

Workflow

Elemental composition:

CH_3

Ionization type:

positive radical, $\text{CH}_3^{\bullet+}$

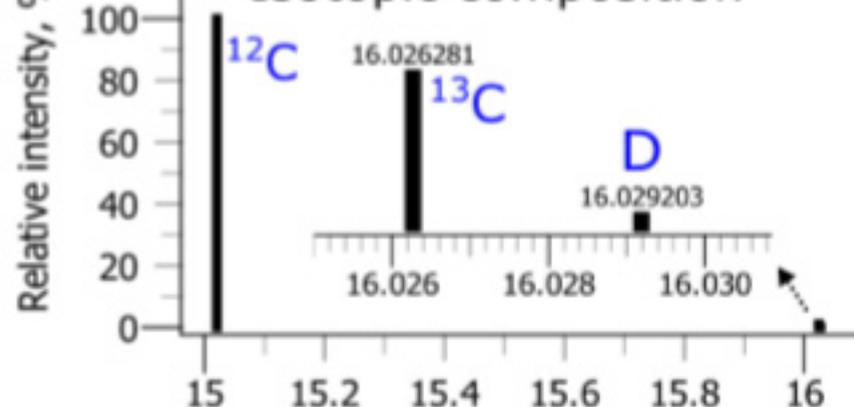
Number of isotopologues:

1 - 2,

relative intensity threshold

a

Isotopic composition



b

Frequencies calculation

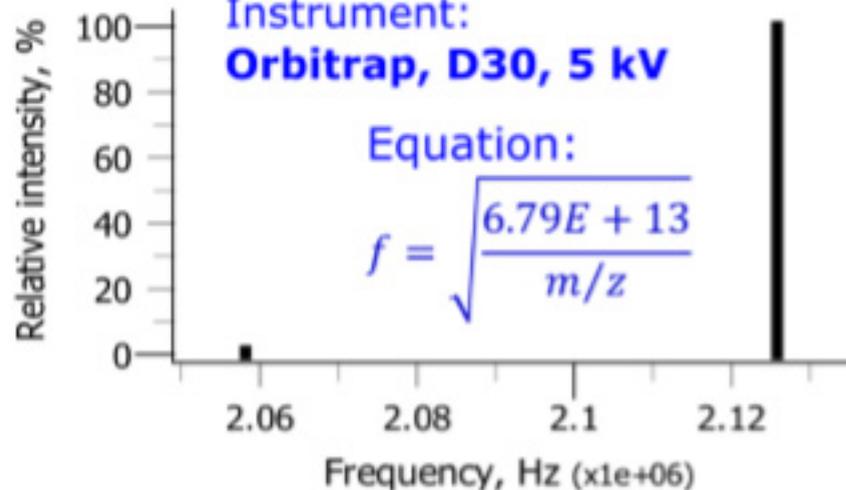
Instrument:

Orbitrap, D30, 5 kV

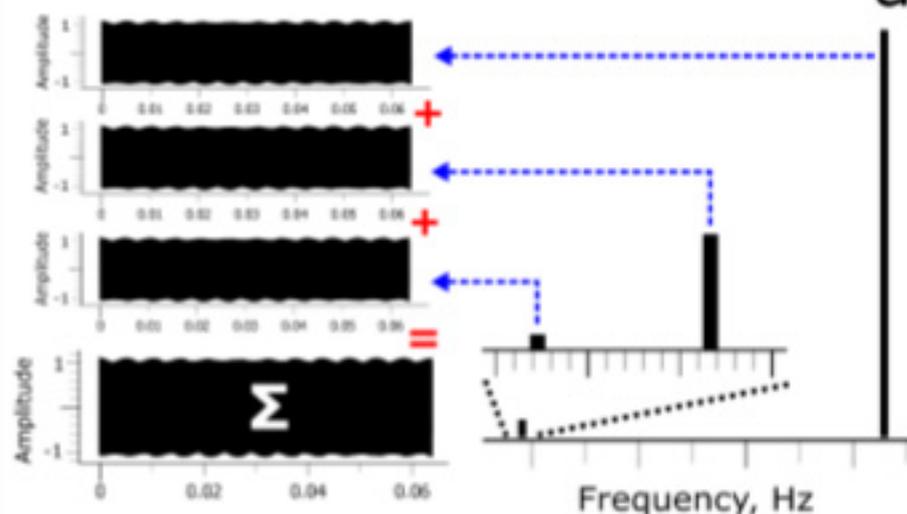
Equation:

$$f = \sqrt{\frac{6.79E + 13}{m/z}}$$

c



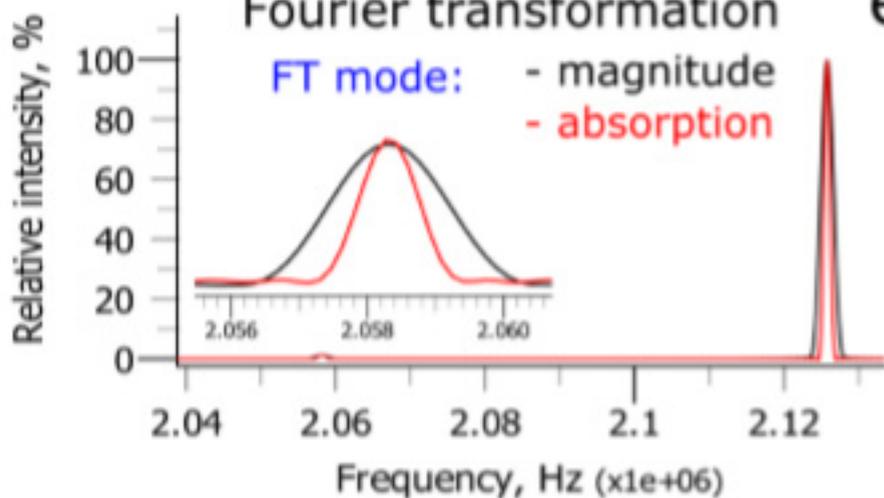
Transients calculation



d

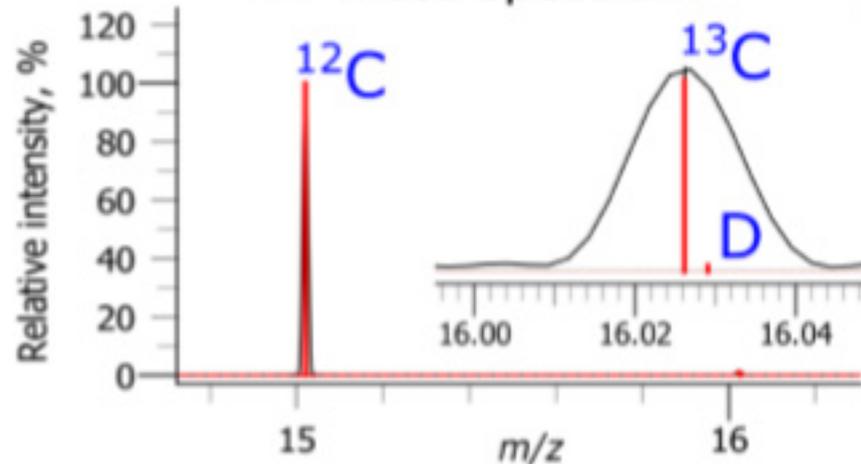
Fourier transformation

FT mode: - magnitude
- absorption



e

FT mass spectrum



f