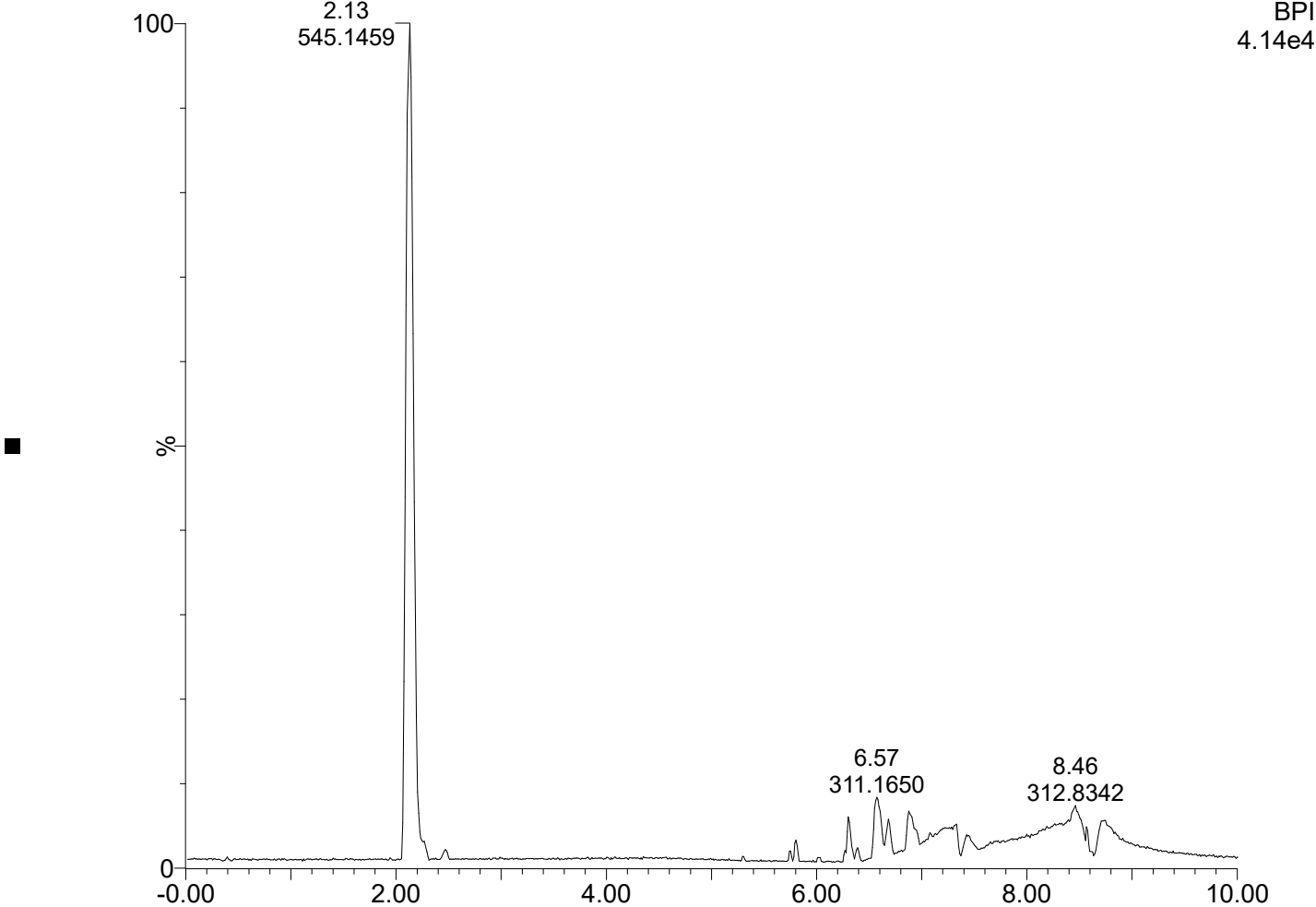


COMPOUND NO. S9 (METHOD A)

