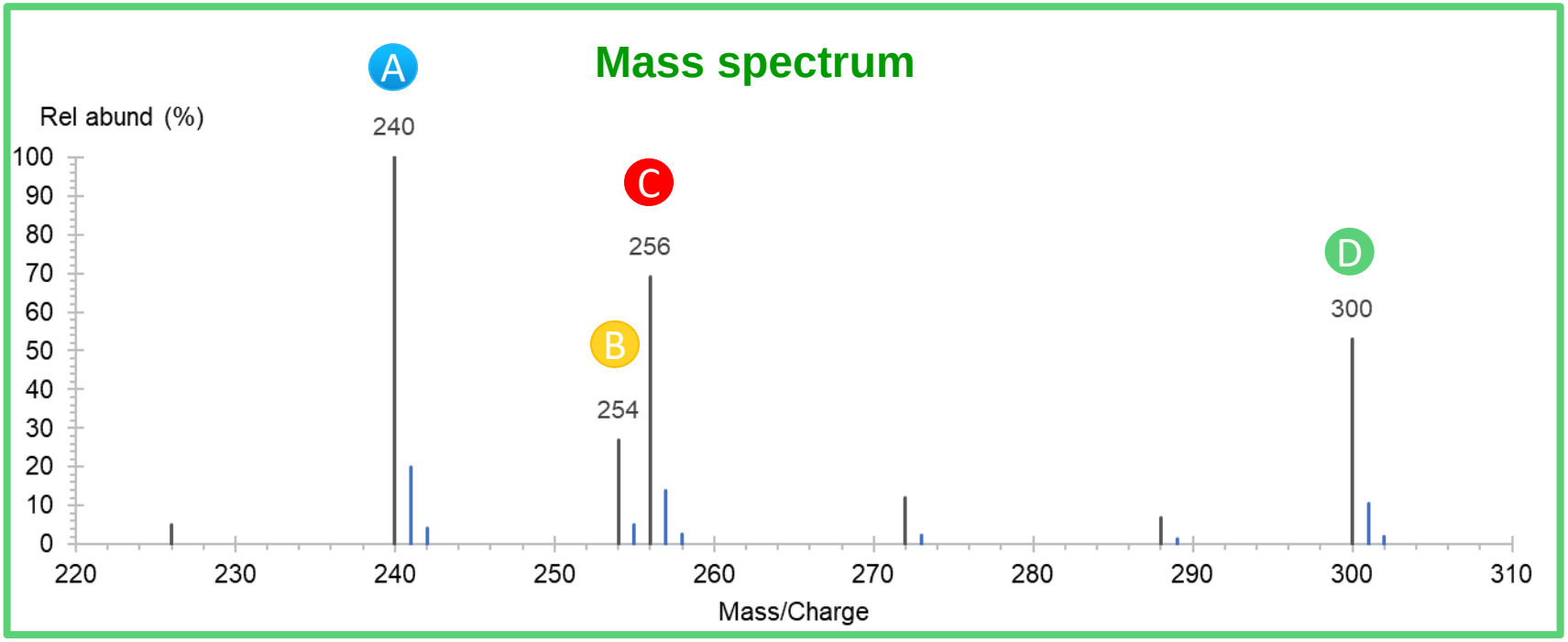
Principle of mass spectrometry



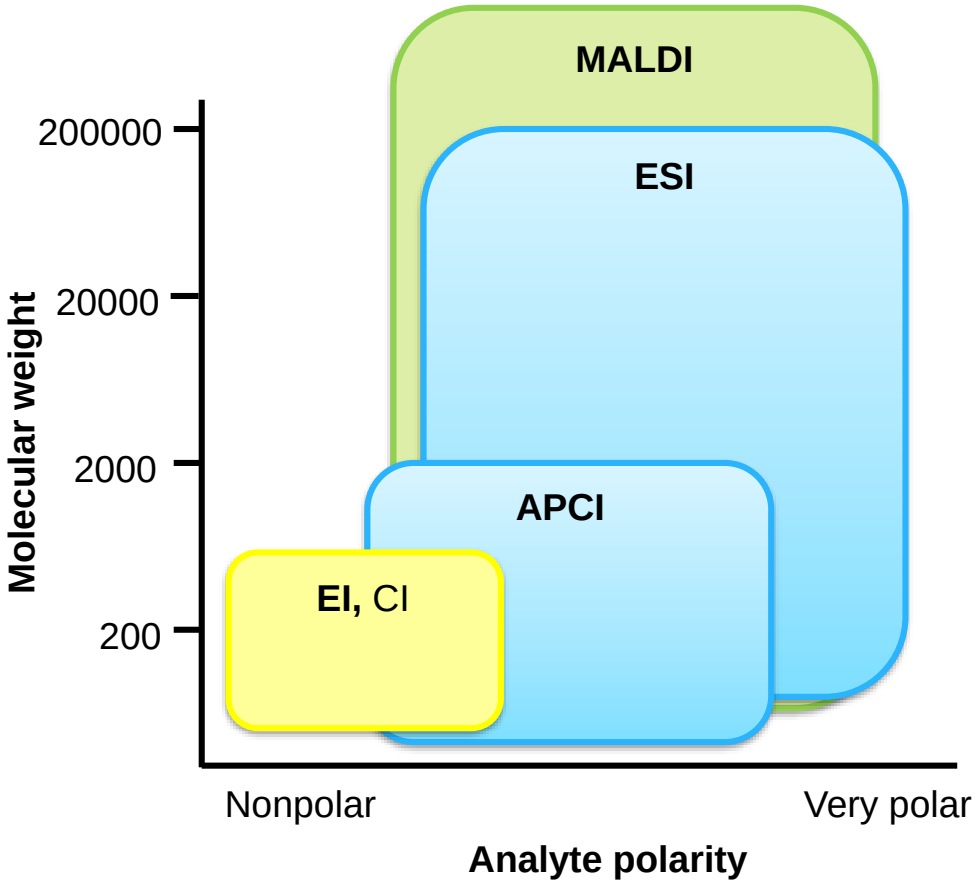
Information obtained with MS

MS provides information about

- **mass-to-charge (*m/z*) ratio – ratio of molecular mass** and **charge**, from which molecular mass of the compound can be deduced (elemental composition),
- **fragments** – information about structure,
- **isotope ratio**.



Ionisation sources



The **suitability of a ionisation source** is determined by

– **the nature of the sample:**
- the molecular mass of analyte,
- the polarity of the compounds,
- the stability of the sample,
- the solubility of the sample;

– **the type of information required**
- information about the composition
  - main components vs trace analysis
  - information about the contaminants
- information about the changes in the material
  - ageing,
  - polymerisation, etc.

* More information about the ionisation techniques and ion formation can be found in additional materials.

