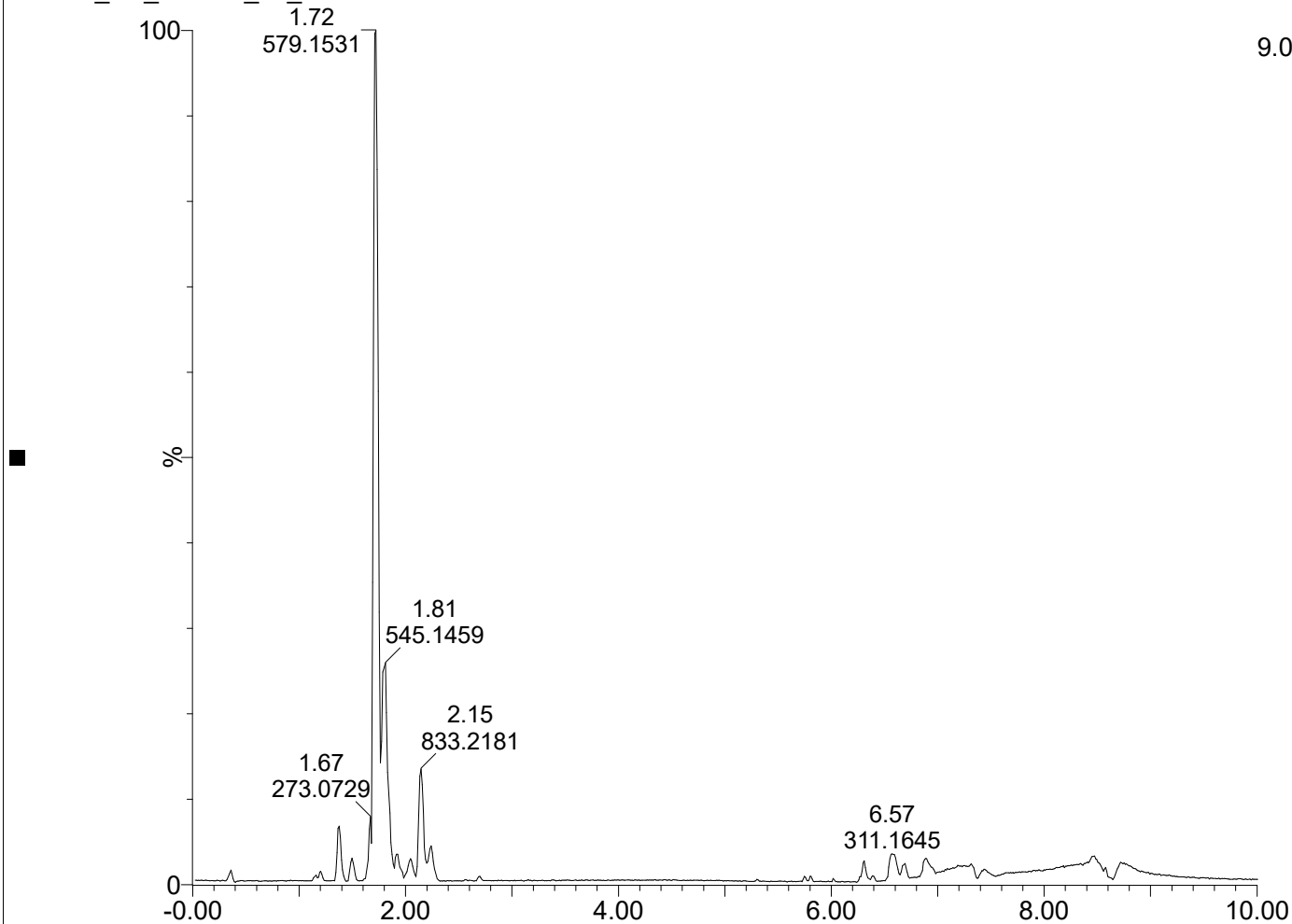


COMPOUND NO. S6 (METHOD A)

