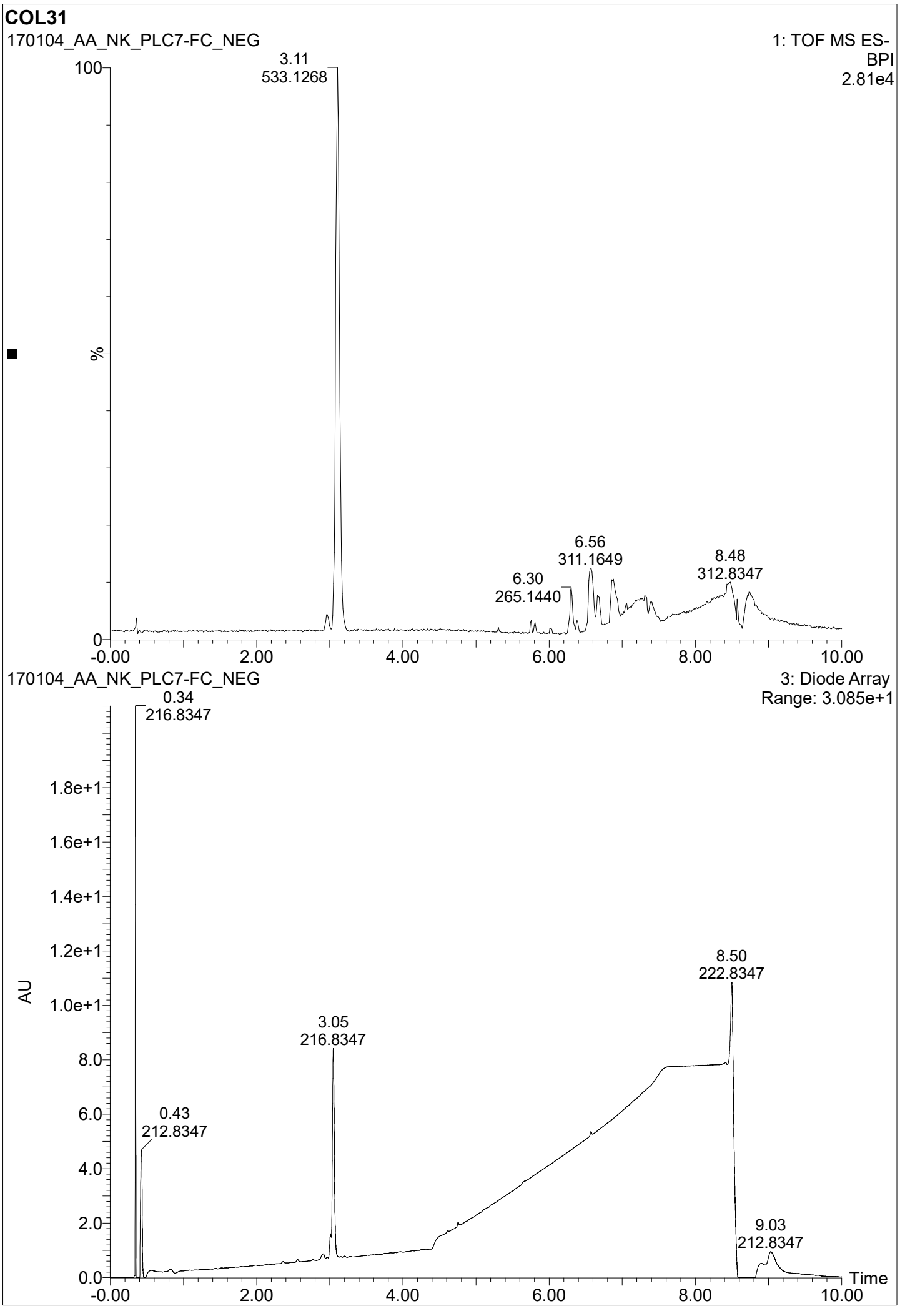
COMPOUND NO. S21 (METHOD A)



