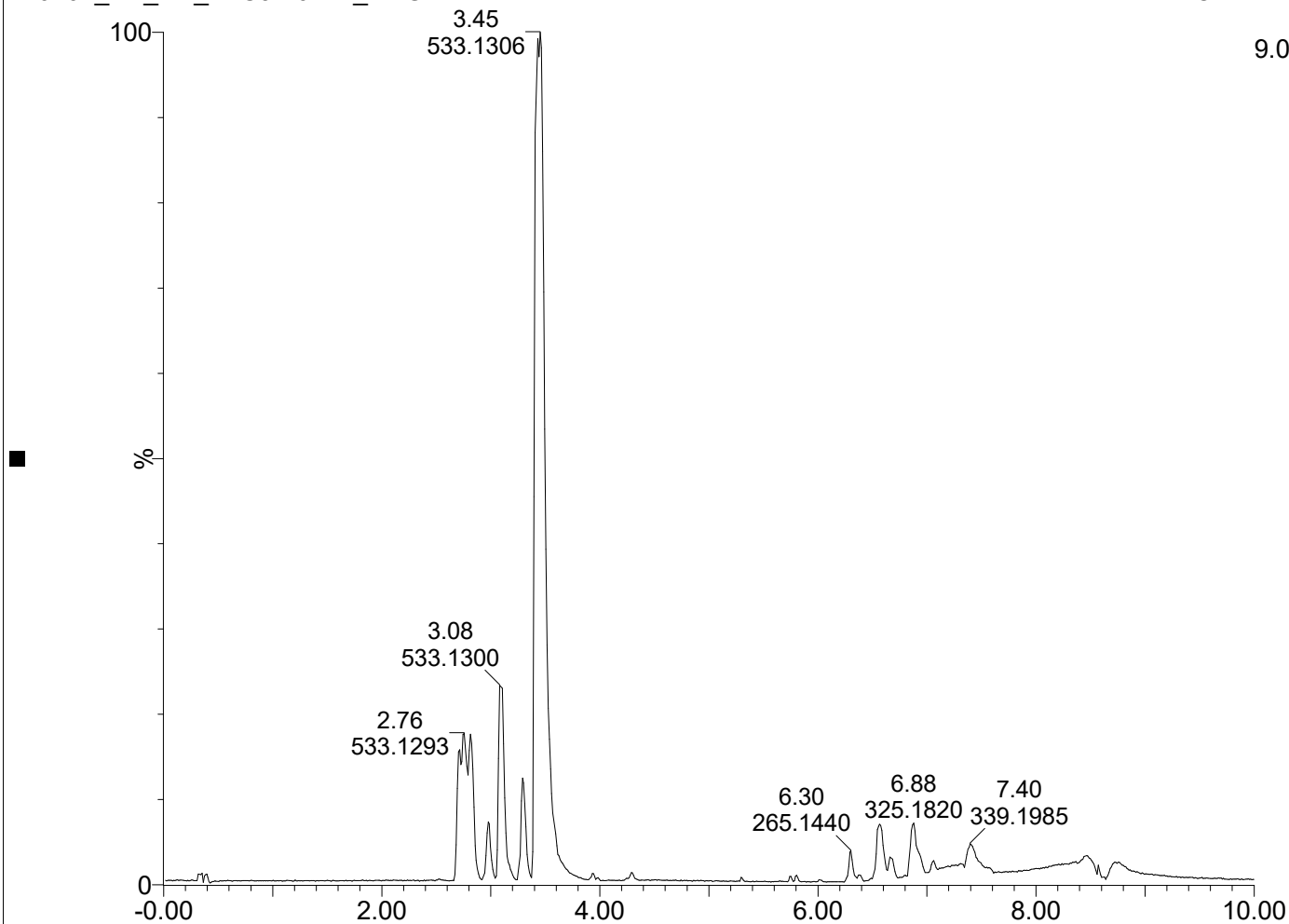


COMPOUND NO. S23 (METHOD A)

