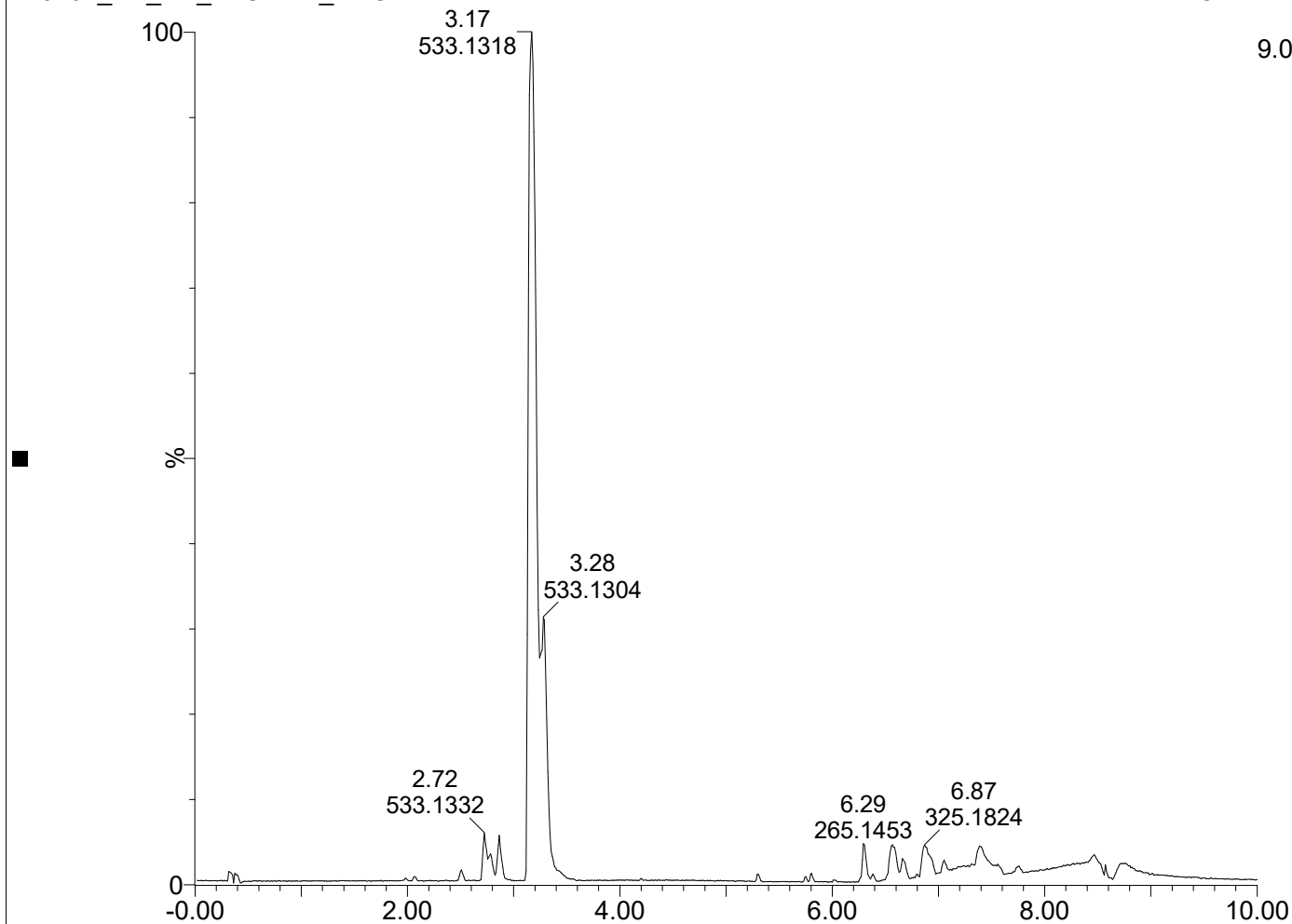


COMPOUND NO. S22 (METHOD A)

