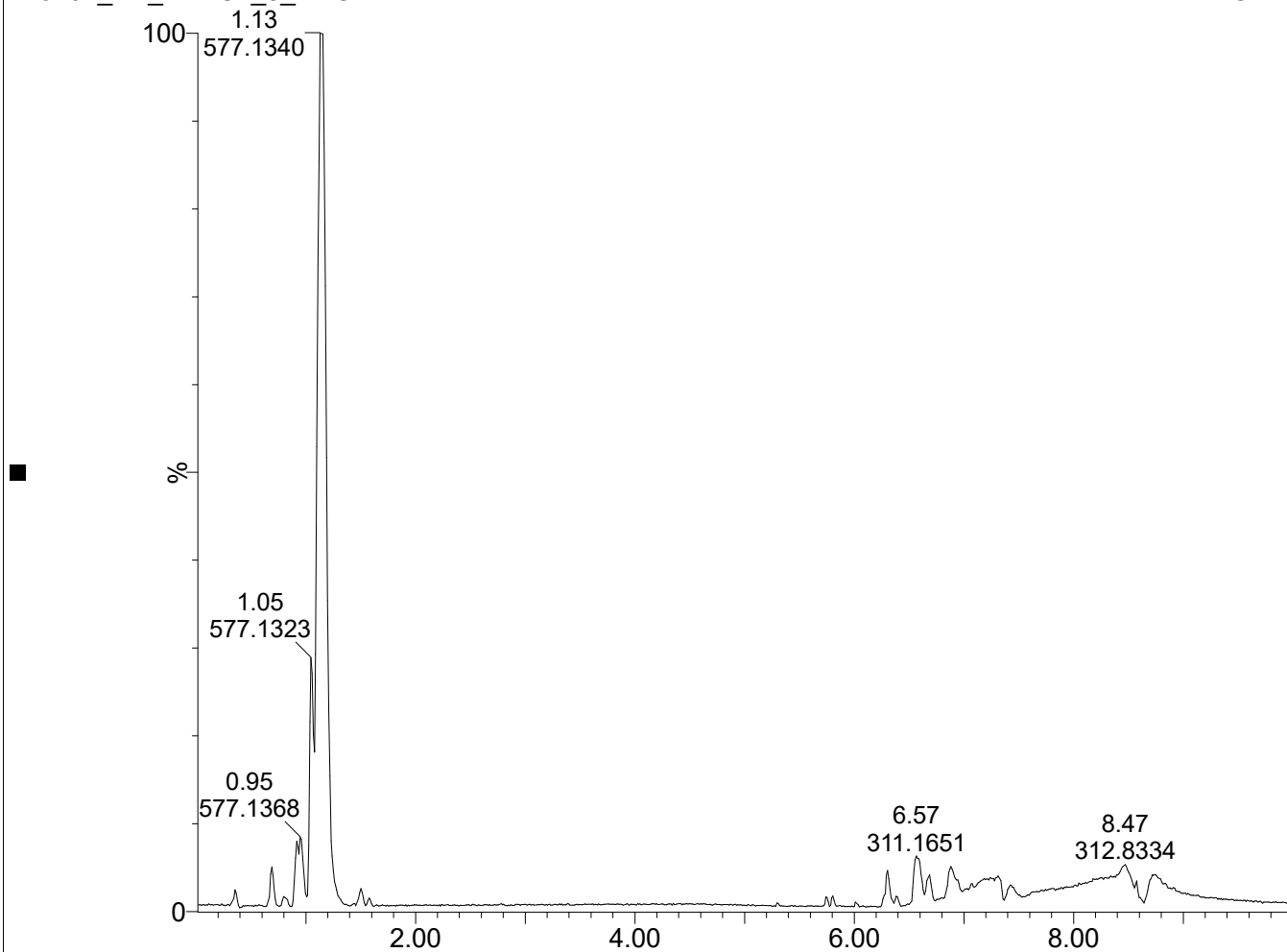


COMPOUND NO. S2 (METHOD A)