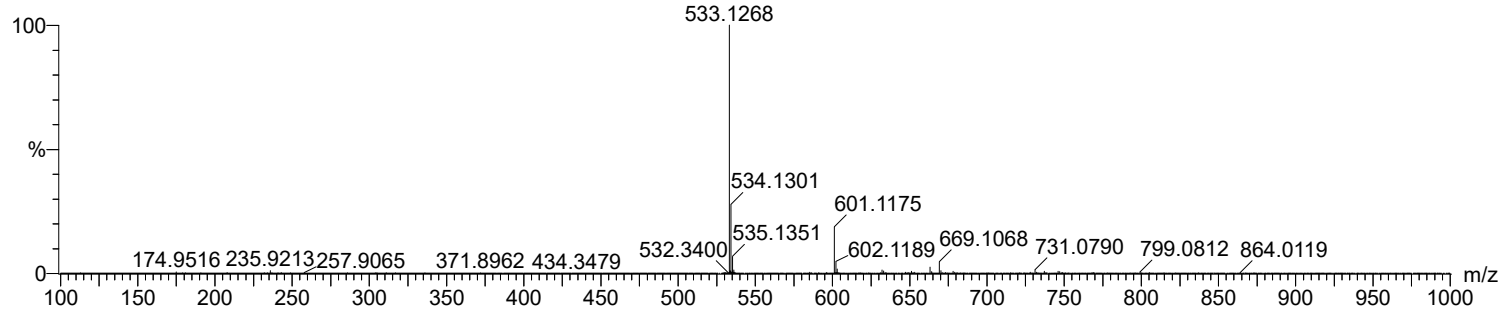
Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

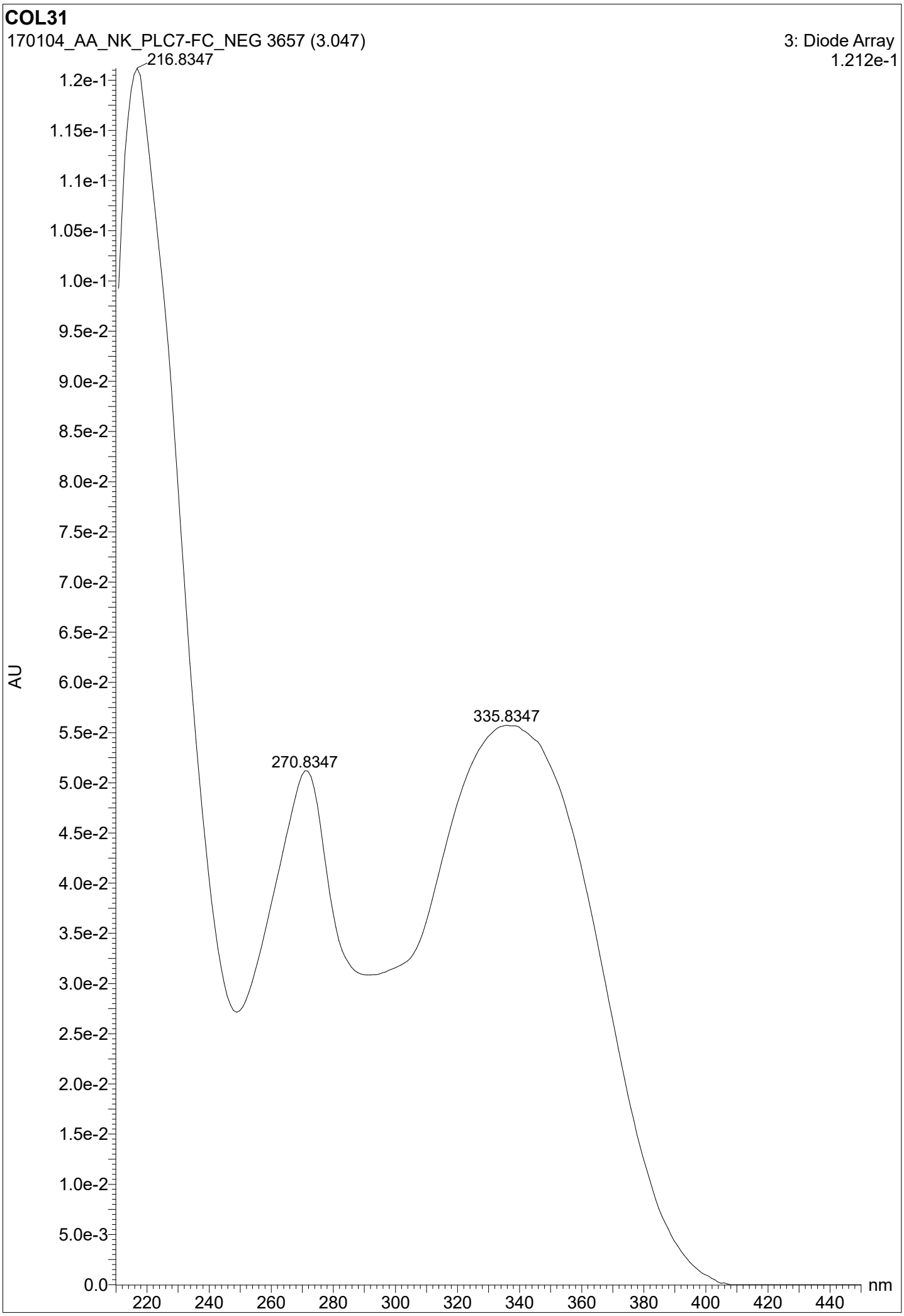
Monoisotopic Mass, Even Electron Ions
141 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

