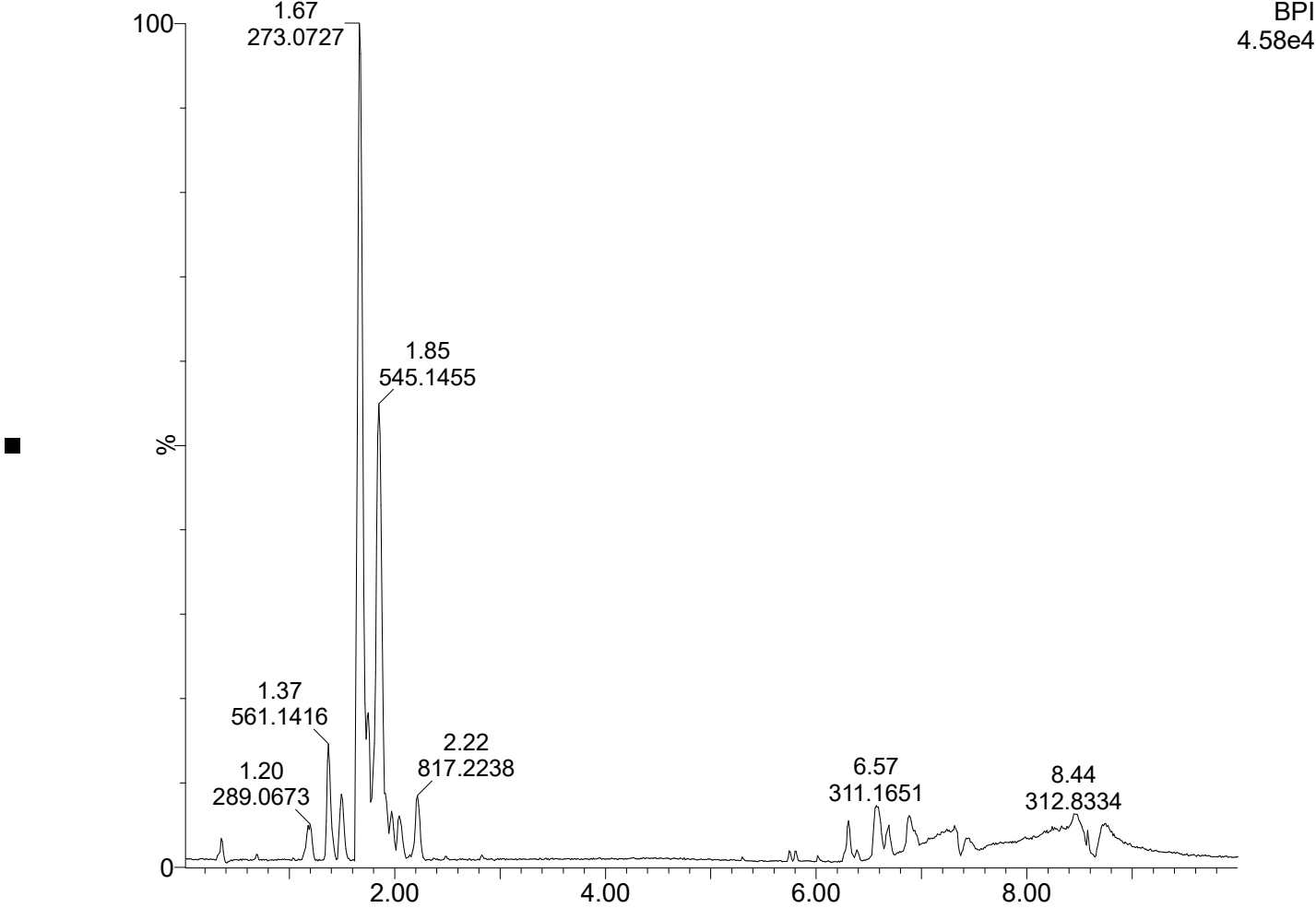


COMPOUND NO. S5 (METHOD A)

