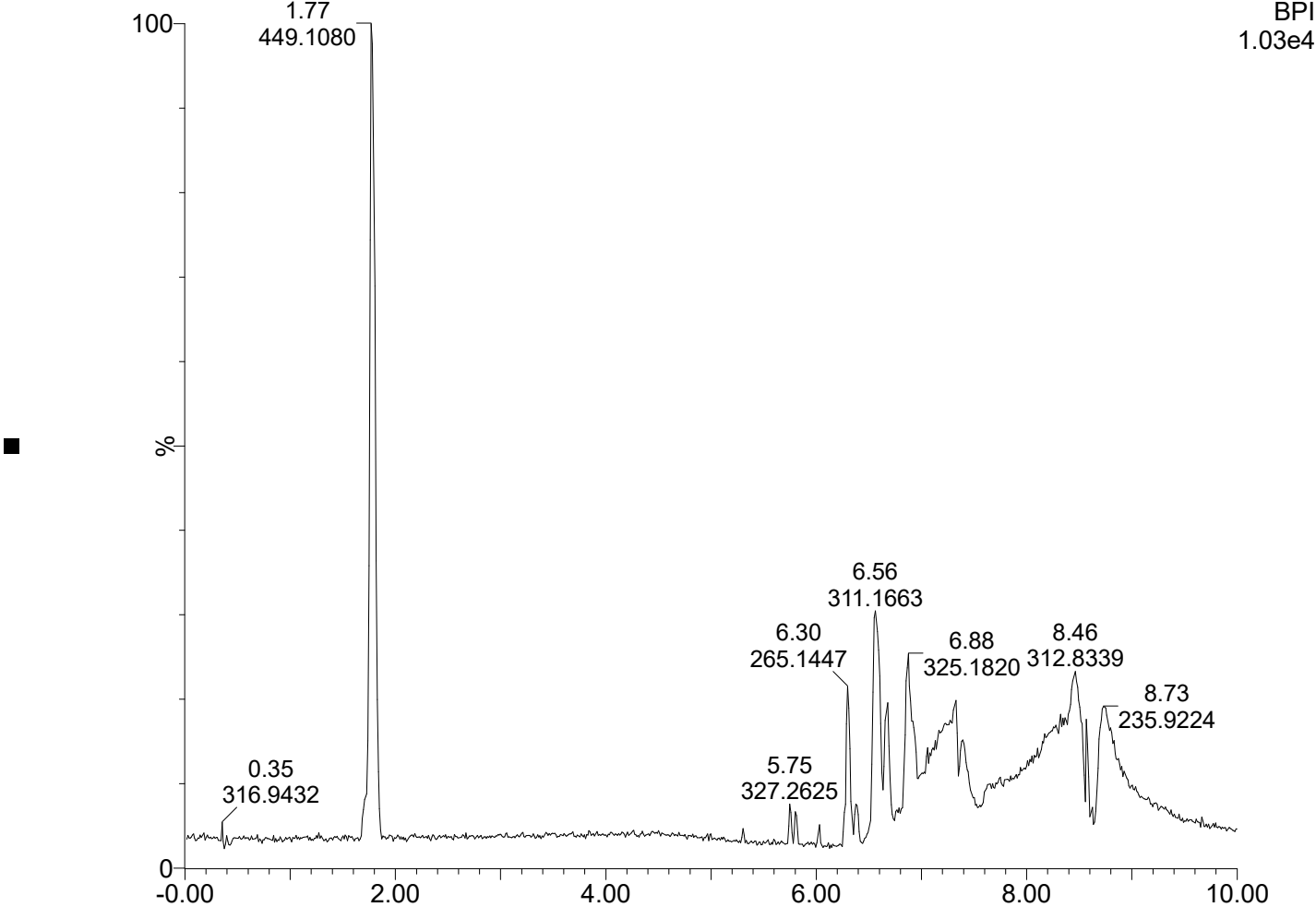


COMPOUND NO. S7 (METHOD A)