COL31

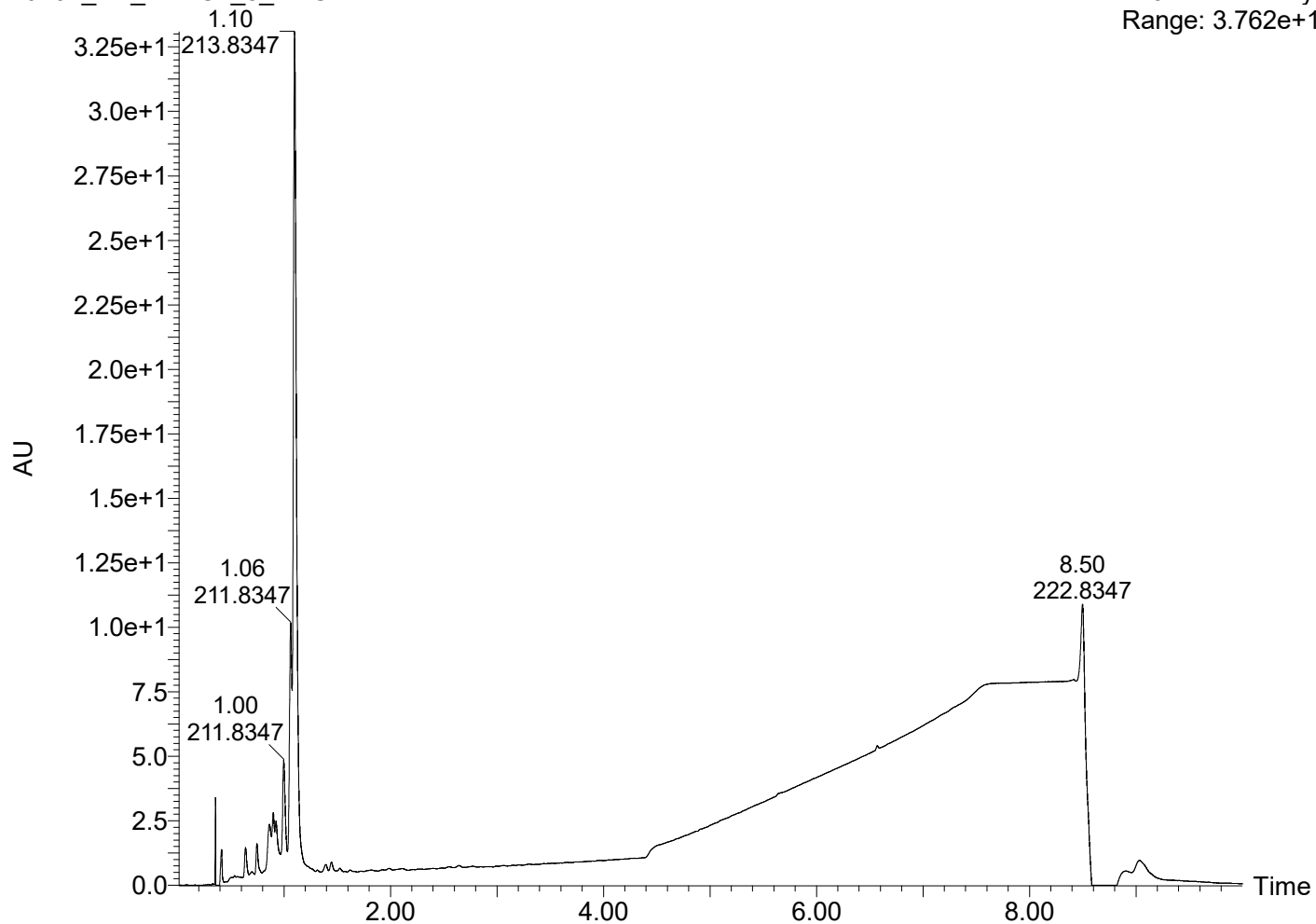
170104_AA_MPLC1_8_NEG

1: TOF MS ES-
BPI
5.16e4



170104_AA_MPLC1_8_NEG

3: Diode Array
Range: 3.762e+1



Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

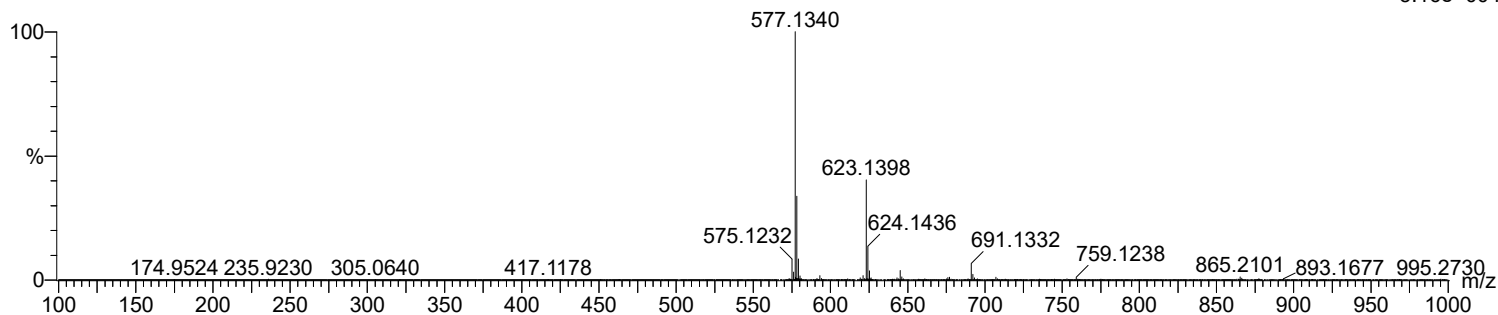
119968 formula(e) evaluated with 943 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-6 Cl: 0-8 Br: 0-8

COL31

170104_AA_MPLC1_8_NEG 98 (1.131)