COL31
170104_AA_NK_PLC7-FC_NEG 267 (3.107)

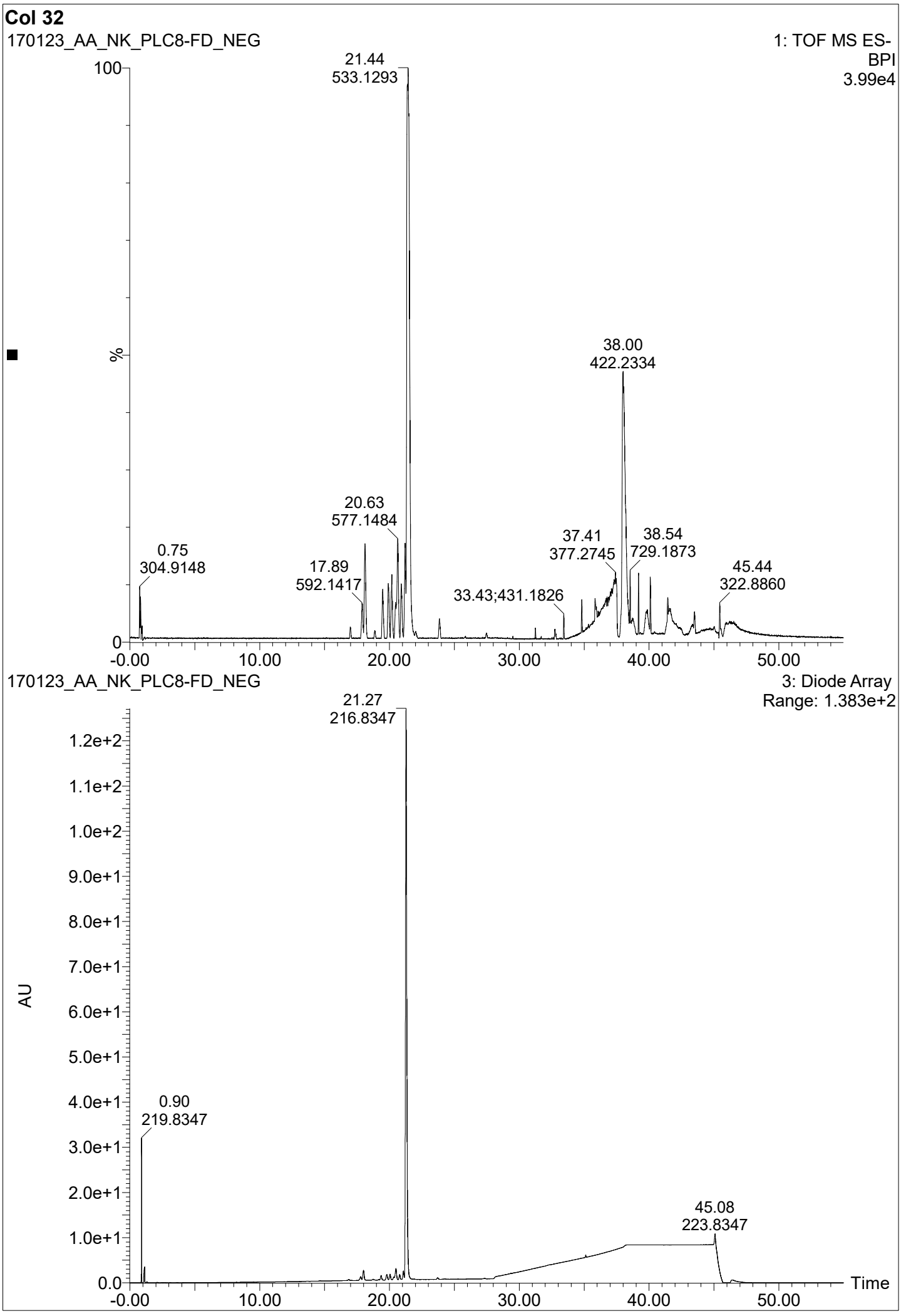
1: TOF MS ES-
2.81e+004



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
533.1268	533.1295	-2.7	-5.1	13.5	207.0	0.001	99.95	C25 H25 O13
	533.1236	3.2	6.0	22.5	214.6	7.631	0.05	C32 H21 O8
	533.1330	-6.2	-11.6	35.5	218.4	11.401	0.00	C43 H17
	533.1201	6.7	12.6	0.5	219.1	12.113	0.00	C14 H29 O21


COL31
170104_AA_NK_PLC7-FC_NEG 3657 (3.047)
