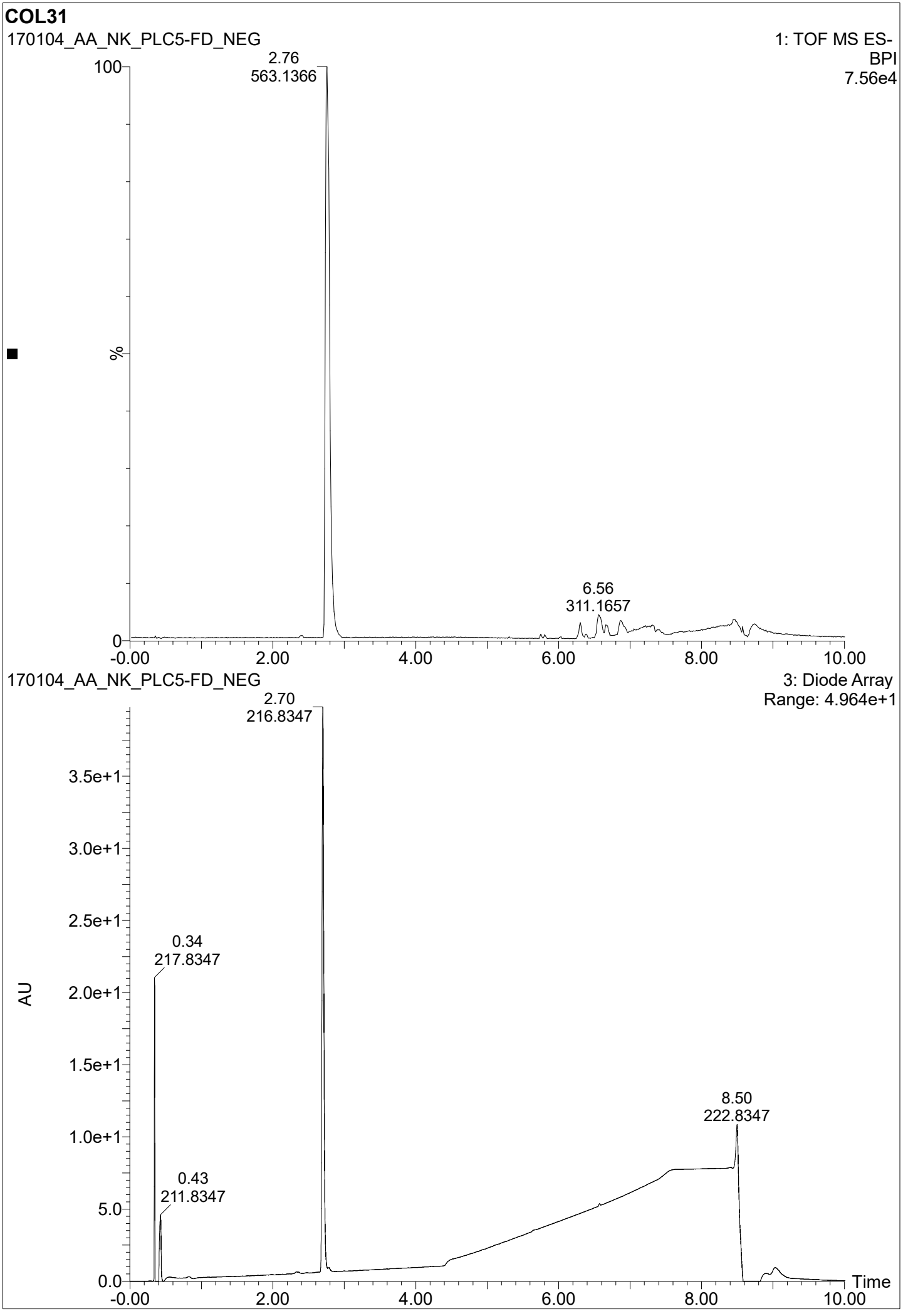
COMPOUND NO. S16 (METHOD A)