COL31

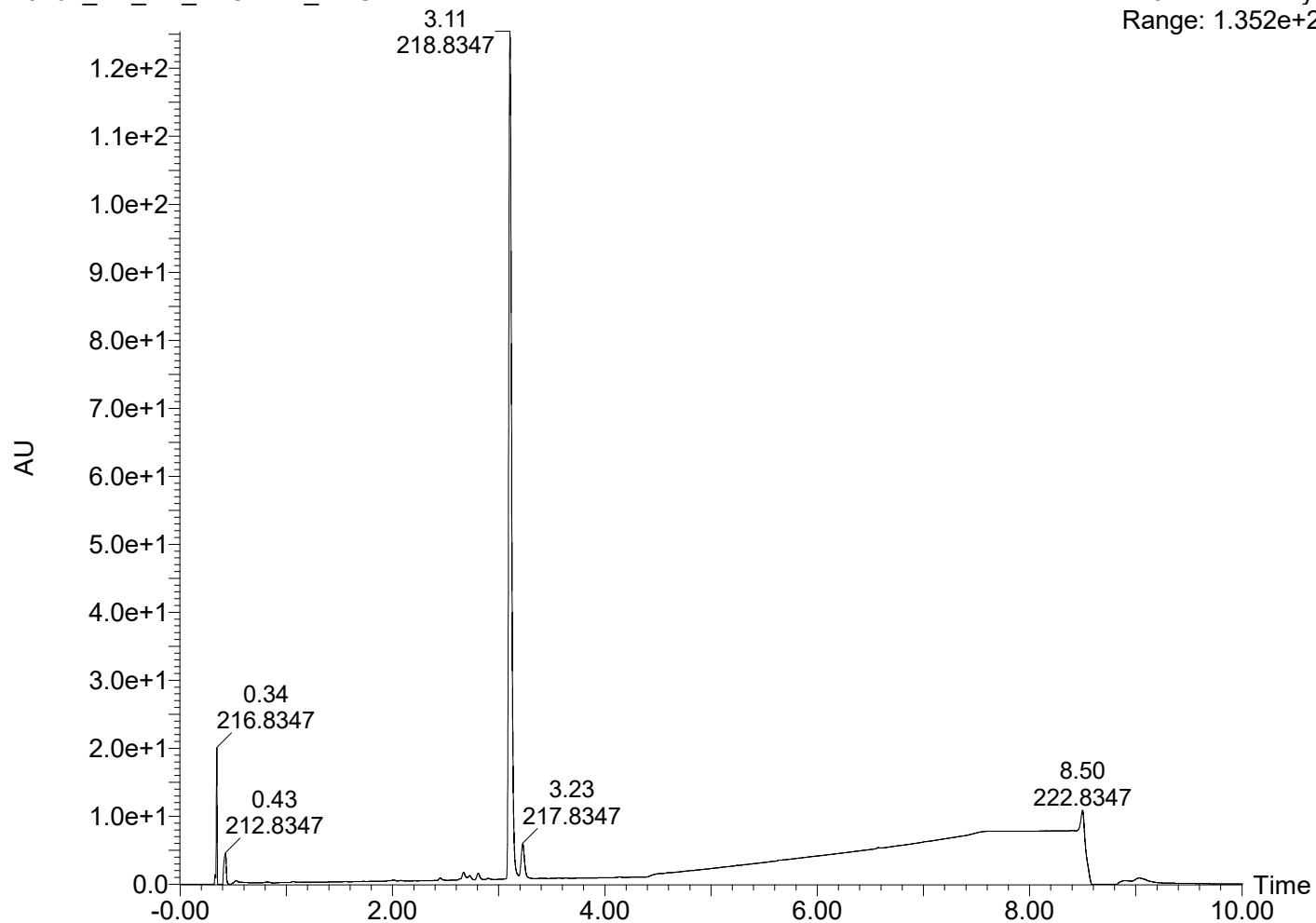
170104_AA_NK_PLC7-FD_NEG

1: TOF MS ES-
BPI
9.03e4



170104_AA_NK_PLC7-FD_NEG

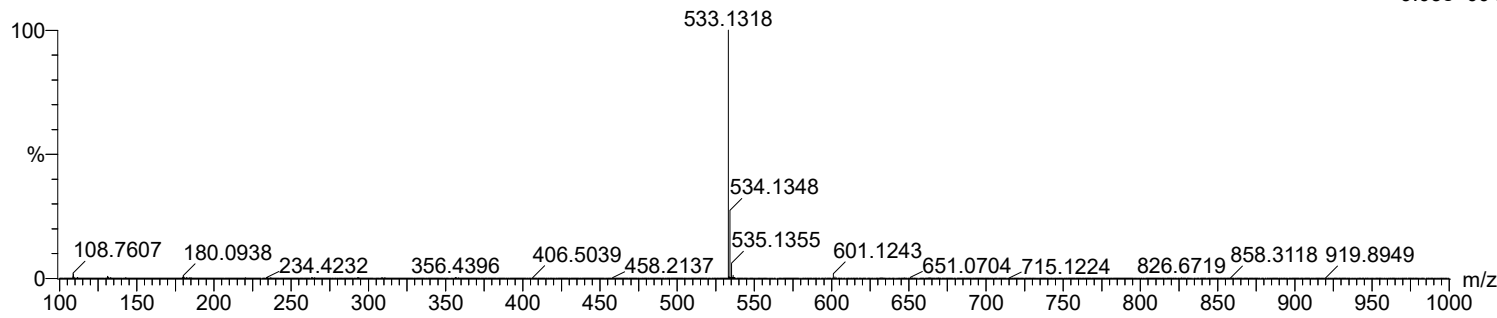
3: Diode Array
Range: 1.352e+2



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
141 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
COL31
170104_AA_NK_PLC7-FD_NEG 273 (3.169)