COL31

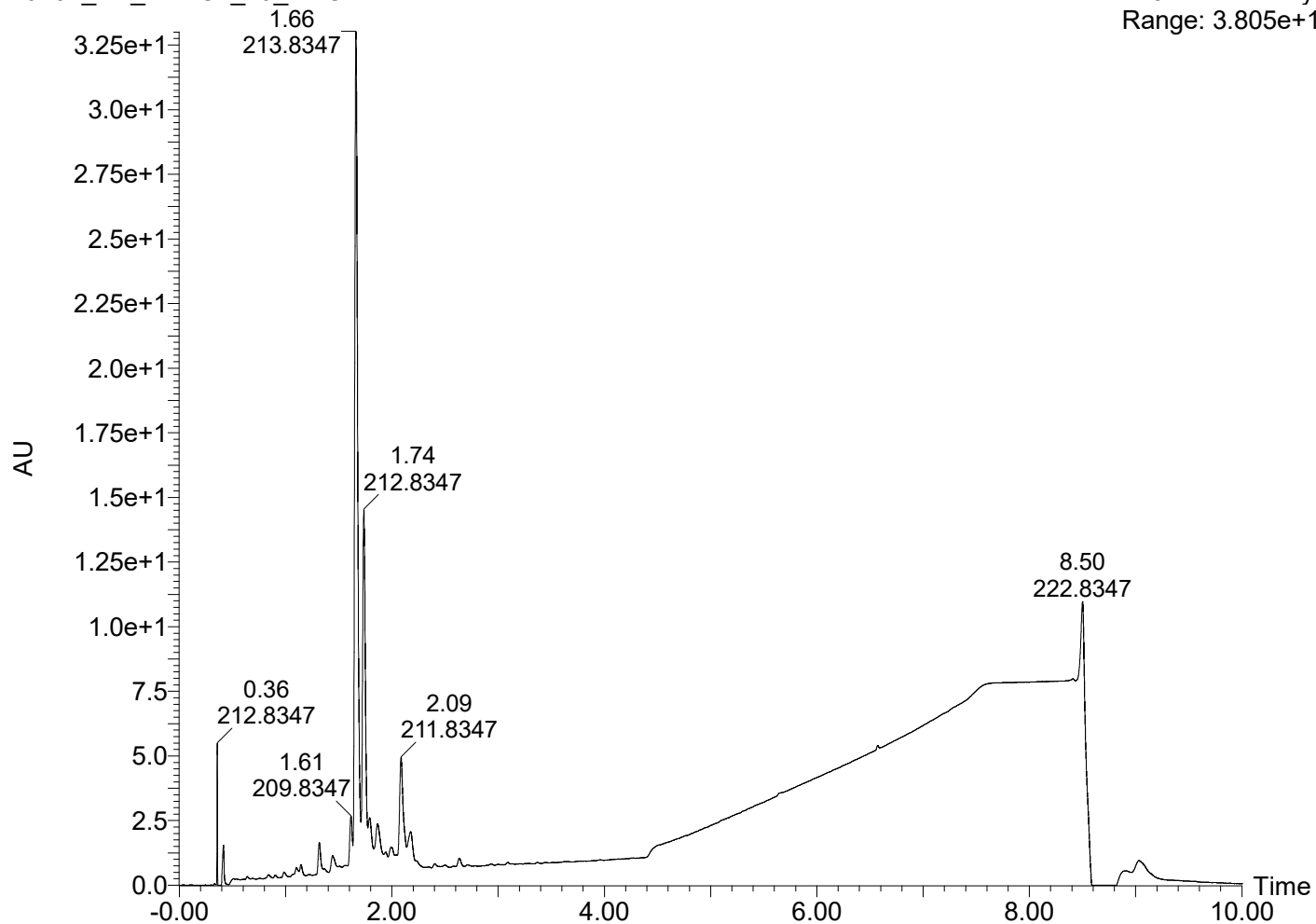
170104_AA_MPLC1_19_NEG

1: TOF MS ES-
BPI
9.00e4



170104_AA_MPLC1_19_NEG

3: Diode Array
Range: 3.805e+1



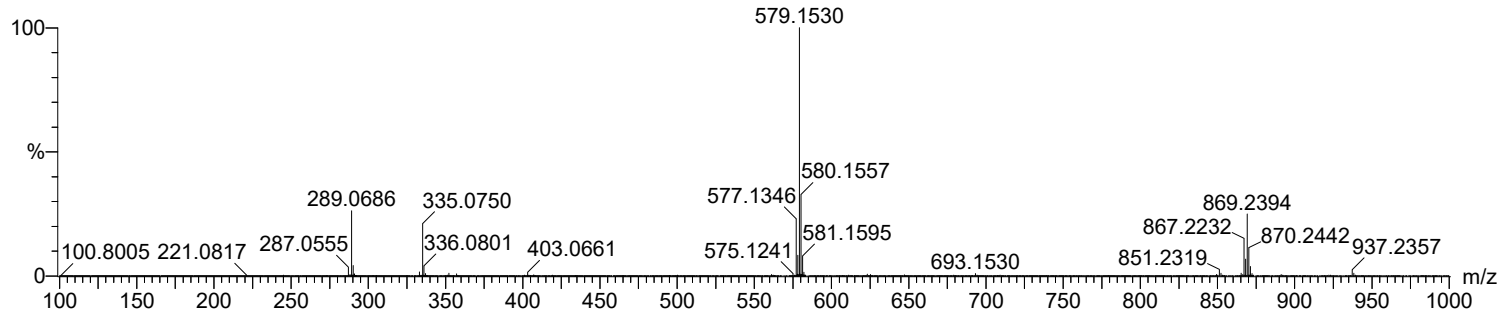
Single Mass Analysis

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