COL31

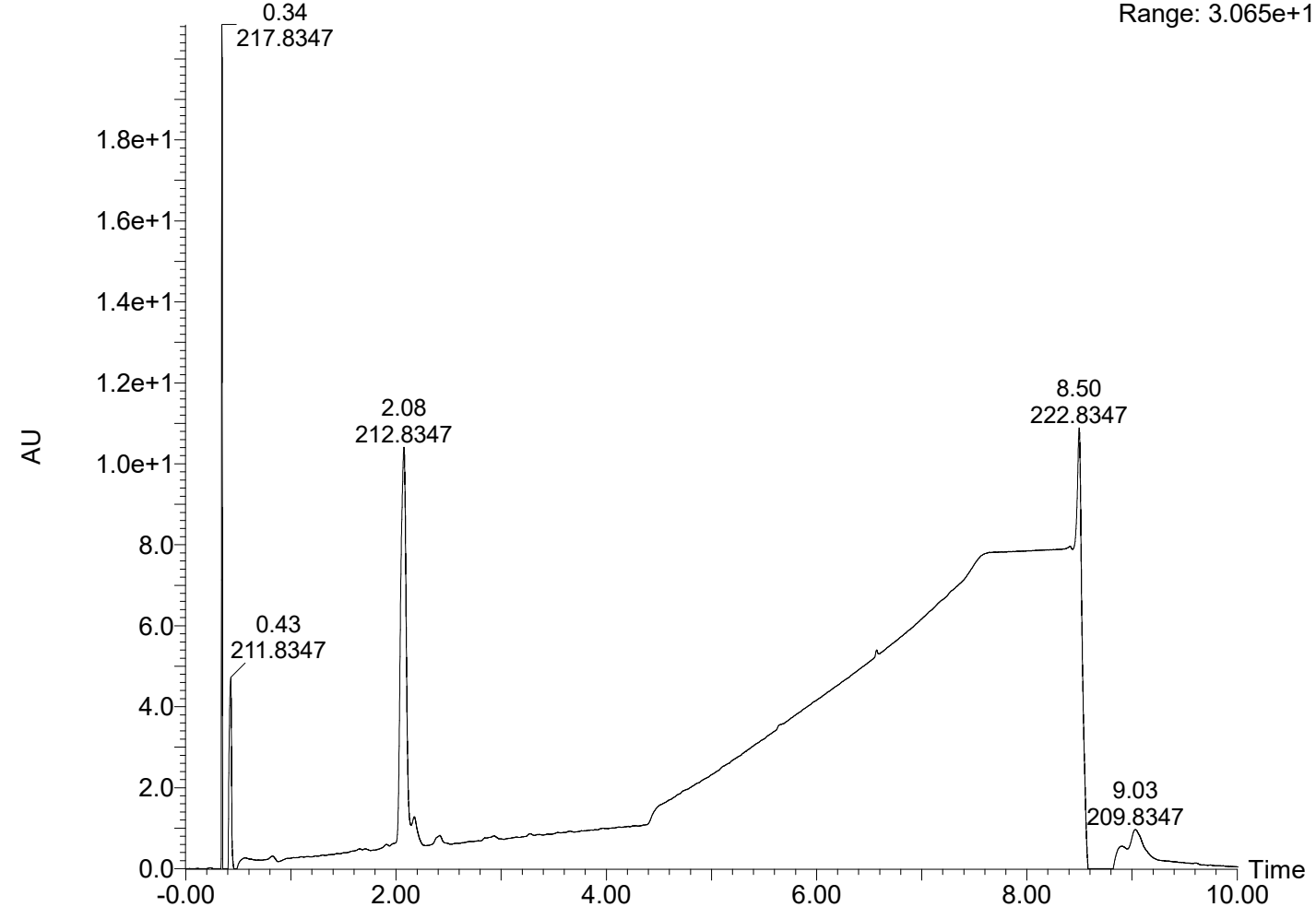
170104\_AA\_MPLC1\_22-5\_NEG

1: TOF MS ES-  
BPI  
4.14e4



170104\_AA\_MPLC1\_22-5\_NEG

3: Diode Array  
Range: 3.065e+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