COL31

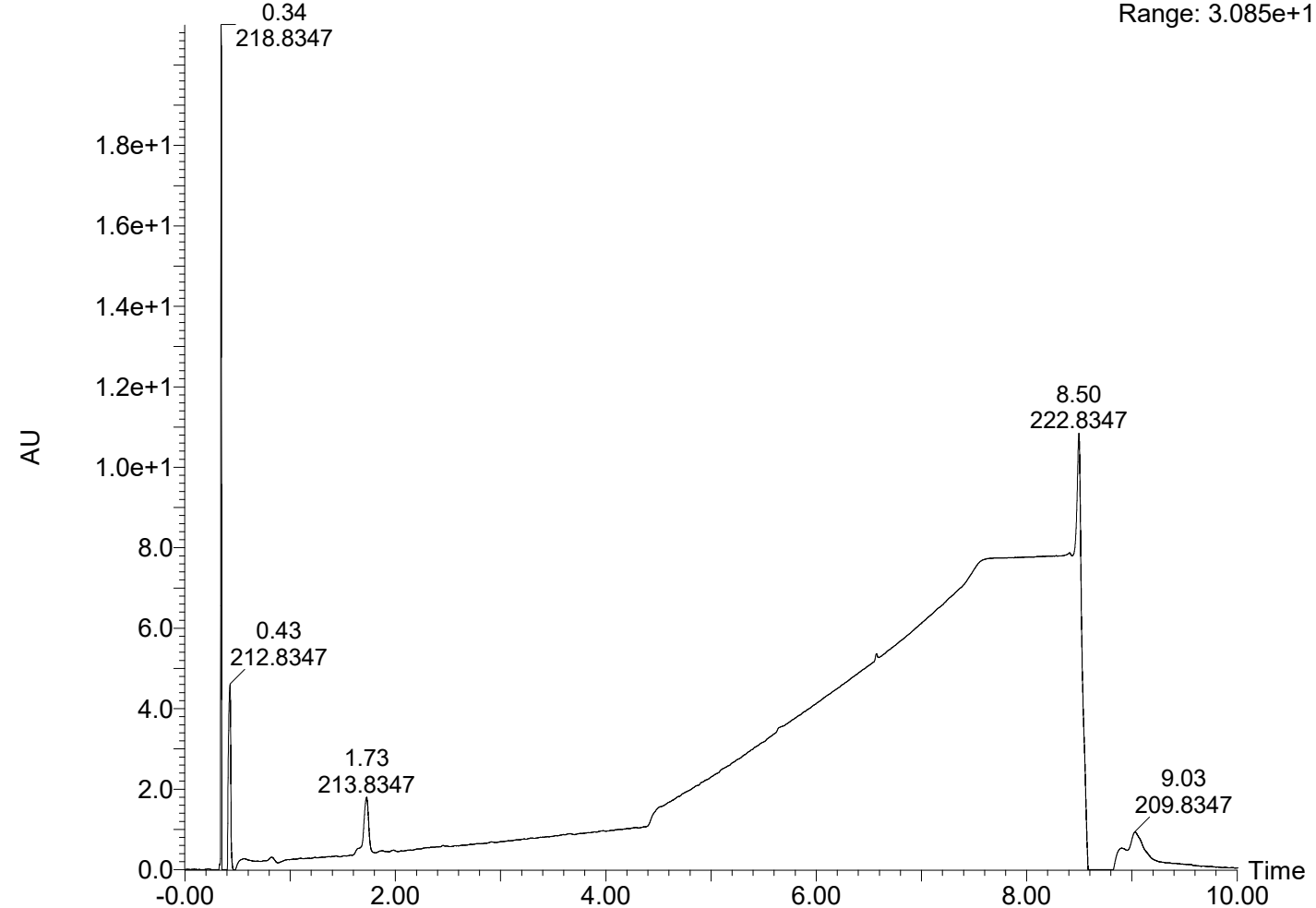
170104_AA_NK_PLC5-FC-3AA_NEG

1: TOF MS ES-
BPI
1.03e4



170104_AA_NK_PLC5-FC-3AA_NEG

3: Diode Array
Range: 3.085e+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

