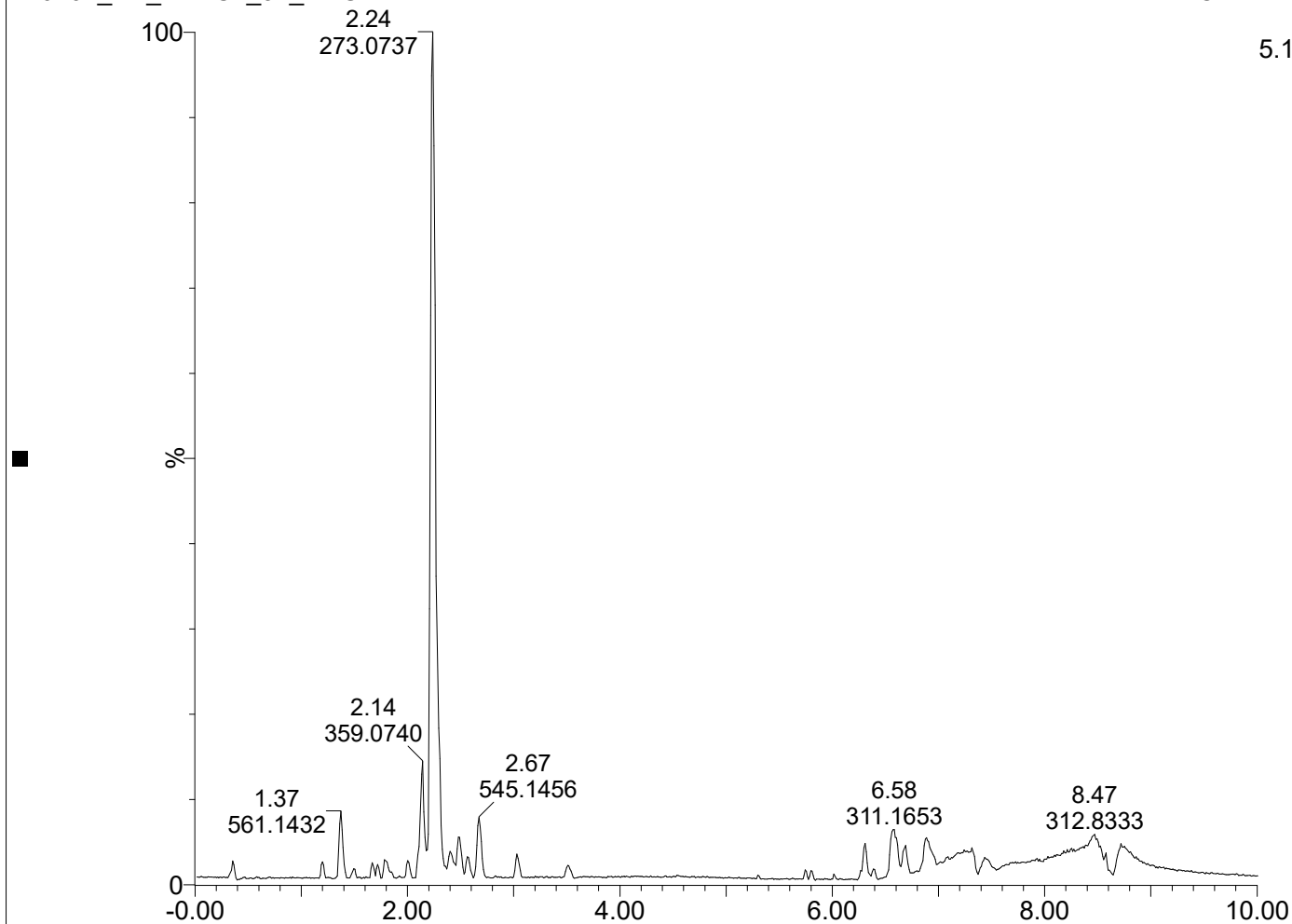


COMPOUND NO. S10 (METHOD A)

