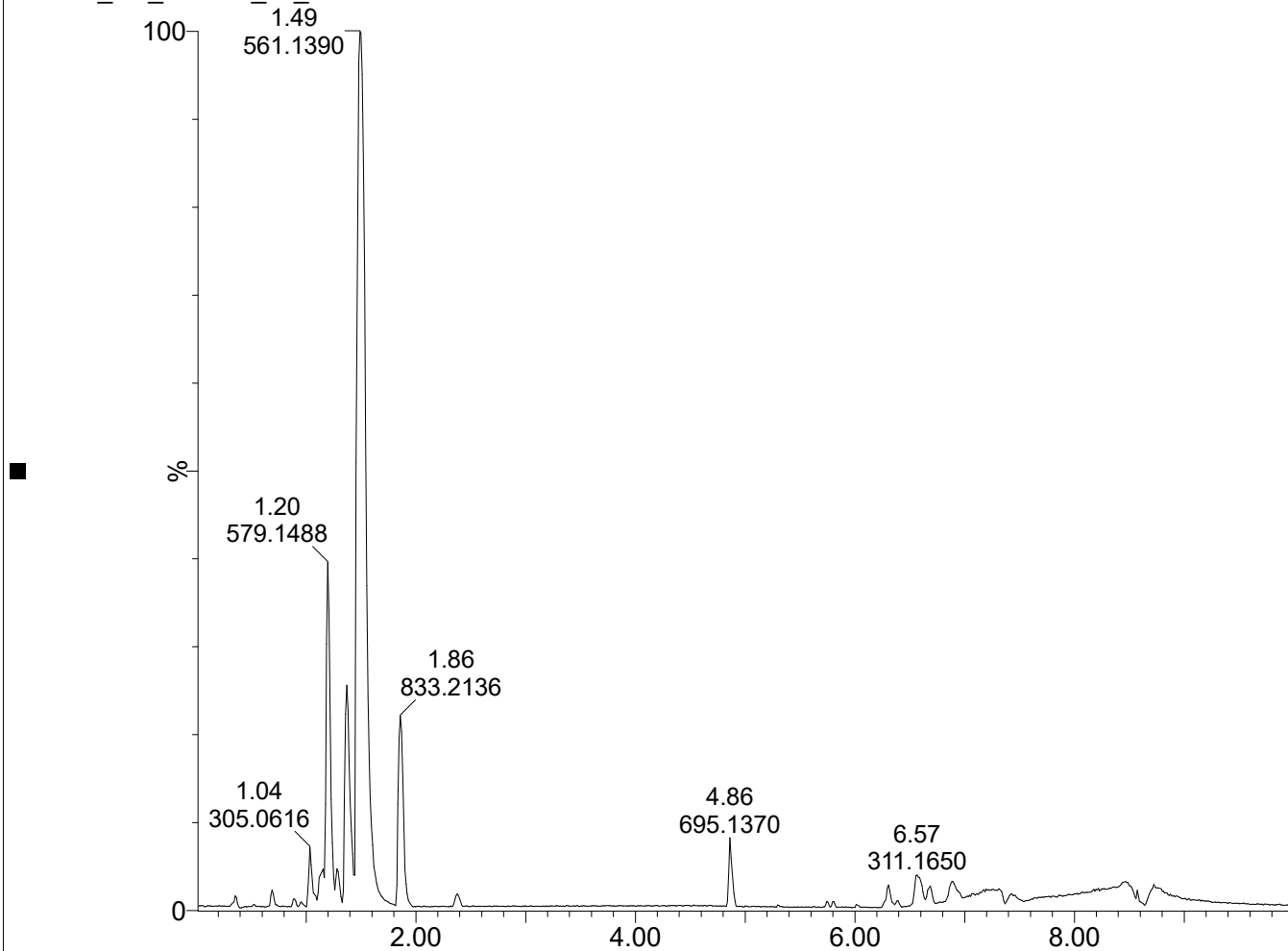


COMPOUND NO. S4 (METHOD A)