COL31

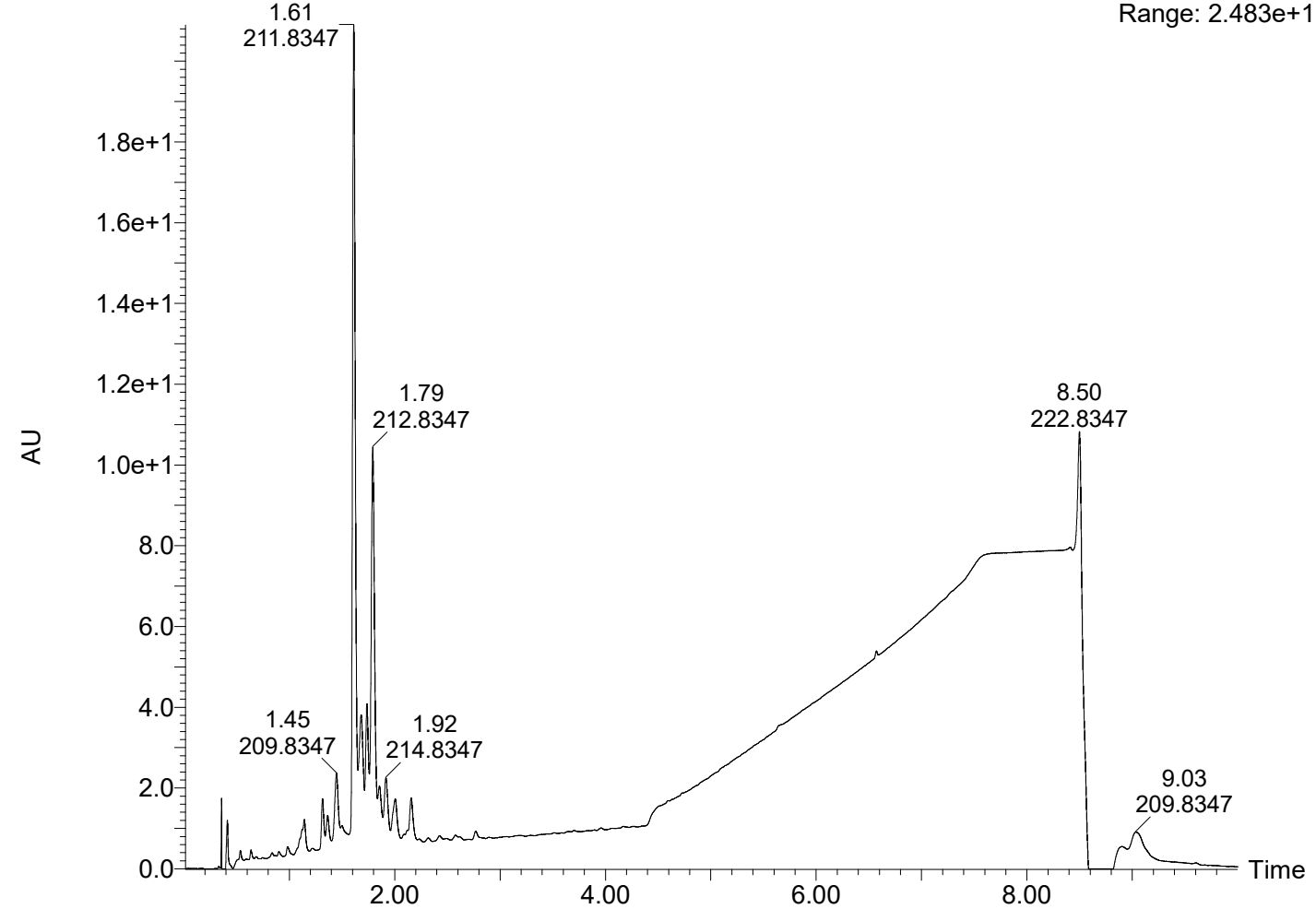
170104\_AA\_MPLC1\_17\_NEG

1: TOF MS ES-  
BPI  
4.58e4



170104\_AA\_MPLC1\_17\_NEG

3: Diode Array  
Range: 2.483e+1



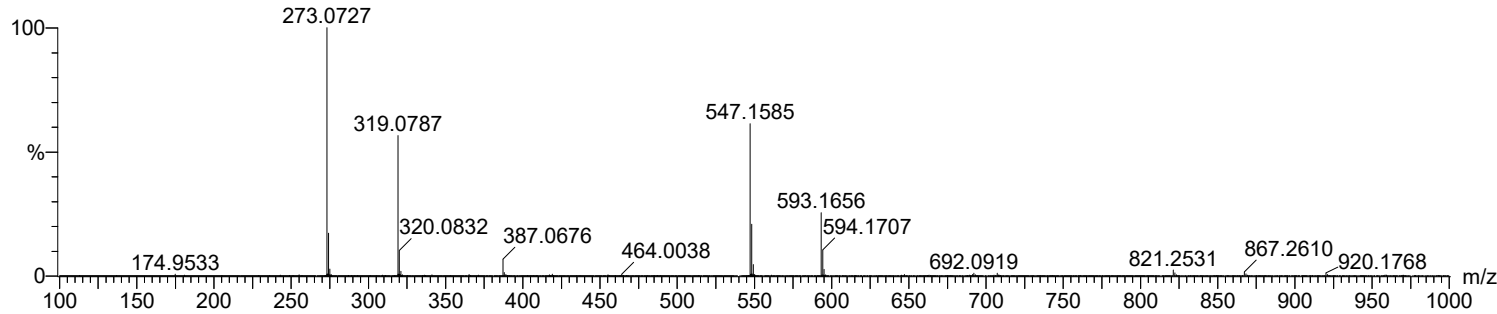
Single Mass Analysis

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  