1: TOF MS ES-
9.03e+004



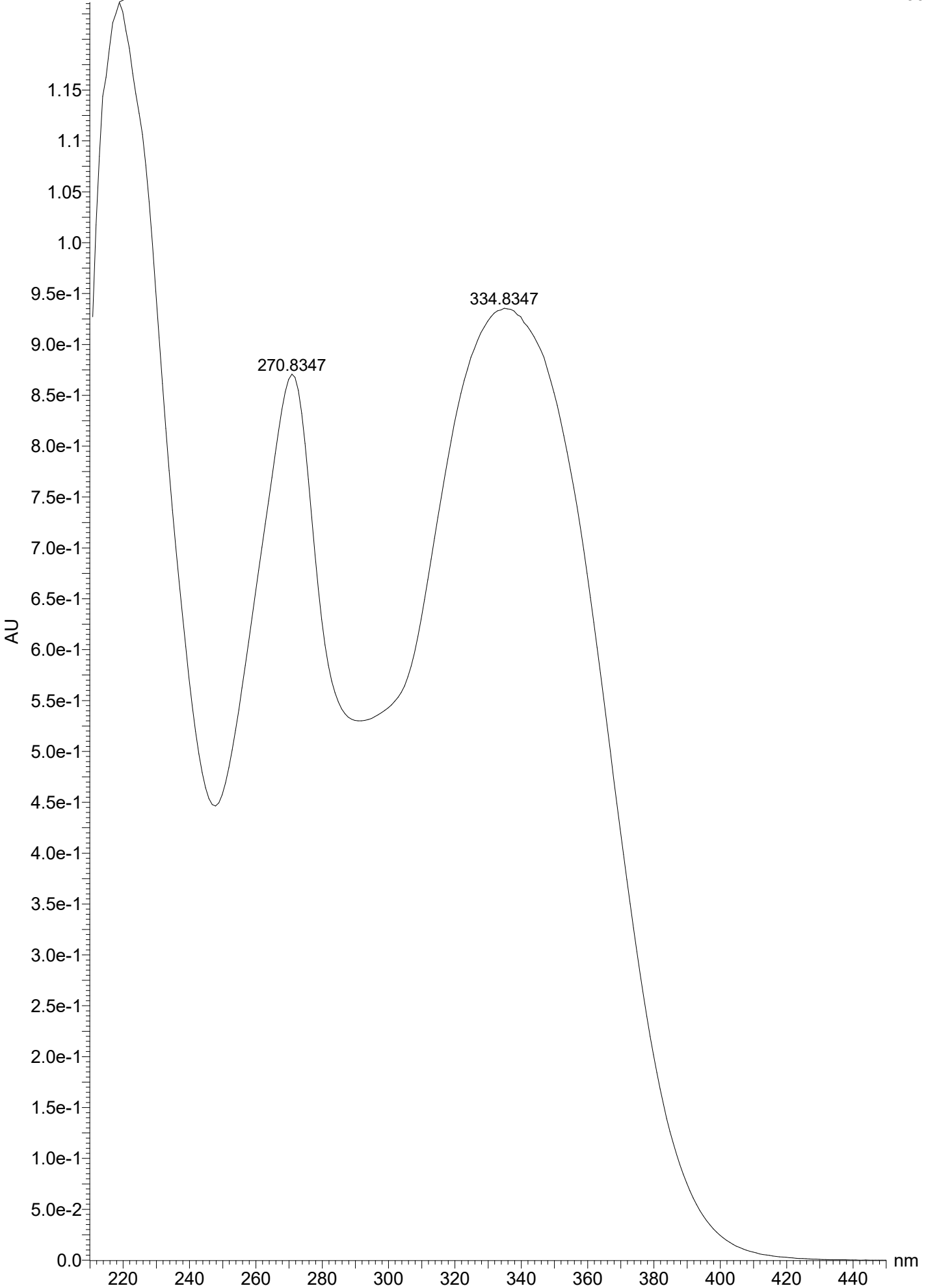
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
533.1318	533.1295	2.3	4.3	13.5	228.3	0.001	99.90	C25 H25 O13
533.1354		-3.6	-6.8	4.5	235.2	6.886	0.10	C18 H29 O18
533.1389		-7.1	-13.3	26.5	239.8	11.460	0.00	C36 H21 O5
533.1330		-1.2	-2.3	35.5	241.0	12.675	0.00	C43 H17