COL31

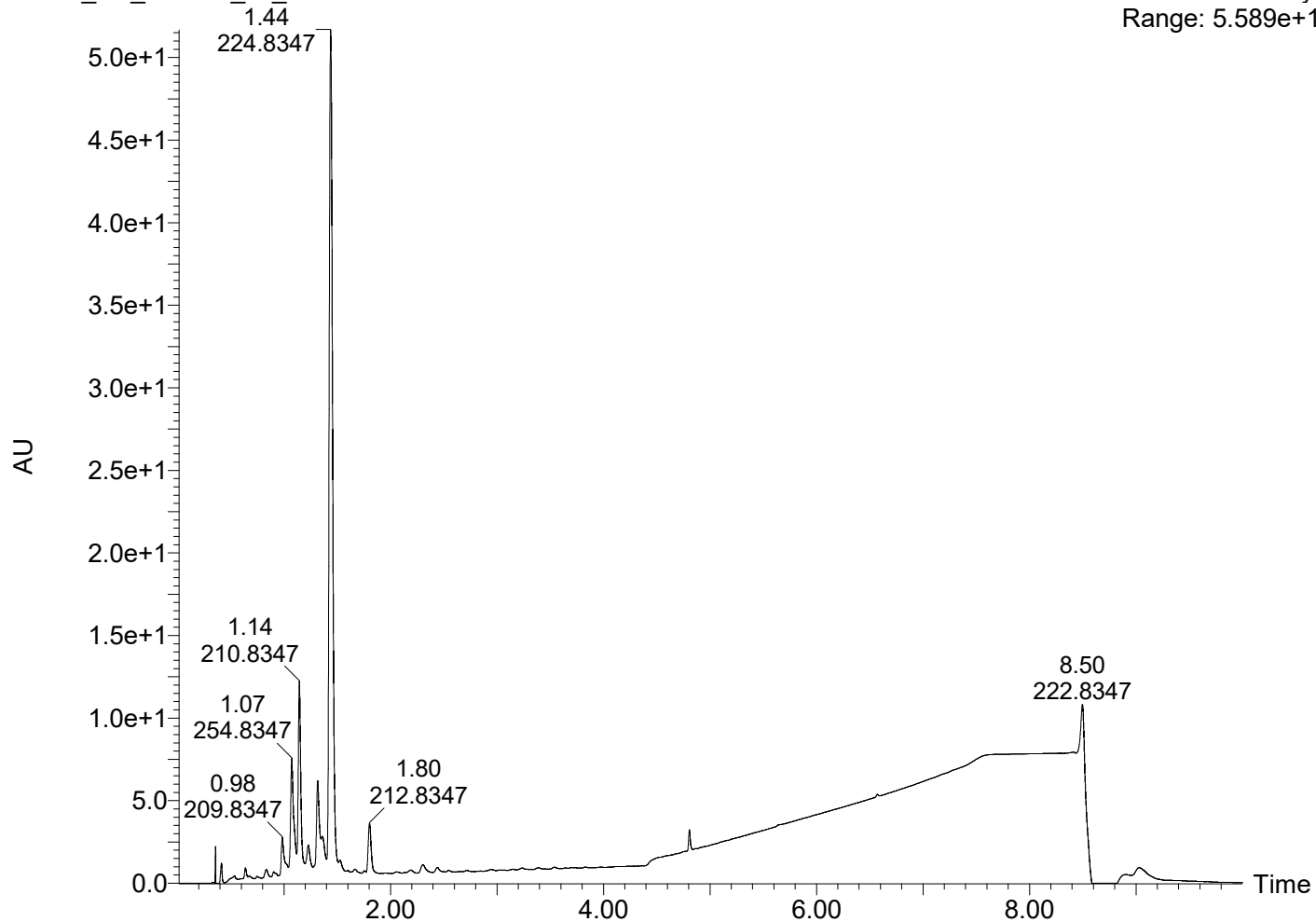
170104_AA_MPLC1_11_NEG

1: TOF MS ES-
BPI
8.38e4



170104_AA_MPLC1_11_NEG

3: Diode Array
Range: 5.589e+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

