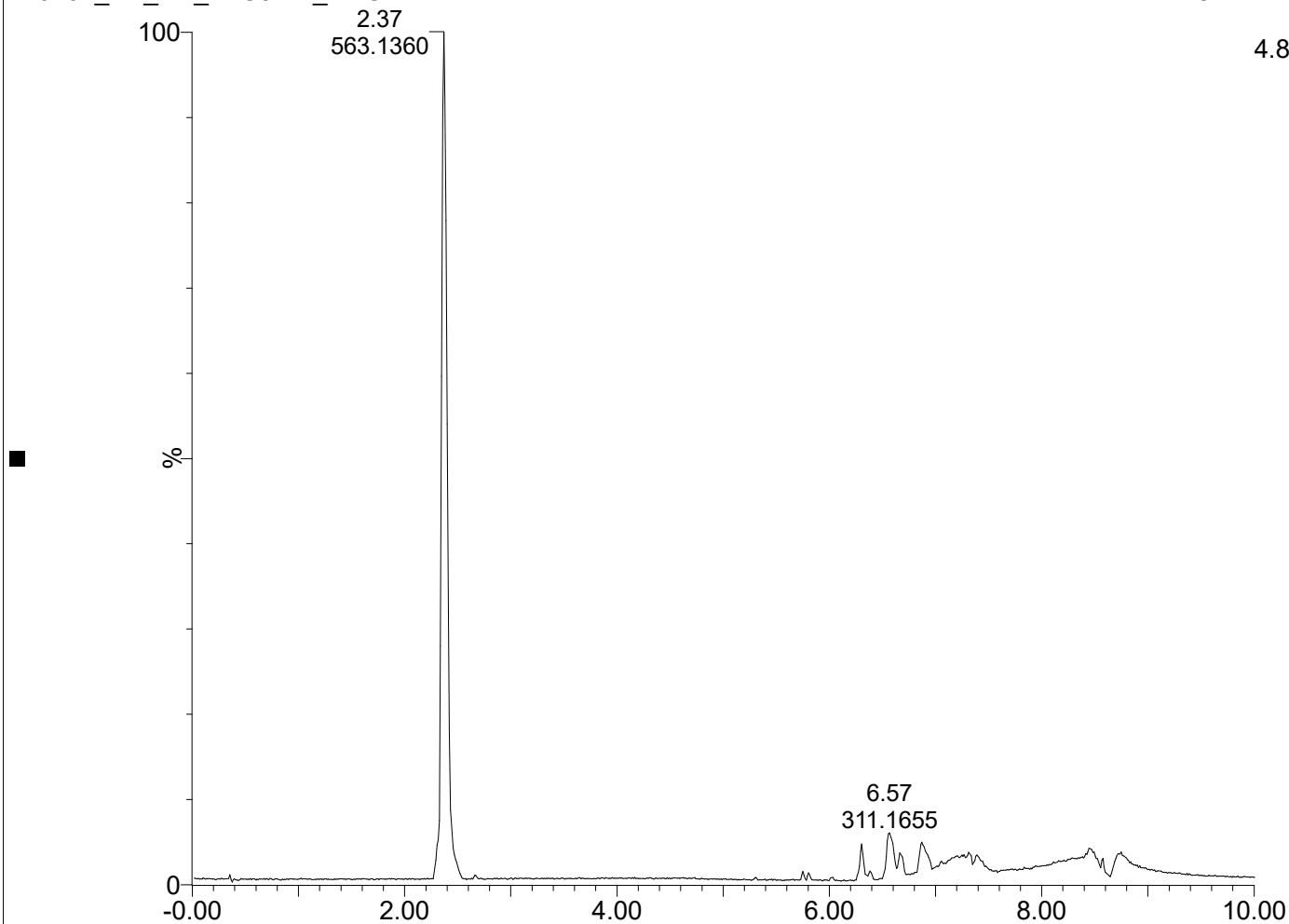


COMPOUND NO. S11 (METHOD A)

