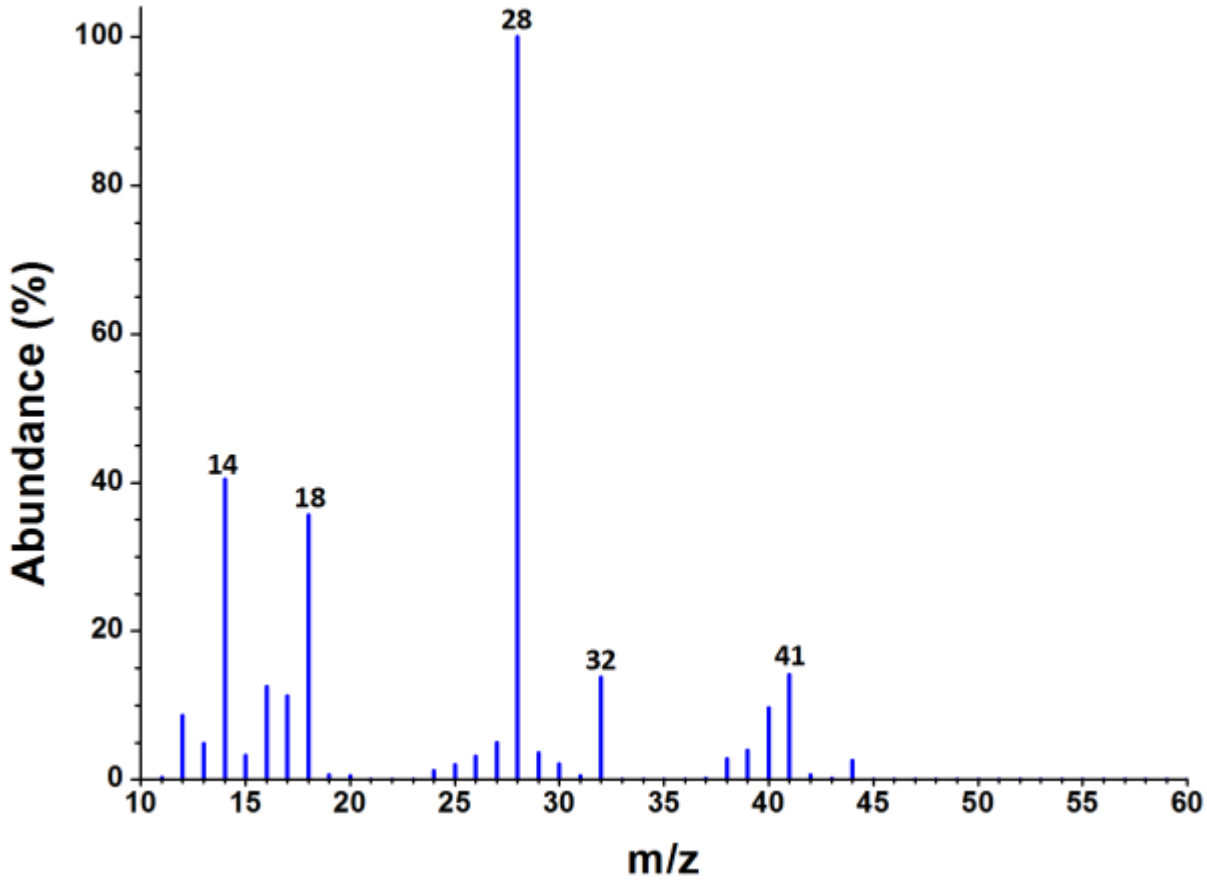
RHODES UNIVERSITY

Mass Spectrometry

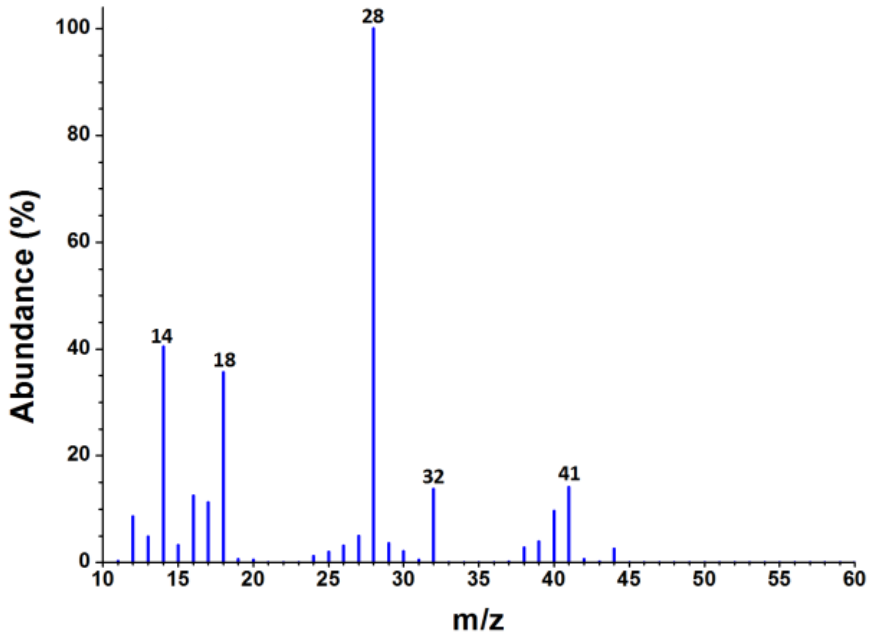


Keamogetse Tshenkeng

Mass Spectrometry

- Mass spectrometry (MS) – analytical technique in which samples are ionized into charged molecules and their ratio of mass-to-charge (m/z) is then measured

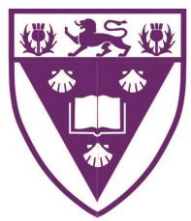
Mass spectrum → relative abundance / intensity vs mass-to-charge ratio