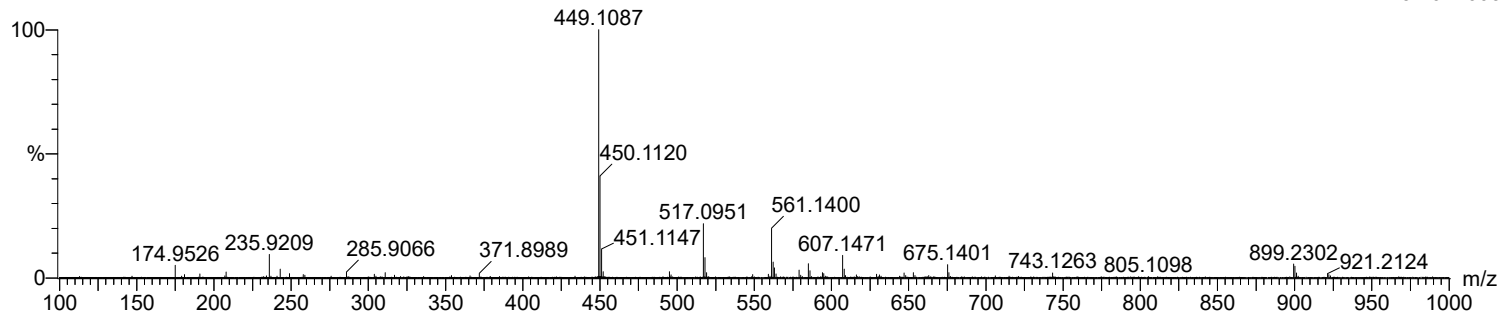
38432 formula(e) evaluated with 291 results within limits (up to 5 best isotopic matches for each mass)

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_NK_PLC5-FC-3AA_NEG 151 (1.749)

1: TOF MS ES-
3.70e+003



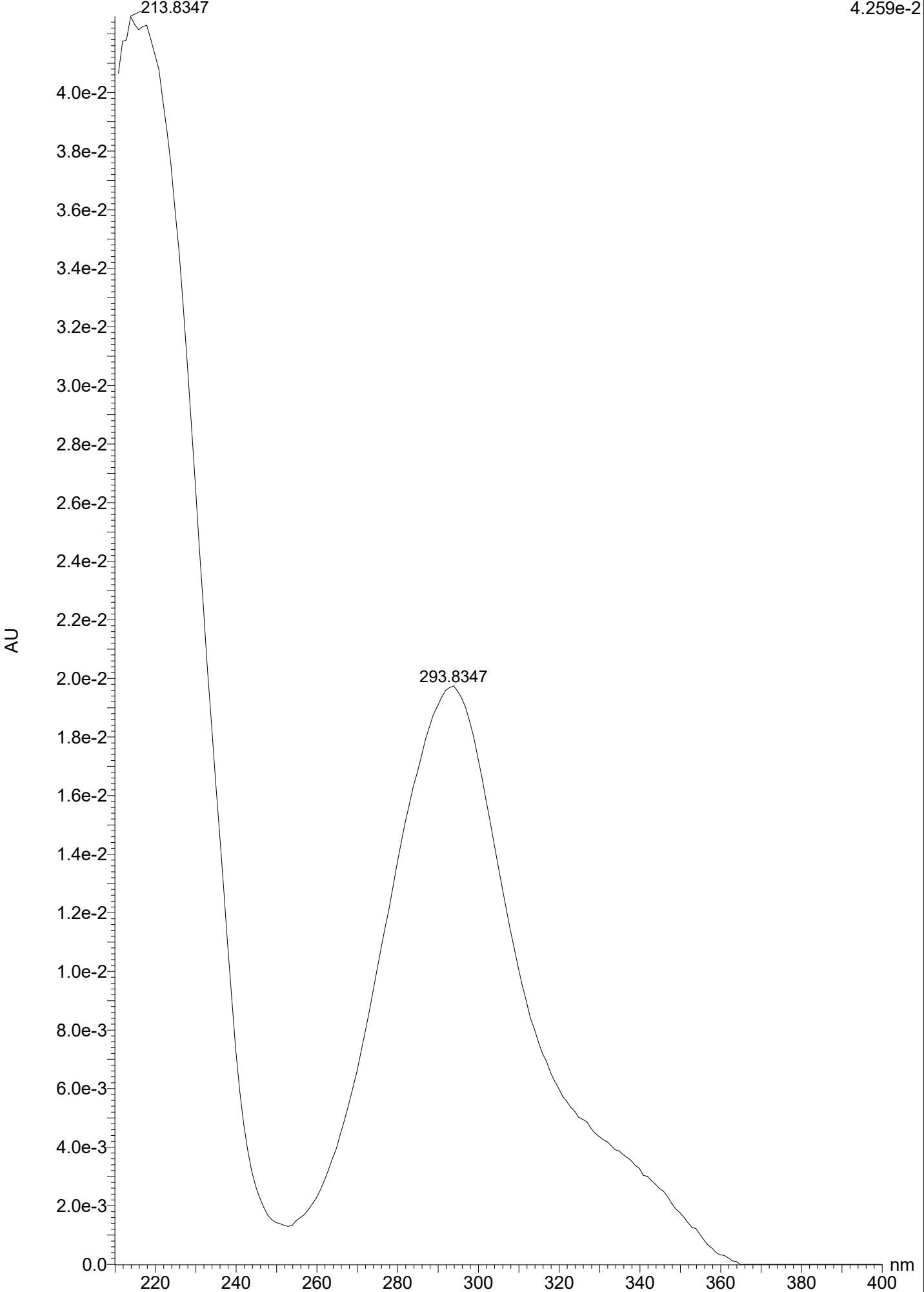
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
449.1087	449.1084	0.3	0.7	11.5	119.0	3.661	2.57	C21 H21 O11
	449.1079	0.8	1.8	29.5	115.7	0.369	69.12	C34 H13 N2
	449.1097	-1.0	-2.2	16.5	118.8	3.449	3.18	C22 H17 N4 O7
	449.1111	-2.4	-5.3	21.5	119.0	3.717	2.43	C23 H13 N8 O3
	449.1112	-2.5	-5.6	24.5	116.8	1.483	22.70	C31 H17 N2 S

