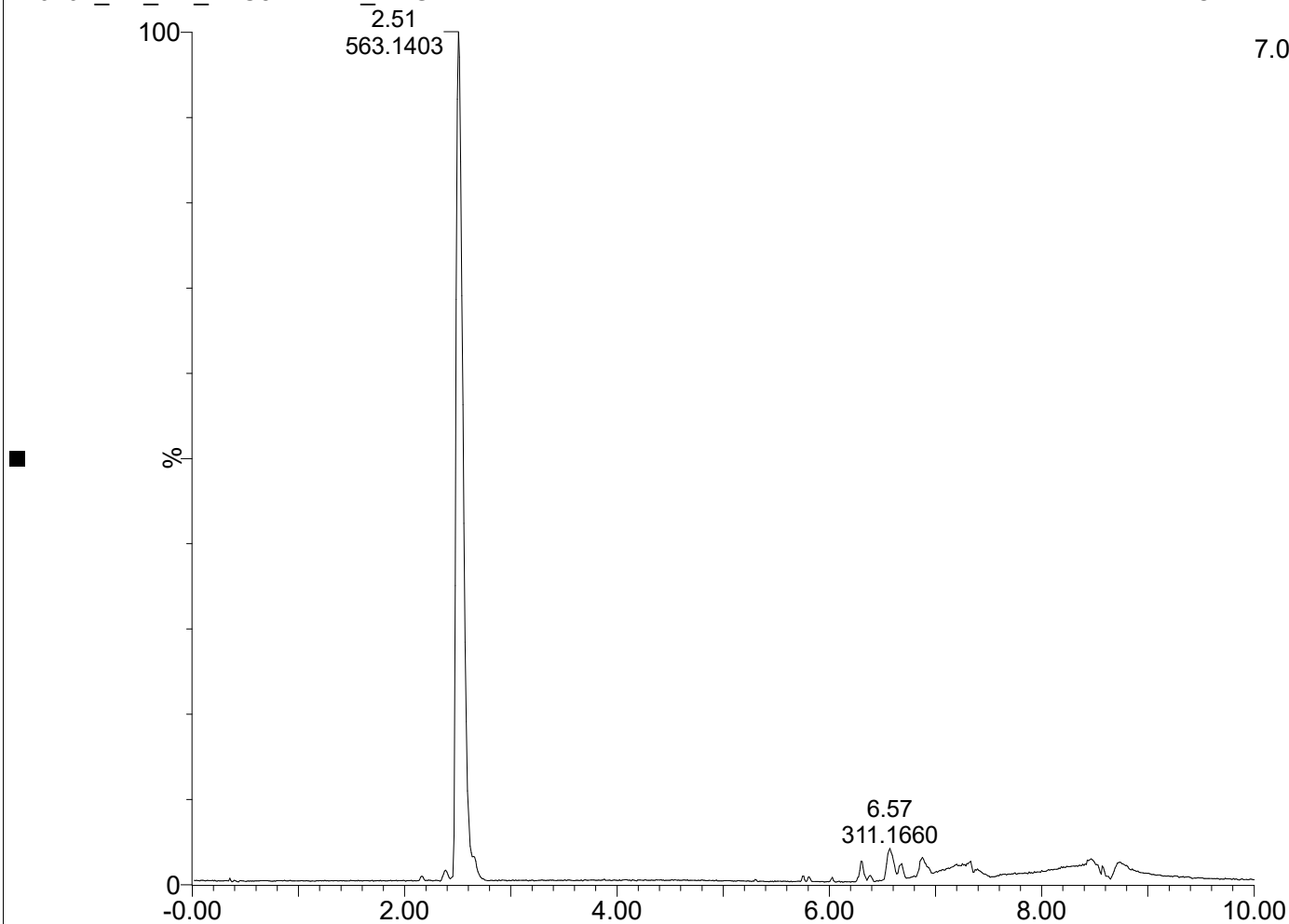


COMPOUND NO. S14 (METHOD A)

