

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -2.0, max = 17.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

369 formula(e) evaluated with 1 results within limits (all results (uj to 1000) for each mass)

Elements Used:

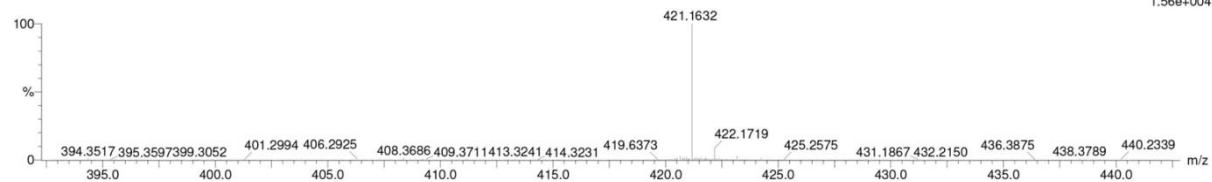
C: 0-500 H: 0-1000 N: 0-5 O: 0-5 S: 0-1

03-Jan-2023

2001014 673 (4.068) Cm (668:677-627:631)

1:19

1: TOF MS ES+
1.56e+004



Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
421.1632	421.1646	-1.4	-3.3	13.5	627.2	0.0	C23 H24 N4 O2 S

Fig.1S. HRMS spectrum