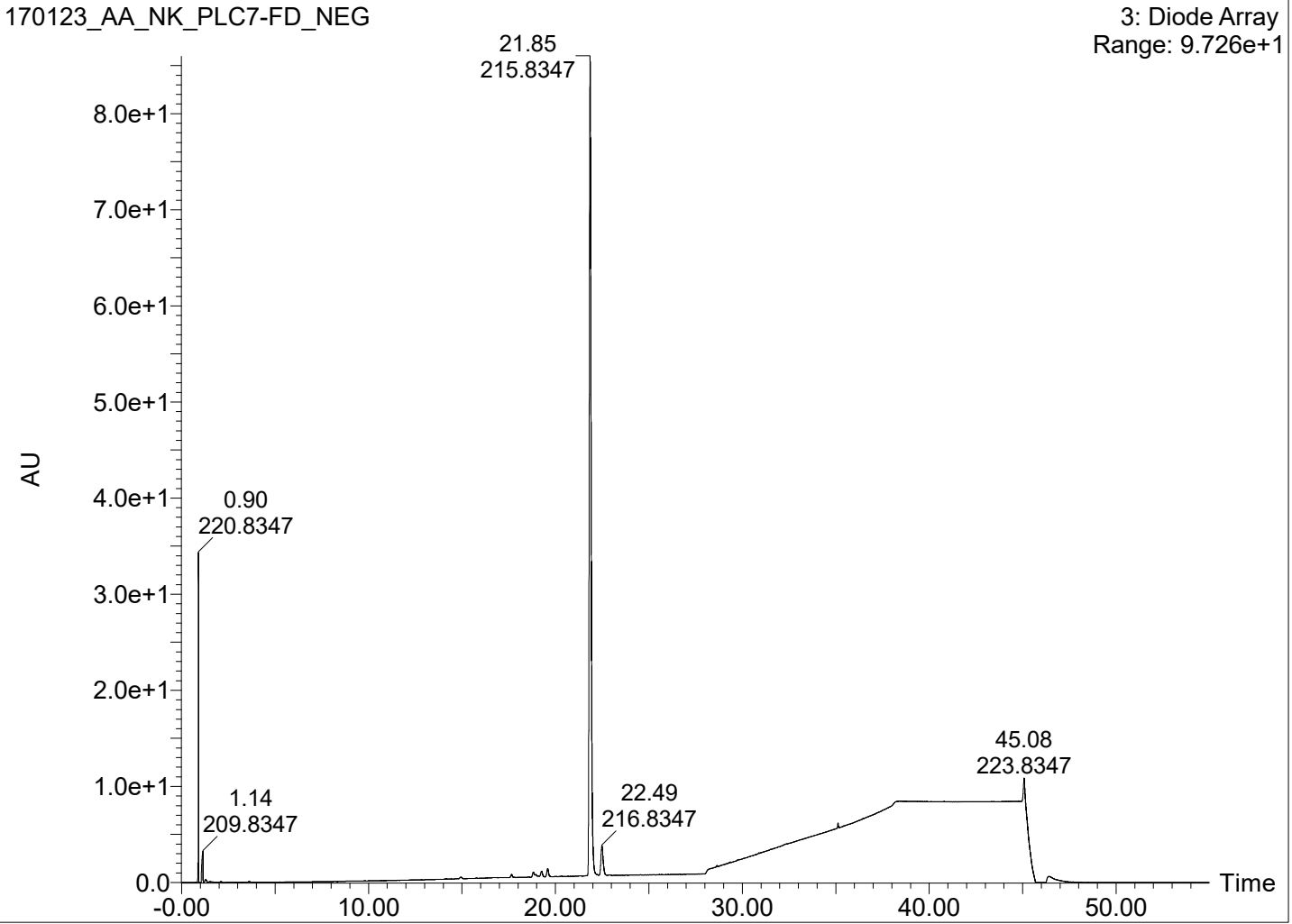