COL31

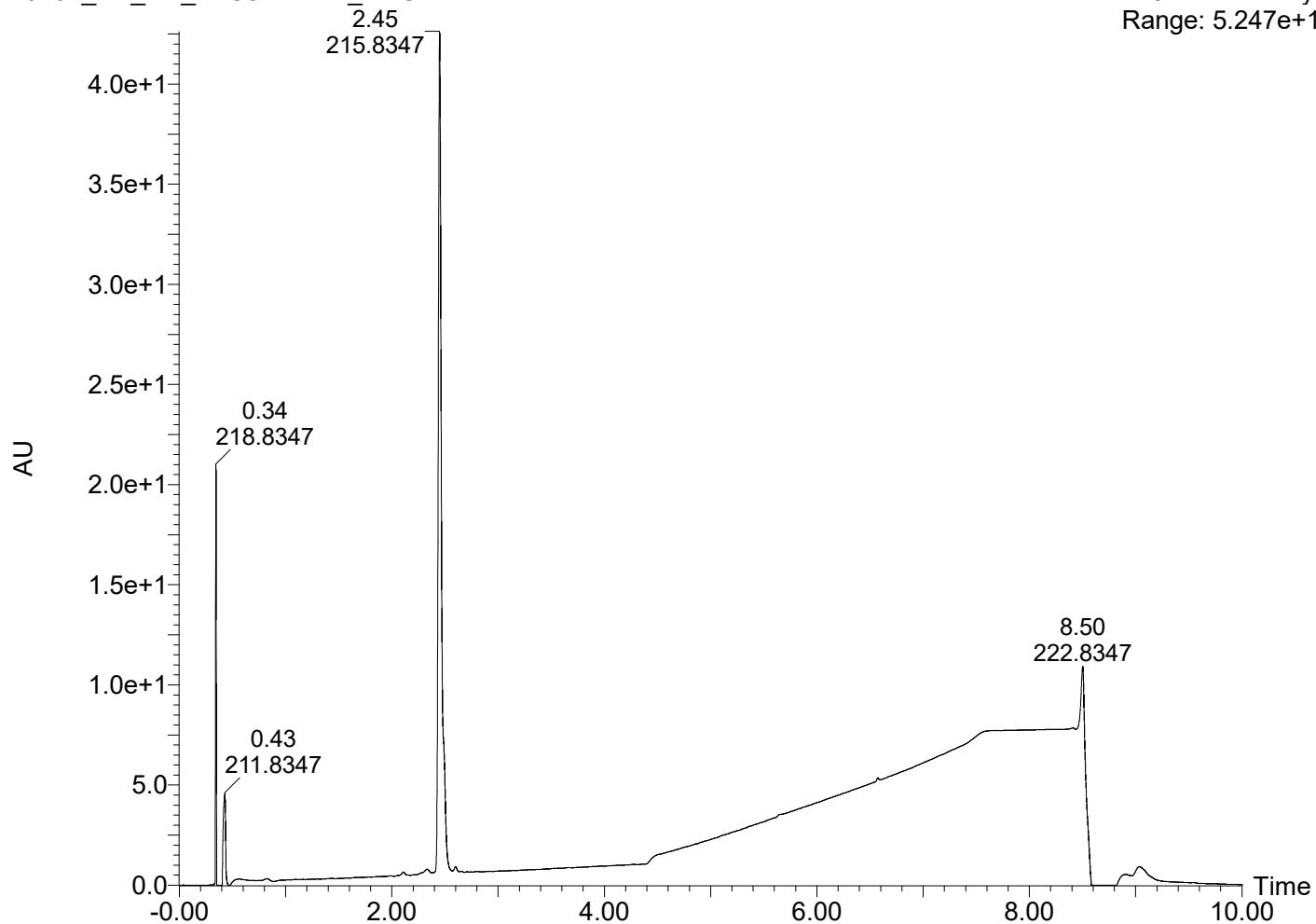
170104_AA_NK_PLC5-FB-1-2_NEG

1: TOF MS ES-
BPI
7.08e4



170104_AA_NK_PLC5-FB-1-2_NEG

3: Diode Array
Range: 5.247e+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