1: TOF MS ES-
5.16e+004

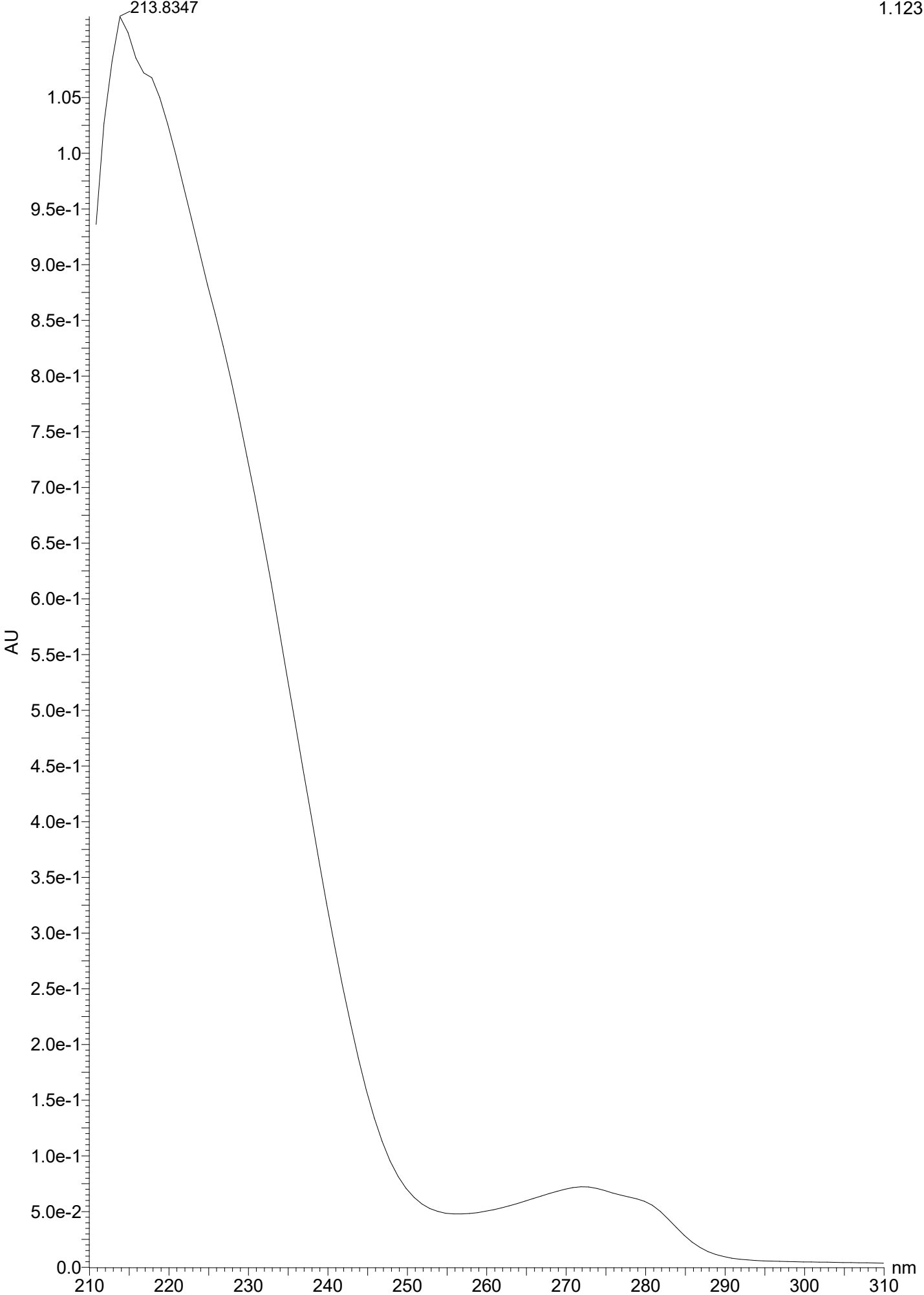
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1340	577.1346	-0.6	-1.0	18.5	202.7	0.088	91.57	C30 H25 O12
577.1359		-1.9	-3.3	23.5	205.2	2.629	7.21	C31 H21 N4 O8
577.1333		0.7	1.2	24.5	207.9	5.314	0.49	C27 H17 N10 O6
577.1319		2.1	3.6	19.5	208.2	5.625	0.36	C26 H21 N6 O10
577.1373		-3.3	-5.7	28.5	208.2	5.629	0.36	C32 H17 N8 O4