COL31

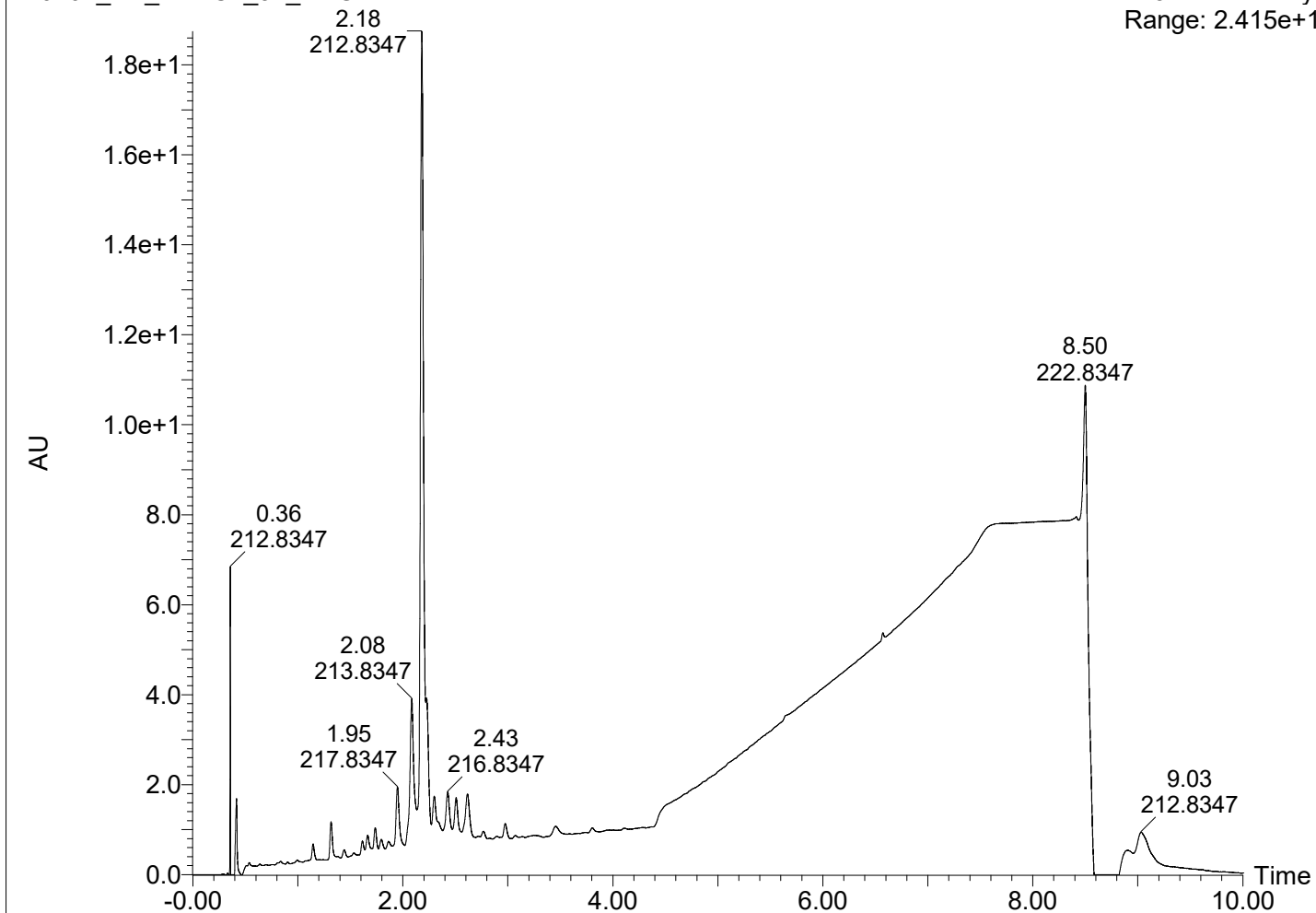
170104_AA_MPLC1_31_NEG

1: TOF MS ES-
BPI
5.11e4



170104_AA_MPLC1_31_NEG

3: Diode Array
Range: 2.415e+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