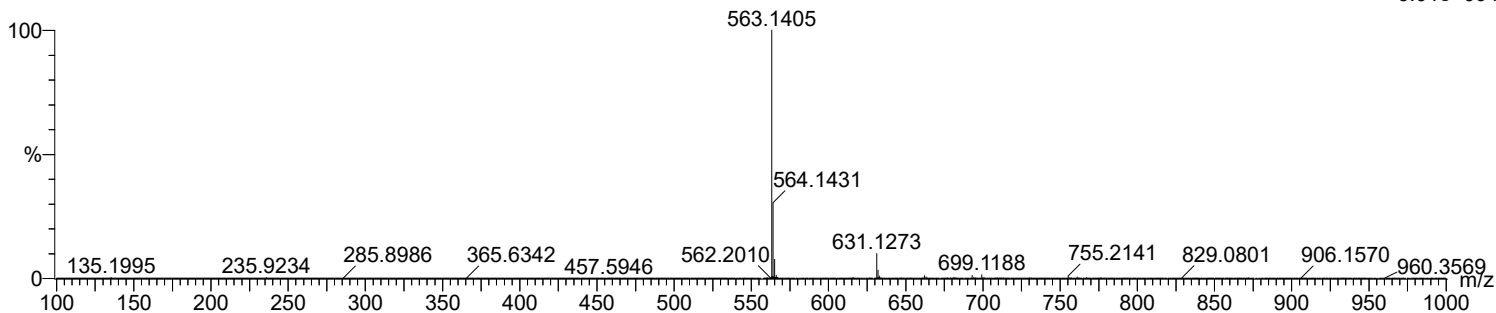
161 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104_AA_NK_PLC5-FB-1-2_NEG 218 (2.528)

1: TOF MS ES-
6.01e+004

Minimum: -1.5

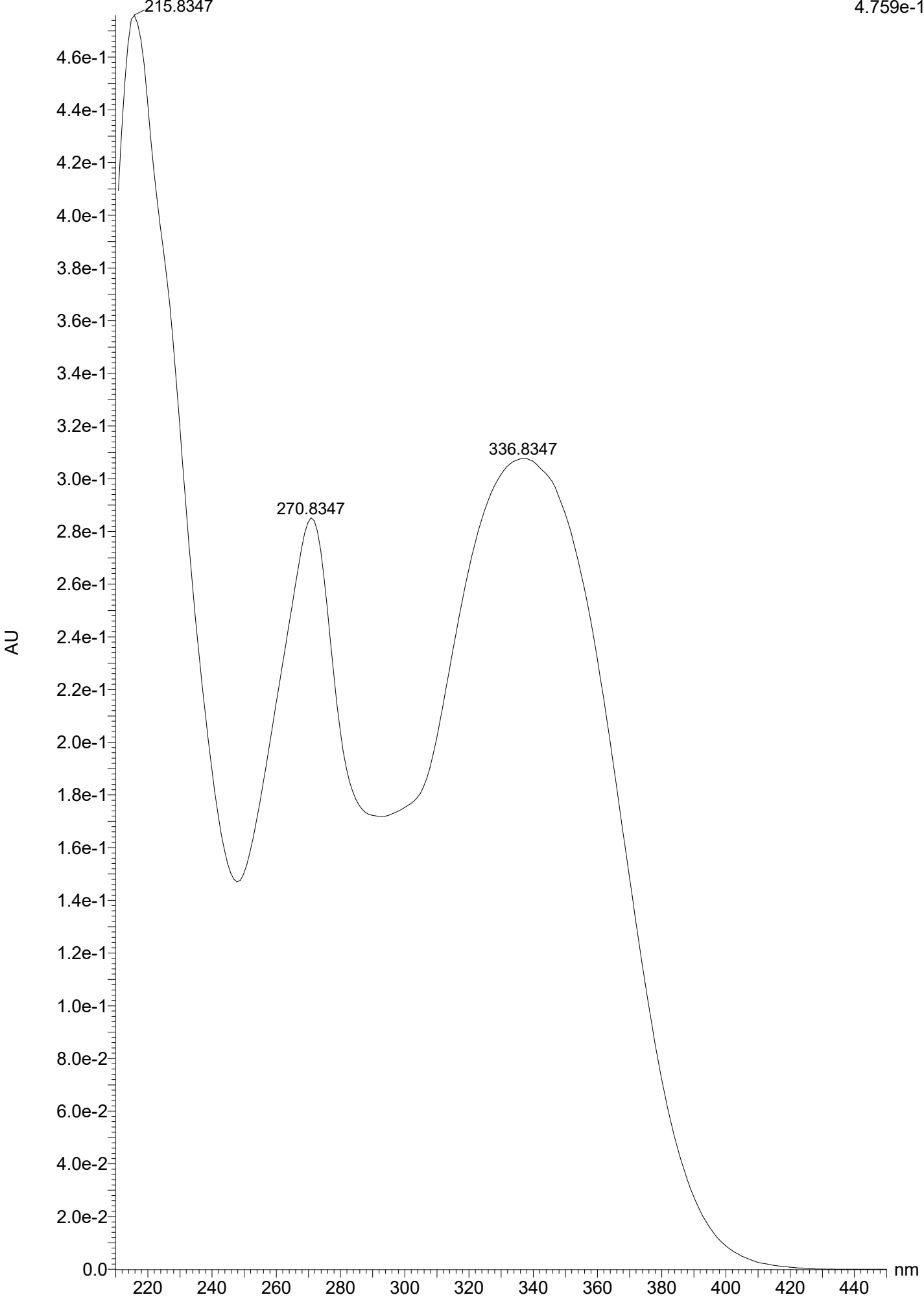
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
563.1405	563.1401	0.4	0.7	13.5	208.2	0.012	98.82	C26 H27 O14
	563.1342	6.3	11.2	22.5	212.8	4.563	1.04	C33 H23 O9
	563.1436	-3.1	-5.5	35.5	215.3	7.062	0.09	C44 H19 O
	563.1460	-5.5	-9.8	4.5	215.8	7.567	0.05	C19 H31 O19