Q. et al., *Applied Mechanics & Materials*, **2013**, 529.

Mass Spectrometer Components

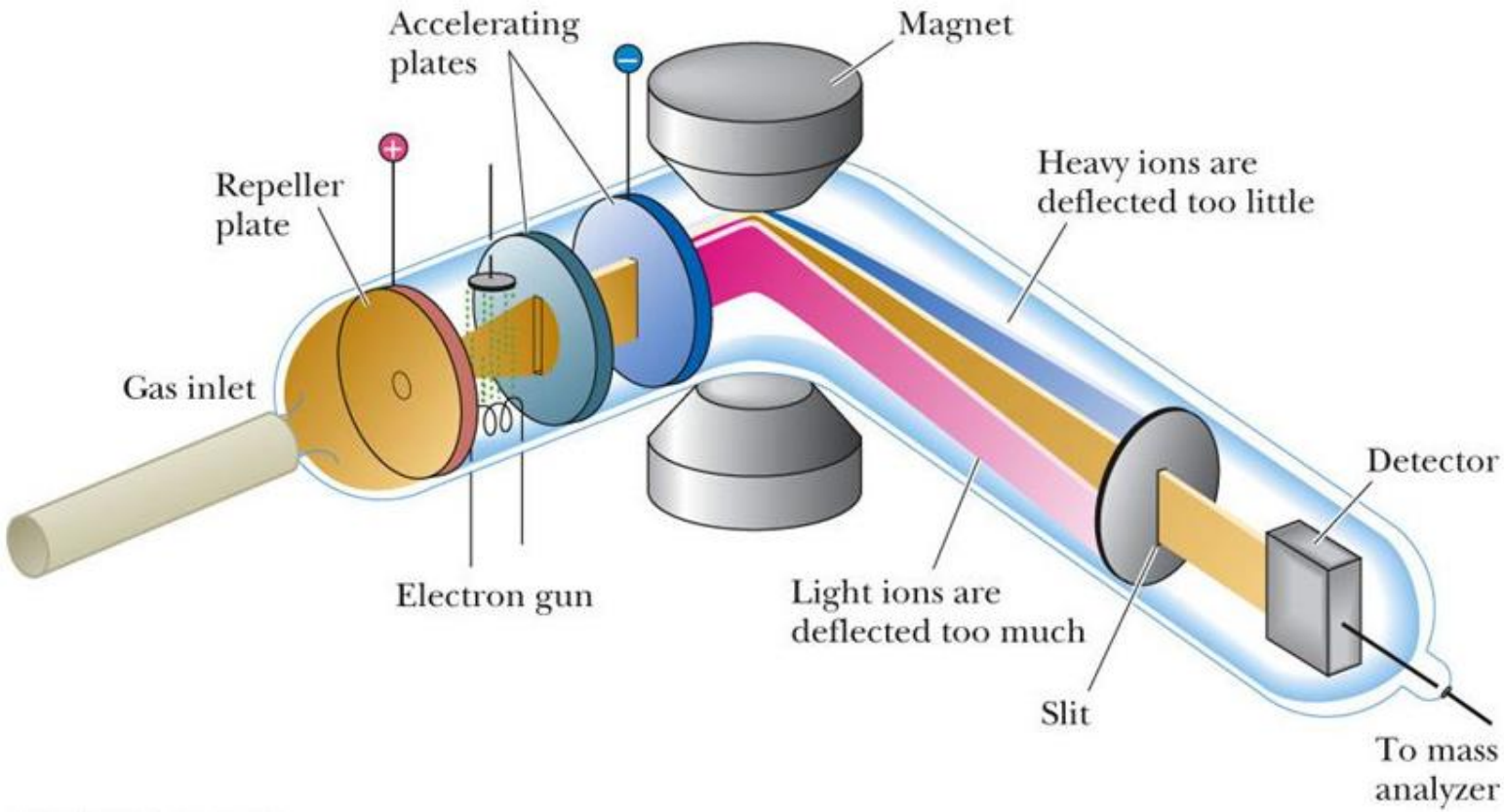
- Inlet system – introduces sample to MS system
- Ionization source – produces gaseous ions from the sample being studied
- Mass analyser – resolves the ions into their characteristic mass components according to their mass-to-charge ratio
- Detector – detects the ions and records the relative abundance of each of the resolved ionic species



