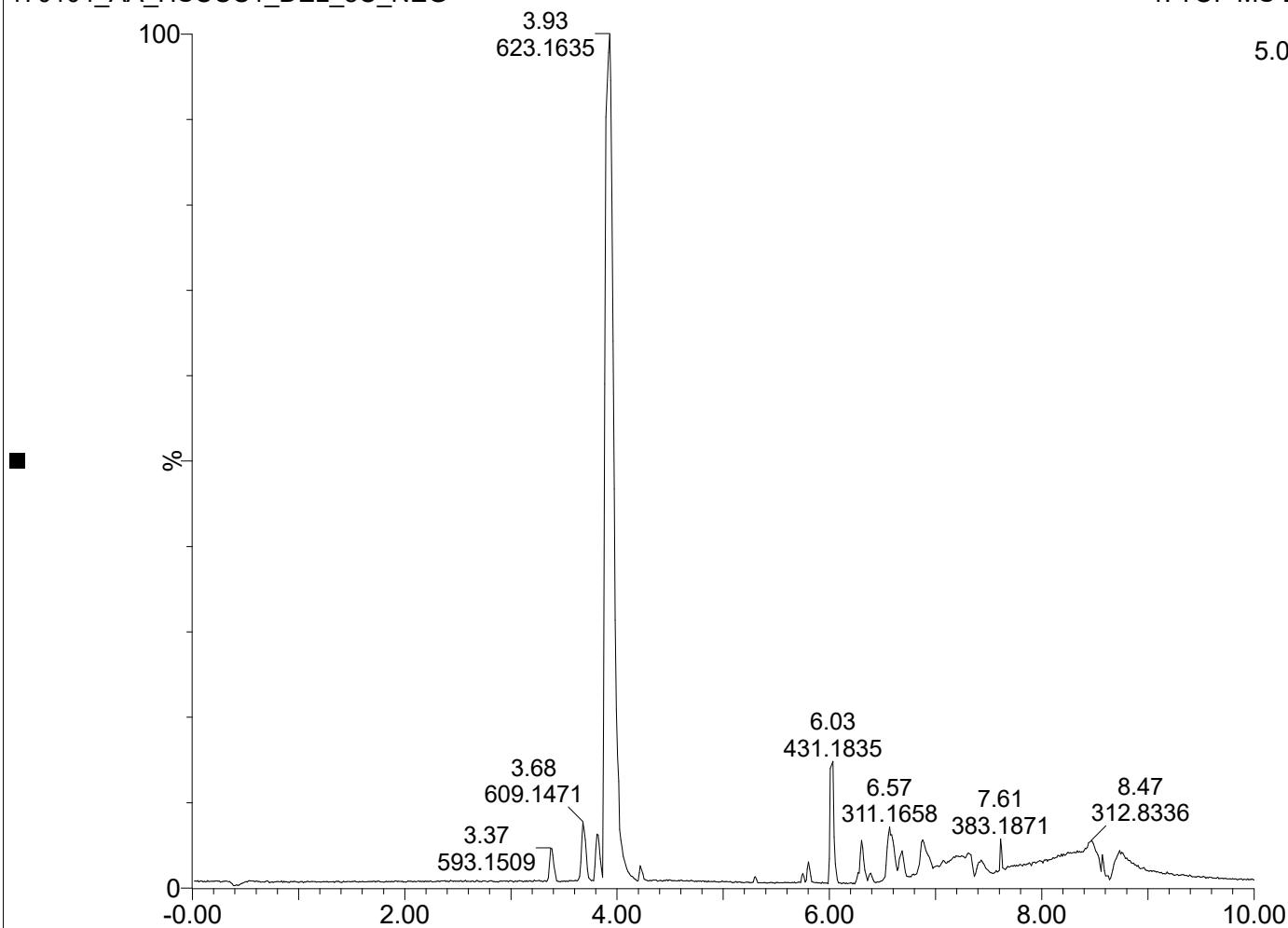


COMPOUND NO. S24 (METHOD A)