COL31

170104_AA_NK_PLC5-FB-1-2_NEG 2939 (2.448)

3: Diode Array
4.759e-1

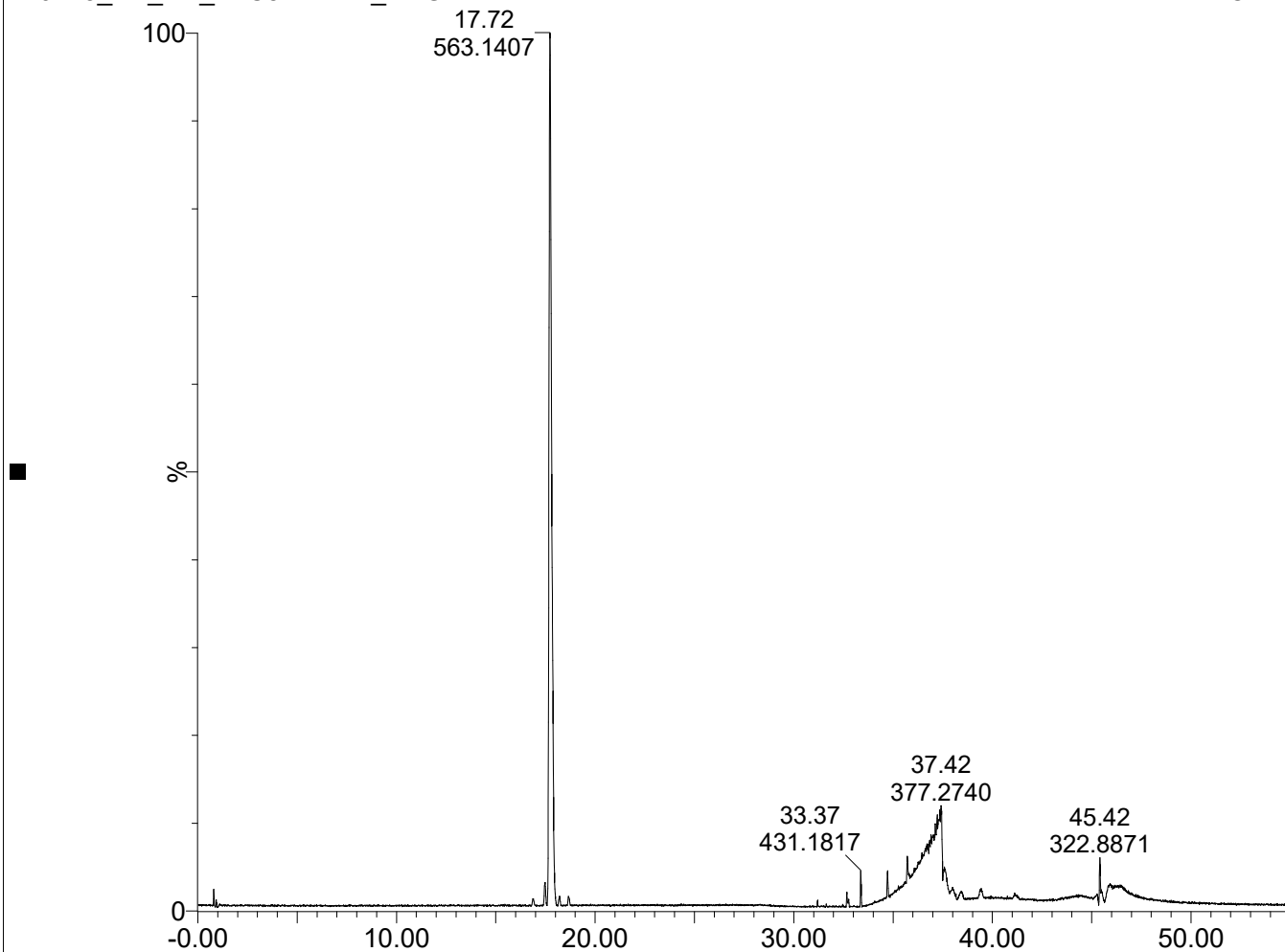


COMPOUND NO. S14 (METHOD B)