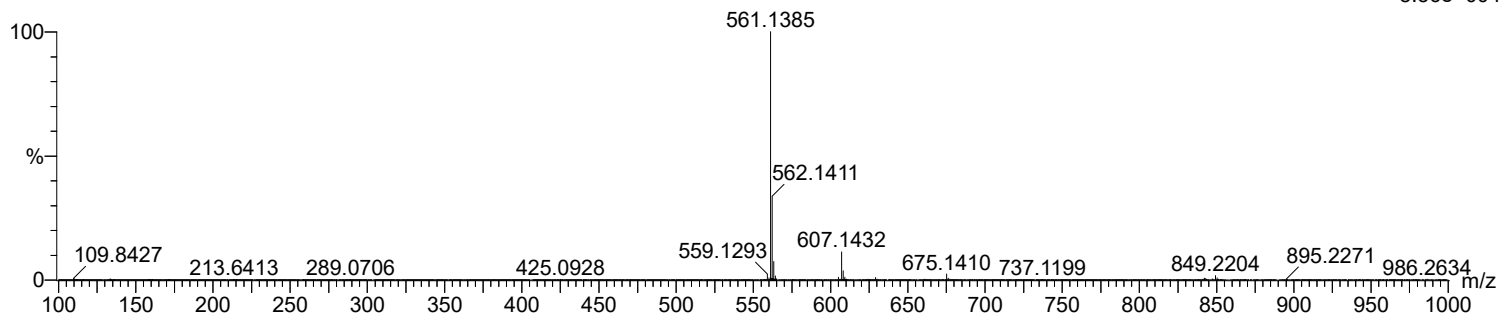
105549 formula(e) evaluated with 794 results within limits (up to 5 best isotopic matches for each mass)

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_11_NEG 129 (1.500)

1: TOF MS ES-
8.36e+004

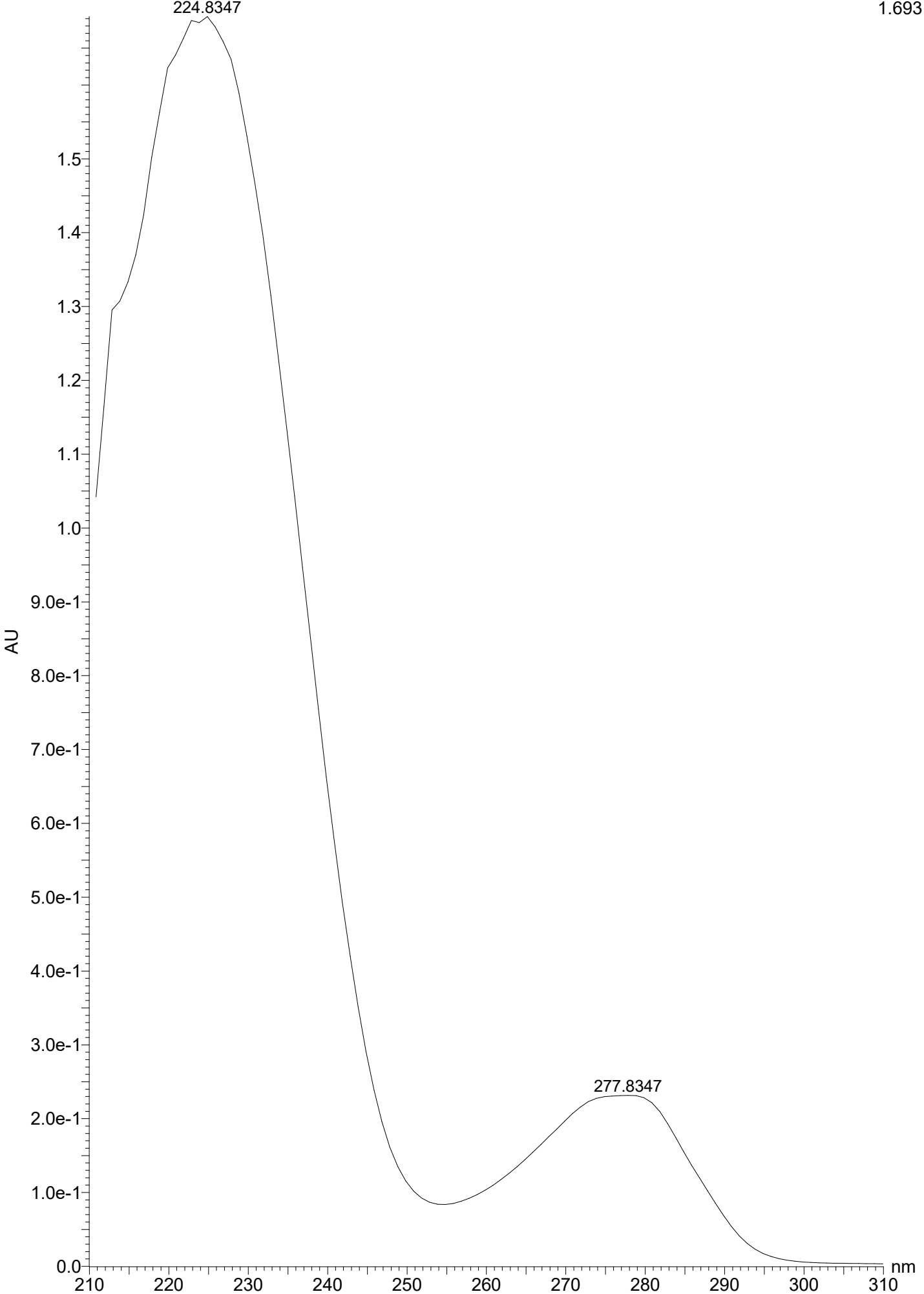
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
561.1385	561.1397	-1.2	-2.1	18.5	210.4	0.024	97.59	C30 H25 O11
	561.1410	-2.5	-4.5	23.5	214.6	4.156	1.57	C31 H21 N4 O7
	561.1383	0.2	0.4	24.5	215.5	5.120	0.60	C27 H17 N10 O5
	561.1370	1.5	2.7	19.5	216.9	6.450	0.16	C26 H21 N6 O9
	561.1397	-1.2	-2.1	29.5	217.4	7.020	0.09	C28 H13 N14 O