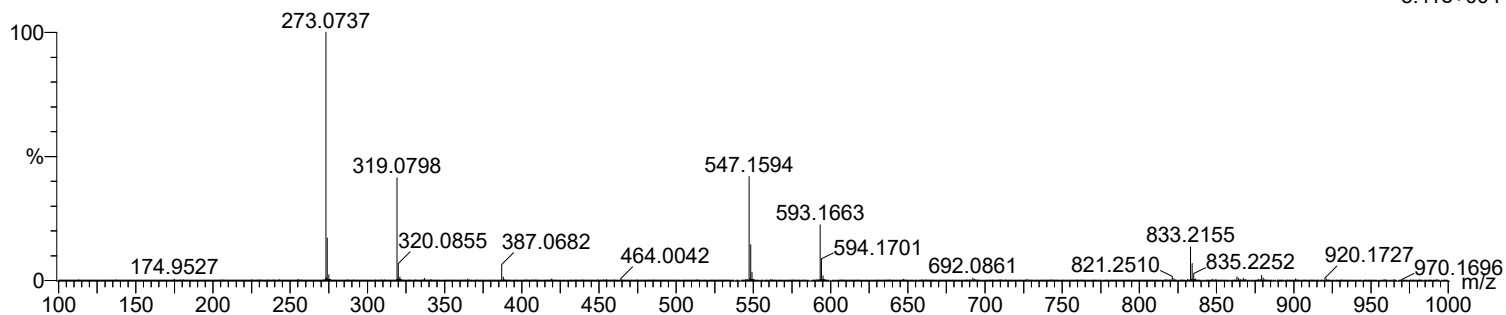
46 formula(e) evaluated with 2 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104_AA_MPLC1_31_NEG 193 (2.238)

1: TOF MS ES-
5.11e+004

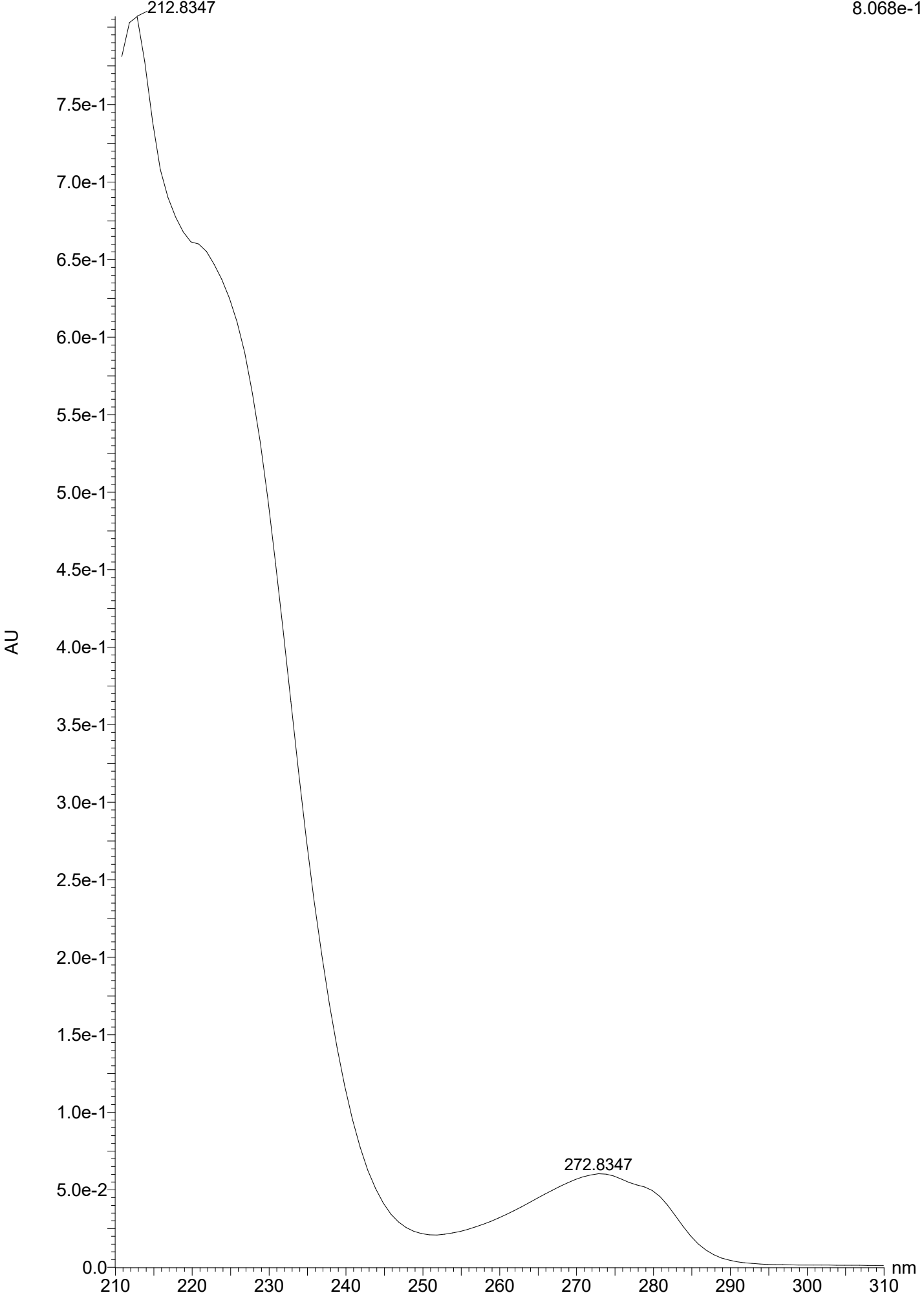
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
273.0737	273.0763	-2.6	-9.5	9.5	458.8	0.000	100.00	C15 H13 O5
	273.0704	3.3	12.1	18.5	468.8	10.008	0.00	C22 H9