COL31

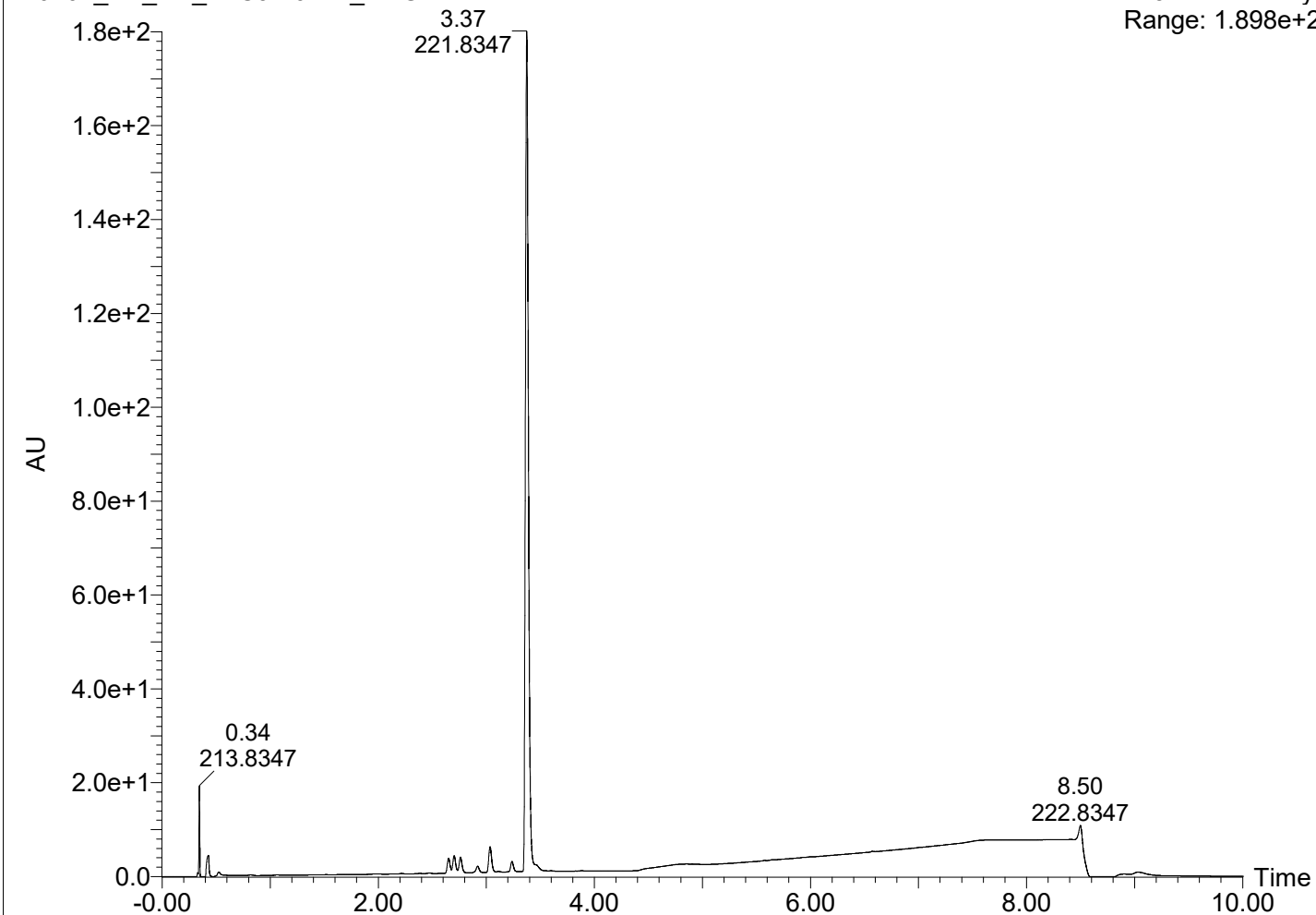
170104\_AA\_NK\_PLC9-10-FD\_NEG

1: TOF MS ES-  
BPI  
9.03e4



170104\_AA\_NK\_PLC9-10-FD\_NEG

3: Diode Array  
Range: 1.898e+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