Mass analysers

MS techniques can be classified according to their ***m/z* resolution**

–shows how well the instrument can distinguish ions with similar *m/z* value

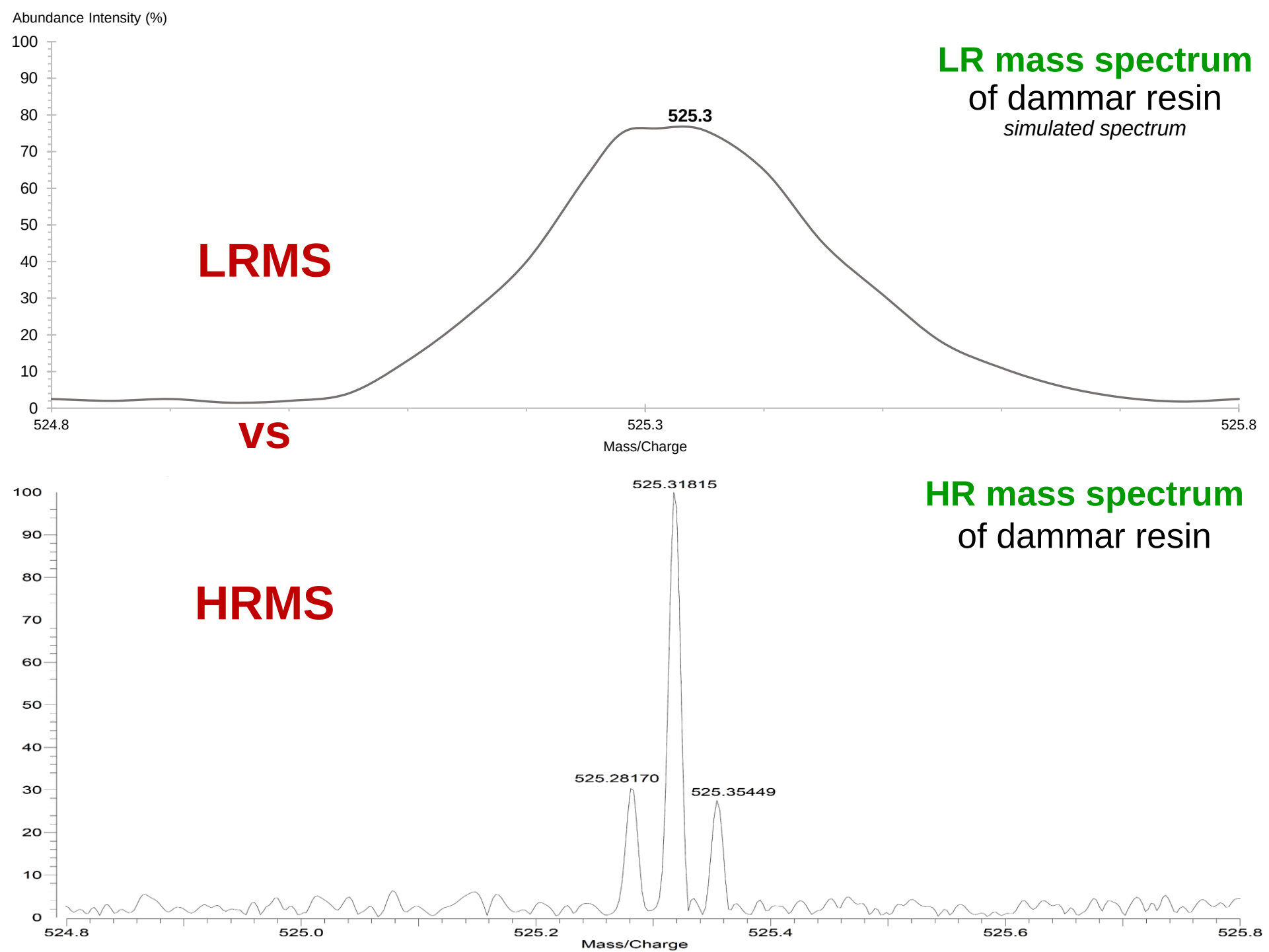
Low Resolution MS (LRMS)

- Provides unit resolution, i.e. compounds with similar *m/z* values appear as one peak in the mass spectrum.
- **Instruments:**
  - Quadrupole (Q), incl. tandem Q
  - Ion Trap (IT)
  - Time of Flight (ToF)

High Resolution MS (HRMS)

- Provides results with high *m/z* accuracy and therefore, distinguishes ions with very similar *m/z* values.
- **Instruments:**
  - FT-ICR-MS
  - Orbitrap
  - Time of Flight (ToF)

* More information about different mass analysers can be found in additional materials.


Abundance Intensity (%)
100
90
80
70
60
50
40
30
20
10
0
525.3
524.8
525.3
525.8
Mass/Charge
LR mass spectrum
of dammar resin
simulated spectrum
LRMS
vs
HRMS
525.31815
525.28170
525.35449
524.8
525.0
525.2
525.4
525.6
525.8
Mass/Charge
HR mass spectrum
of dammar resin

LRMS vs HRMS

Analysis of **dammar resin**

with **MALDI-FT-ICR-MS**

Vahur, S.; Teearu, A.; Haljasorg, T.; Burk, P.; Leito, I.; Kaljurand, I. J. Mass Spectrom, 2012, 47(3), 392 - 409.

Summary

MS – diverse and powerful group of methods suitable for the analysis of **different types of materials**.

Different **mass analysers** are compatible with various **ionisation sources**.

MS is one of the most sensitive analytical techniques – useful for **small samples** and **trace analysis**.

MS provides information about **molecular mass**, **structure**, and **isotope ratios**.