COL31

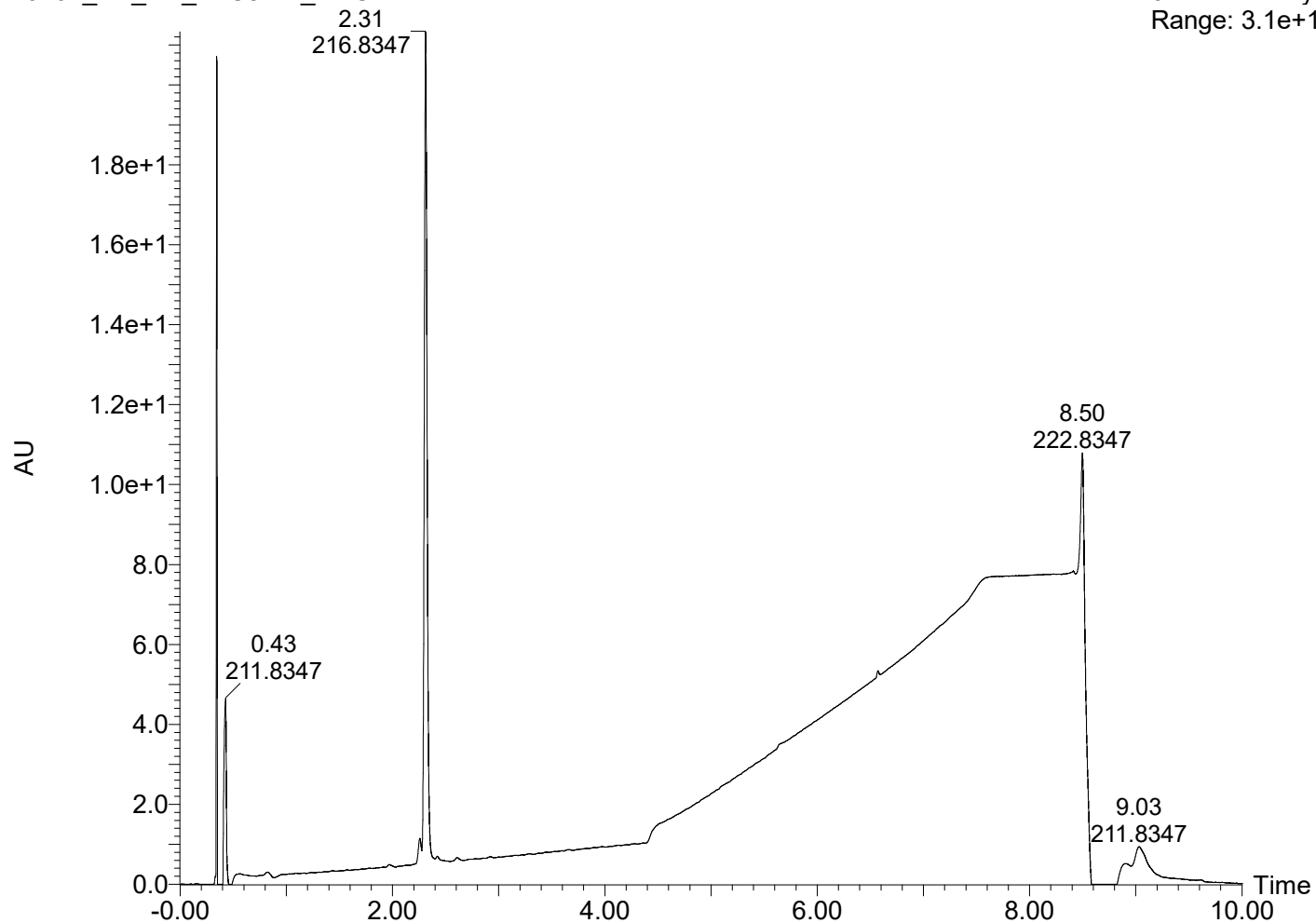
170104_AA_NK_PLC5-FA_NEG

1: TOF MS ES-
BPI
4.88e4



170104_AA_NK_PLC5-FA_NEG

3: Diode Array
Range: 3.1e+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

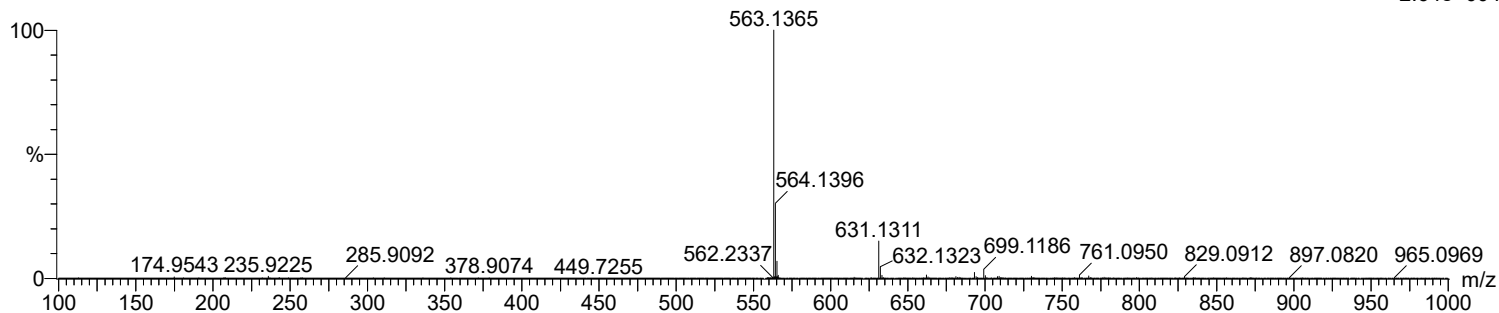