4399 formula(e) evaluated with 33 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\_17\_NEG 143 (1.666)

1: TOF MS ES-  
4.58e+004



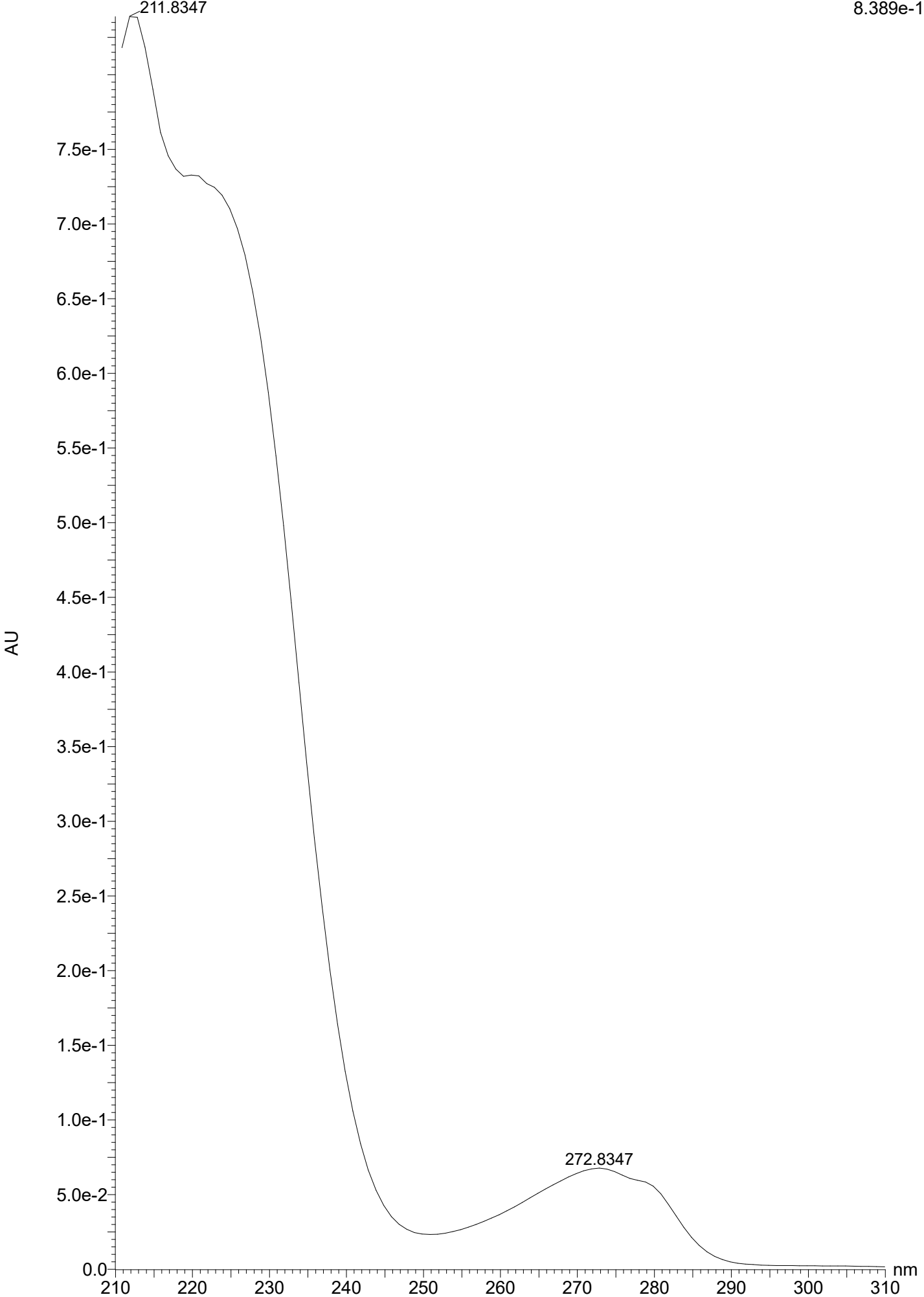
Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
273.0727	273.0763	-3.6	-13.2	9.5	407.5	0.019	98.10	C15 H13 O5
	273.0704	2.3	8.4	18.5	411.8	4.316	1.33	C22 H9
	273.0736	-0.9	-3.3	10.5	413.1	5.600	0.37	C11 H9 N6 O3
	273.0723	0.4	1.5	5.5	413.7	6.268	0.19	C10 H13 N2 O7
	273.0696	3.1	11.4	6.5	418.0	10.503	0.00	C6 H9 N8 O5