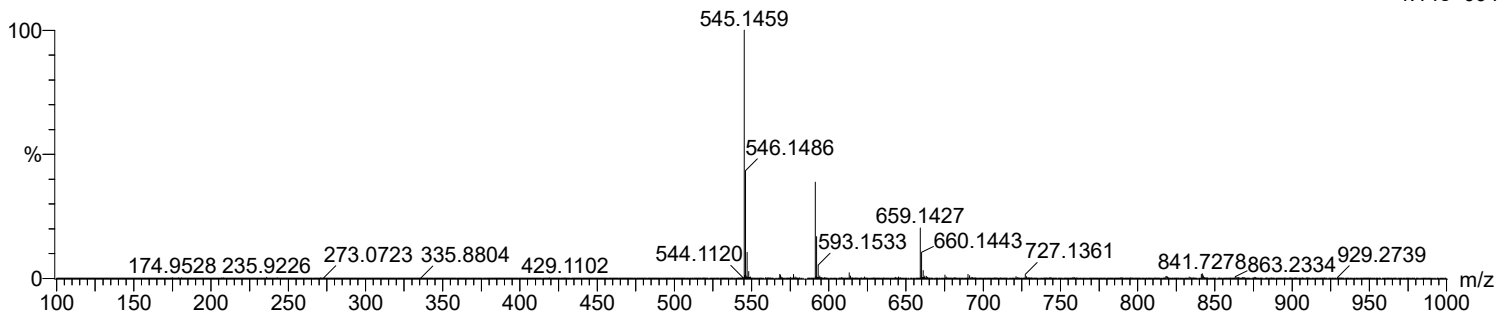
147 formula(e) evaluated with 3 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104\_AA\_MPLC1\_22-5\_NEG 183 (2.131)

1: TOF MS ES-  
4.14e+004

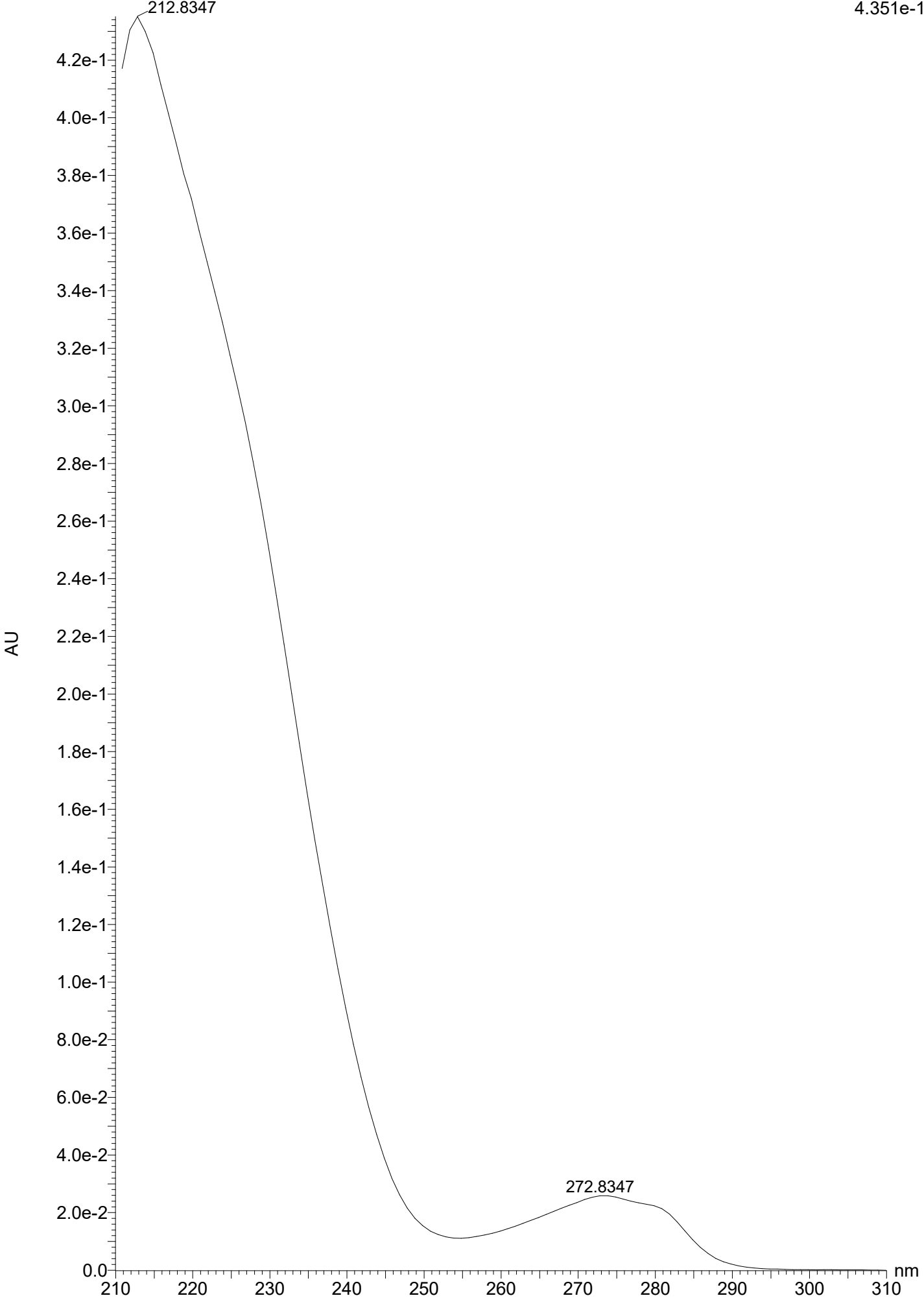
Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
545.1459	545.1448	1.1	2.0	18.5	212.2	2.068	12.65	C30 H25 O10
	545.1506	-4.7	-8.6	9.5	215.9	5.755	0.32	C23 H29 O15
	545.1389	7.0	12.8	27.5	210.2	0.139	87.04	C37 H21 O5