161 formula(e) evaluated with 5 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104_AA_NK_PLC5-FA_NEG 207 (2.400)

1: TOF MS ES-
2.64e+004

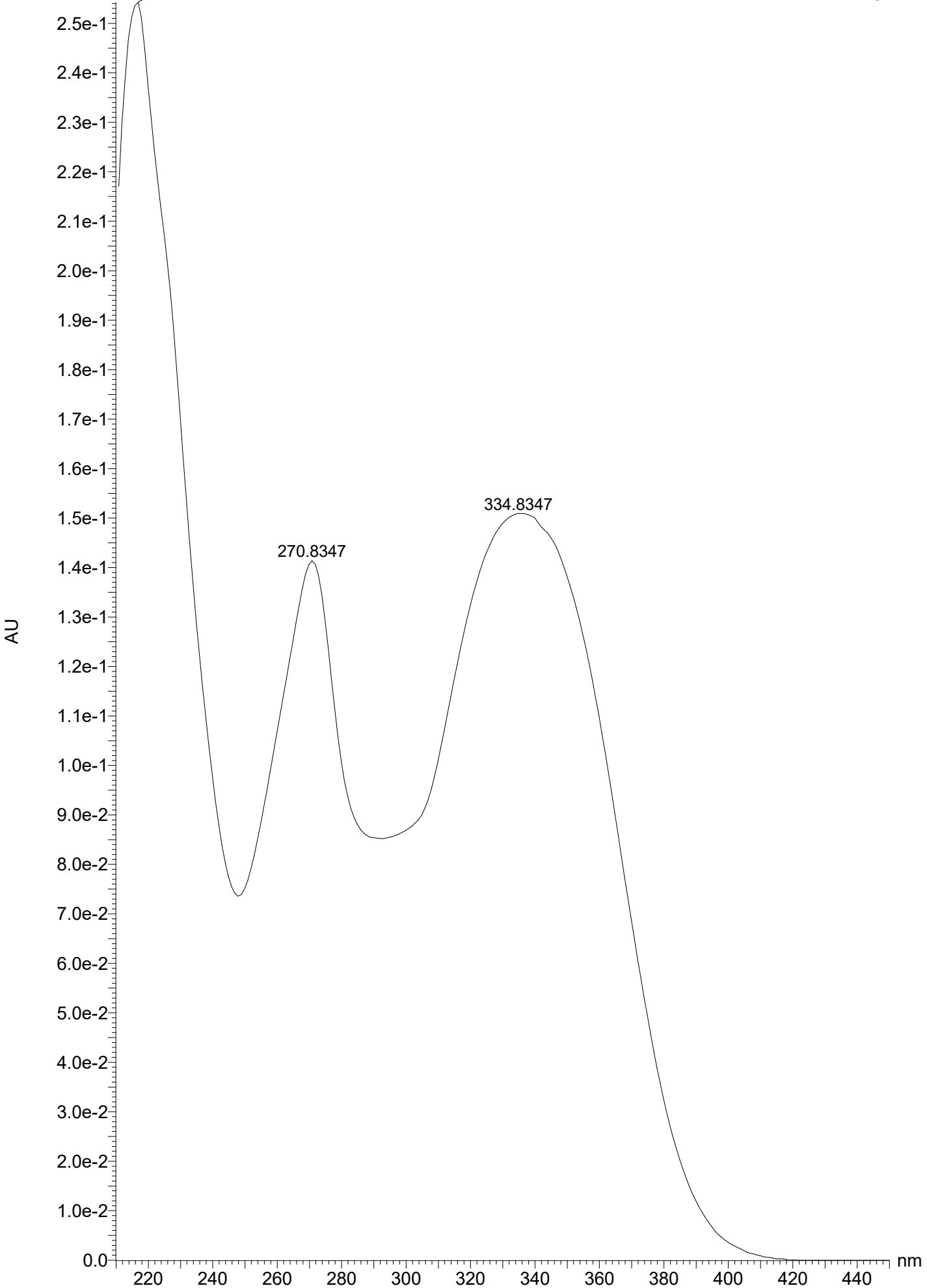
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
563.1365	563.1401	-3.6	-6.4	13.5	170.3	0.003	99.69	C26 H27 O14
563.1342		2.3	4.1	22.5	176.1	5.770	0.31	C33 H23 O9
563.1307		5.8	10.3	0.5	181.6	11.278	0.00	C15 H31 O22
563.1283		8.2	14.6	31.5	181.8	11.515	0.00	C40 H19 O4
563.1436		-7.1	-12.6	35.5	182.5	12.171	0.00	C44 H19 O