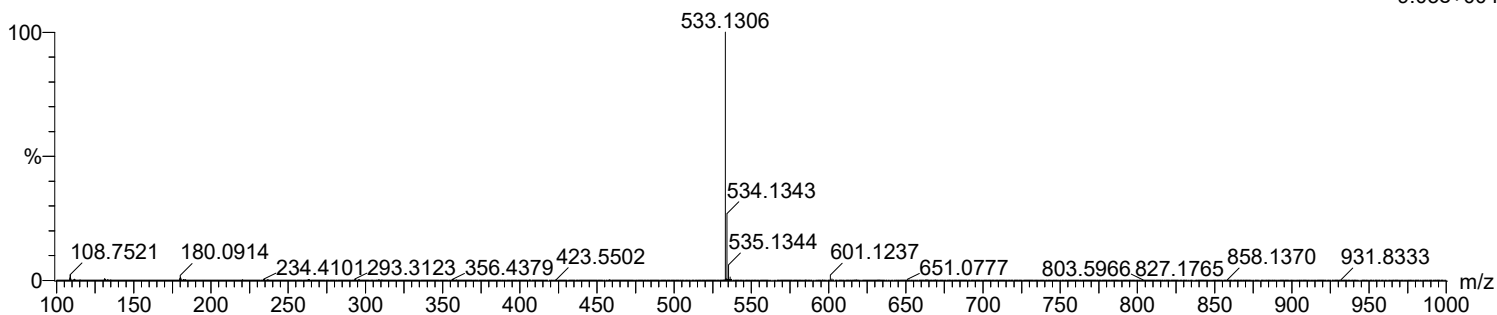
141 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