5588 formula(e) evaluated with 42 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_19_NEG 148 (1.722)

1: TOF MS ES-
9.00e+004



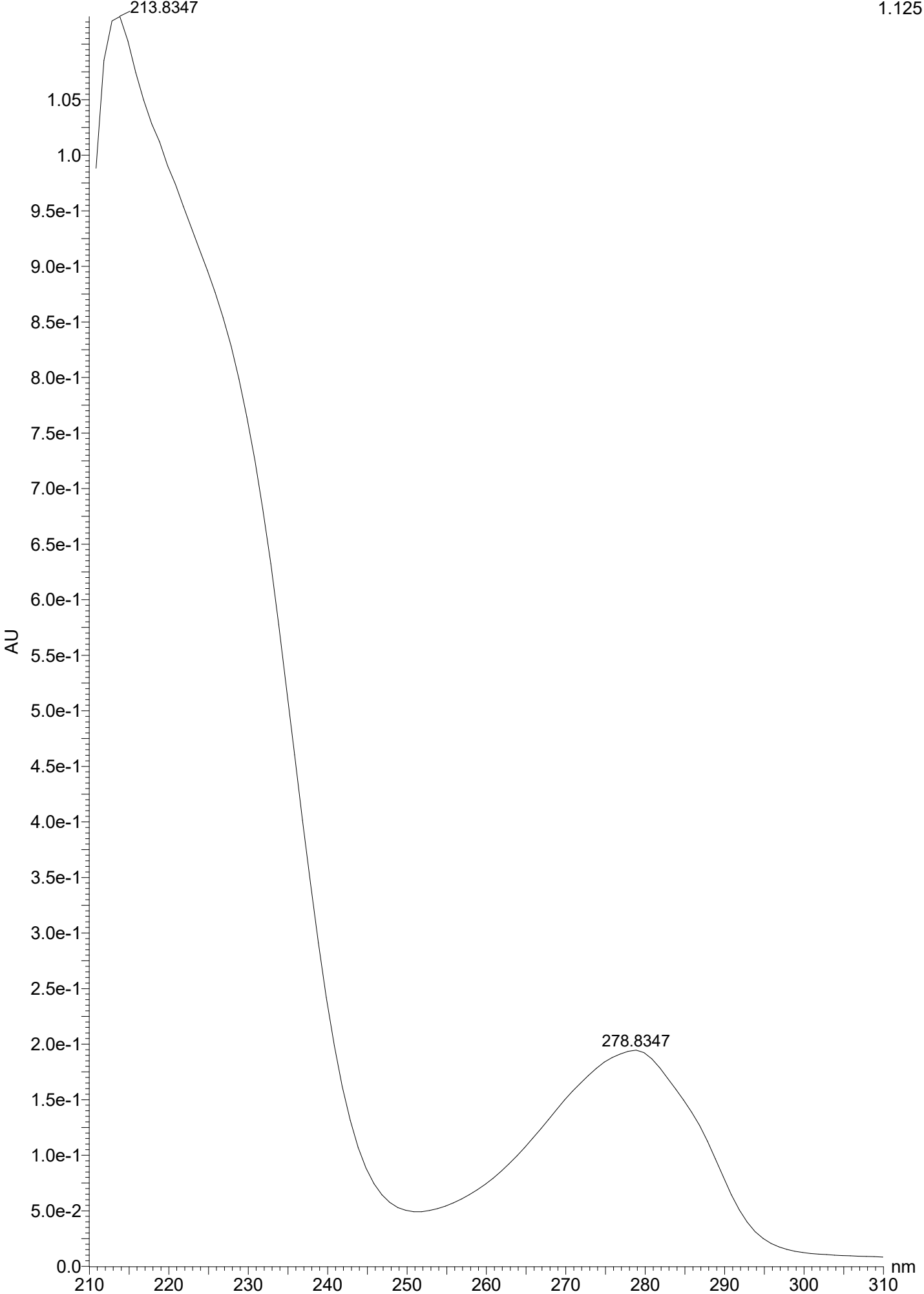
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
289.0686	289.0712	-2.6	-9.0	9.5	401.3	0.060	94.18	C15 H13 O6
289.0685		0.1	0.3	10.5	405.0	3.785	2.27	C11 H9 N6 O4
289.0726		-4.0	-13.8	14.5	405.3	4.070	1.71	C16 H9 N4 O2
289.0672		1.4	4.8	5.5	405.5	4.274	1.39	C10 H13 N2 O8
289.0699		-1.3	-4.5	15.5	406.6	5.397	0.45	C12 H5 N10