COL31

170104_AA_NK_PLC5-FC-3AA_NEG 2073 (1.727)

3: Diode Array
4.259e-2

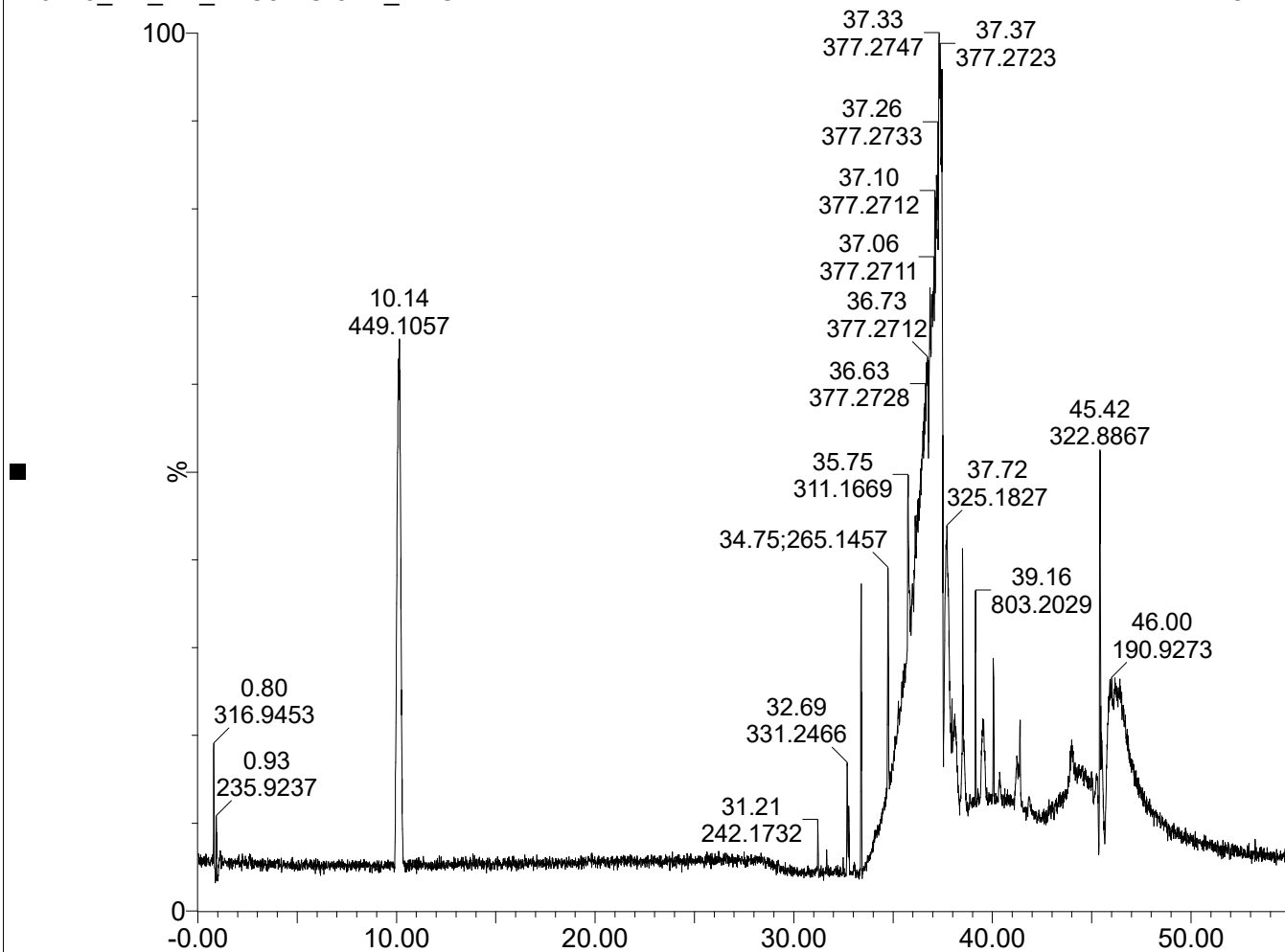


COMPOUND NO. S7 (METHOD B)