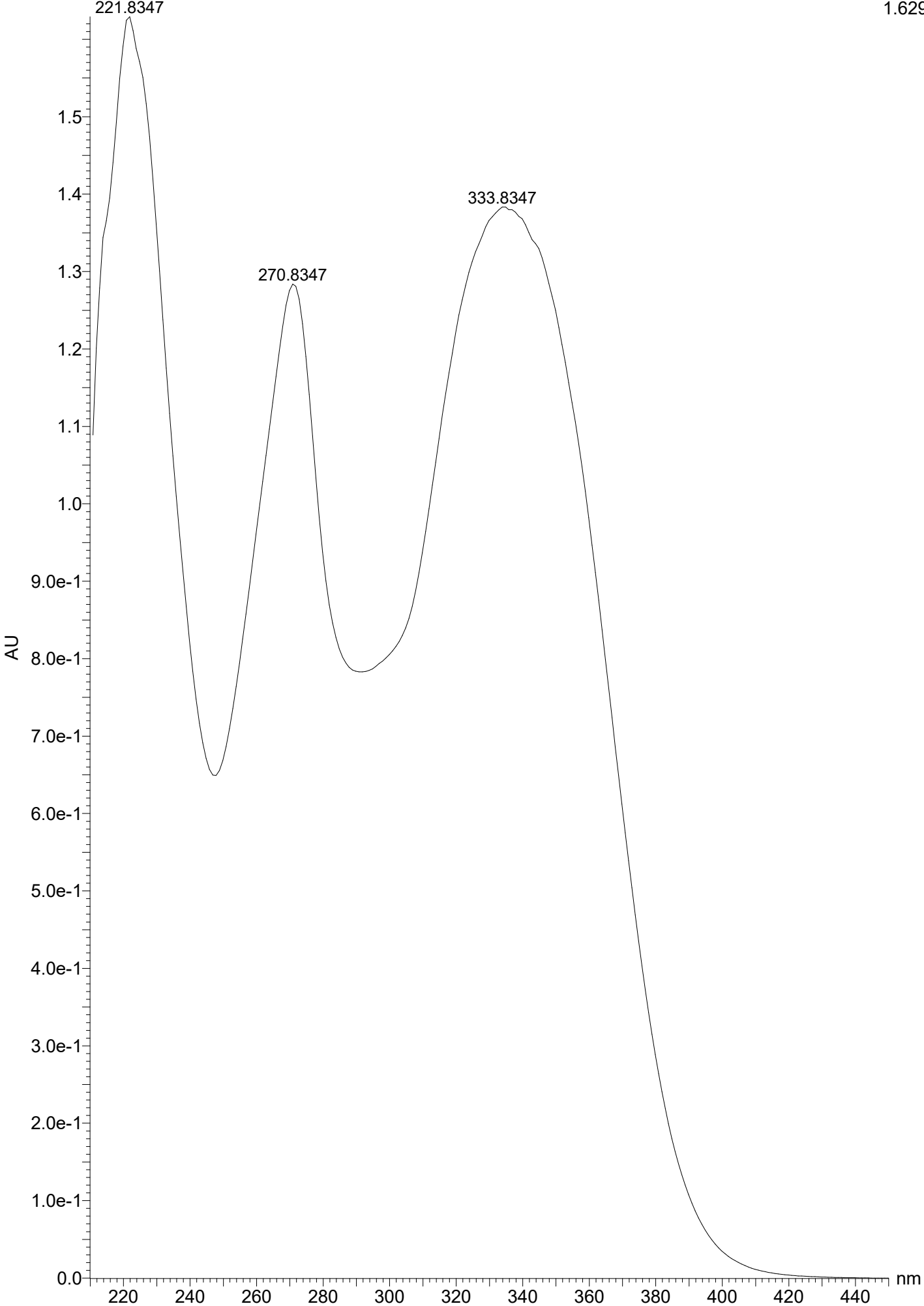
COL31

170104\_AA\_NK\_PLC9-10-FD\_NEG 297 (3.453)

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
533.1306	533.1295	1.1	2.1	13.5	235.6	0.001	99.86	C25 H25 O13
533.1354		-4.8	-9.0	4.5	242.2	6.674	0.13	C18 H29 O18
533.1236		7.0	13.1	22.5	244.9	9.299	0.01	C32 H21 O8
533.1330		-2.4	-4.5	35.5	248.1	12.489	0.00	C43 H17