COL31

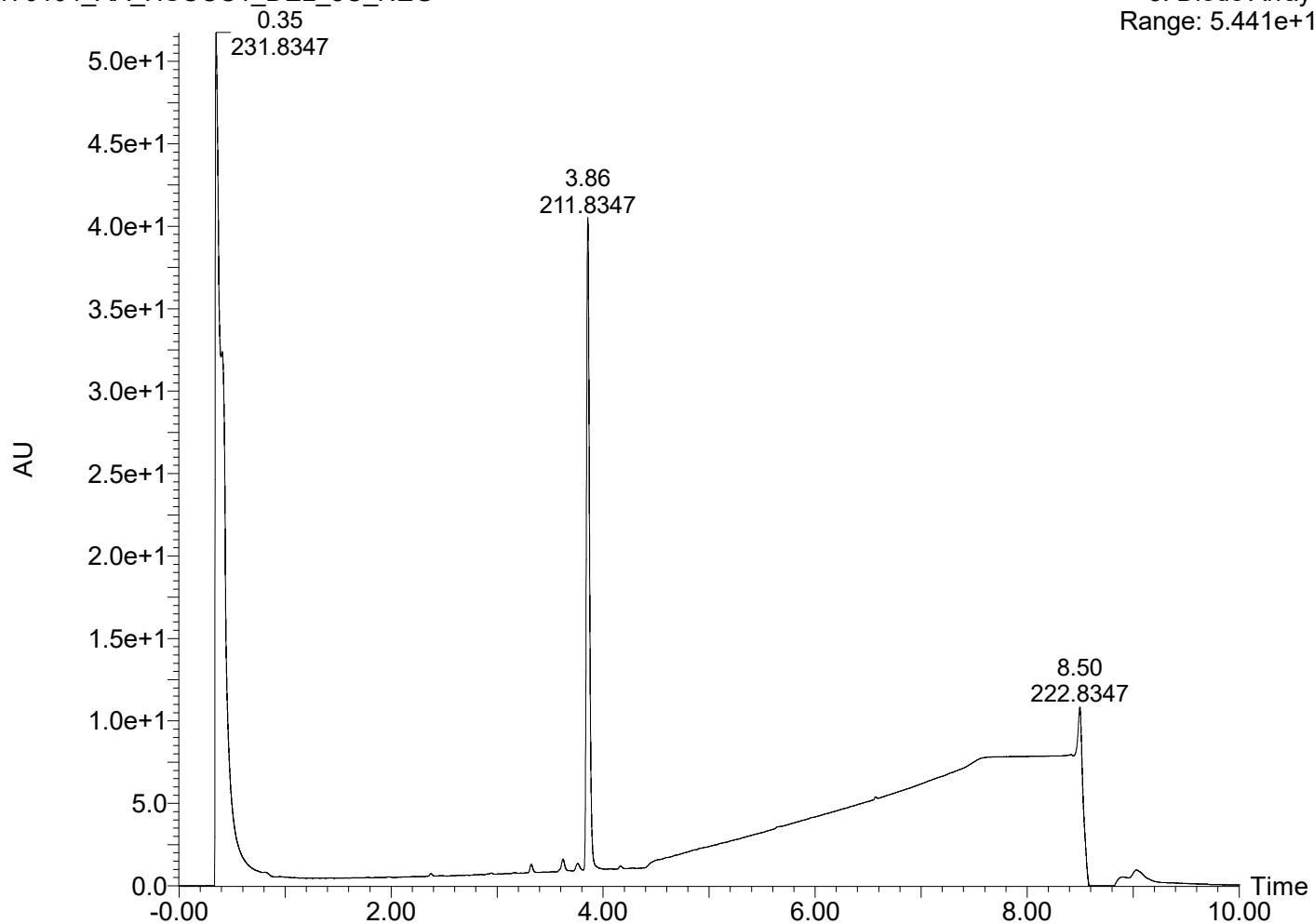
170104_AA_HSCCC1_DEL_8C_NEG

1: TOF MS ES-
BPI
5.03e4



170104_AA_HSCCC1_DEL_8C_NEG

3: Diode Array
Range: 5.441e+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

