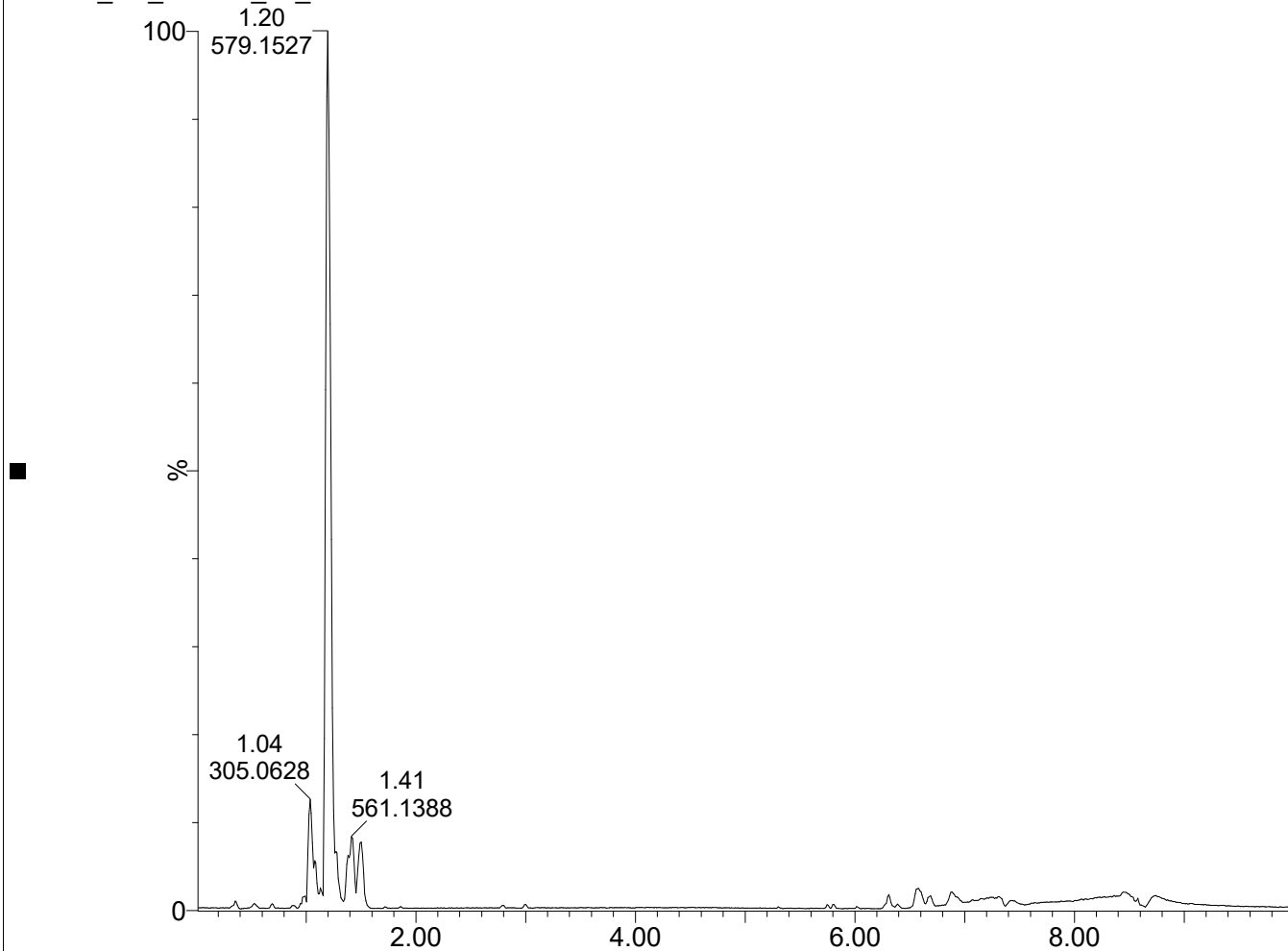


COMPOUND NO. S3 (METHOD A)