COL31

170104_AA_MPLC1_31_NEG 2616 (2.179)

3: Diode Array
8.068e-1

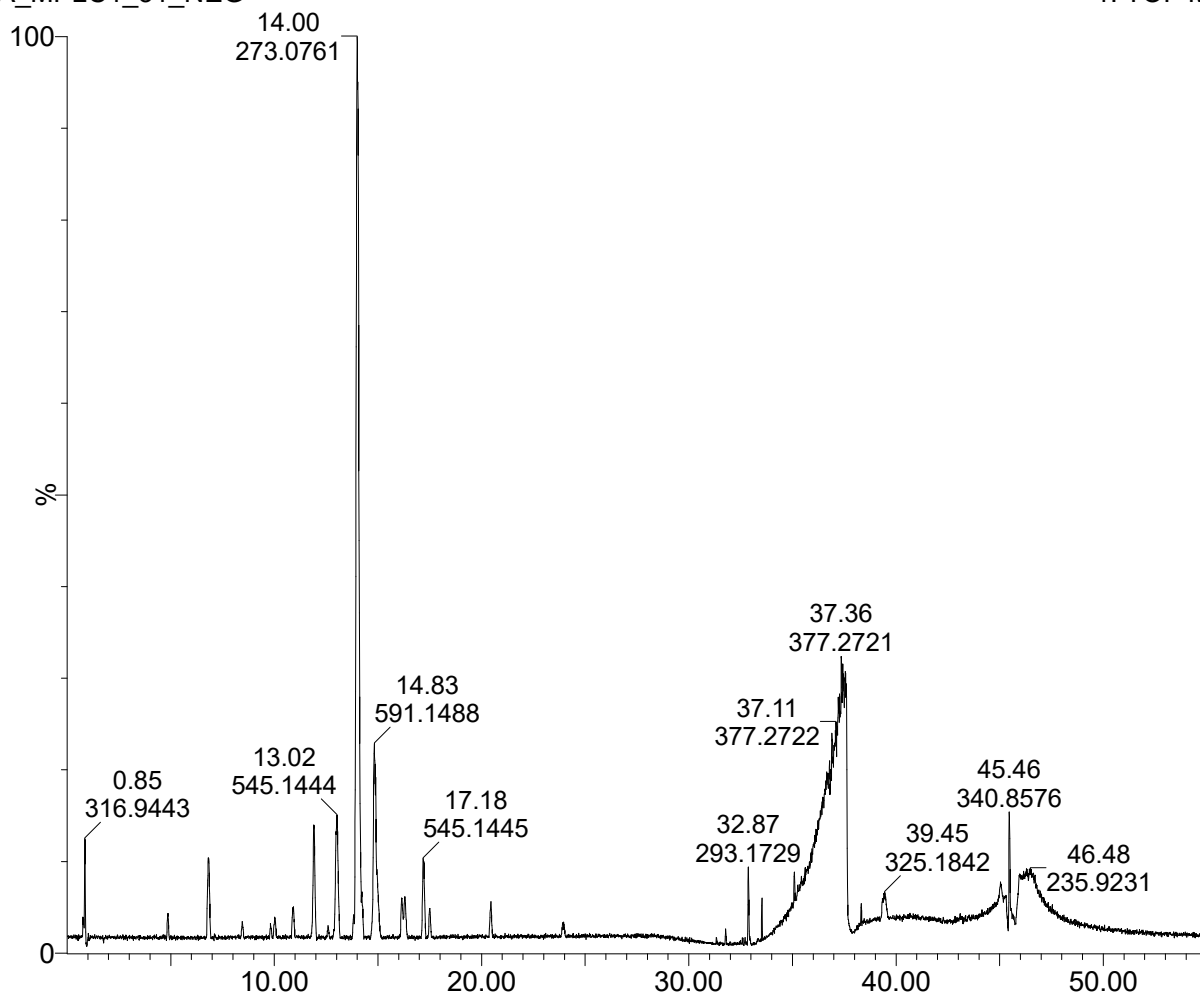


COMPOUND NO. S10 (METHOD B)