COL31

170104_AA_MPLC1_11_NEG 1728 (1.439)

3: Diode Array
1.693

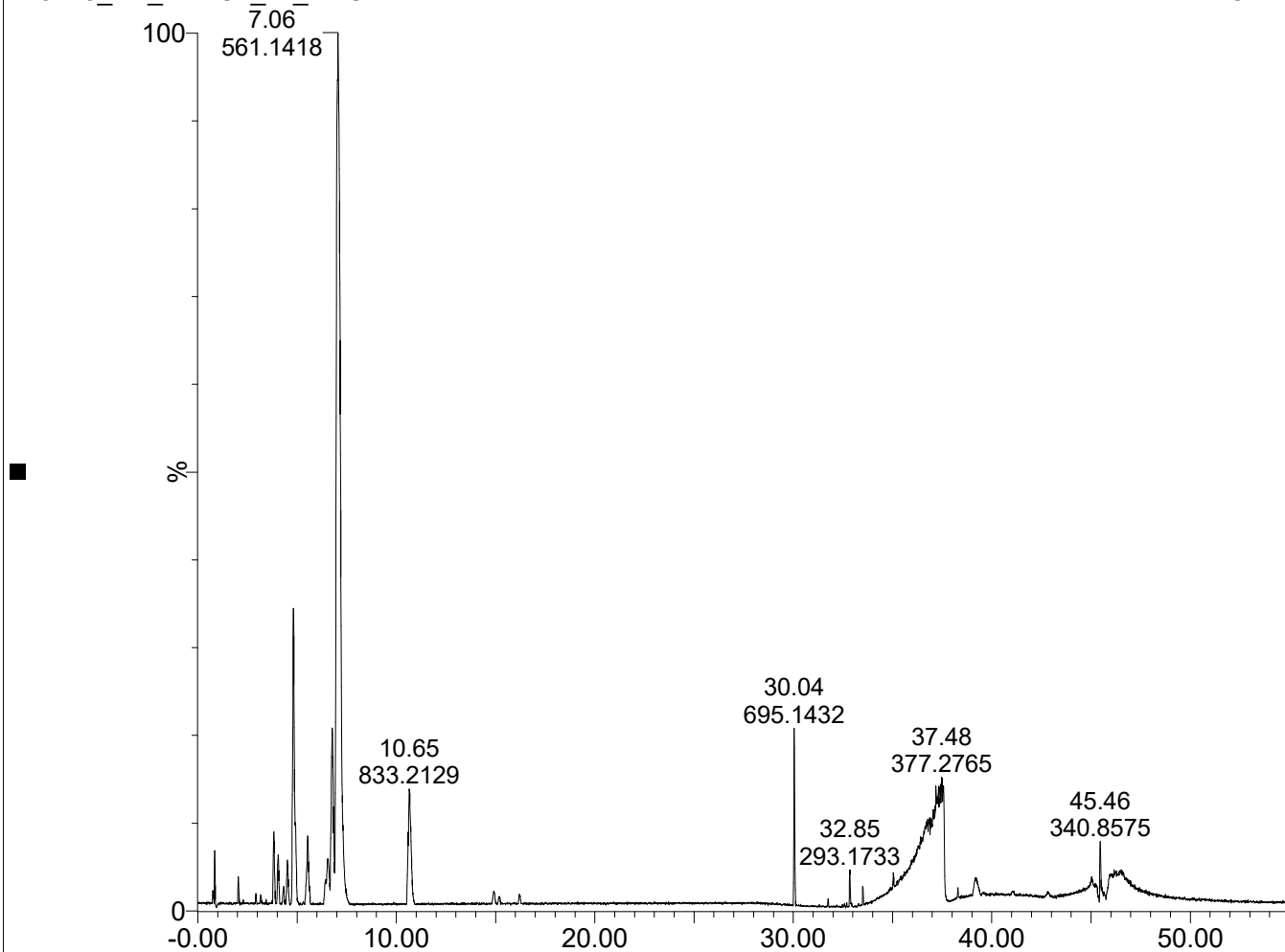


COMPOUND NO. S4 (METHOD B)