Col 32

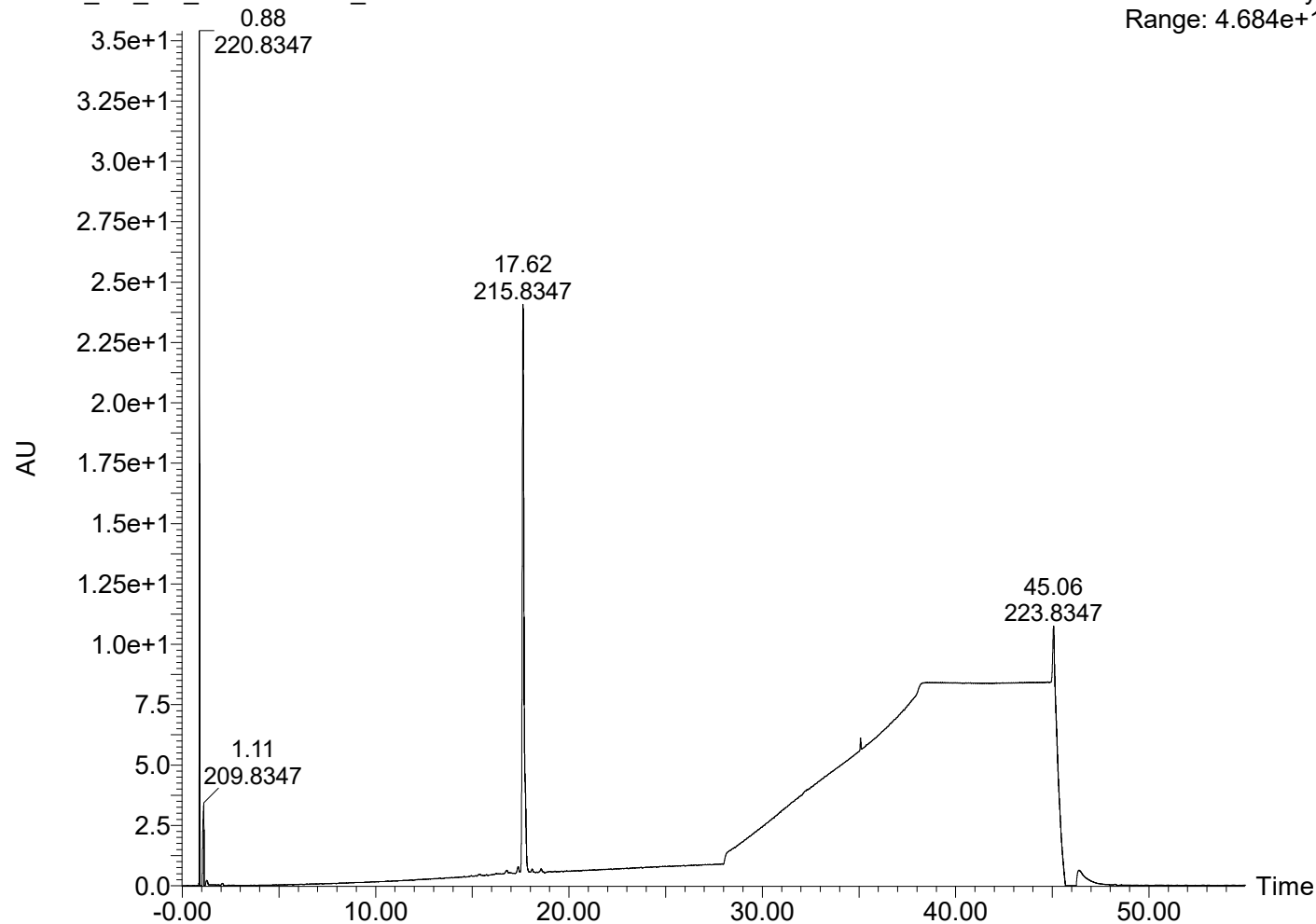
170123_AA_NK_PLC5-FB-1-2_NEG

1: TOF MS ES-
BPI
4.27e4



170123_AA_NK_PLC5-FB-1-2_NEG

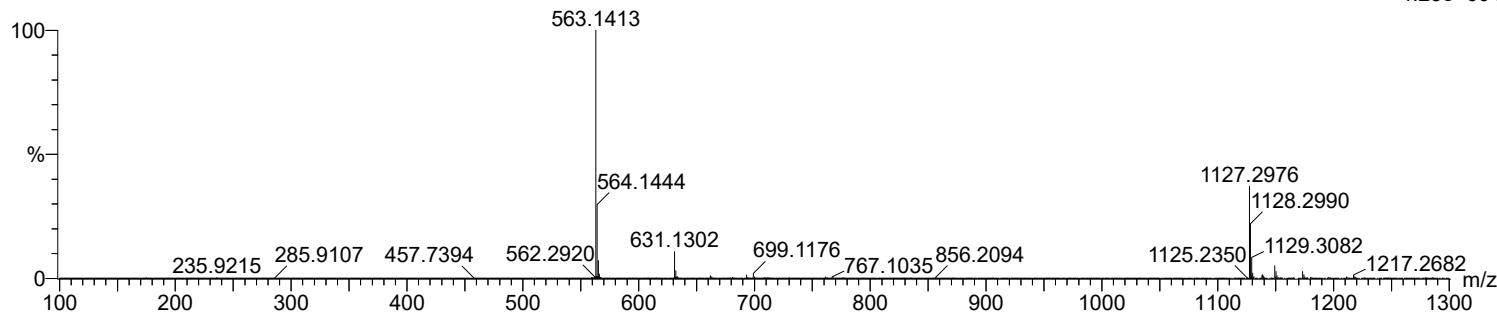
3: Diode Array
Range: 4.684e+1



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
161 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
170123_AA_NK_PLC5-FB-1-2_NEG 1510 (17.735)

1: TOF MS ES-
4.25e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
563.1413	563.1401	1.2	2.1	13.5	192.9	0.000	100.00	C26 H27 O14
563.1342		7.1	12.6	22.5	203.5	10.577	0.00	C33 H23 O9
563.1460		-4.7	-8.3	4.5	204.4	11.452	0.00	C19 H31 O19
563.1436		-2.3	-4.1	35.5	204.8	11.861	0.00	C44 H19 O
563.1495		-8.2	-14.6	26.5	205.8	12.901	0.00	C37 H23 O6

Col 32

170123_AA_NK_PLC5-FB-1-2_NEG 21142 (17.620)

3: Diode Array
2.836e-1