COL31

170104\_AA\_MPLC1\_22-5\_NEG 2484 (2.069)

3: Diode Array  
4.351e-1



# COMPOUND NO. S9 (METHOD B)

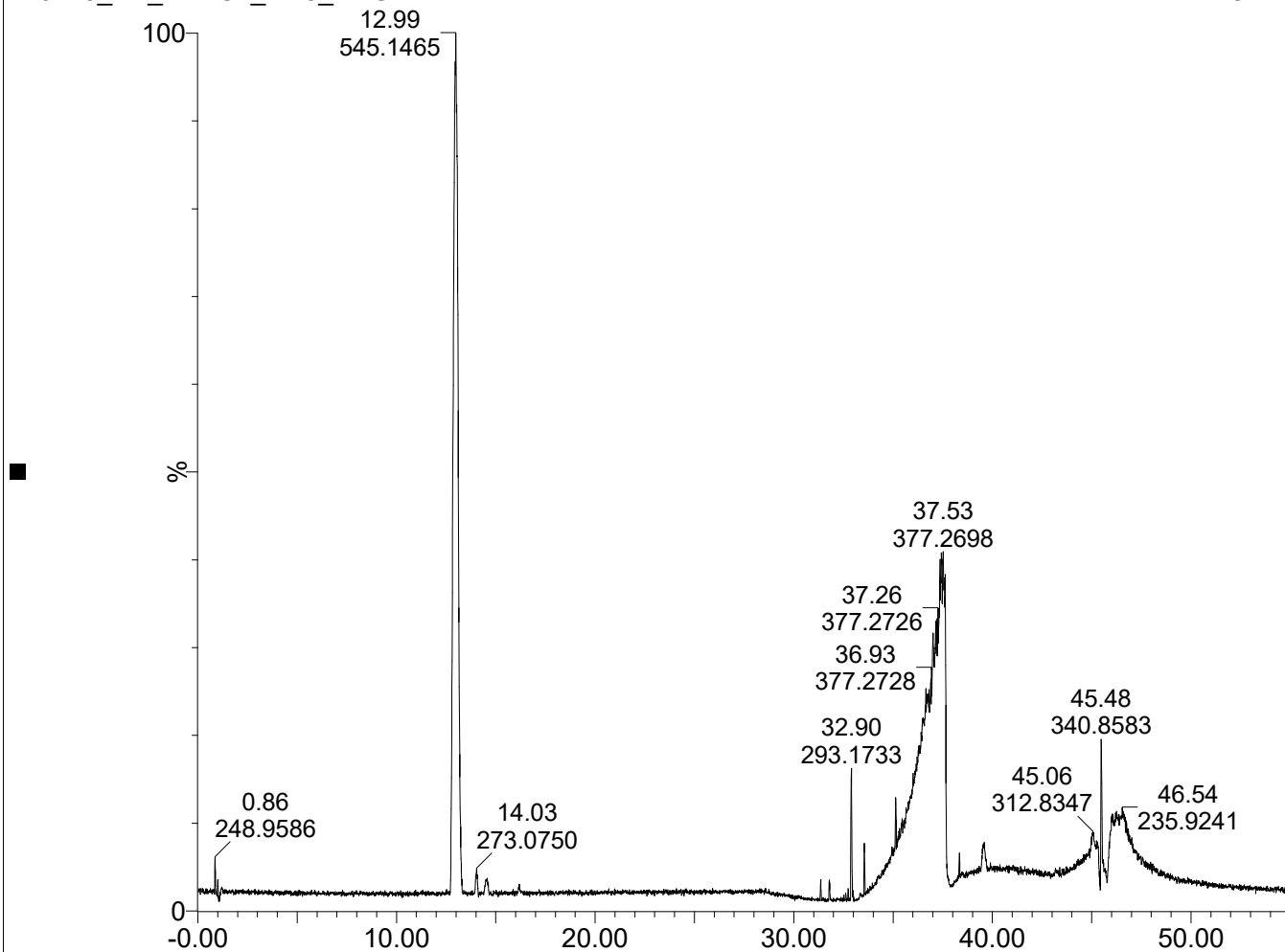
Col 32

170125\_AA\_MPLC1\_22-5\_NEG

1: TOF MS ES-

BPI

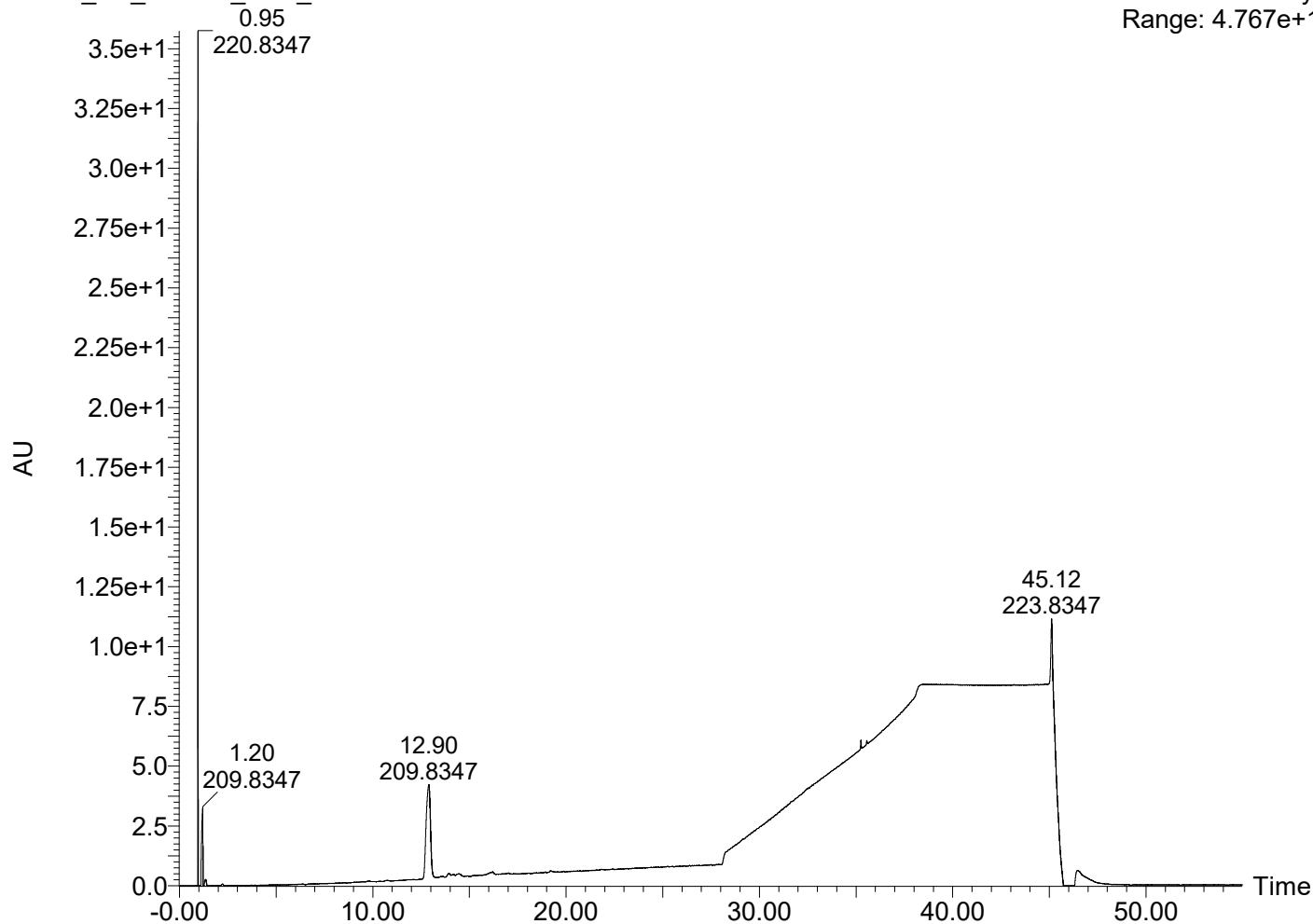
1.24e4



170125\_AA\_MPLC1\_22-5\_NEG

