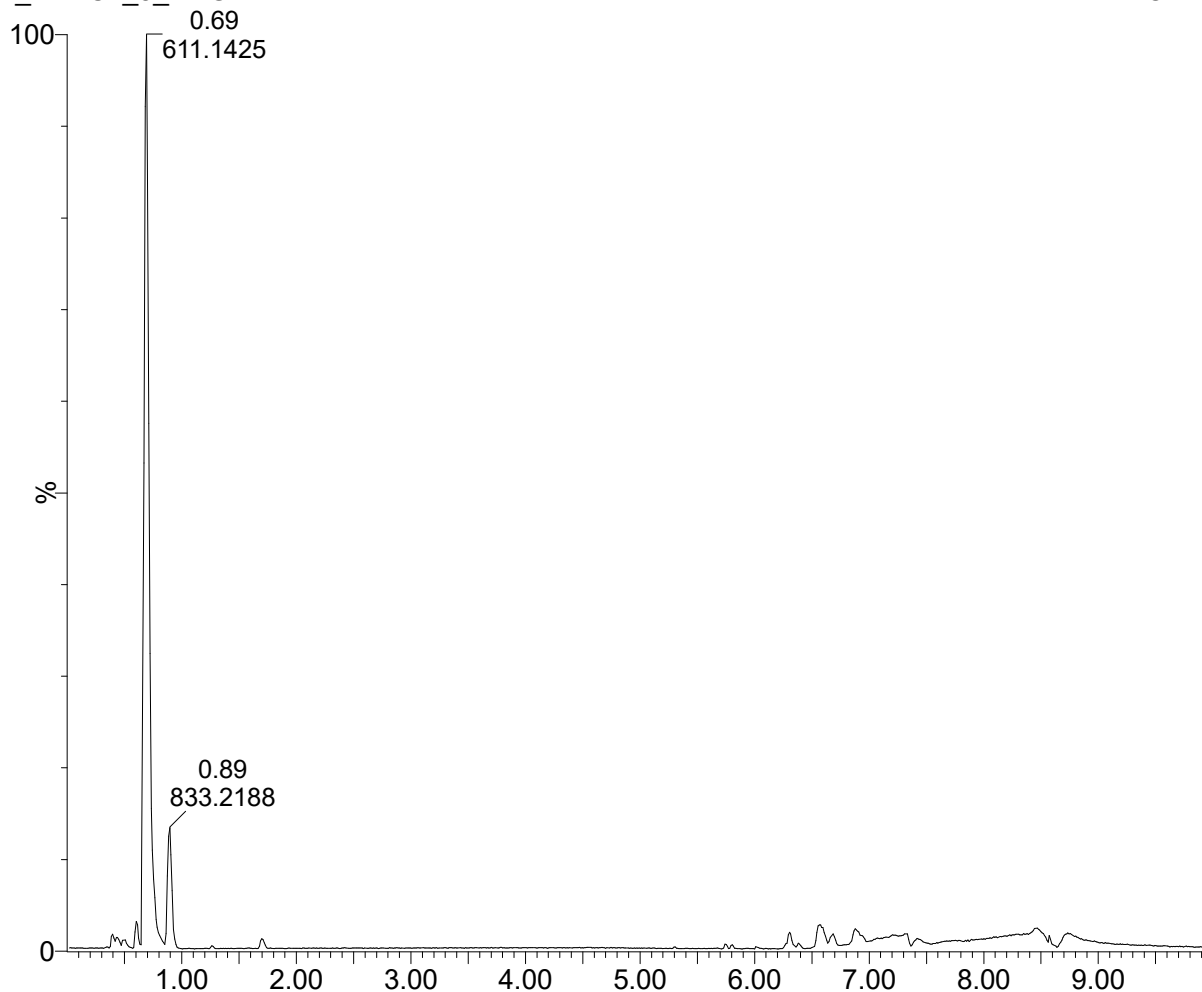


COMPOUND NO. S1 (METHOD A)