Col 32

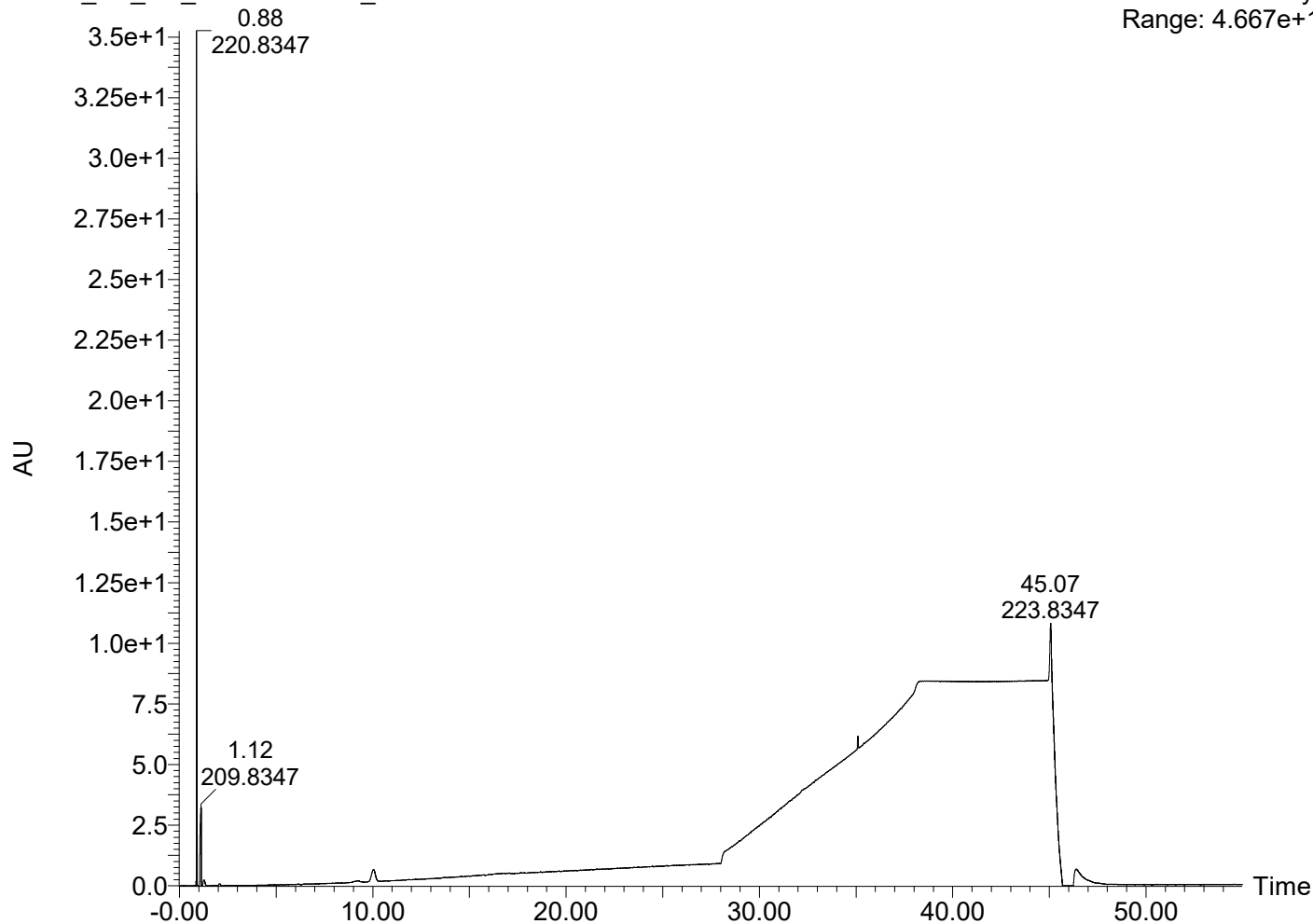
170123_AA_NK_PLC5-FC-3AA_NEG

1: TOF MS ES-
BPI
5.02e3



170123_AA_NK_PLC5-FC-3AA_NEG

3: Diode Array
Range: 4.667e+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

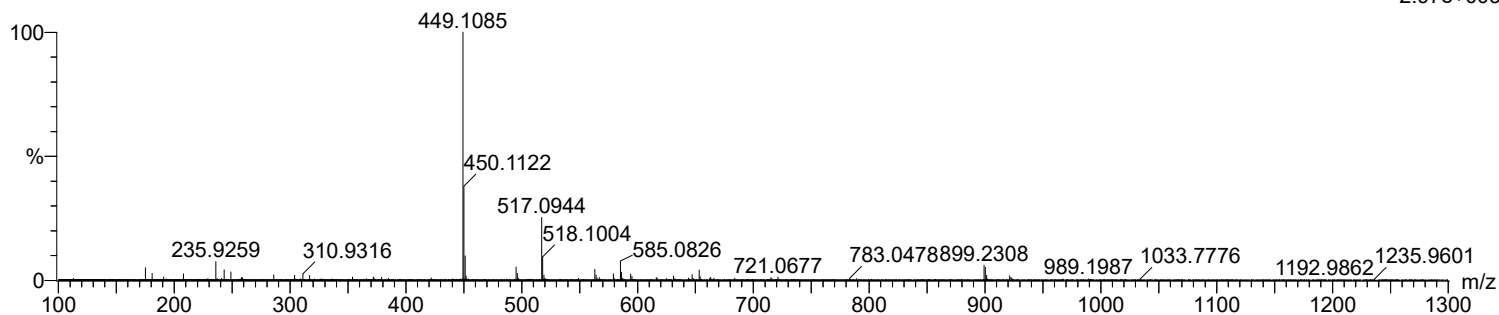
105 formula(e) evaluated with 3 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170123_AA_NK_PLC5-FC-3AA_NEG 858 (10.084)

1: TOF MS ES-
2.97e+003

Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
449.1085	449.1084	0.1	0.2	11.5	112.5	0.361	69.71	C21 H21 O11
	449.1025	6.0	13.4	20.5	113.4	1.234	29.12	C28 H17 O6
	449.1143	-5.8	-12.9	2.5	116.6	4.450	1.17	C14 H25 O16

Col 32

170123_AA_NK_PLC5-FC-3AA_NEG 12035 (10.030)

3: Diode Array
1.55e-2