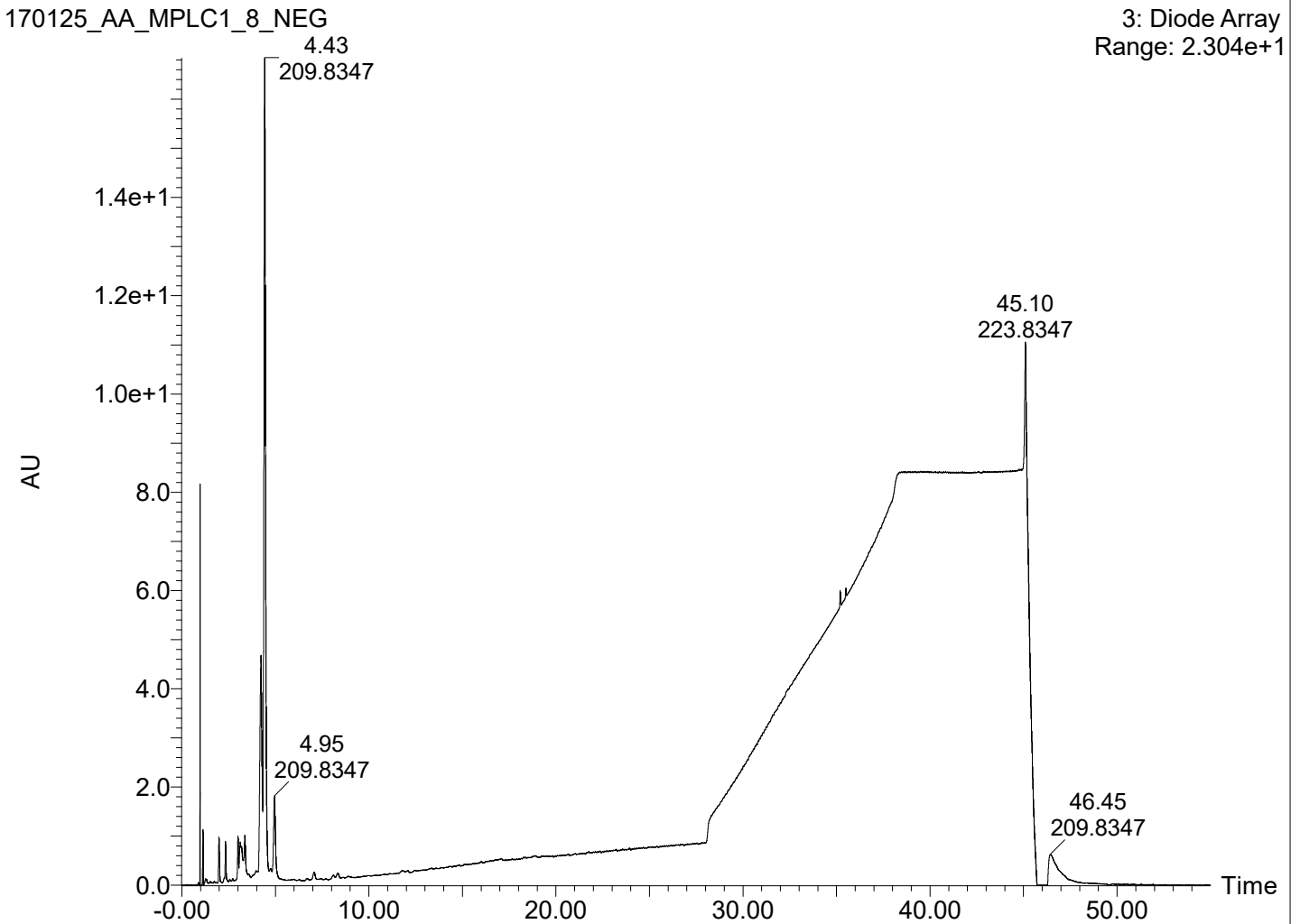