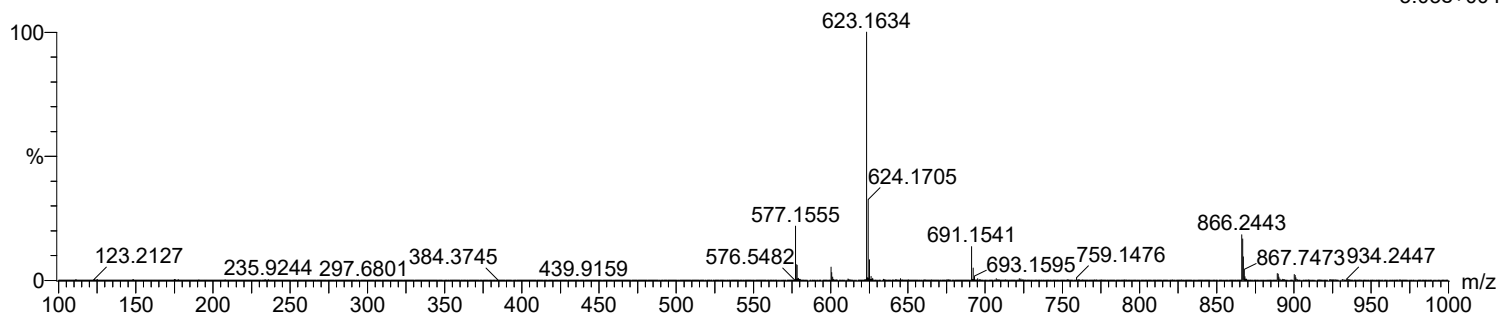
162 formula(e) evaluated with 5 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104_AA_HSCCC1_DEL_8C_NEG 338 (3.930)

1: TOF MS ES-
5.03e+004

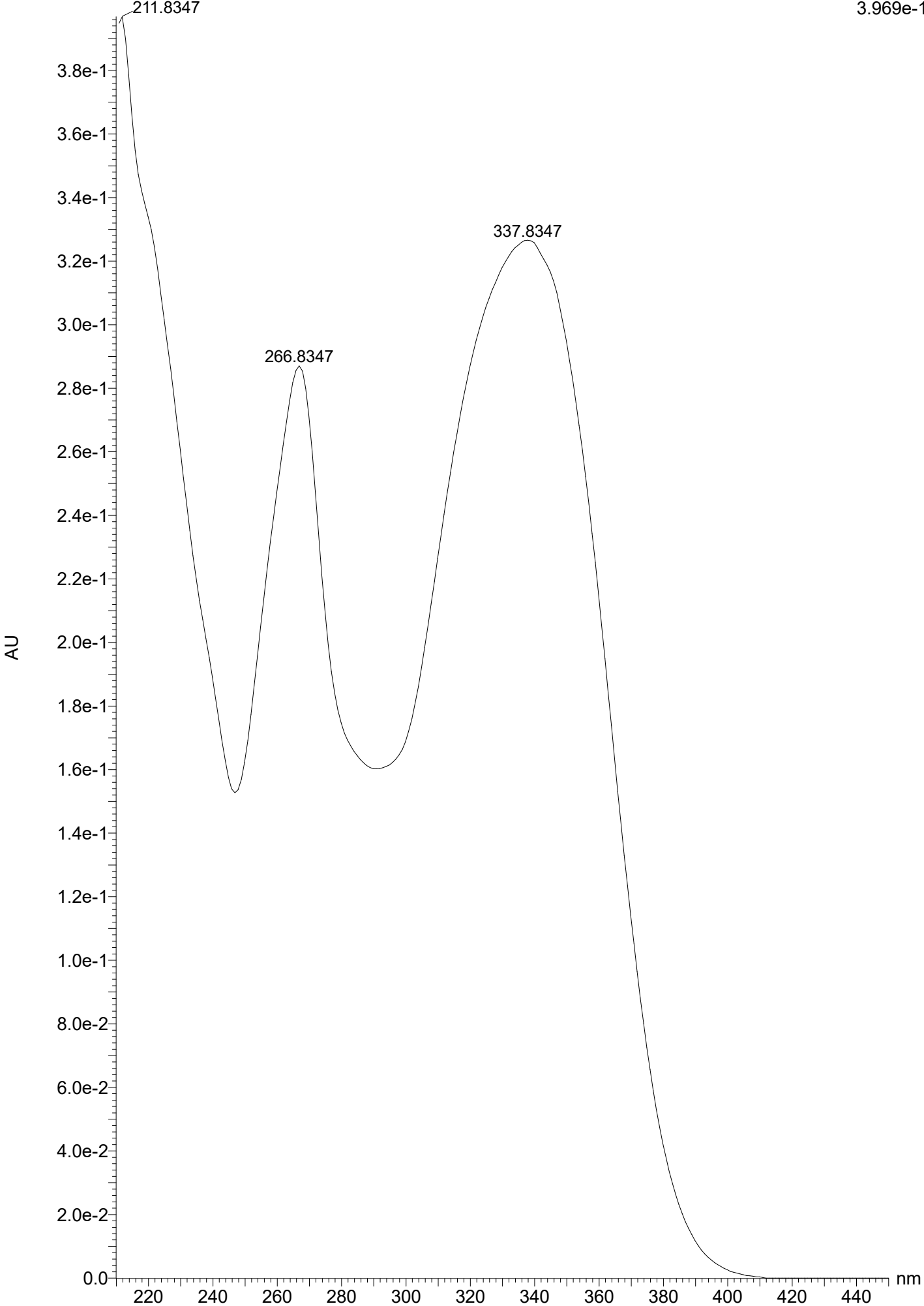
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1569	577.1557	1.2	2.1	13.5	167.9	0.676	50.87	C27 H29 O14
577.1616		-4.7	-8.1	4.5	168.4	1.098	33.37	C20 H33 O19
577.1499		7.0	12.1	22.5	169.6	2.346	9.57	C34 H25 O9
577.1651		-8.2	-14.2	26.5	170.6	3.360	3.47	C38 H25 O6
577.1592		-2.3	-4.0	35.5	170.9	3.606	2.72	C45 H21 O