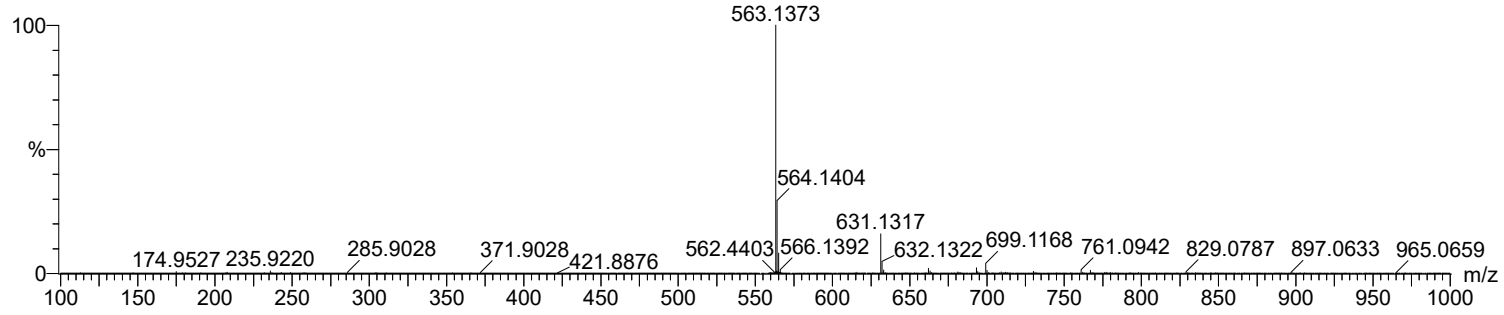
Single Mass Analysis

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

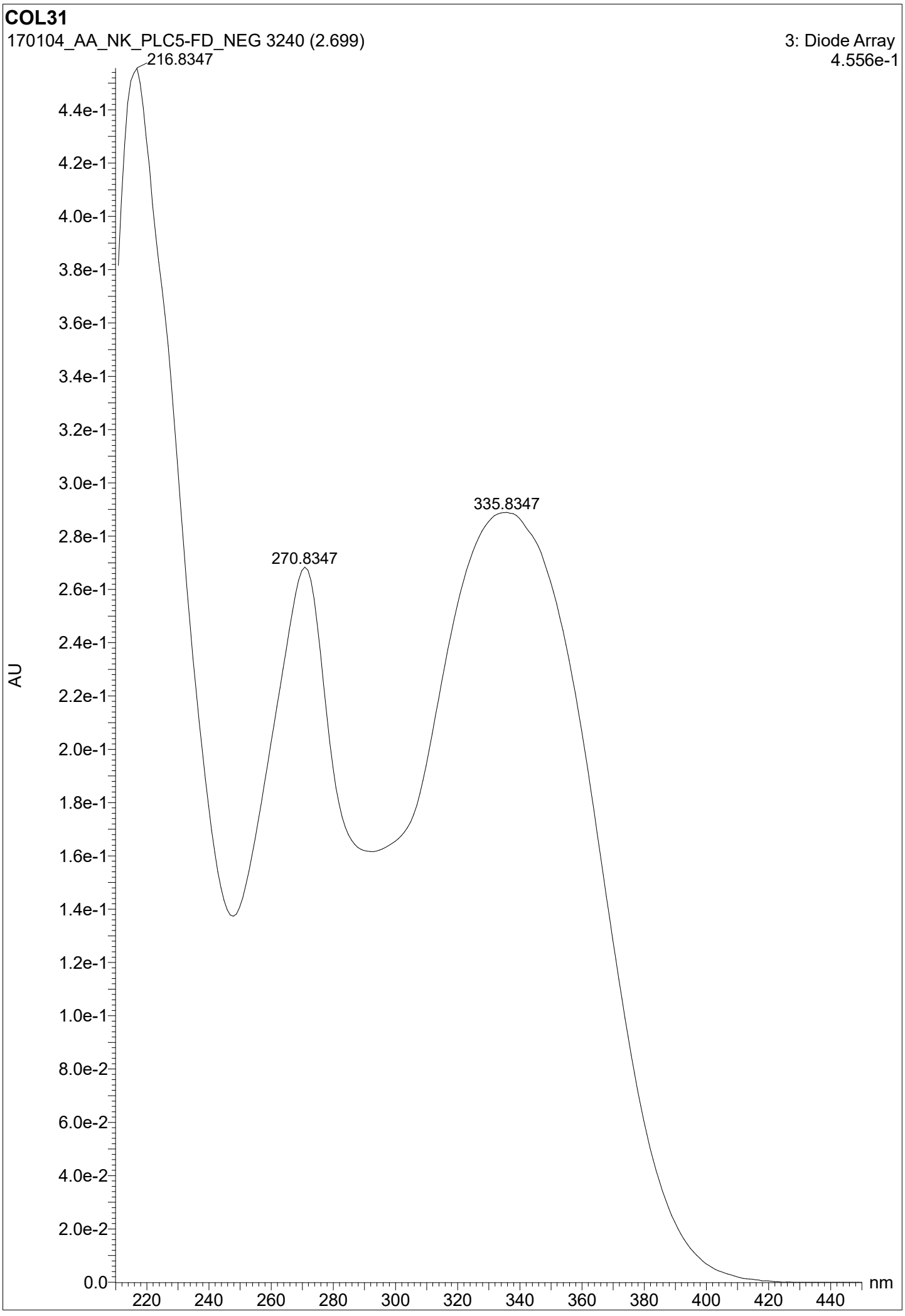
Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