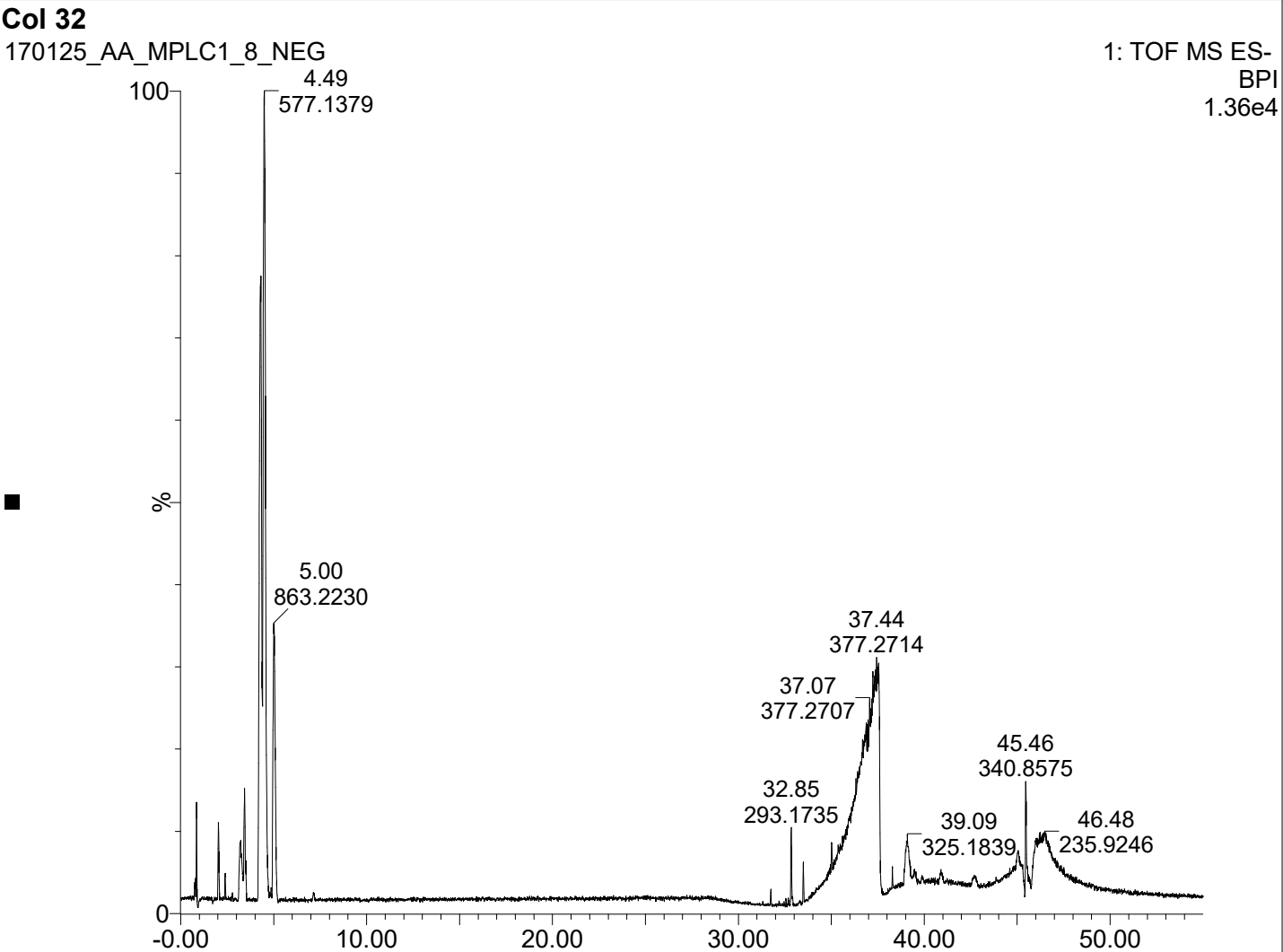
COL31