COL31

170104_AA_MPLC1_19_NEG 1998 (1.664)

3: Diode Array
1.125

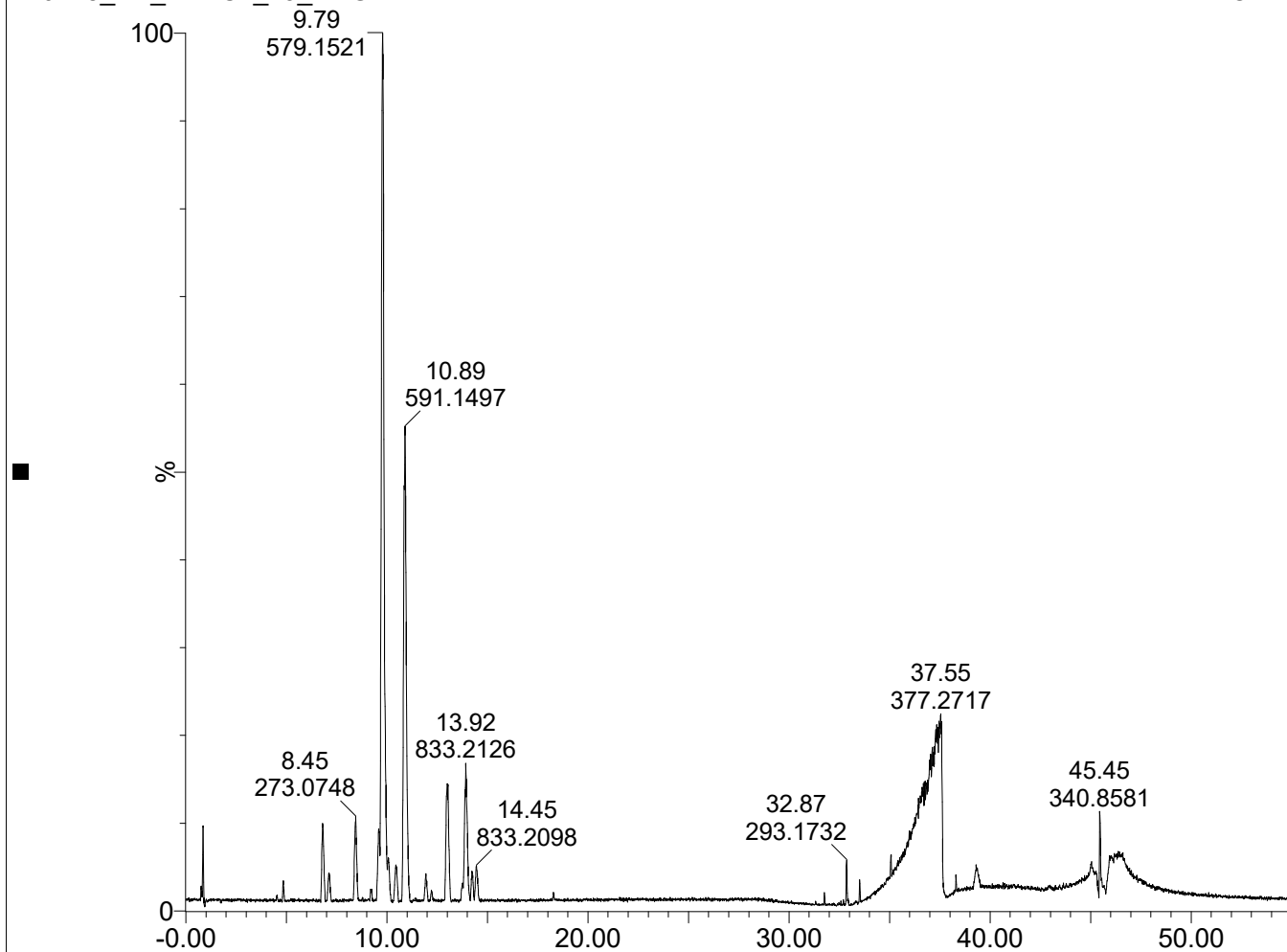


COMPOUND NO. S6 (METHOD B)