Col 32

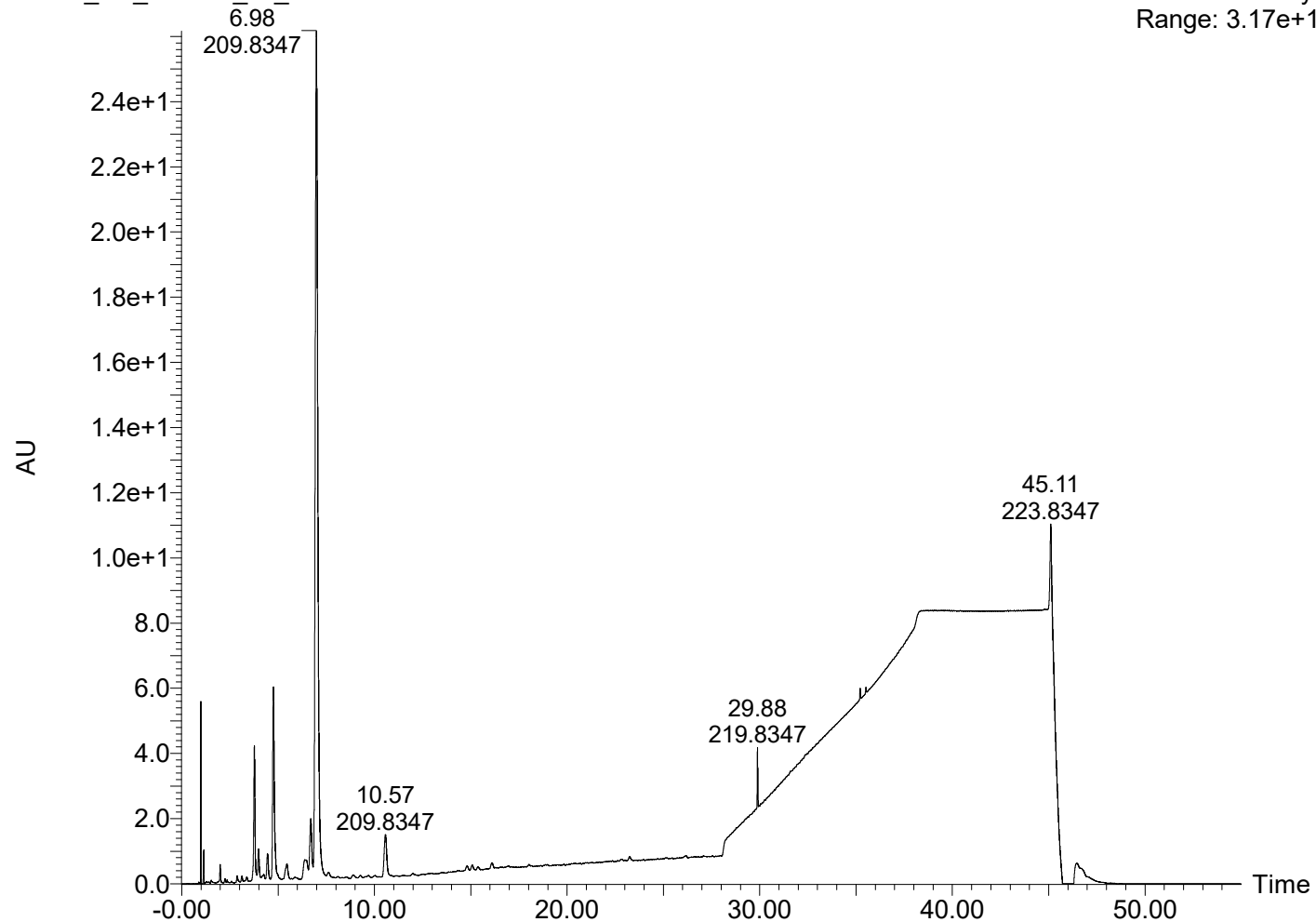
170125_AA_MPLC1_11_NEG

1: TOF MS ES-
BPI
3.00e4



170125_AA_MPLC1_11_NEG

3: Diode Array
Range: 3.17e+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

154 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)

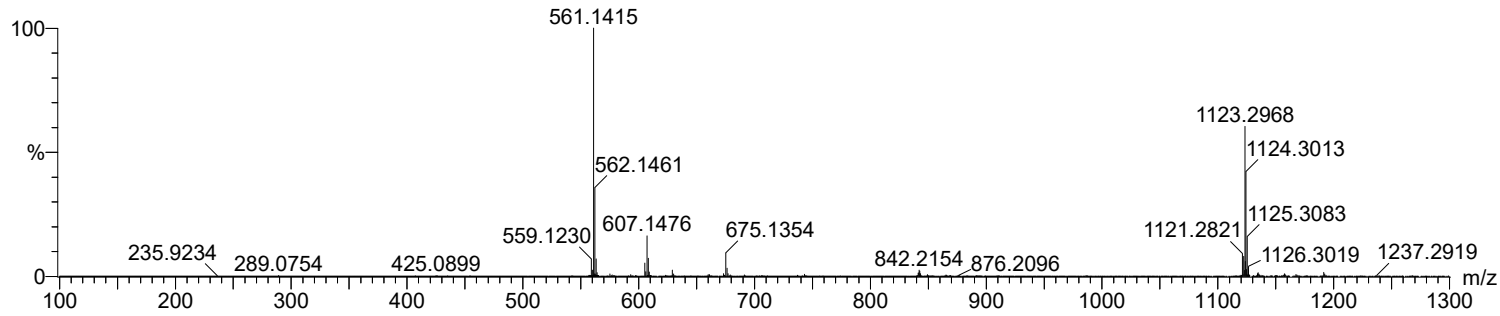
Elements Used:

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

Col 32

170125_AA_MPLC1_11_NEG 601 (7.054)

1: TOF MS ES-
2.97e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
561.1415	561.1397	1.8	3.2	18.5	190.6	0.031	96.92	C30 H25 O11
561.1338		7.7	13.7	27.5	194.5	3.888	2.05	C37 H21 O6
561.1491		-7.6	-13.5	31.5	195.8	5.218	0.54	C41 H21 O3
561.1456		-4.1	-7.3	9.5	195.9	5.321	0.49	C23 H29 O16

Col 32

170125_AA_MPLC1_11_NEG 8368 (6.973)

3: Diode Array
1.029