COL31

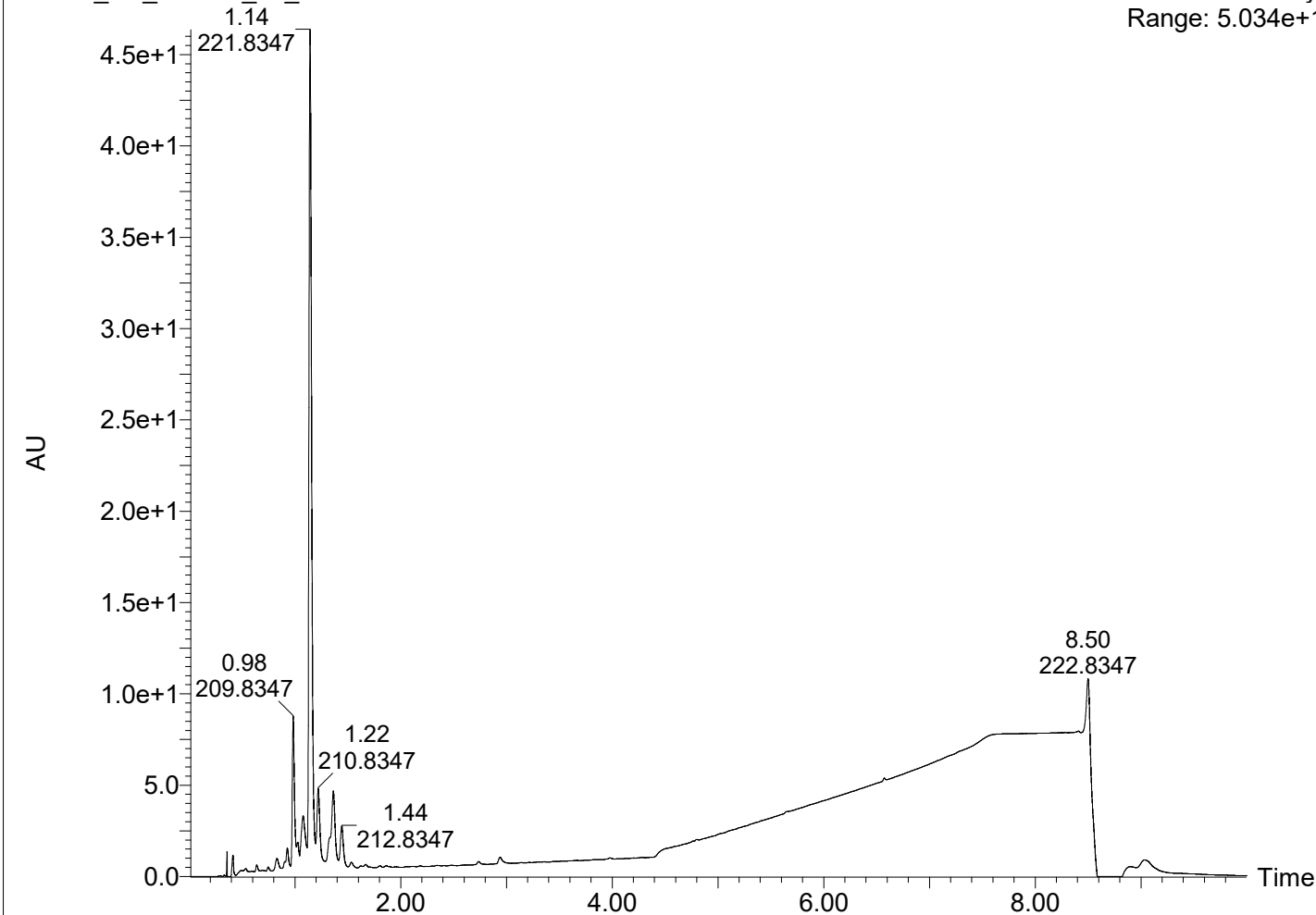
170104_AA_MPLC1_10_NEG

1: TOF MS ES-
BPI
1.33e5



170104_AA_MPLC1_10_NEG

3: Diode Array
Range: 5.034e+1



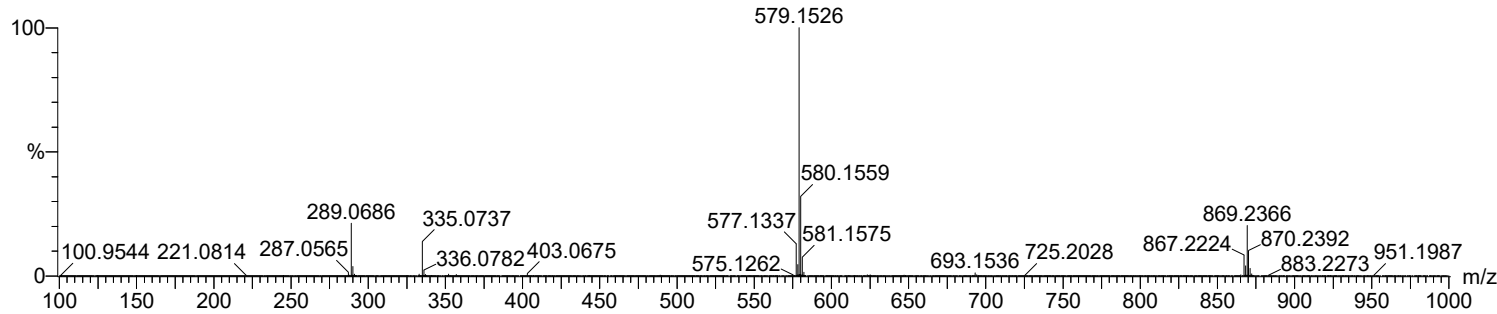
Single Mass Analysis

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