COL31

170104_AA_HSCCC1_DEL_8C_NEG 4630 (3.857)

3: Diode Array
3.969e-1

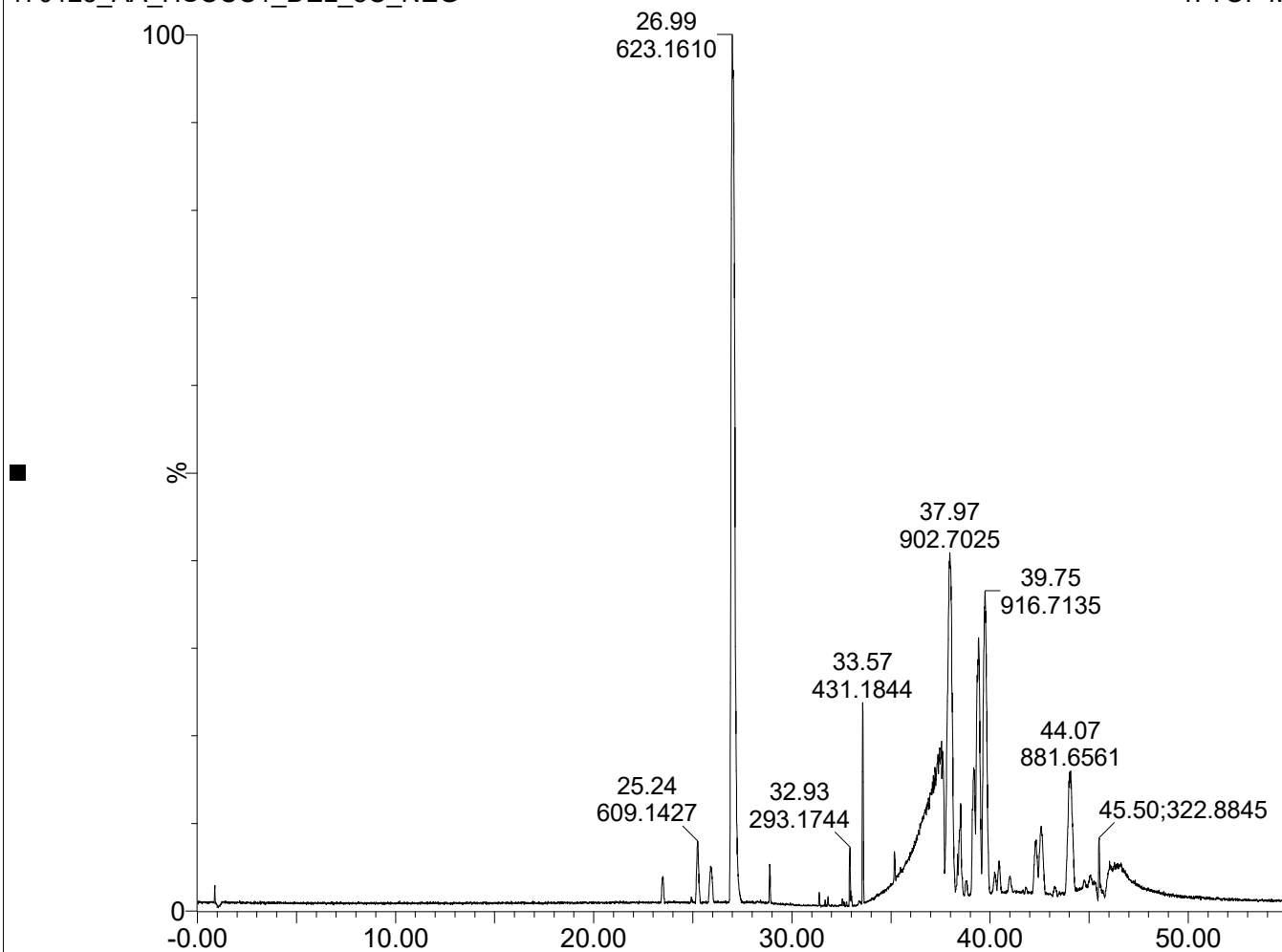


COMPOUND NO. S24 (METHOD B)