Col 32

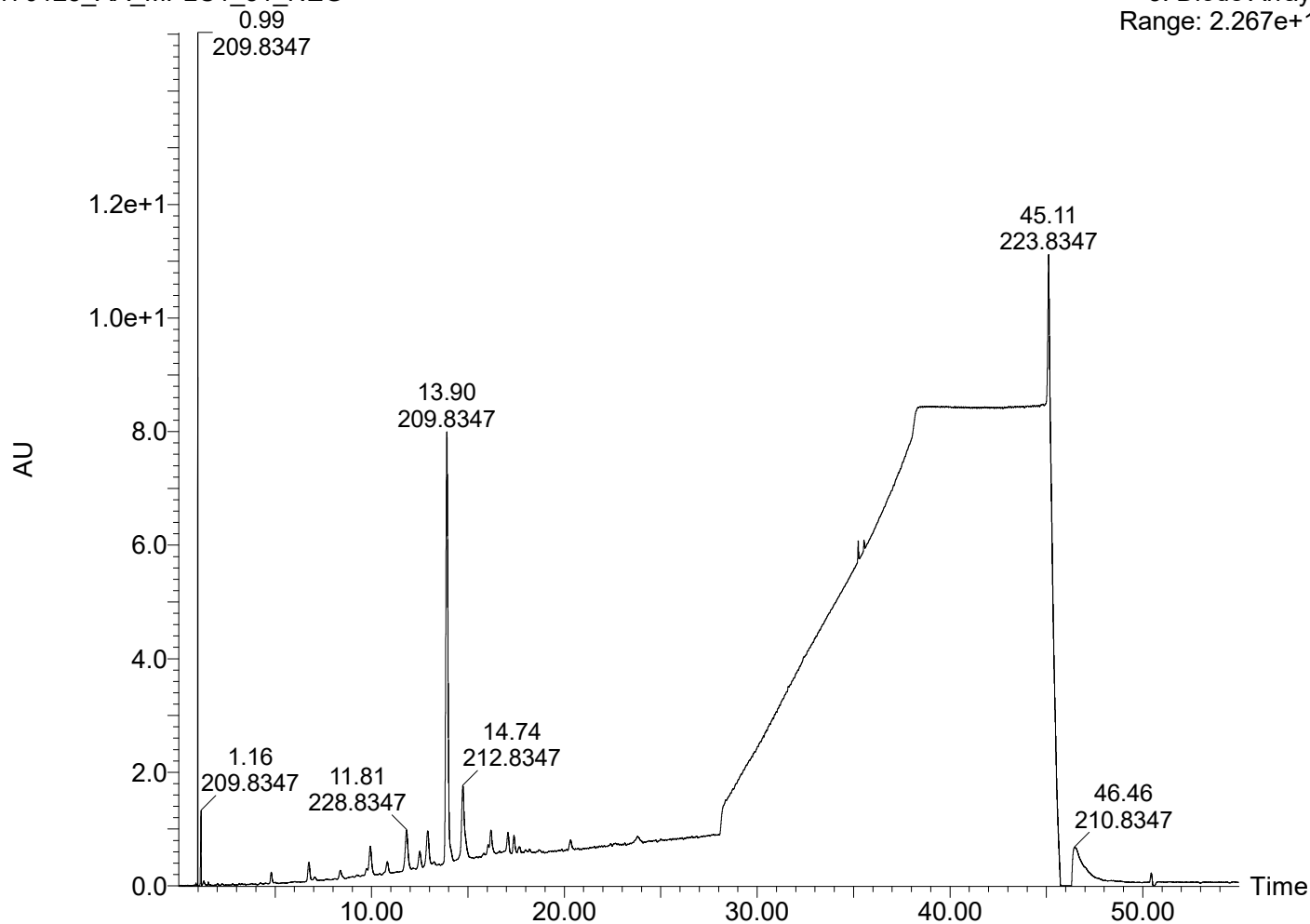
170125_AA_MPLC1_31_NEG

1: TOF MS ES-
BPI
1.56e4



170125_AA_MPLC1_31_NEG

3: Diode Array
Range: 2.267e+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

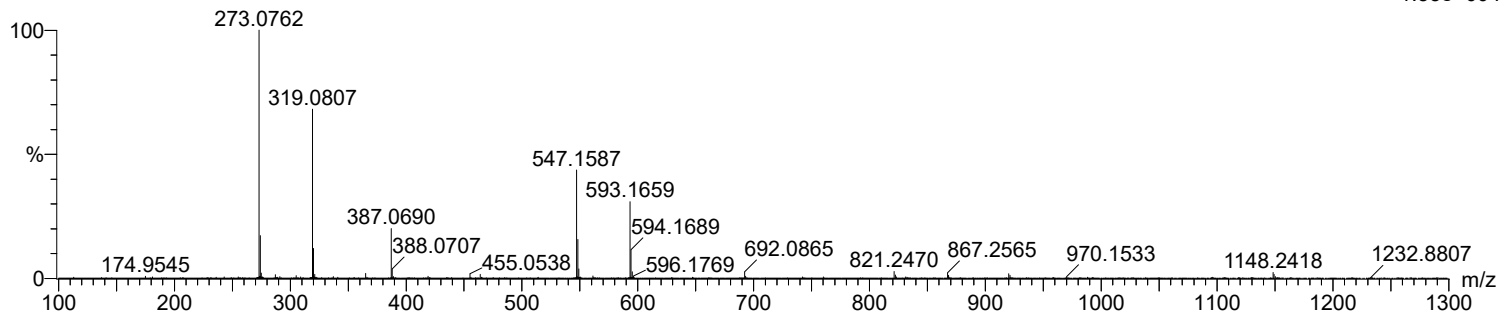
46 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170125_AA_MPLC1_31_NEG 1192 (14.006)

1: TOF MS ES-
1.55e+004

Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
273.0762	273.0763	-0.1	-0.4	9.5	325.6	n/a	n/a	C15 H13 O5

Col 32

170125_AA_MPLC1_31_NEG 16676 (13.898)

3: Diode Array
4.287e-1