COL31
170104_AA_NK_PLC5-FD_NEG 241 (2.804)

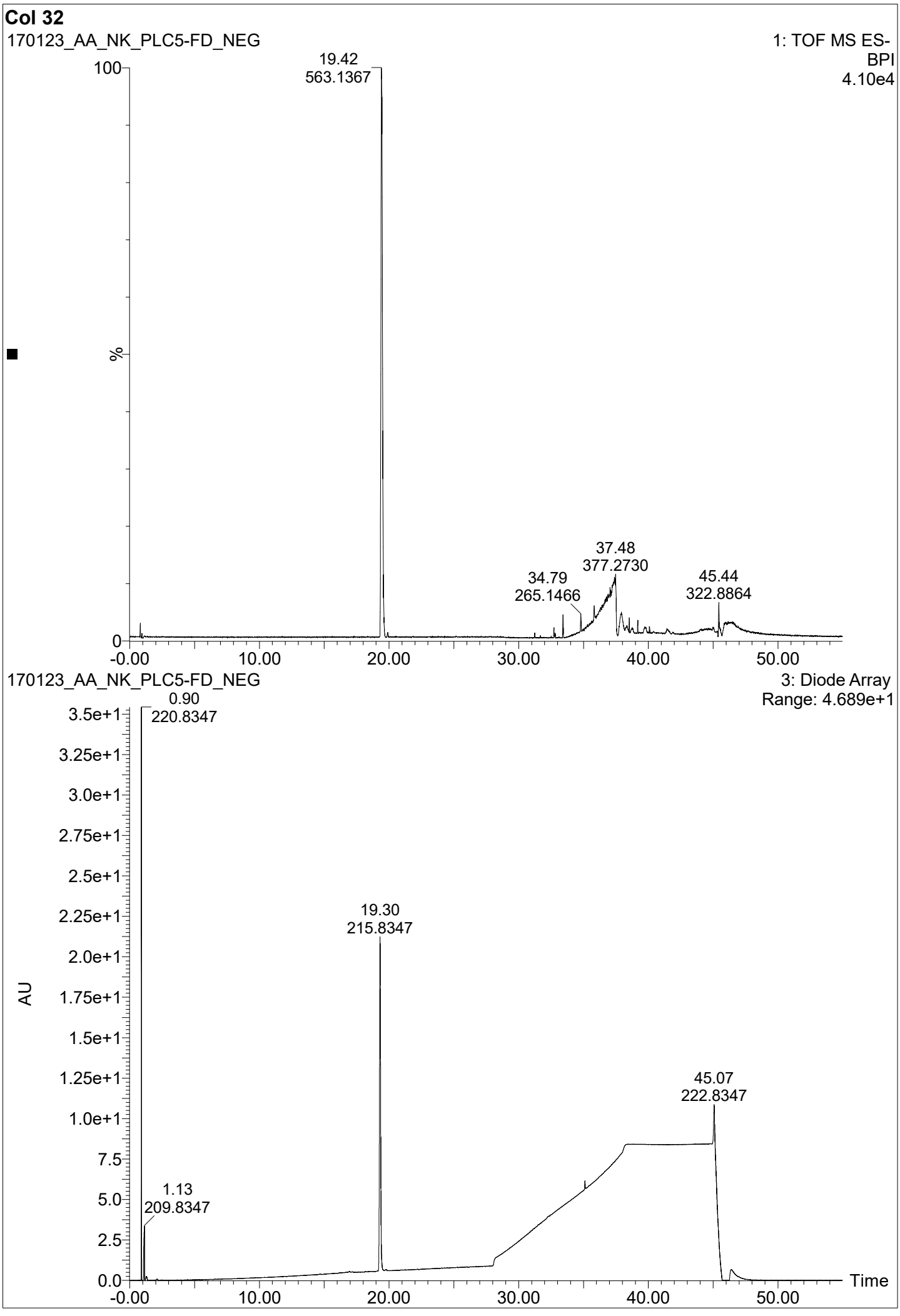
1: TOF MS ES-
2.76e+004



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
563.1373	563.1401	-2.8	-5.0	13.5	199.0	0.021	97.94	C26 H27 O14
	563.1342	3.1	5.5	22.5	202.8	3.898	2.03	C33 H23 O9
	563.1307	6.6	11.7	0.5	207.5	8.586	0.02	C15 H31 O22
	563.1436	-6.3	-11.2	35.5	208.4	9.423	0.01	C44 H19 O


COL31
170104_AA_NK_PLC5-FD_NEG 3240 (2.699)
3: Diode Array
4.556e-1
216.8347
270.8347
335.8347
AU
nm
4.4e-1
4.2e-1
4.0e-1
3.8e-1
3.6e-1
3.4e-1
3.2e-1
3.0e-1
2.8e-1
2.6e-1
2.4e-1
2.2e-1
2.0e-1
1.8e-1
1.6e-1
1.4e-1
1.2e-1
1.0e-1
8.0e-2
6.0e-2
4.0e-2
2.0e-2
0.0
220
240
260
280
300
320
340
360
380
400
420
440

COMPOUND NO. S16 (METHOD B)