Col 32

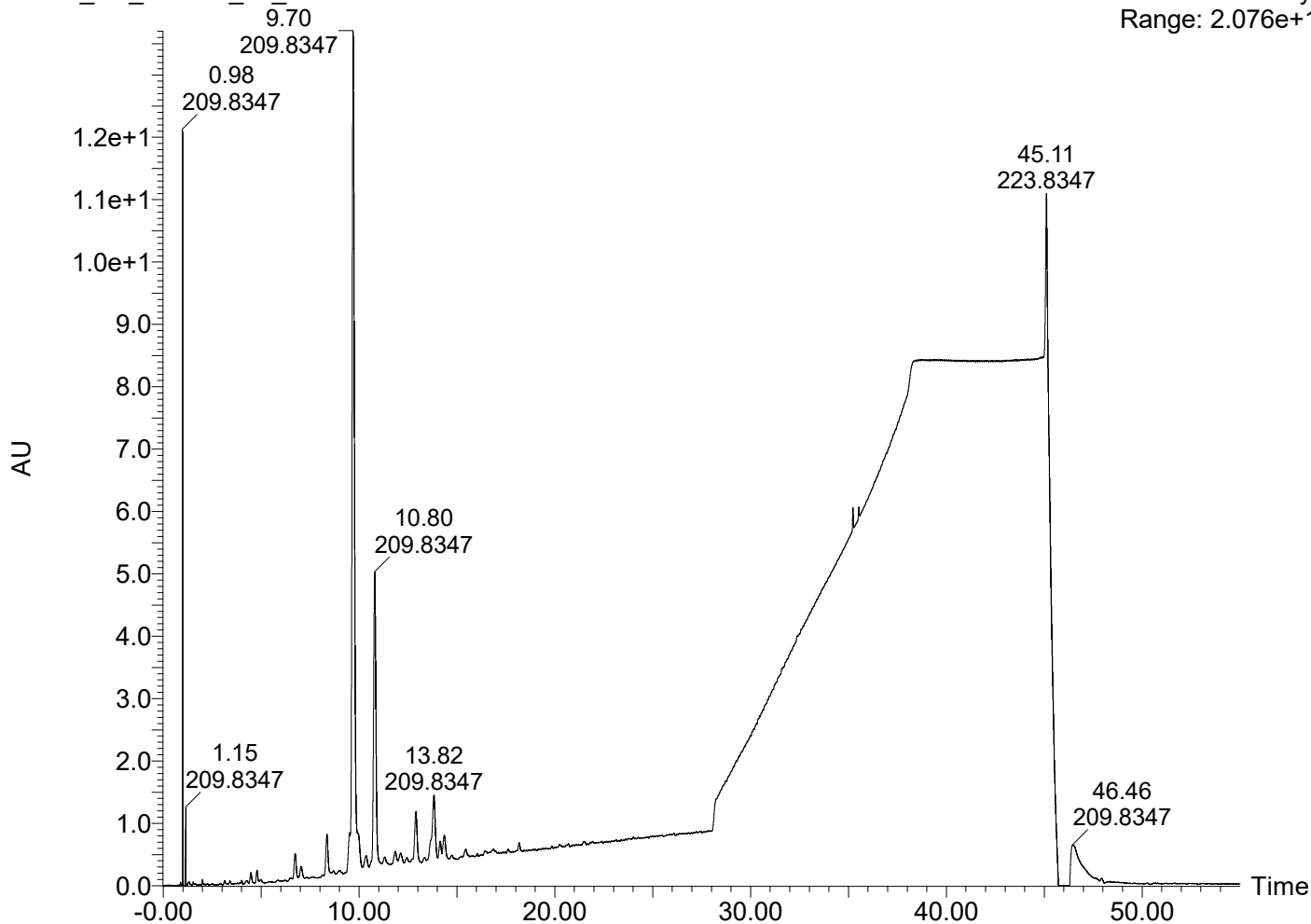
170125_AA_MPLC1_19_NEG

1: TOF MS ES-
BPI
2.14e4



170125_AA_MPLC1_19_NEG

3: Diode Array
Range: 2.076e+1

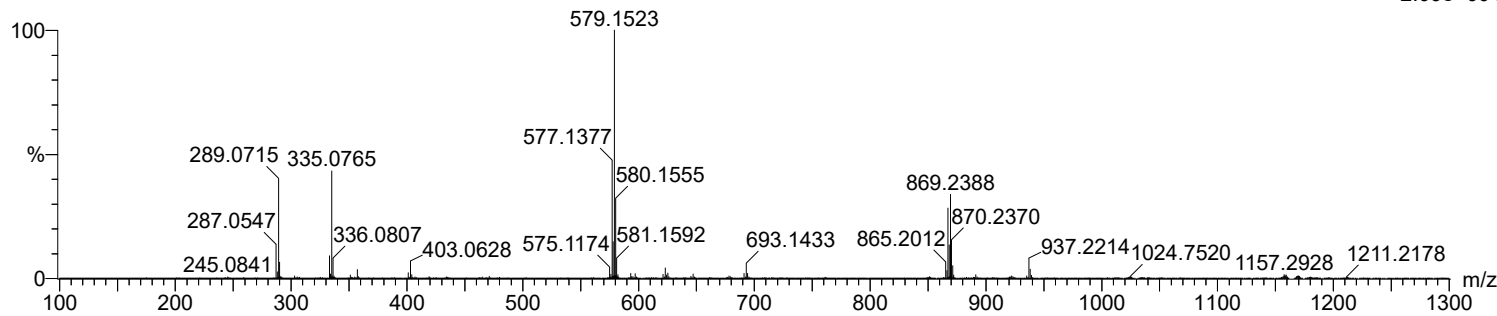


Single Mass Analysis

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
51 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_19_NEG 833 (9.776)

1: TOF MS ES-
2.09e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
289.0715	289.0712	0.3	1.0	9.5	248.8	n/a	n/a	C15 H13 O6

Col 32

170125_AA_MPLC1_19_NEG 11651 (9.709)

3: Diode Array
7.187e-1