COL31

170104_AA_NK_PLC5-FA_NEG 2776 (2.313)

3: Diode Array
2.542e-1

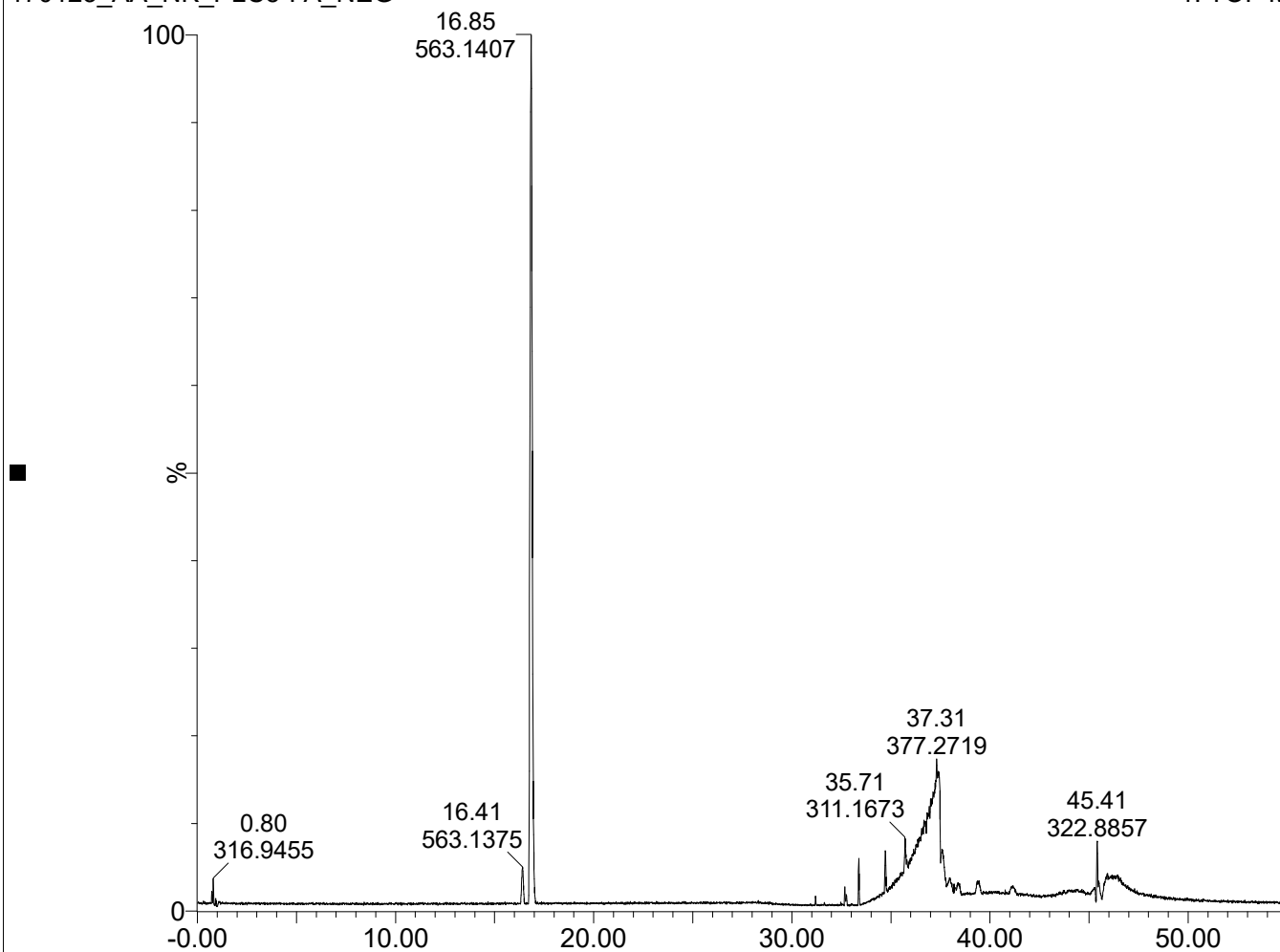


COMPOUND NO. S11 (METHOD B)