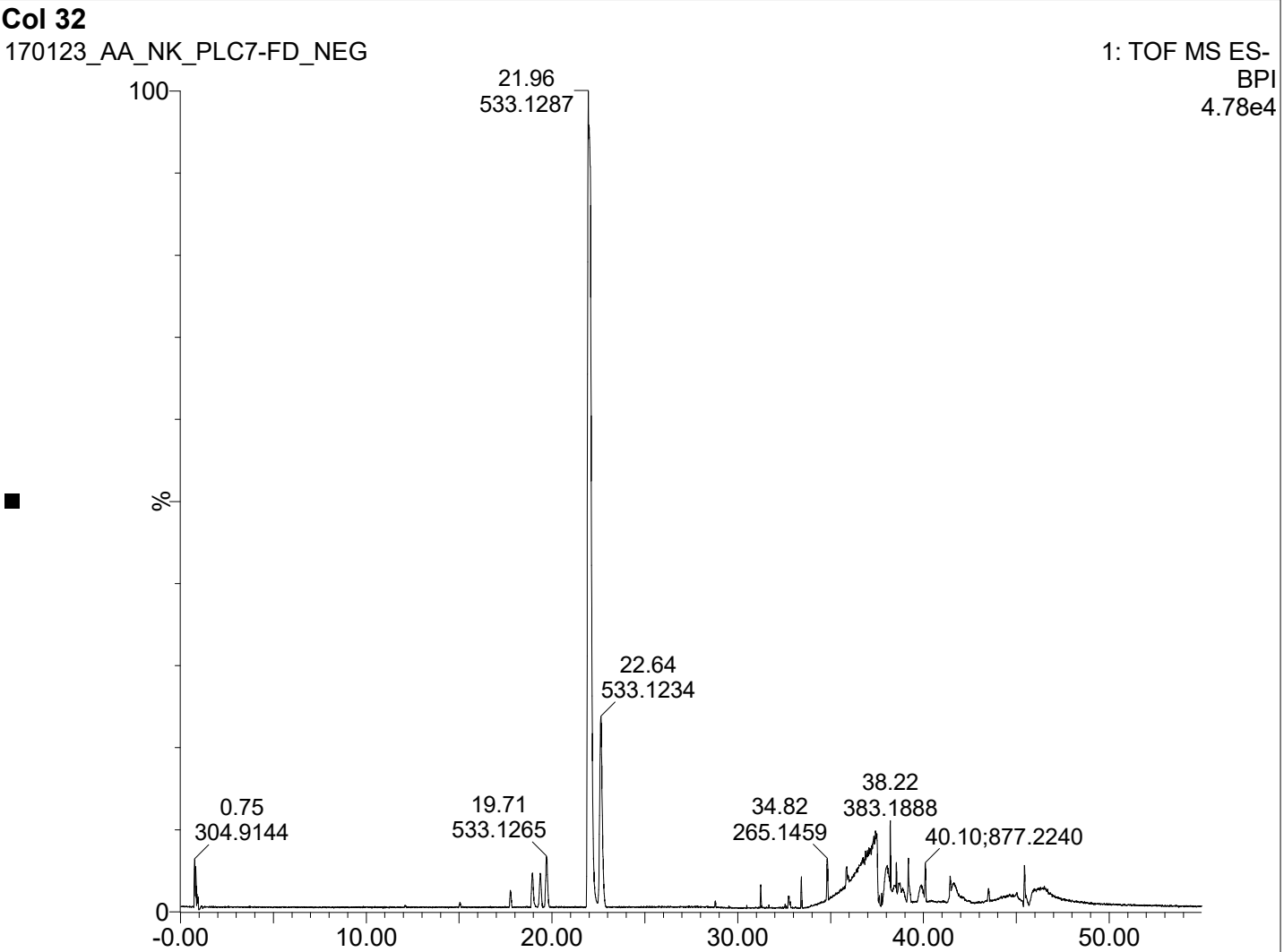
COL31