COL31

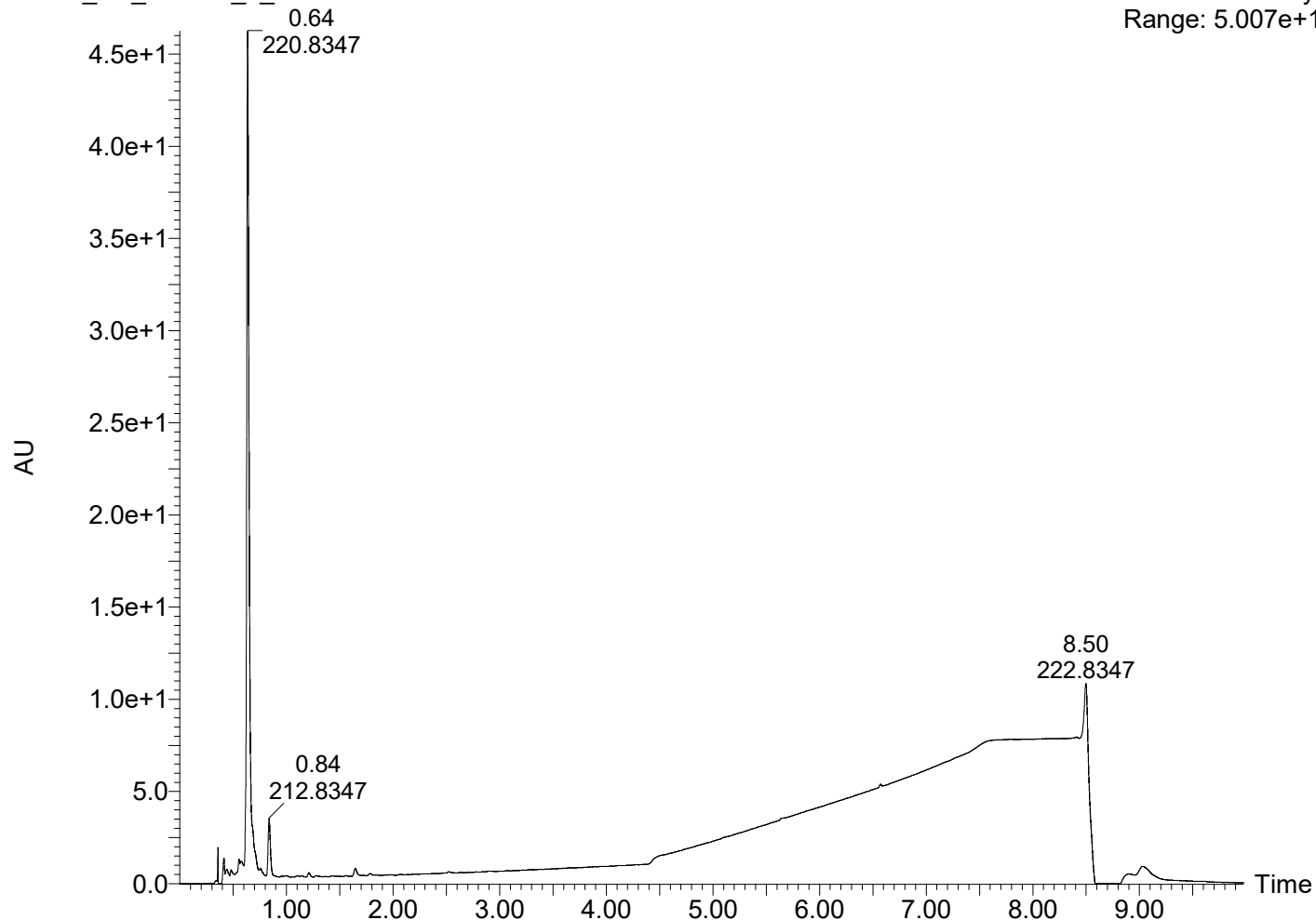
170104_AA_MPLC1_5_NEG

1: TOF MS ES-
BPI
1.09e5



170104_AA_MPLC1_5_NEG

3: Diode Array
Range: 5.007e+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