3: Diode Array
1.212e-1
216.8347
270.8347
335.8347
AU
nm
1.2e-1
1.15e-1
1.1e-1
1.05e-1
1.0e-1
9.5e-2
9.0e-2
8.5e-2
8.0e-2
7.5e-2
7.0e-2
6.5e-2
6.0e-2
5.5e-2
5.0e-2
4.5e-2
4.0e-2
3.5e-2
3.0e-2
2.5e-2
2.0e-2
1.5e-2
1.0e-2
5.0e-3
0.0
220
240
260
280
300
320
340
360
380
400
420
440

COMPOUND NO. S21 (METHOD B)



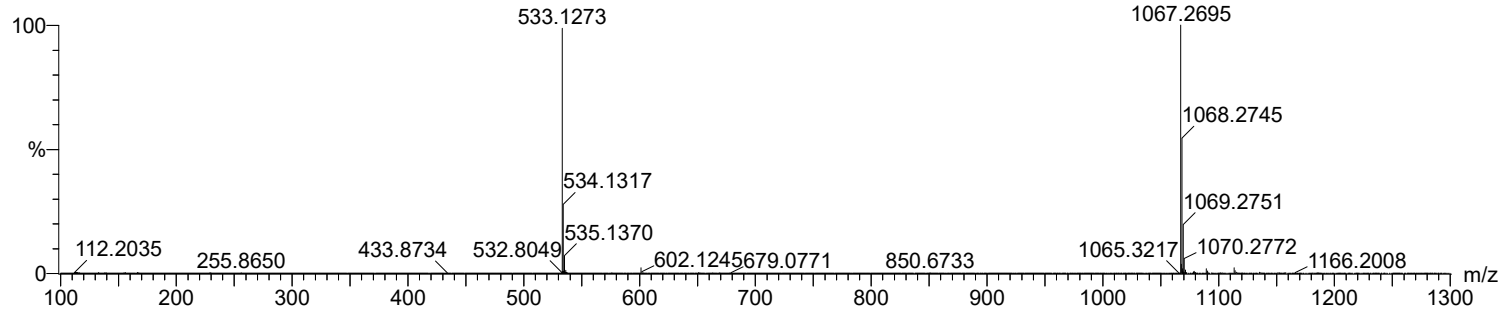
Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