170104_AA_MPLC1_8_NEG 1328 (1.106)

3: Diode Array
1.123



COMPOUND NO. S2 (METHOD B)

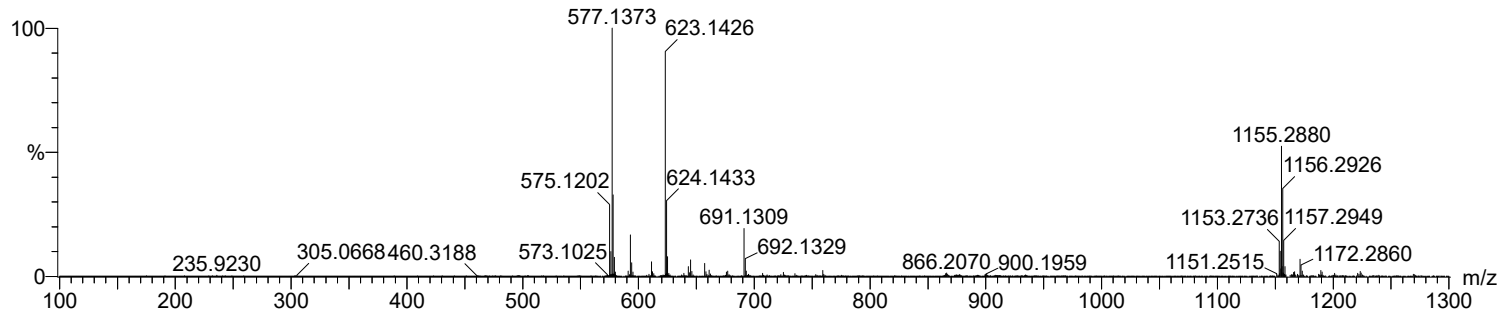


Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
162 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200
Col 32
170125_AA_MPLC1_8_NEG 380 (4.478)

1: TOF MS ES-
1.35e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1373	577.1346	2.7	4.7	18.5	146.2	0.001	99.94	C30 H25 O12
577.1405		-3.2	-5.5	9.5	154.0	7.778	0.04	C23 H29 O17
577.1287		8.6	14.9	27.5	155.0	8.818	0.01	C37 H21 O7
577.1440		-6.7	-11.6	31.5	156.8	10.589	0.00	C41 H21 O4

Col 32

170125_AA_MPLC1_8_NEG 5320 (4.433)

3: Diode Array
7.565e-1