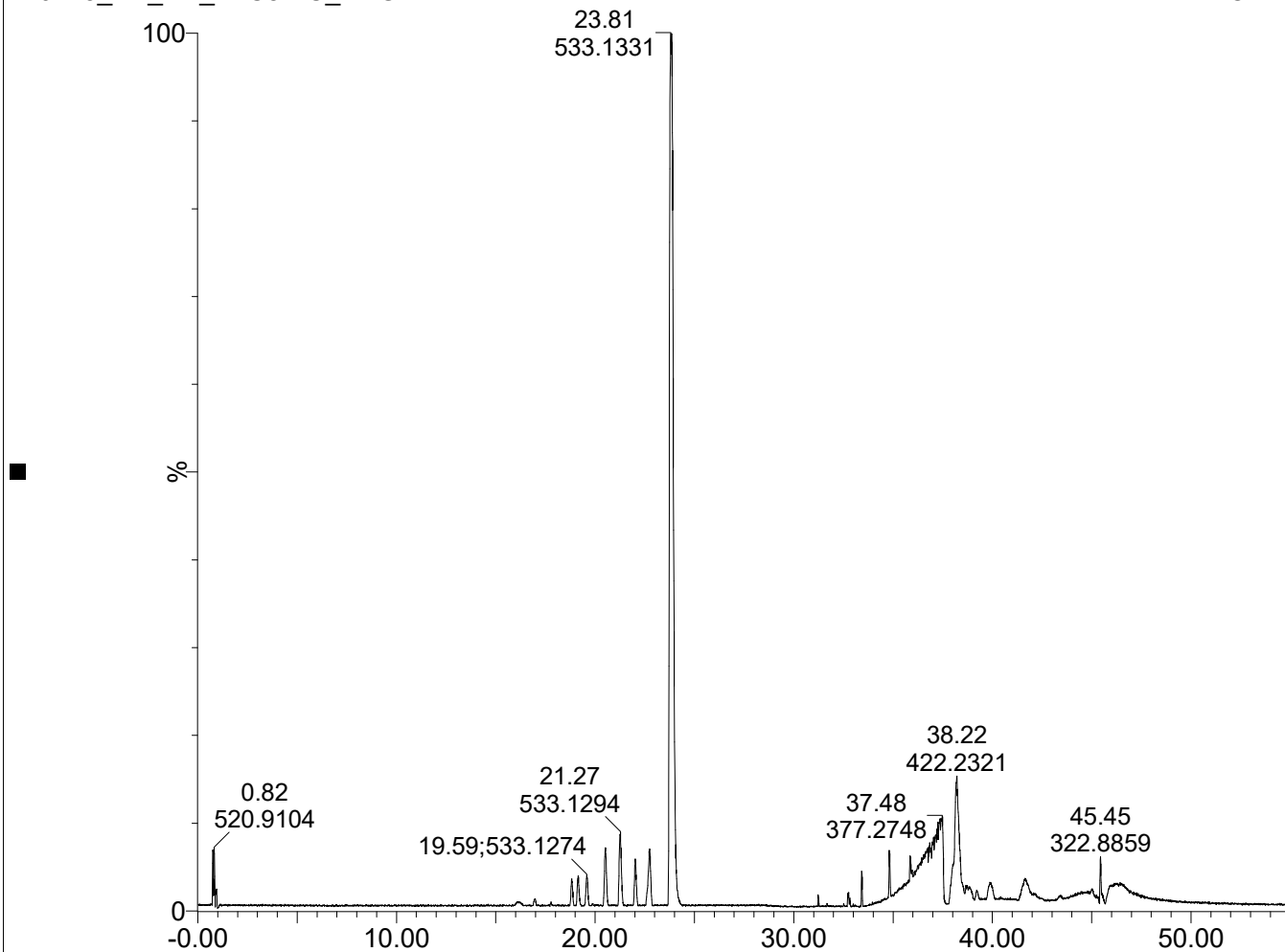


# COMPOUND NO. S23 (METHOD B)

Col 32

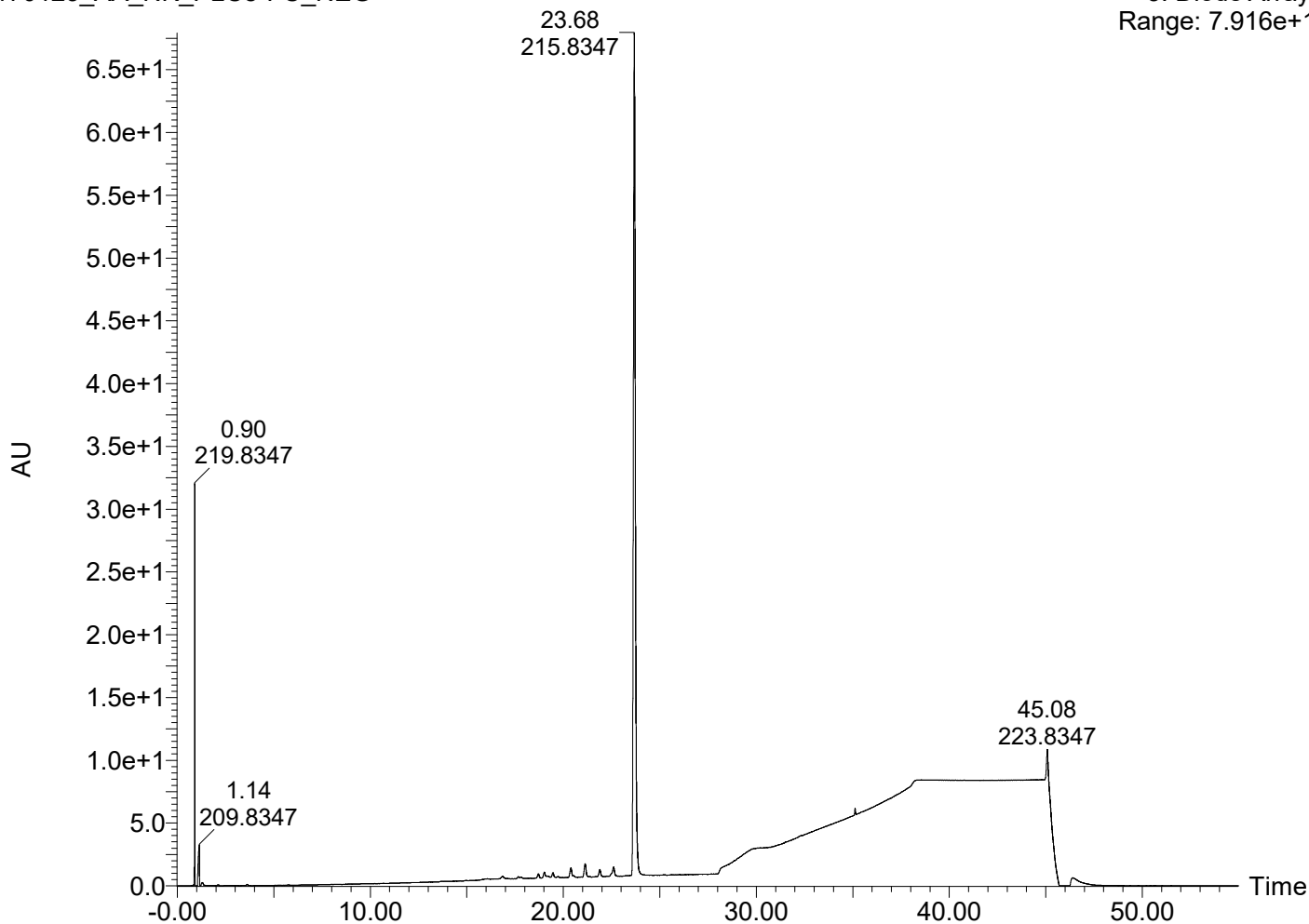
170123\_AA\_NK\_PLC8-FC\_NEG

1: TOF MS ES-  
BPI  
4.37e4



170123\_AA\_NK\_PLC8-FC\_NEG

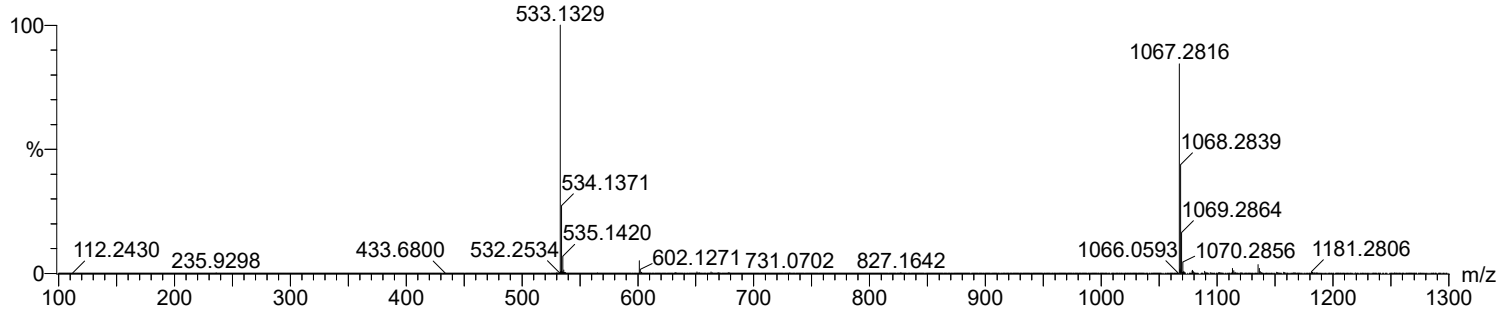
3: Diode Array  
Range: 7.916e+1



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  
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  
Col 32  
170123\_AA\_NK\_PLC8-FC\_NEG 2027 (23.802)

1: TOF MS ES-  
4.33e+004



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
533.1329	533.1295	3.4	6.4	13.5	196.2	0.000	99.96	C25 H25 O13
	533.1354	-2.5	-4.7	4.5	204.4	8.226	0.03	C18 H29 O18
	533.1389	-6.0	-11.3	26.5	205.3	9.140	0.01	C36 H21 O5
	533.1330	-0.1	-0.2	35.5	205.8	9.615	0.01	C43 H17

Col 32

170123\_AA\_NK\_PLC8-FC\_NEG 28401 (23.671)

3: Diode Array  
7.562e-1