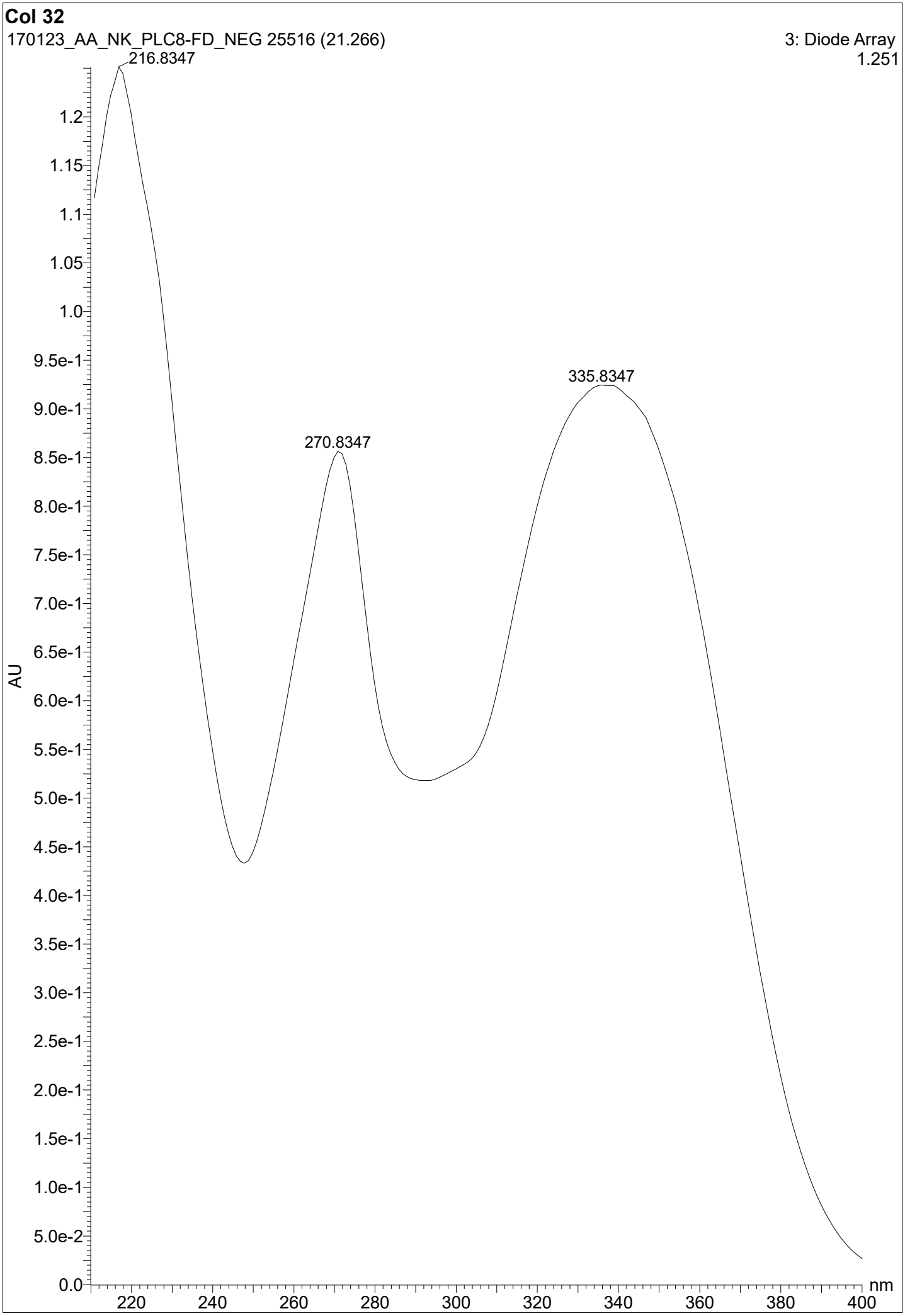
Monoisotopic Mass, Even Electron Ions
141 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Col 32
170123_AA_NK_PLC8-FD_NEG 1821 (21.409)

1: TOF MS ES-
3.88e+004



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
533.1273	533.1295	-2.2	-4.1	13.5	191.9	0.002	99.76	C25 H25 O13
	533.1236	3.7	6.9	22.5	197.9	6.077	0.23	C32 H21 O8
	533.1330	-5.7	-10.7	35.5	201.0	9.098	0.01	C43 H17
	533.1201	7.2	13.5	0.5	202.1	10.179	0.00	C14 H29 O21


Col 32
170123_AA_NK_PLC8-FD_NEG 25516 (21.266)
3: Diode Array
1.251
216.8347
270.8347
335.8347
AU
nm
1.2
1.15
1.1
1.05
1.0
9.5e-1
9.0e-1
8.5e-1
8.0e-1
7.5e-1
7.0e-1
6.5e-1
6.0e-1
5.5e-1
5.0e-1
4.5e-1
4.0e-1
3.5e-1
3.0e-1
2.5e-1
2.0e-1
1.5e-1
1.0e-1
5.0e-2
0.0
220
240
260
280
300
320
340
360
380
400