COL31

170104\_AA\_MPLC1\_17\_NEG 1935 (1.612)

3: Diode Array  
8.389e-1

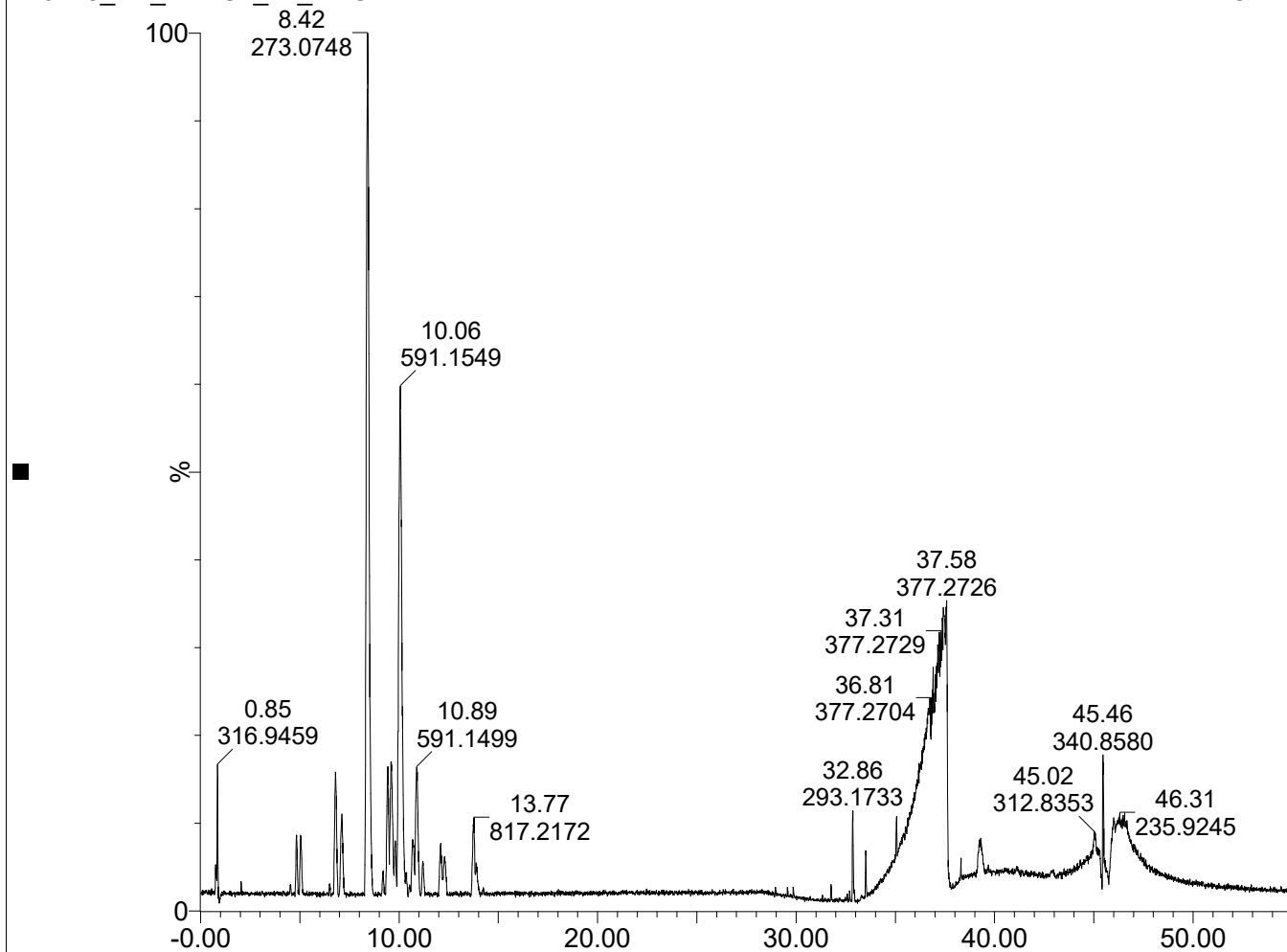


COMPOUND NO. S5 (METHOD B)