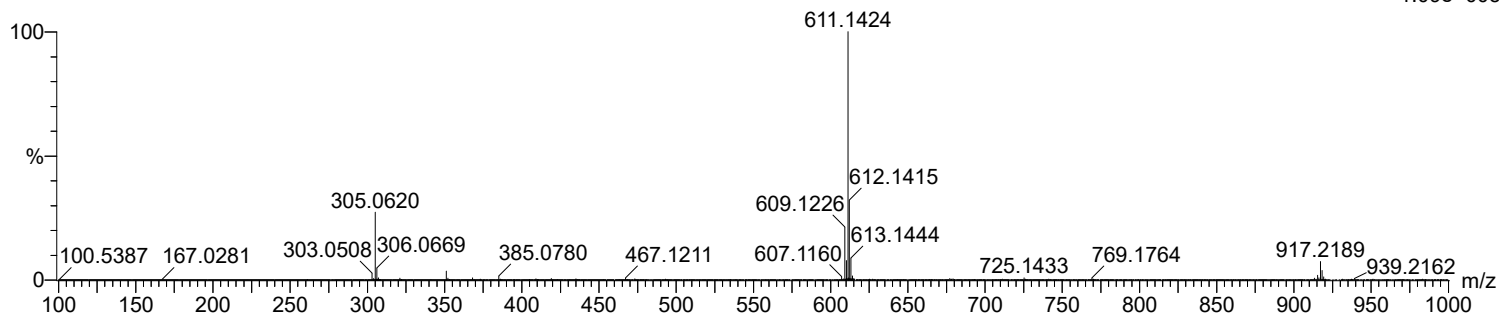
7027 formula(e) evaluated with 62 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-6 Cl: 0-8 Br: 0-8

COL31

170104_AA_MPLC1_5_NEG 59 (0.691)

1: TOF MS ES-
1.09e+005

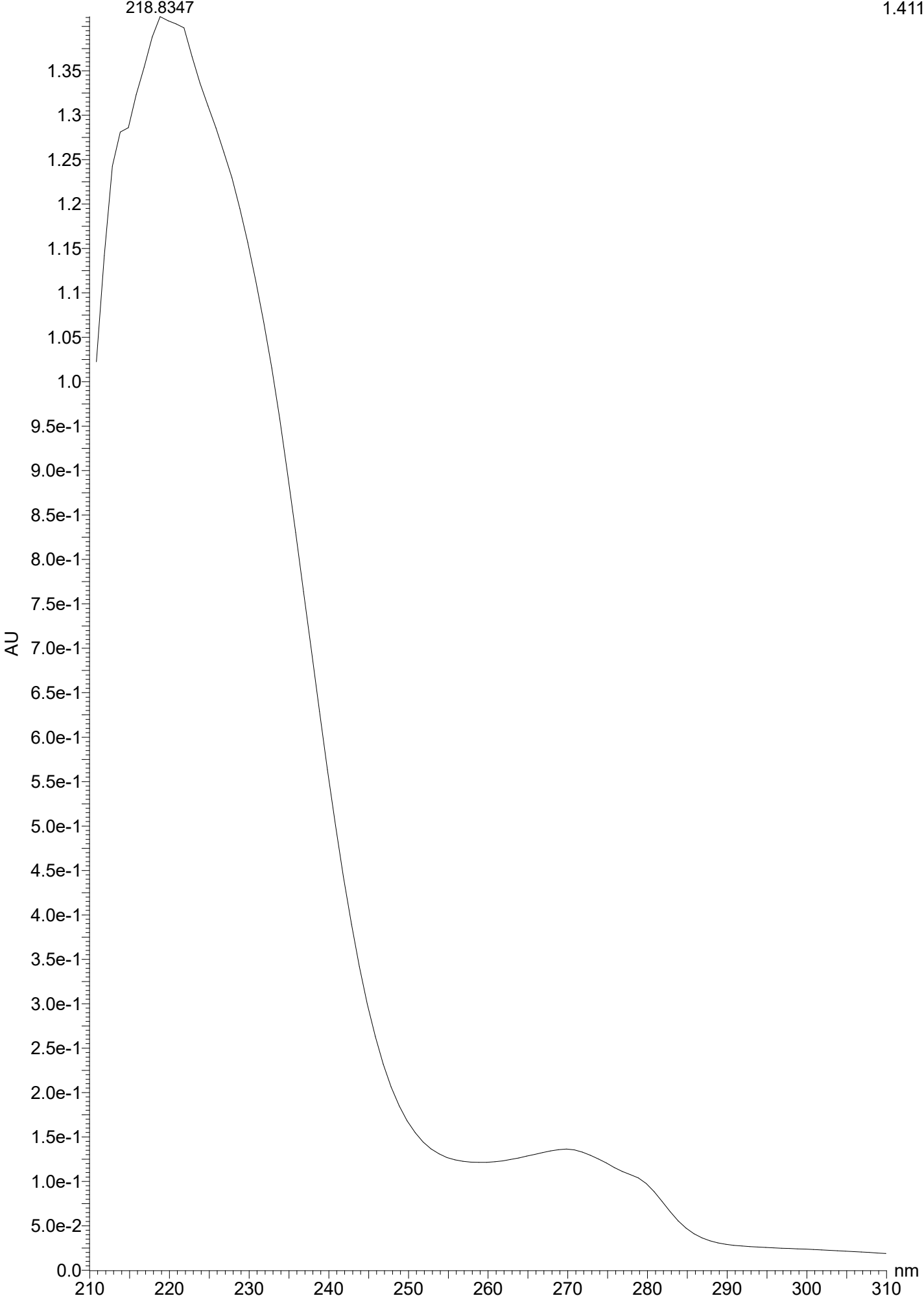
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
305.0620	305.0661	-4.1	-13.4	9.5	356.4	0.004	99.58	C15 H13 O7
	305.0634	-1.4	-4.6	10.5	362.8	6.373	0.17	C11 H9 N6 O5
	305.0621	-0.1	-0.3	5.5	363.2	6.805	0.11	C10 H13 N2 O9
	305.0648	-2.8	-9.2	15.5	363.4	6.963	0.09	C12 H5 N10 O
	305.0576	4.4	14.4	19.5	364.2	7.828	0.04	C18 H5 N6

