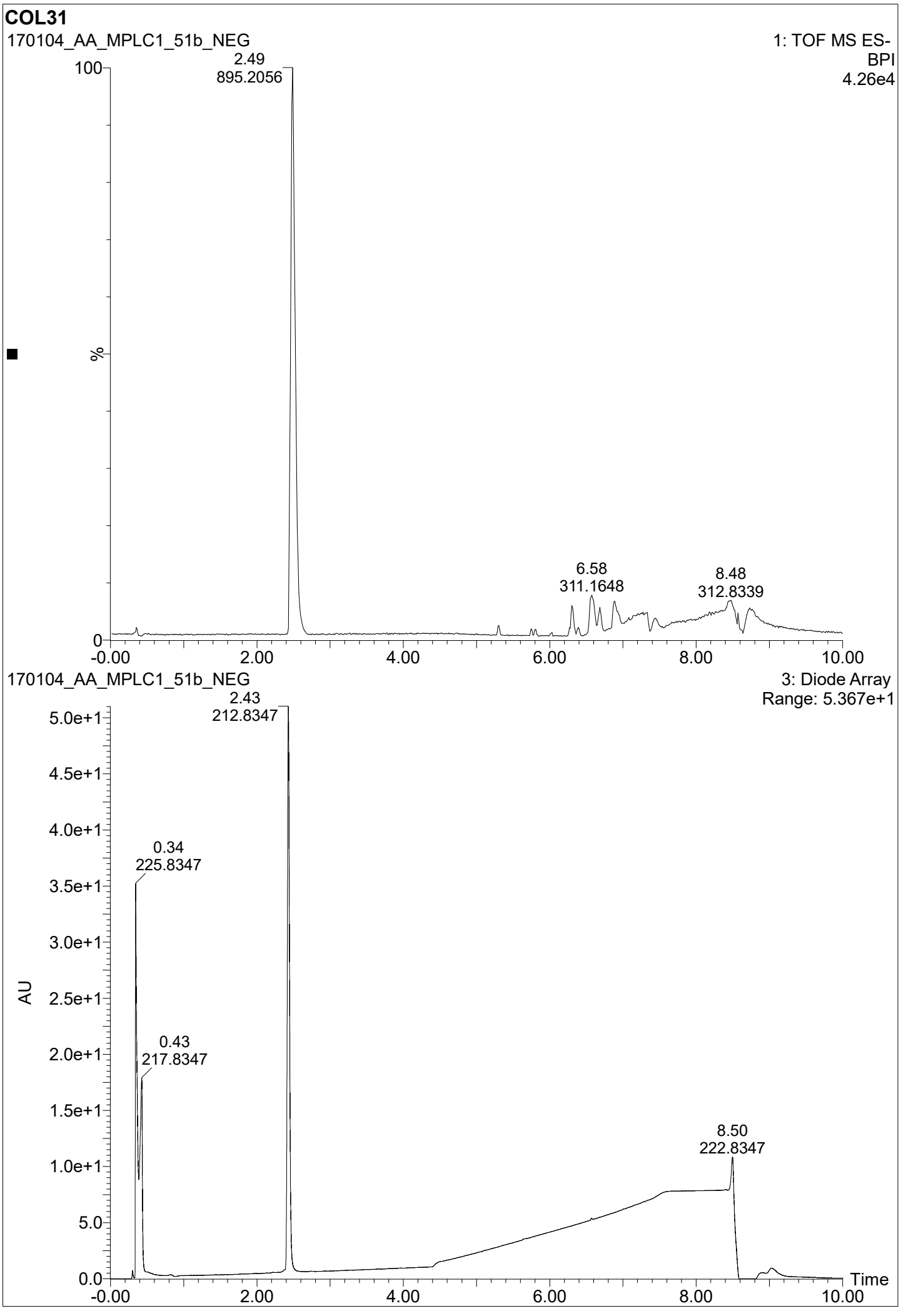
COMPOUND NO. S13 (METHOD A)