5588 formula(e) evaluated with 42 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_10_NEG 103 (1.198)

1: TOF MS ES-
1.33e+005



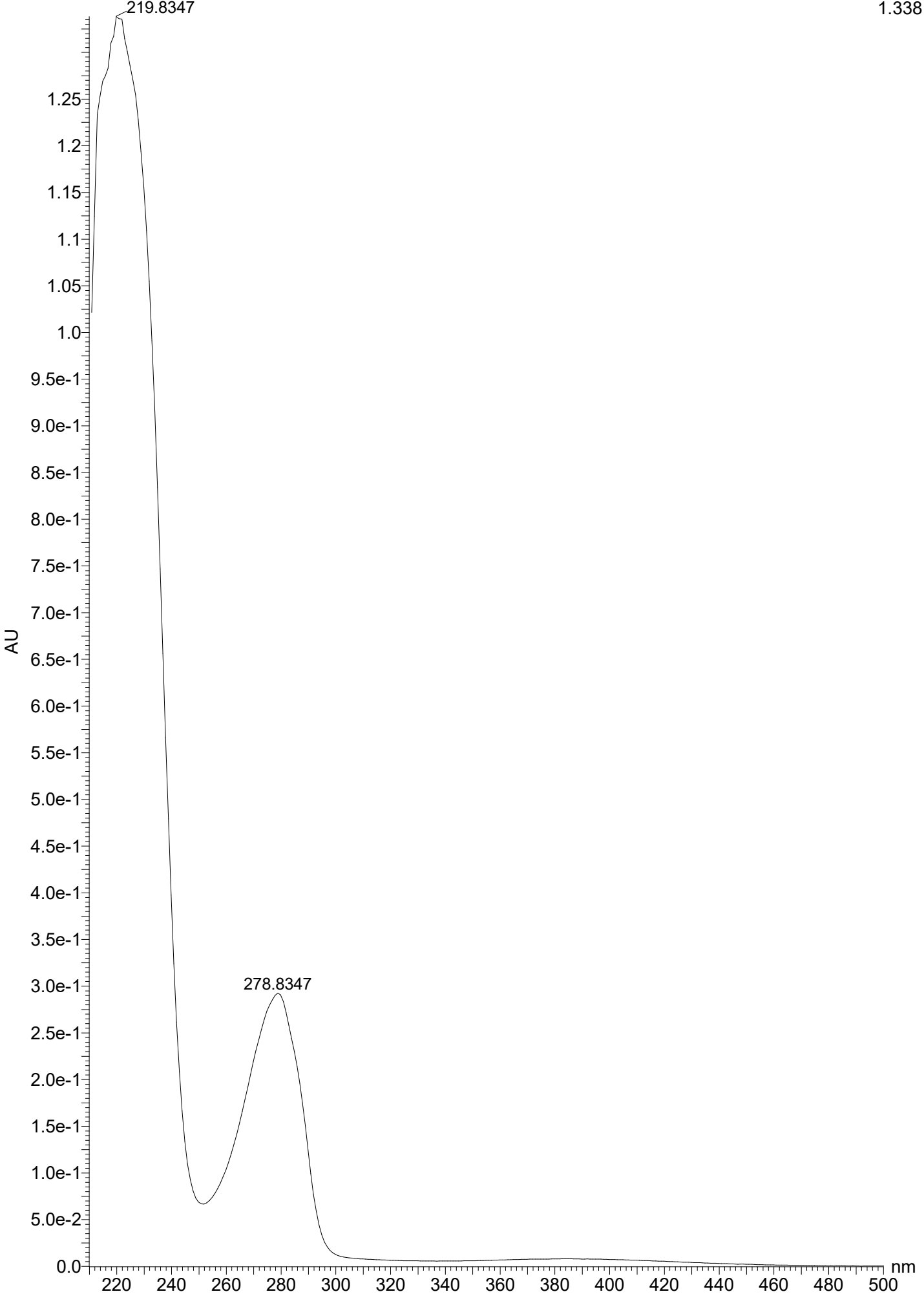
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
289.0686	289.0712	-2.6	-9.0	9.5	417.4	0.269	76.39	C15 H13 O6
	289.0726	-4.0	-13.8	14.5	418.9	1.725	17.81	C16 H9 N4 O2
	289.0653	3.3	11.4	18.5	420.5	3.414	3.29	C22 H9 O
	289.0685	0.1	0.3	10.5	421.3	4.190	1.52	C11 H9 N6 O4
	289.0699	-1.3	-4.5	15.5	421.7	4.610	1.00	C12 H5 N10