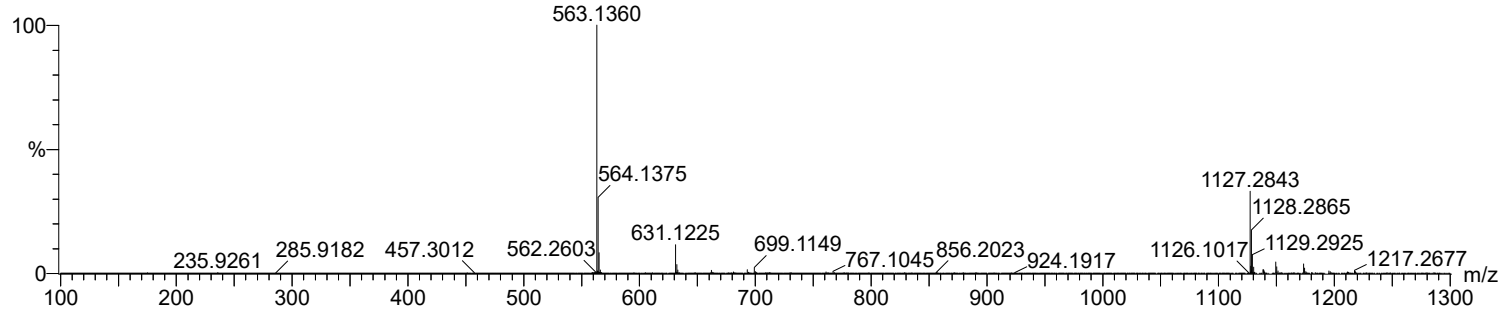
Single Mass Analysis

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

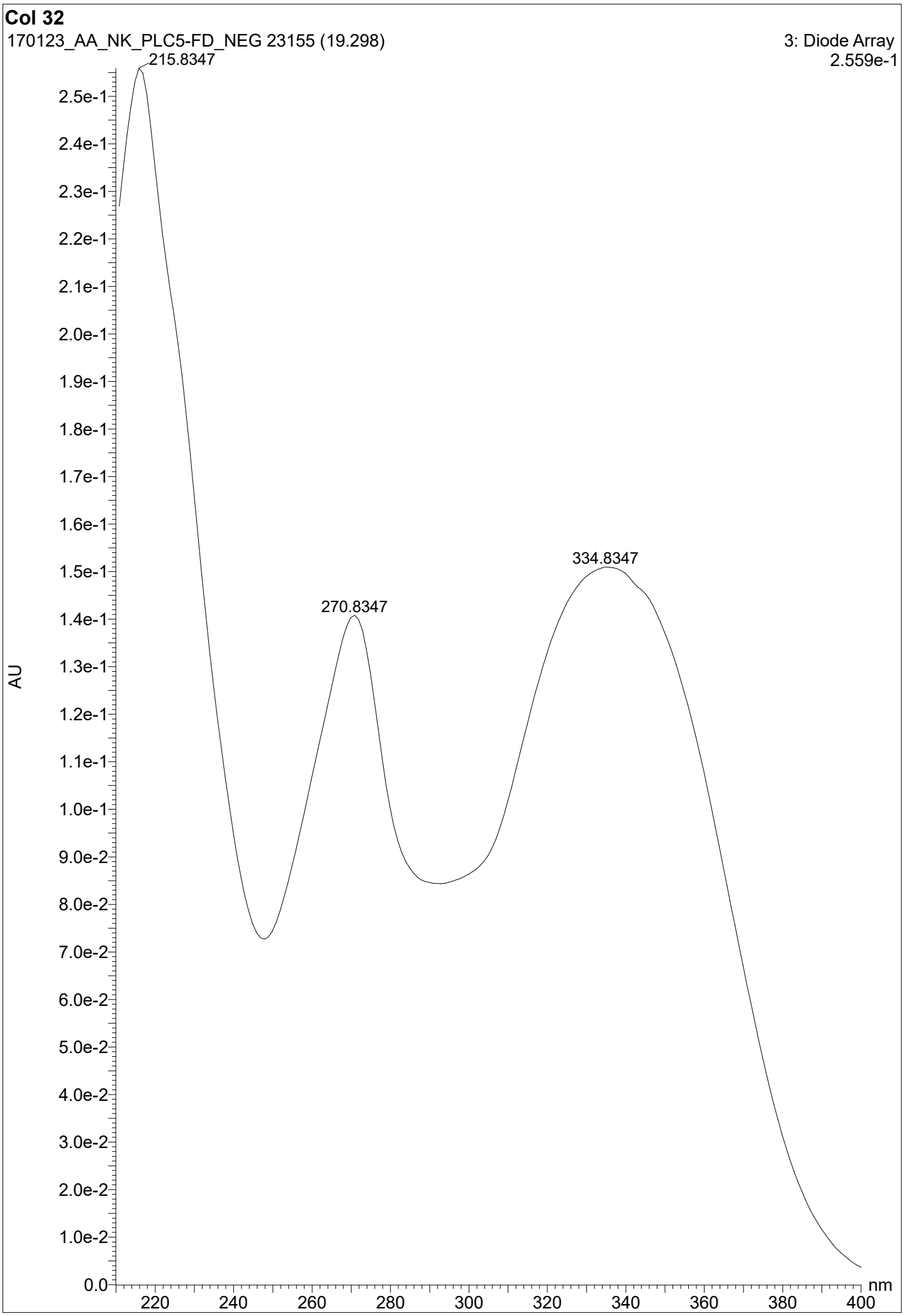
Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 5 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Col 32
170123_AA_NK_PLC5-FD_NEG 1653 (19.441)

1: TOF MS ES-
3.93e+004



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
563.1360	563.1401	-4.1	-7.3	13.5	189.5	0.140	86.97	C26 H27 O14
	563.1342	1.8	3.2	22.5	191.4	2.090	12.37	C33 H23 O9
	563.1283	7.7	13.7	31.5	194.8	5.434	0.44	C40 H19 O4
	563.1436	-7.6	-13.5	35.5	195.8	6.482	0.15	C44 H19 O
	563.1307	5.3	9.4	0.5	196.6	7.276	0.07	C15 H31 O22


Col 32
170123_AA_NK_PLC5-FD_NEG 23155 (19.298)
3: Diode Array
2.559e-1
215.8347
270.8347
334.8347
AU
nm
2.5e-1
2.4e-1
2.3e-1
2.2e-1
2.1e-1
2.0e-1
1.9e-1
1.8e-1
1.7e-1
1.6e-1
1.5e-1
1.4e-1
1.3e-1
1.2e-1
1.1e-1
1.0e-1
9.0e-2
8.0e-2
7.0e-2
6.0e-2
5.0e-2
4.0e-2
3.0e-2
2.0e-2
1.0e-2
0.0
220
240
260
280
300
320
340
360
380
400