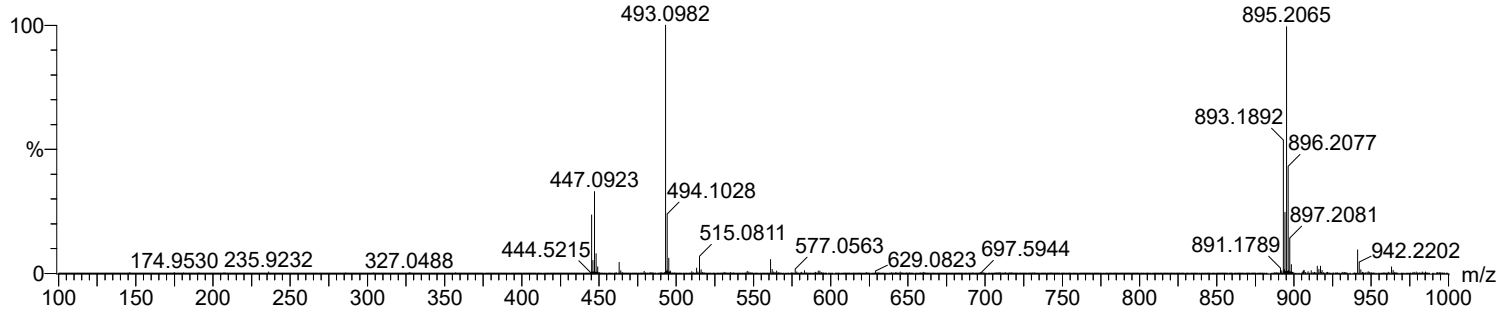
Single Mass Analysis

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

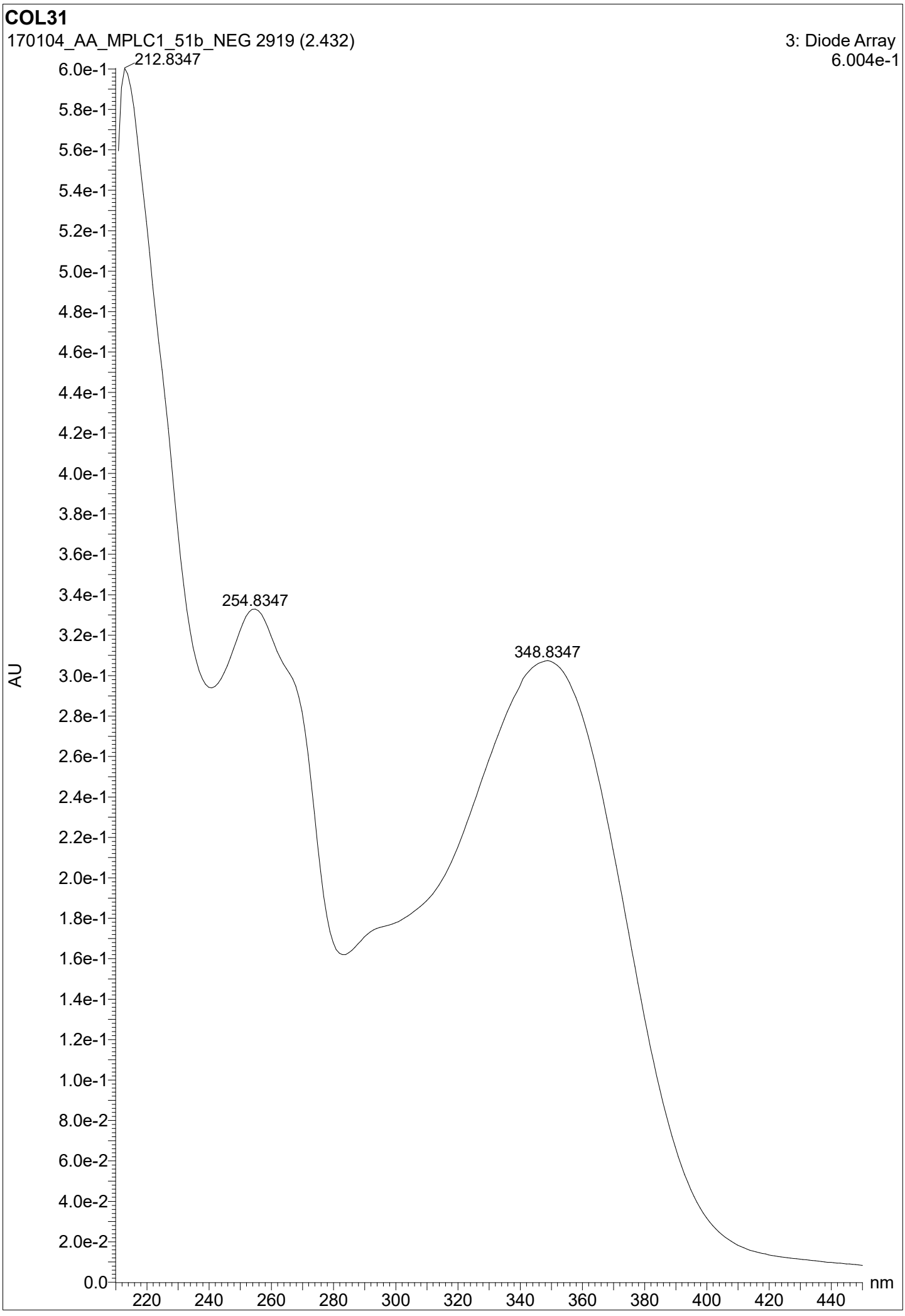
Monoisotopic Mass, Even Electron Ions
108 formula(e) evaluated with 3 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