170104_AA_NK_PLC7-FD_NEG 3728 (3.106)

3: Diode Array
1.236



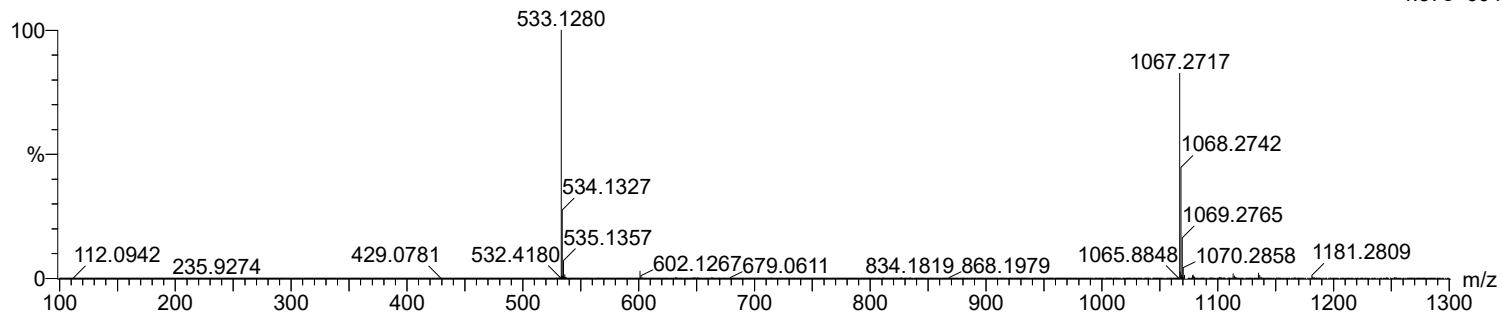
COMPOUND NO. S22 (METHOD B)



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
141 formula(e) evaluated with 5 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_PLC7-FD_NEG 1873 (21.998)

1: TOF MS ES-
4.57e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
533.1280	533.1295	-1.5	-2.8	13.5	211.9	0.001	99.90	C25 H25 O13
	533.1236	4.4	8.3	22.5	219.1	7.217	0.07	C32 H21 O8
	533.1354	-7.4	-13.9	4.5	220.4	8.587	0.02	C18 H29 O18
	533.1330	-5.0	-9.4	35.5	221.8	9.975	0.00	C43 H17
	533.1201	7.9	14.8	0.5	223.1	11.238	0.00	C14 H29 O21

Col 32

170123_AA_NK_PLC7-FD_NEG 26212 (21.846)

3: Diode Array
9.178e-1