COL31

170104_AA_MPLC1_5_NEG 767 (0.638)

3: Diode Array
1.411

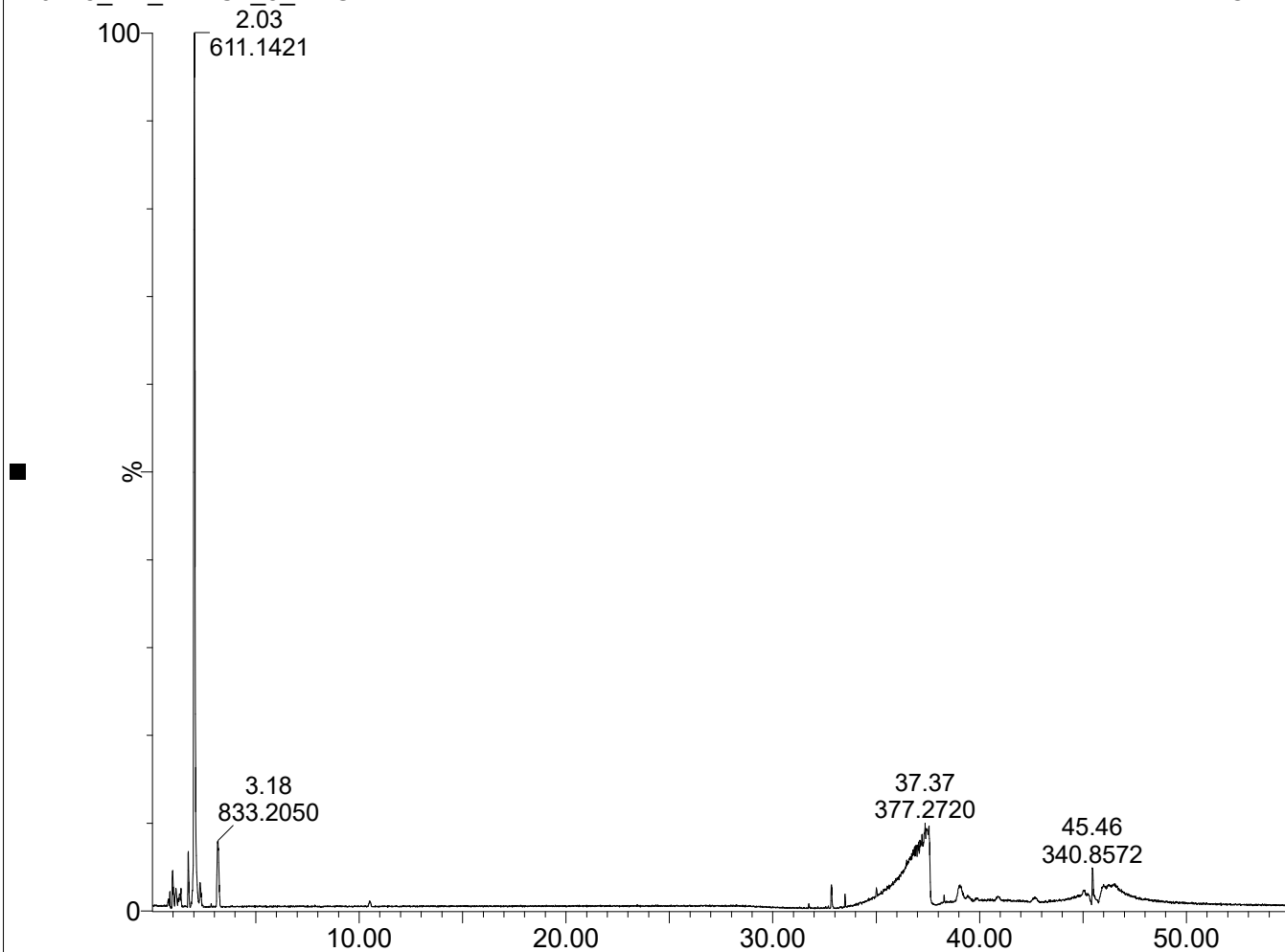


COMPOUND NO. S1 (METHOD B)