Col 32

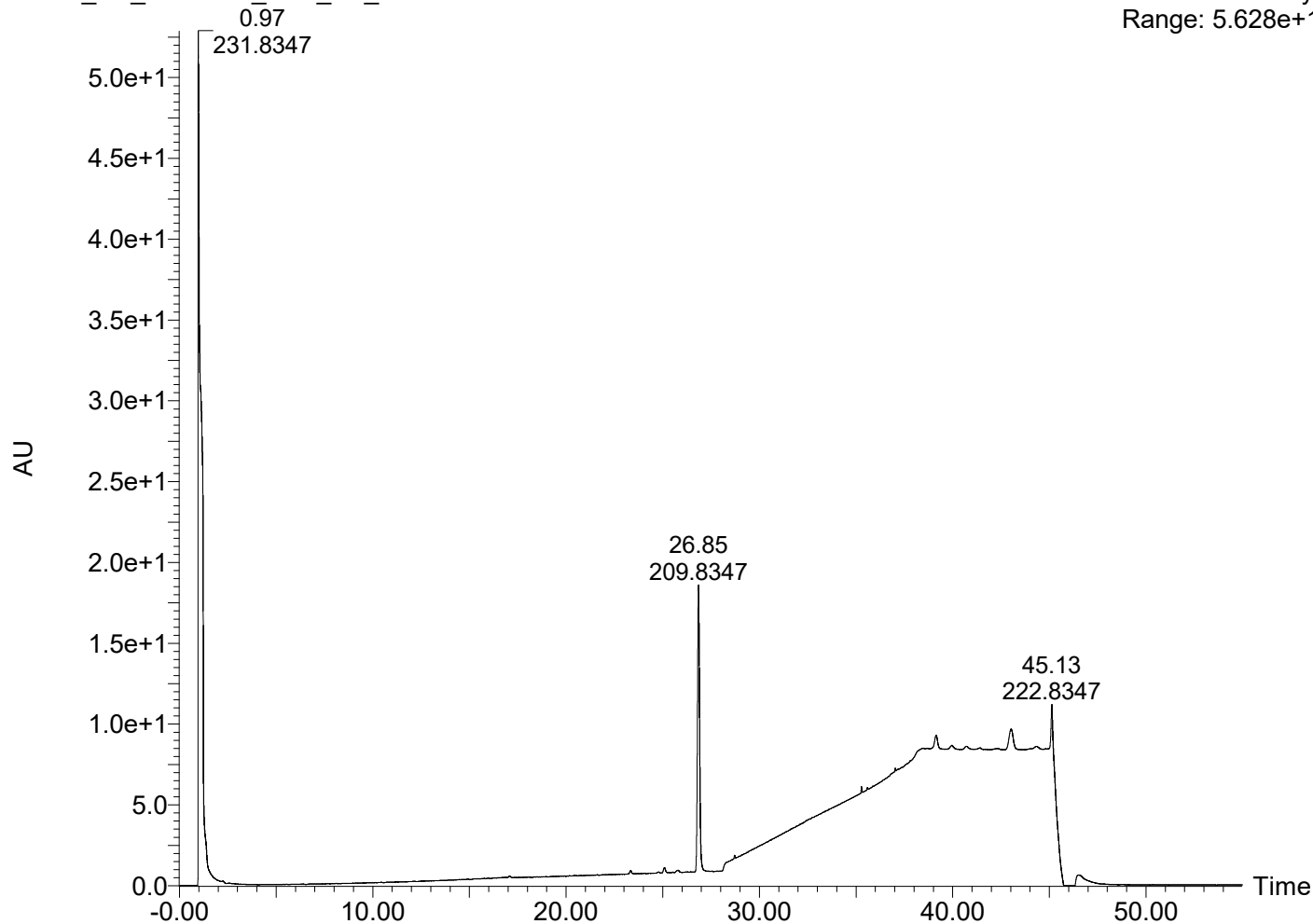
170125_AA_HSCCC1_DEL_8C_NEG

1: TOF MS ES-
BPI
2.55e4



170125_AA_HSCCC1_DEL_8C_NEG

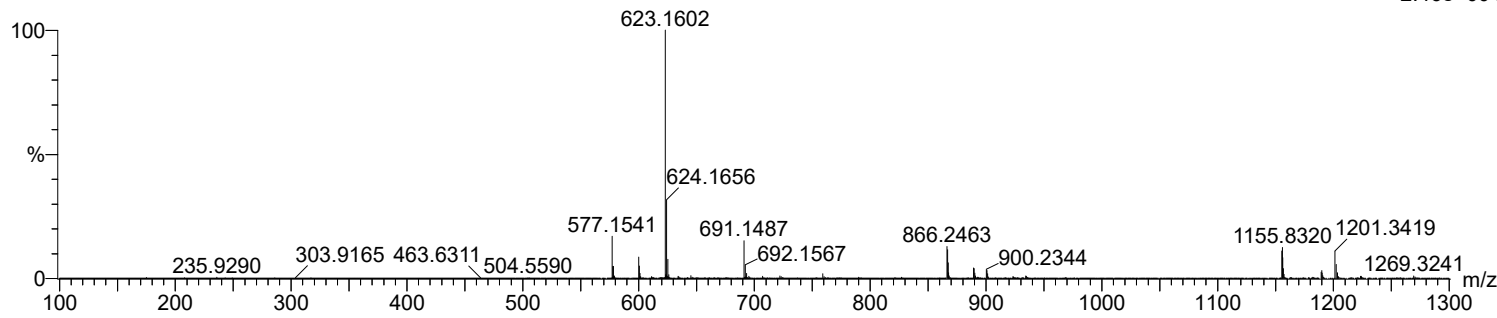
3: Diode Array
Range: 5.628e+1



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
162 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
170125_AA_HSCCC1_DEL_8C_NEG 2297 (27.011)

1: TOF MS ES-
2.46e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1541	577.1557	-1.6	-2.8	13.5	157.2	0.136	87.33	C27 H29 O14
577.1616		-7.5	-13.0	4.5	159.4	2.330	9.73	C20 H33 O19
577.1499		4.2	7.3	22.5	161.0	3.936	1.95	C34 H25 O9
577.1463		7.8	13.5	0.5	161.9	4.806	0.82	C16 H33 O22
577.1592		-5.1	-8.8	35.5	163.5	6.358	0.17	C45 H21 O

Col 32

170125_AA_HSCCC1_DEL_8C_NEG 32210 (26.846)

3: Diode Array
2.108e-1