How does a Mass Spectrometer work?

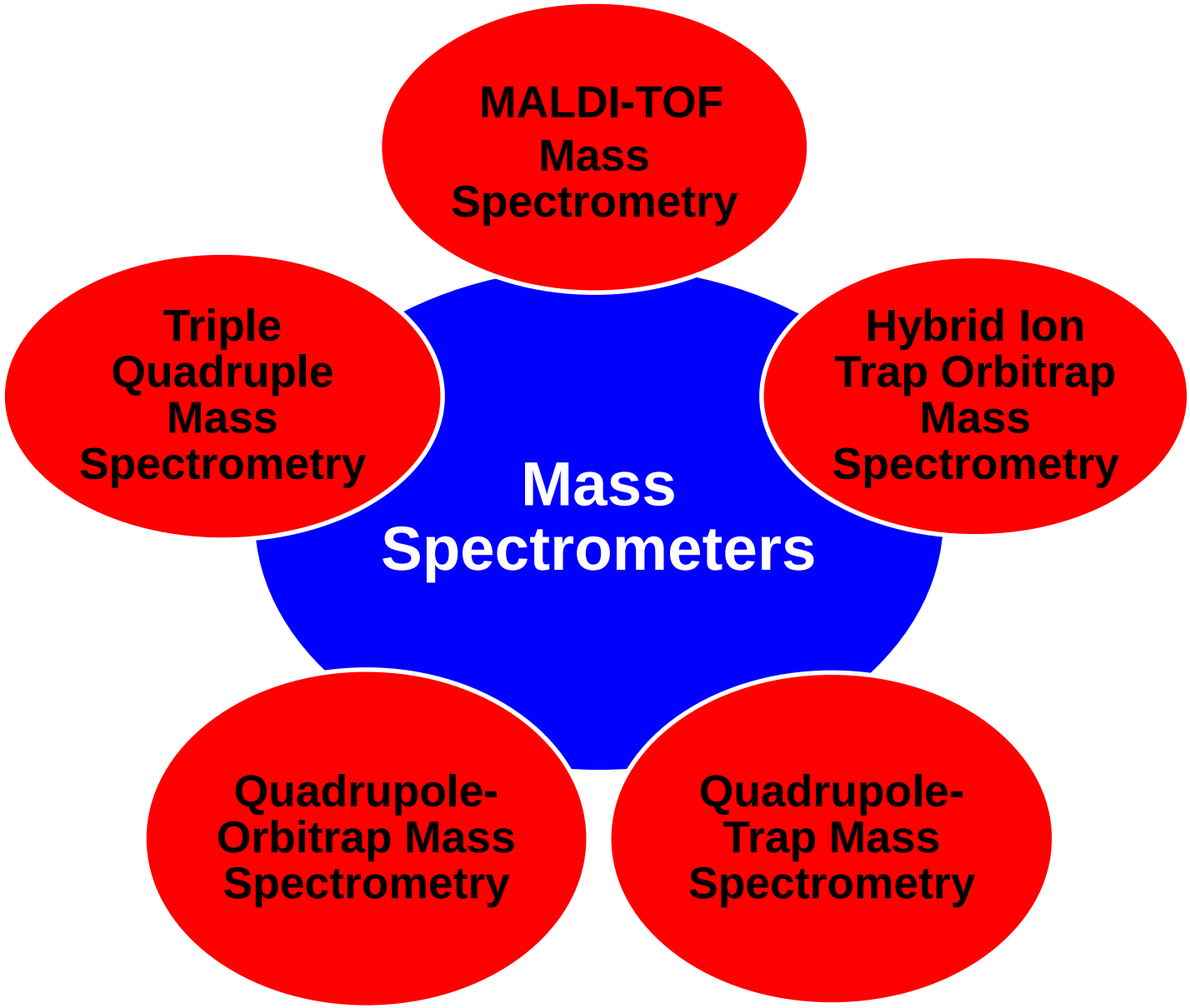
- A sample is ionized (eg. by bombarding it with electrons)
- Some of the samples molecules break into charged fragments or simply become charged without fragmenting
- These ions are then separated according to their mass-to-charge ratio