3: Diode Array

Range: 4.767e+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

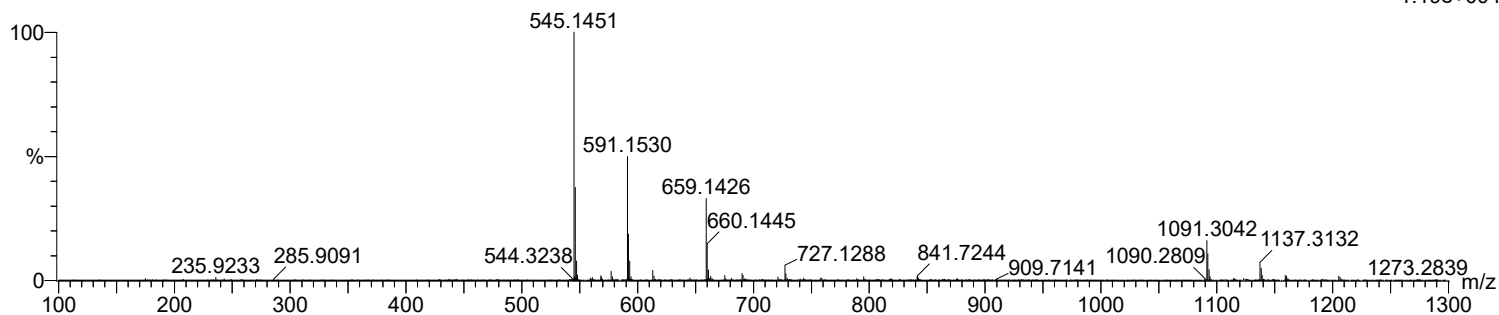
147 formula(e) evaluated with 3 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170125\_AA\_MPLC1\_22-5\_NEG 1103 (12.964)

1: TOF MS ES-  
1.19e+004

Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
545.1451	545.1448	0.3	0.6	18.5	180.2	0.386	67.95	C30 H25 O10
	545.1389	6.2	11.4	27.5	181.0	1.151	31.63	C37 H21 O5
	545.1506	-5.5	-10.1	9.5	185.3	5.480	0.42	C23 H29 O15

Col 32

170125\_AA\_MPLC1\_22-5\_NEG 15454 (12.879)

3: Diode Array  
1.897e-1

