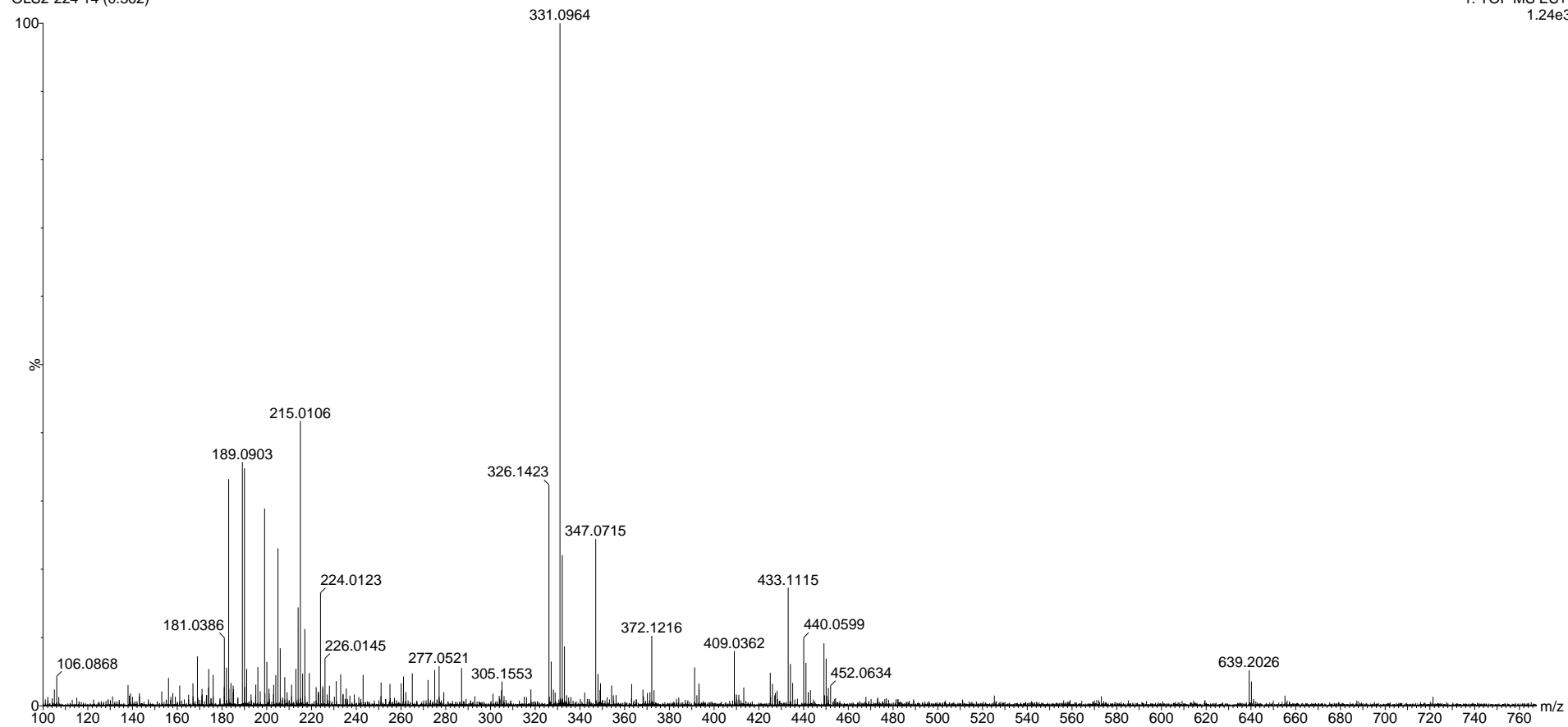


OLS2-224  
OLS2-224 14 (0.362)

29-Feb-2024  
1: TOF MS ES+  
1.24e3



Theoretical mass for  $[M+H]^+$ : 309.1161

Elemental Composition Report for 326m/z

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 1-20   H: 0-60   N: 0-1   O: 1-10   Na: 0-1   S: 1-1

Minimum: -1.5

Maximum: 5.0   5.0   100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
326.1423	326.1426	-0.3	-0.9	5.5	92.1	0.0	C16 H24 N O4 S [M+NH4]+ adduct

Elemental Composition Report for 331m/z

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 1-20   H: 0-60   N: 0-1   O: 1-10   Na: 0-1   S: 1-1

Minimum: -1.5

Maximum: 5.0   5.0   100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
331.0964	331.0980	-1.6	-4.8	6.5	116.9	0.0	C16 H20 O4 Na S [M+Na]+ adduct