How does a Mass Spectrometer work?



Mass Spectrometry Uses

- Quantify known materials
- Identify unknown compounds within sample
- Elucidate structure and chemical properties of different molecules
- Know the fragmentation of the molecule

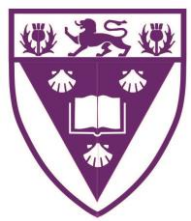

MALDI-TOF Mass Spectrometry
Triple Quadruple Mass Spectrometry
Hybrid Ion Trap Orbitrap Mass Spectrometry
Mass Spectrometers
Quadrupole-Orbitrap Mass Spectrometry
Quadrupole-Trap Mass Spectrometry

MALDI-TOF Mass Spectrometer

- Matrix-assisted laser desorption/ionization (MALDI) - time-of-flight (TOF) mass spectrometer (MS)

  - MALDI: soft ionization that involves a laser striking a matrix of small molecules to make the analyte molecules into the gas phase

  - TOF: ions of different m/z are dispersed in time during their flight along a field-free drift path of known length



MALDI-TOF Mass Spectrometer

MALDI-TOF Mass Spectrometer

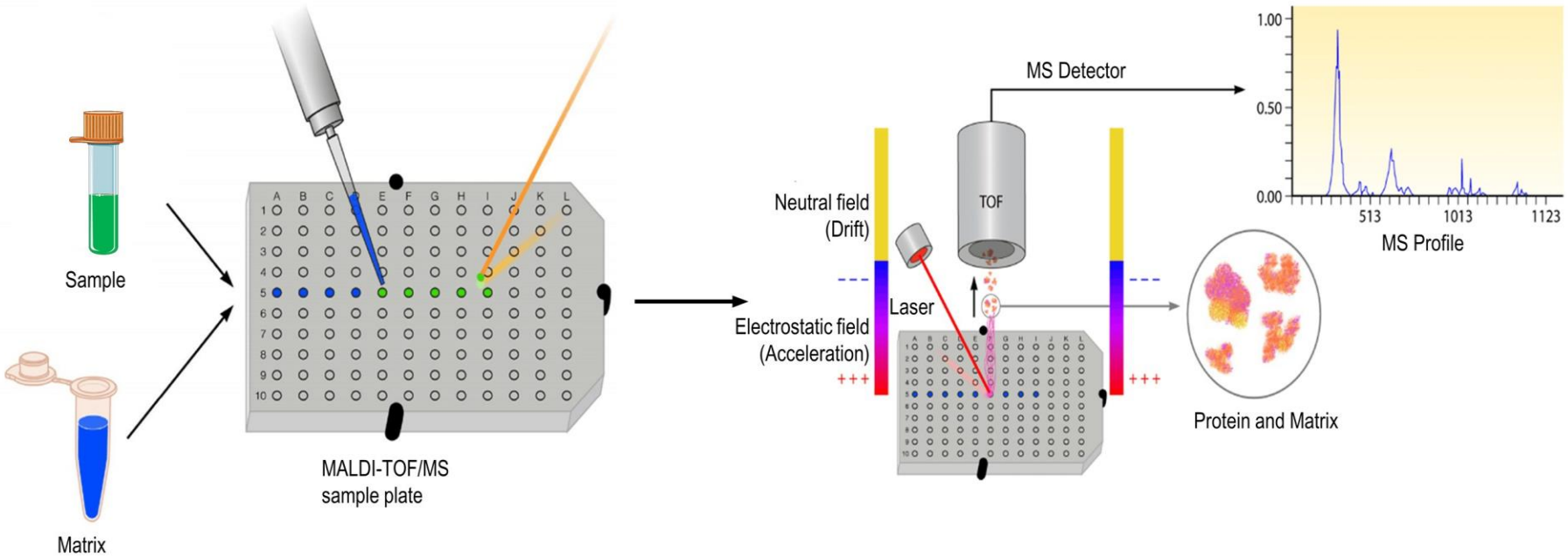
- Inlet system – MS sample plate

- Ionization source – MALDI

  Matrix – compound that promotes the formation of ions (eg. α-cyano-4-hydroxycinnamic acid, 3,5-dimethoxy-4-hydroxycinnamic acid and 2,5-dihydroxybenzoic acid