Col 32

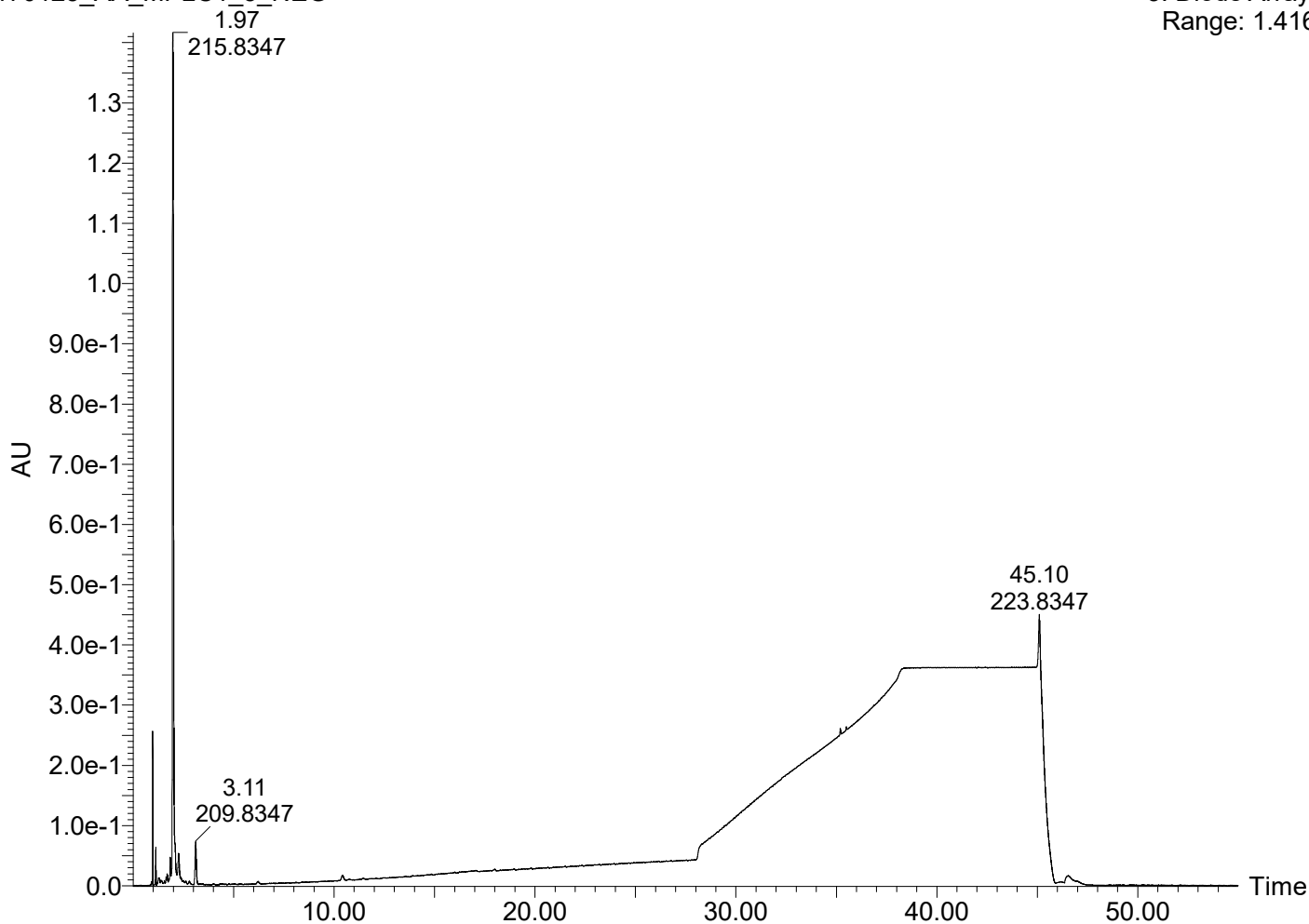
170125_AA_MPLC1_5_NEG

1: TOF MS ES-
BPI
4.20e4



170125_AA_MPLC1_5_NEG

3: Diode Array
Range: 1.416



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

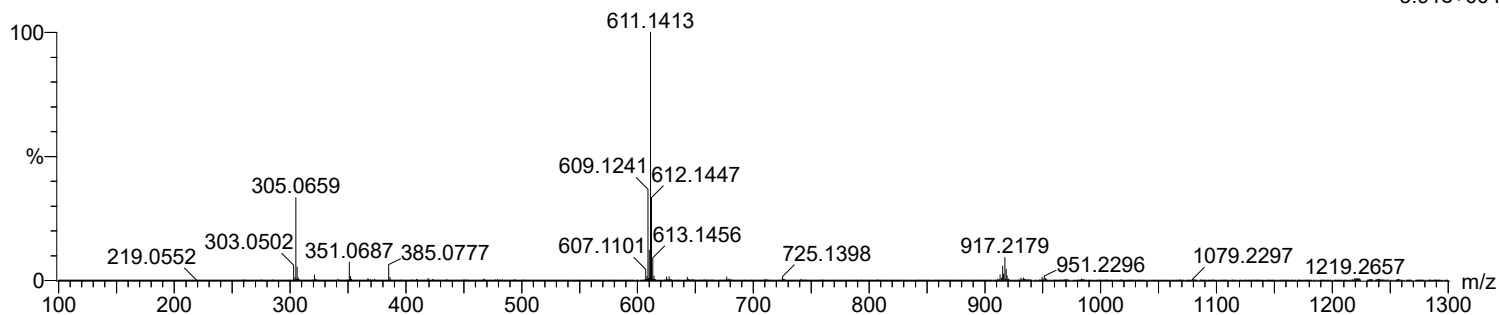
56 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170125_AA_MPLC1_5_NEG 171 (2.018)

1: TOF MS ES-
3.91e+004

Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
305.0659	305.0661	-0.2	-0.7	9.5	266.5	n/a	n/a	C15 H13 O7

Col 32

170125_AA_MPLC1_5_NEG 2376 (1.979)

3: Diode Array
1.404