Col 32

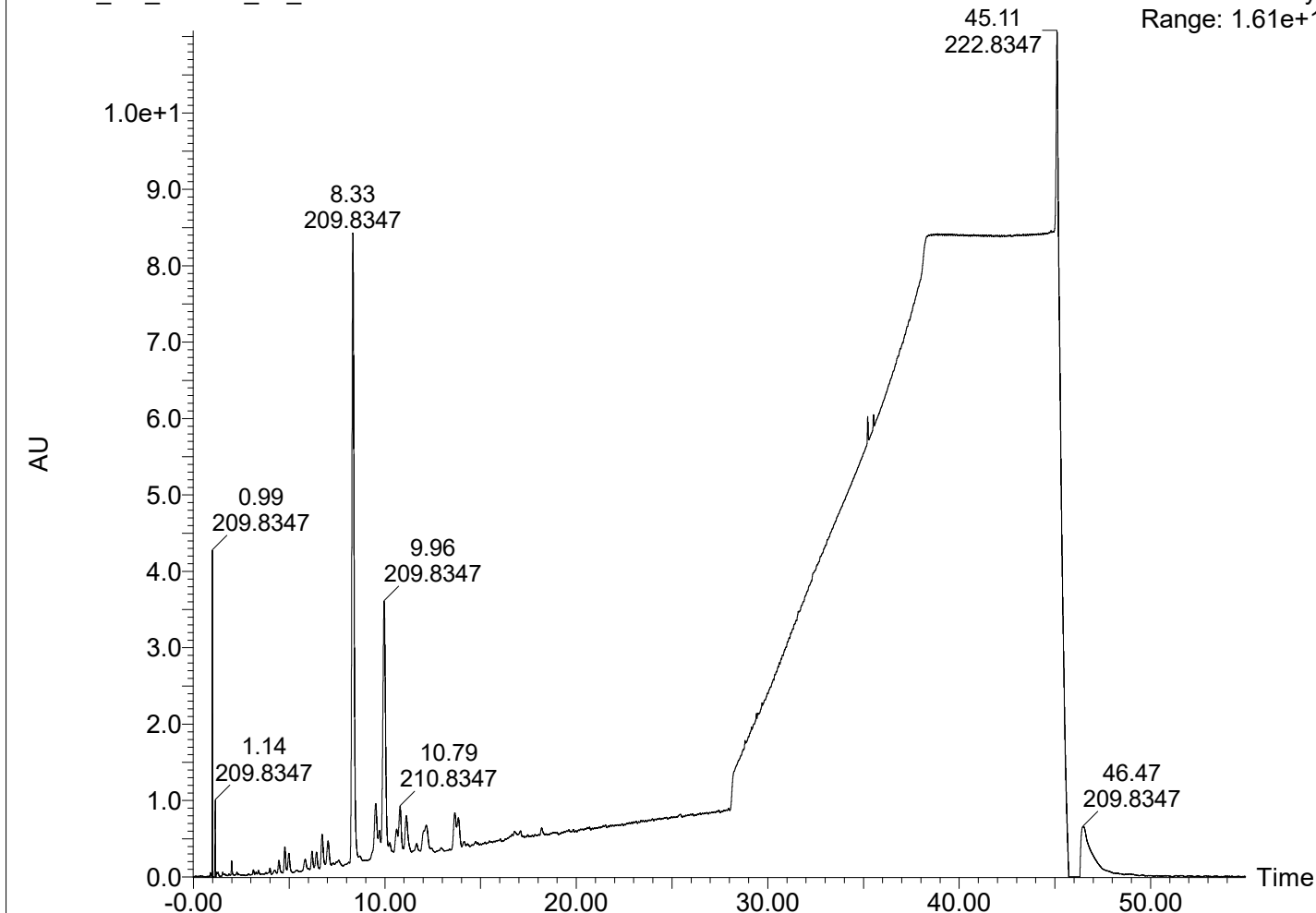
170125\_AA\_MPLC1\_17\_NEG

1: TOF MS ES-  
BPI  
1.30e4



170125\_AA\_MPLC1\_17\_NEG

3: Diode Array  
Range: 1.61e+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

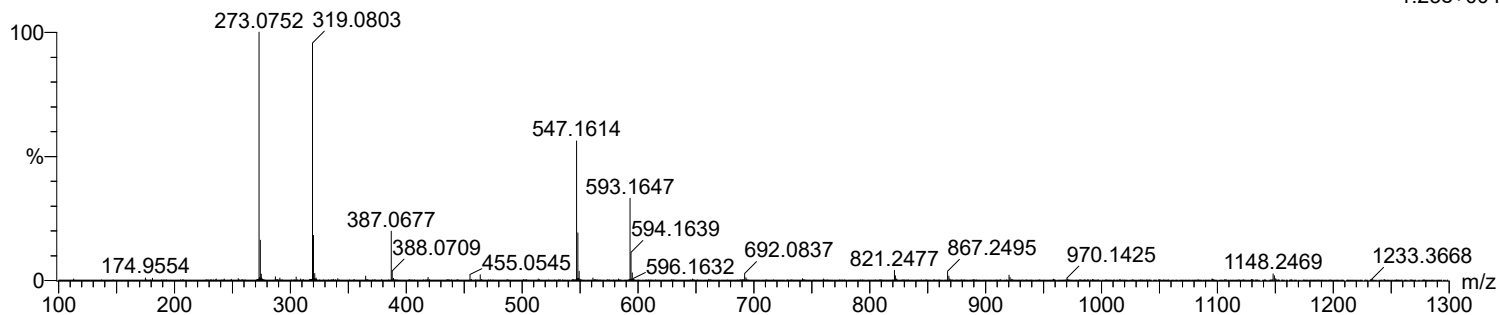
46 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170125\_AA\_MPLC1\_17\_NEG 718 (8.434)

1: TOF MS ES-  
1.23e+004

Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
273.0752	273.0763	-1.1	-4.0	9.5	291.8	n/a	n/a	C15 H13 O5

Col 32

170125\_AA\_MPLC1\_17\_NEG 9981 (8.318)

3: Diode Array  
4.22e-1