COL31

170104_AA_MPLC1_10_NEG 1377 (1.147)

3: Diode Array
1.338



COMPOUND NO. S3 (METHOD B)

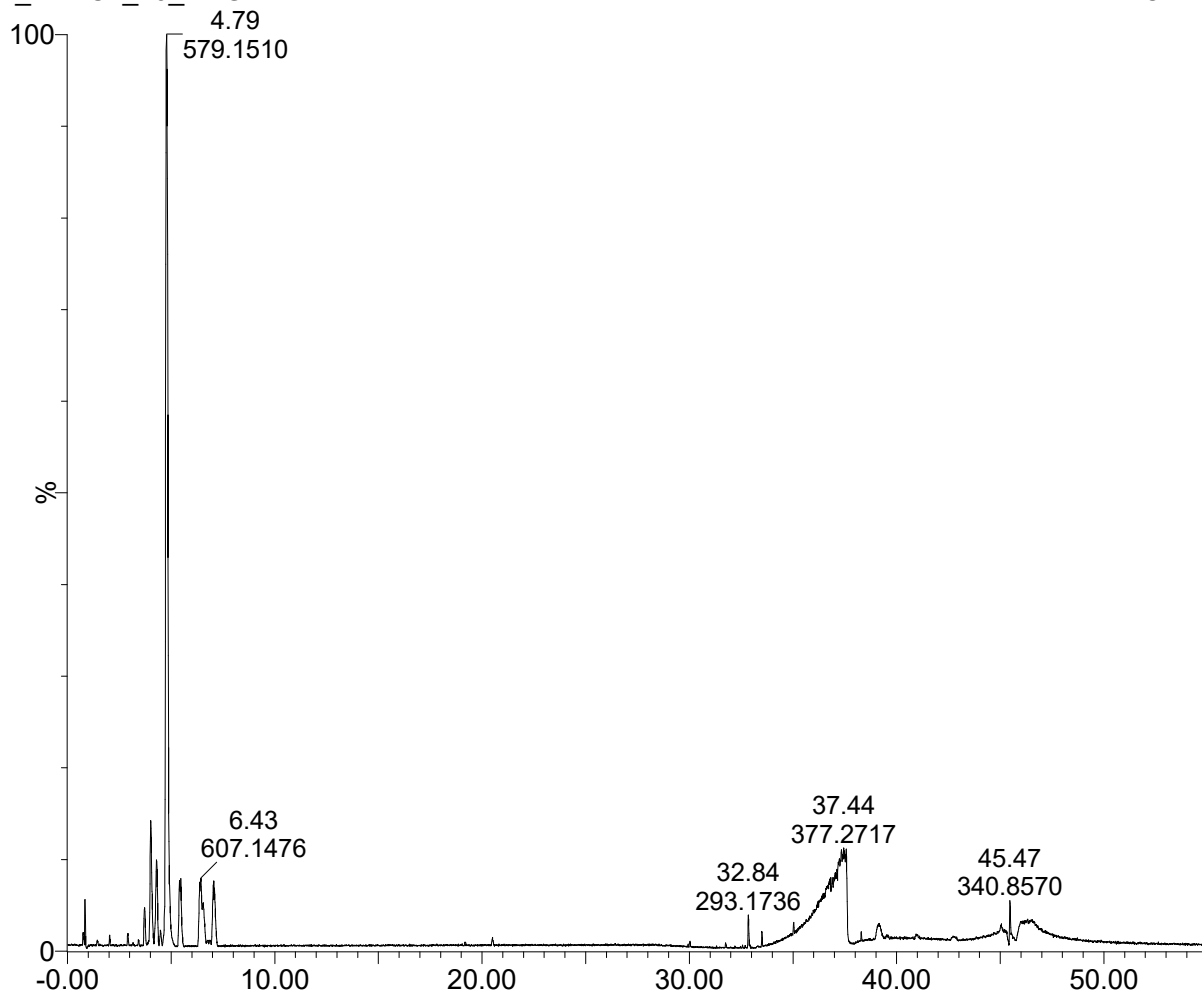
Col 32

170125_AA_MPLC1_10_NEG

1: TOF MS ES-

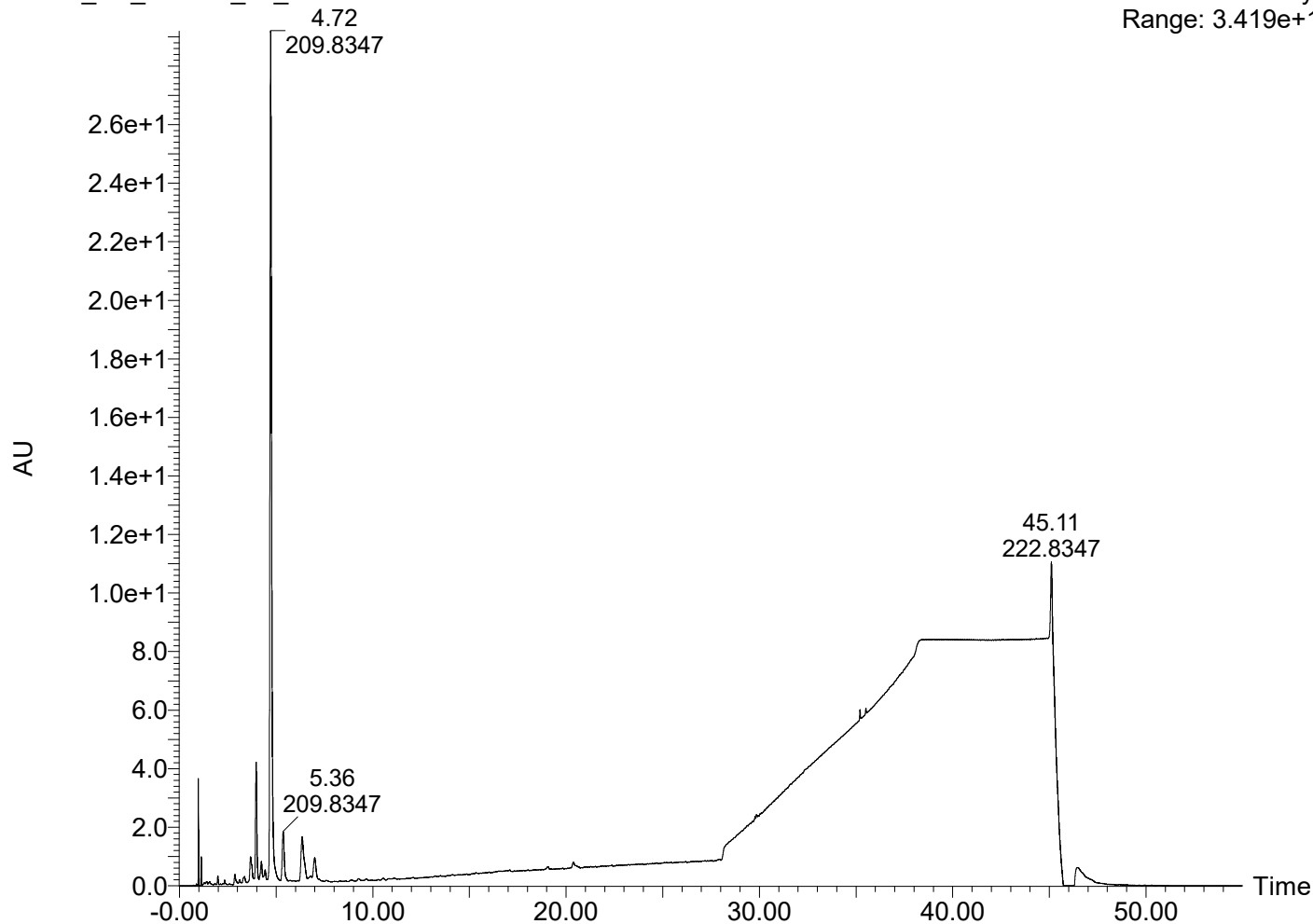
BPI

3.91e4



170125_AA_MPLC1_10_NEG

3: Diode Array
Range: 3.419e+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

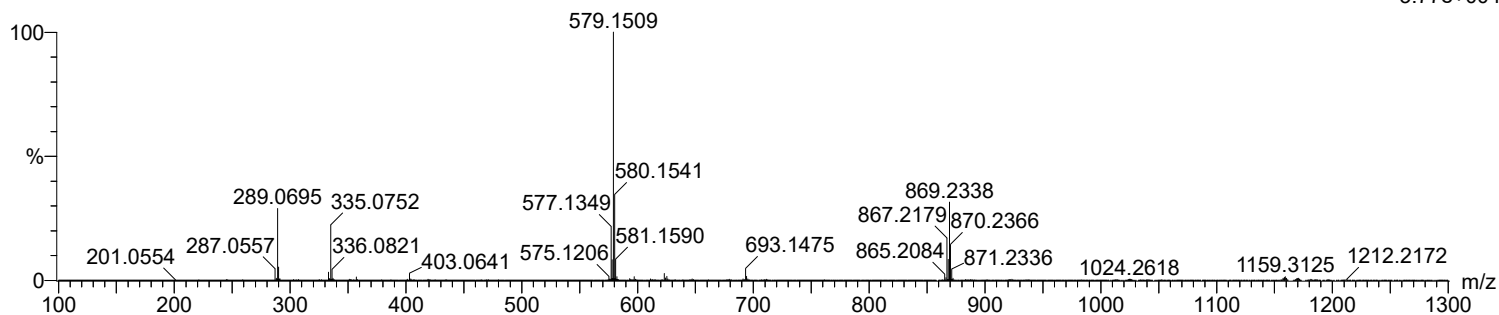
51 formula(e) evaluated with 2 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Col 32

170125_AA_MPLC1_10_NEG 408 (4.799)

1: TOF MS ES-
3.77e+004

Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
289.0695	289.0712	-1.7	-5.9	9.5	282.3	0.004	99.59	C15 H13 O6
	289.0653	4.2	14.5	18.5	287.8	5.509	0.41	C22 H9 O

Col 32

170125_AA_MPLC1_10_NEG 5657 (4.713)

3: Diode Array
1.198