- Mass analyser –TOF

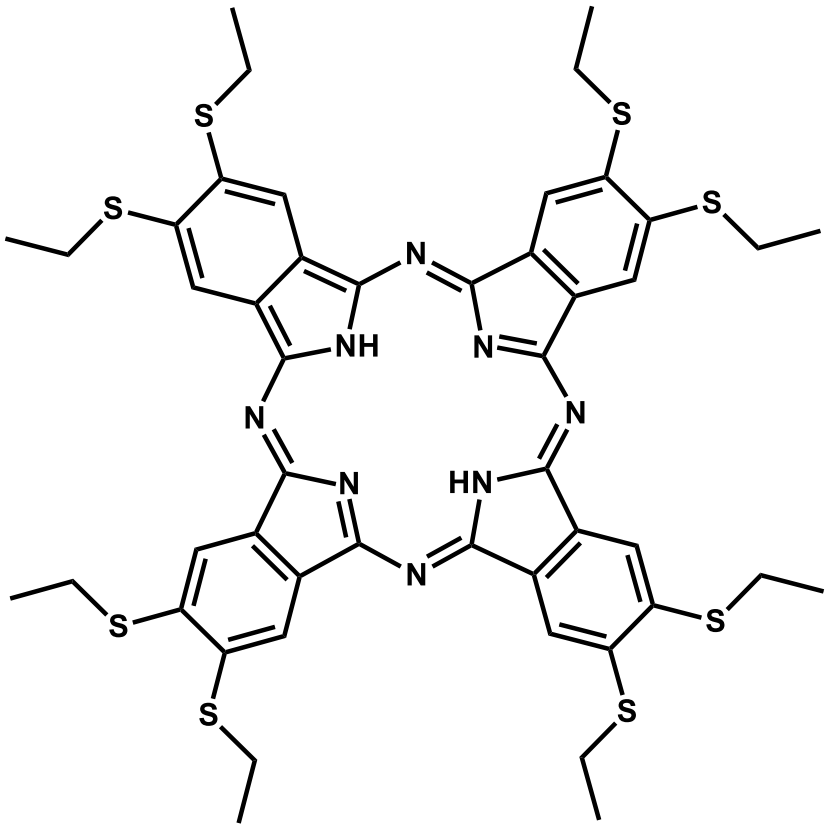
MALDI-TOF MS



https://www.creative-proteomics.com/technology/maldi-tof-mass-spectrometry.htm

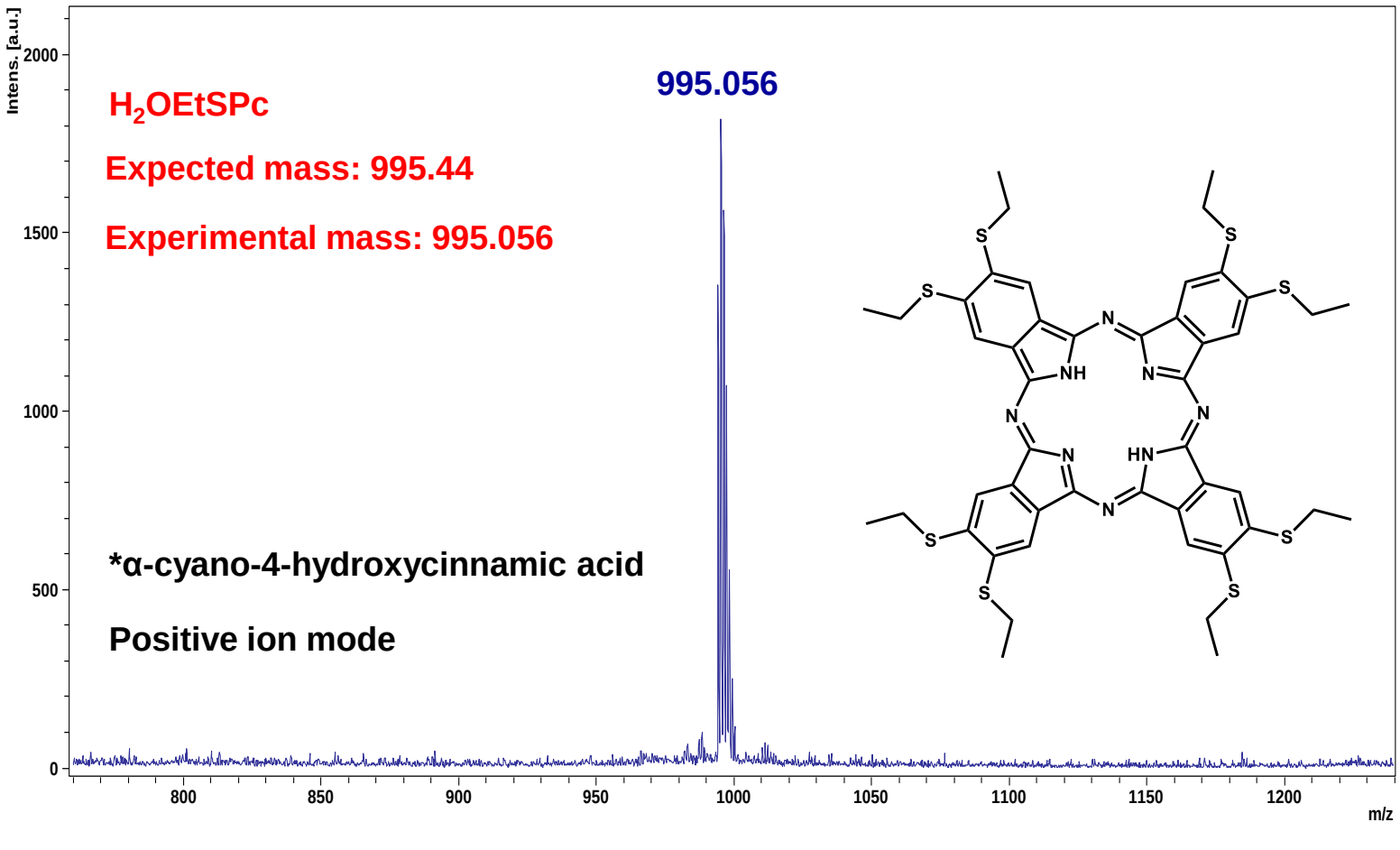
Respondent

- Rhulani

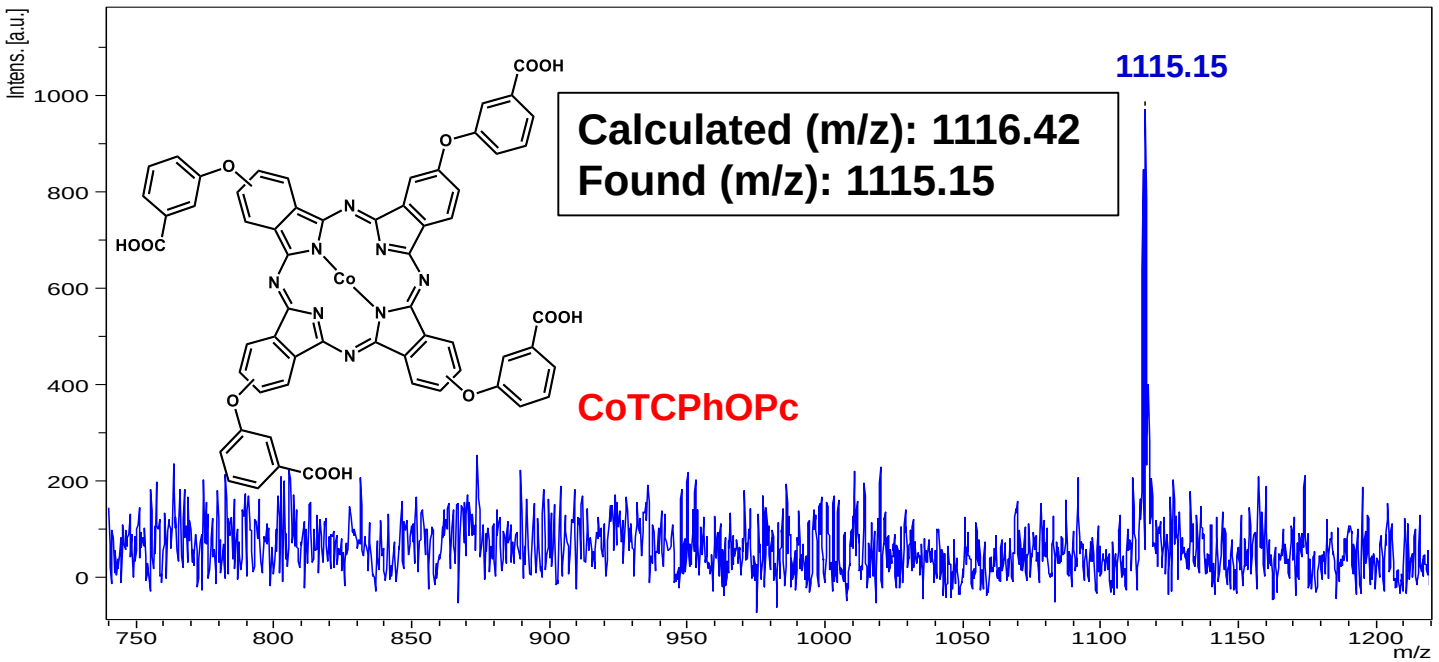


Metal Free Octa Ethyl Sulfide Phthalocyanine (H_2OEtSPc)

Respondent


Intens. [a.u.]
2000
1500
1000
500
0
995.056
H2OEtSPc
Expected mass: 995.44
Experimental mass: 995.056
*α-cyano-4-hydroxycinnamic acid
Positive ion mode
800
850
900
950
1000
1050
1100
1150
1200
m/z

Mass Spectrum

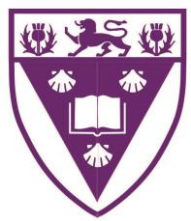


*α-cyano-4-hydroxycinnamic acid

Positive ion mode

Applications

- Environmental monitoring and analysis – soil, water and air pollutants, water quality
- Geochemistry – age determination, soil and rock composition, oil and gas surveying
- Chemical and Petrochemical industry – quality control
- Identify structures of biomolecules – carbohydrates, nucleic acids
- Monitoring gases in patients breath during surgery



Acknowledgements

- Dist Prof T. Nyokong
- Dr P. N. Mashazi
- F3 and F5
- S22 / CNI

Thank you