COL31
170104_AA_MPLC1_51b_NEG 212 (2.467)

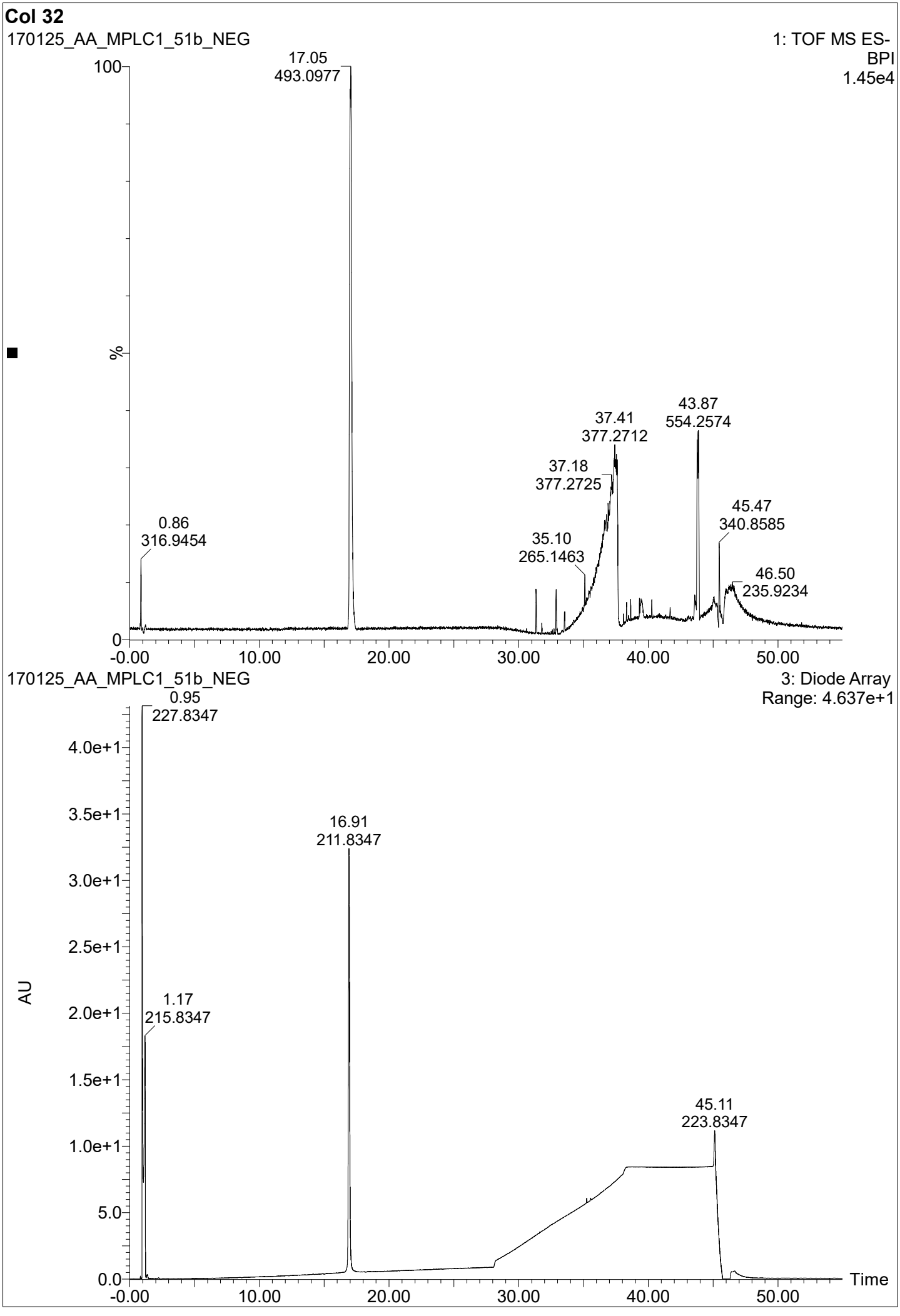
1: TOF MS ES-
2.97e+004



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.0923	447.0927	-0.4	-0.9	12.5	221.9	0.252	77.70	C21 H19 O11
	447.0869	5.4	12.1	21.5	223.3	1.696	18.34	C28 H15 O6
	447.0986	-6.3	-14.1	3.5	224.9	3.230	3.96	C14 H23 O16


COL31
170104_AA_MPLC1_51b_NEG 2919 (2.432)
3: Diode Array
6.004e-1
212.8347
254.8347
348.8347
AU
nm
6.0e-1
5.8e-1
5.6e-1
5.4e-1
5.2e-1
5.0e-1
4.8e-1
4.6e-1
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. S13 (METHOD B)



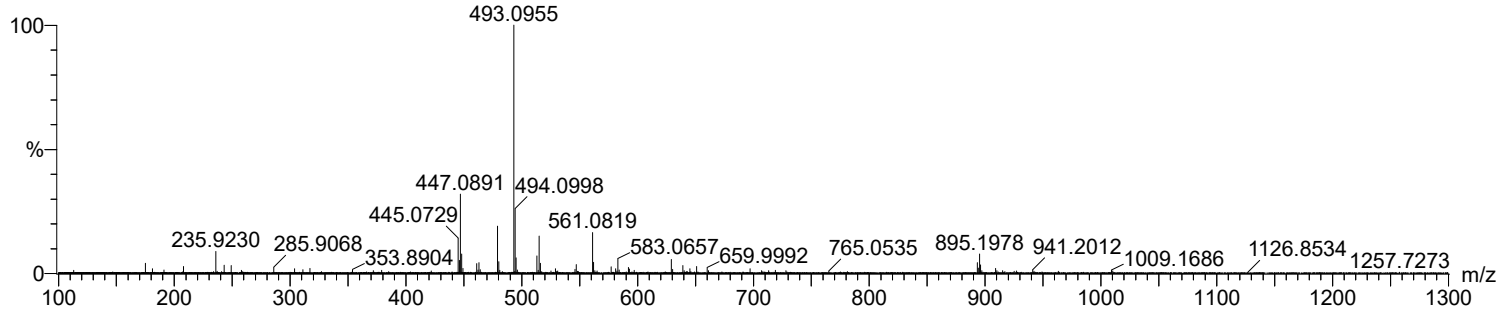
Single Mass Analysis

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

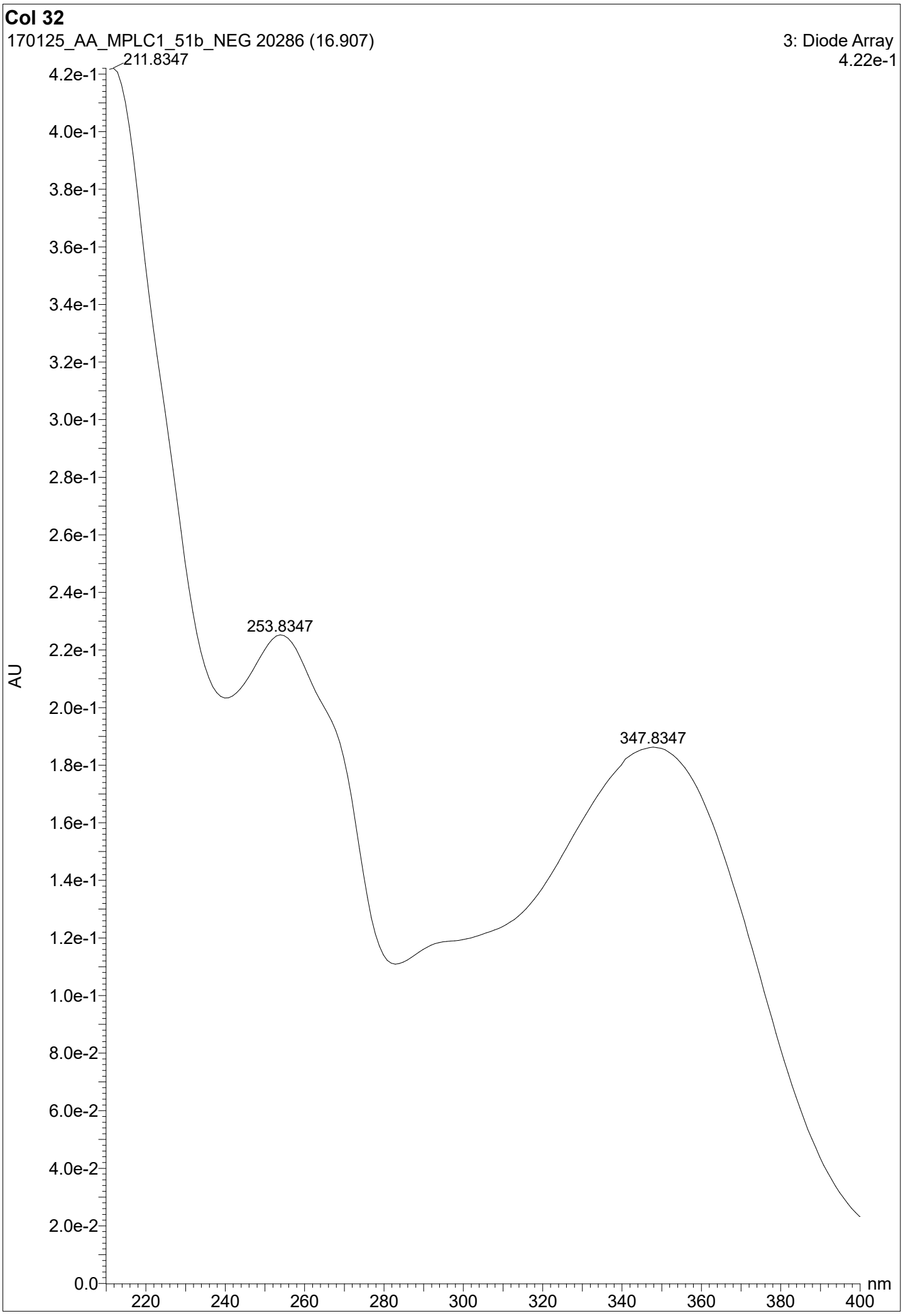
Monoisotopic Mass, Even Electron Ions
108 formula(e) evaluated with 3 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Col 32
170125_AA_MPLC1_51b_NEG 1464 (17.188)

1: TOF MS ES-
2.61e+003



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.0891	447.0927	-3.6	-8.1	12.5	68.2	0.112	89.39	C21 H19 O11
	447.0869	2.2	4.9	21.5	70.4	2.254	10.50	C28 H15 O6
	447.0834	5.7	12.7	-0.5	74.9	6.799	0.11	C10 H23 O19


Col 32
170125_AA_MPLC1_51b_NEG 20286 (16.907)
3: Diode Array
4.22e-1
211.8347
253.8347
347.8347
AU
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
nm