Col 32

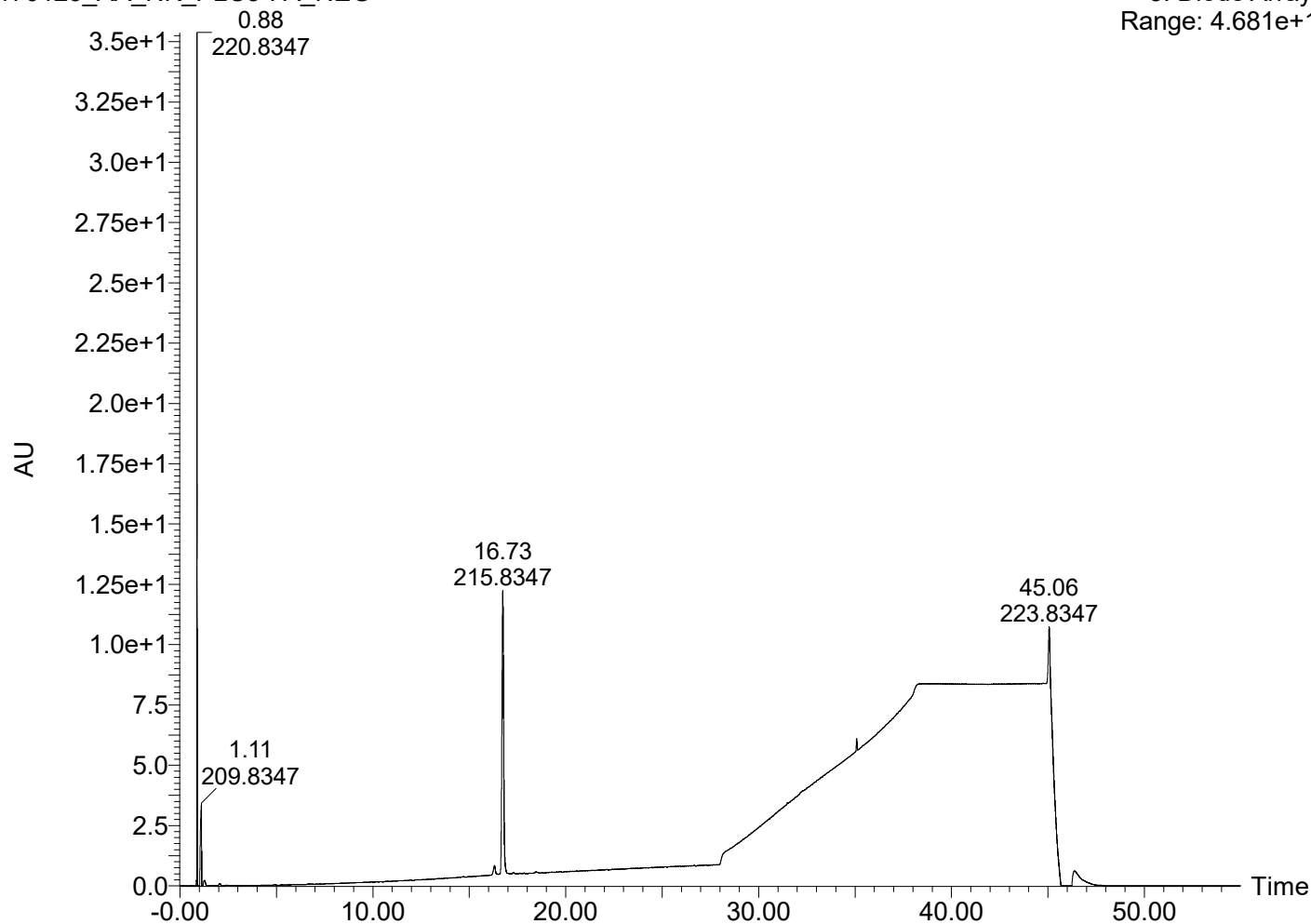
170123_AA_NK_PLC5-FA_NEG

1: TOF MS ES-
BPI
3.04e4



170123_AA_NK_PLC5-FA_NEG

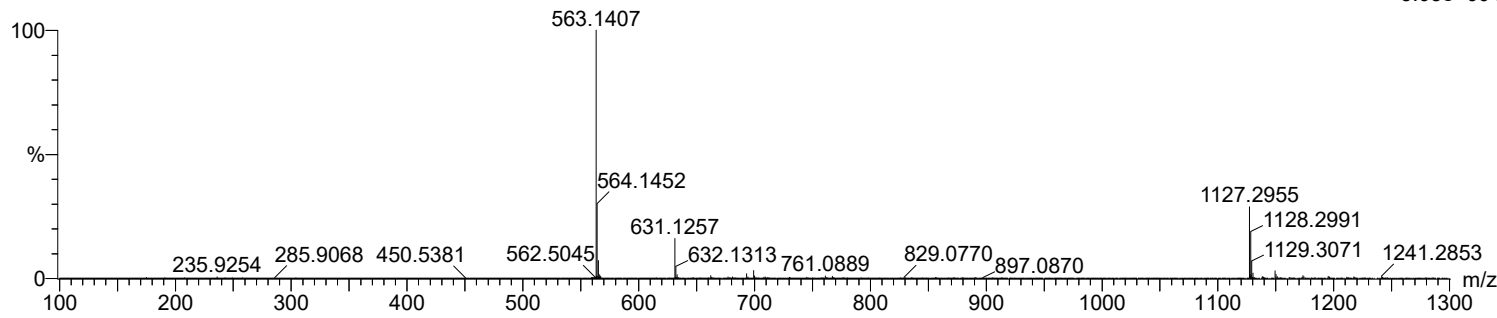
3: Diode Array
Range: 4.681e+1



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
Col 32
170123_AA_NK_PLC5-FA_NEG 1435 (16.850)

1: TOF MS ES-
3.05e+004



Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
563.1407	563.1401	0.6	1.1	13.5	182.9	0.000	99.99	C26 H27 O14
	563.1342	6.5	11.5	22.5	192.3	9.453	0.01	C33 H23 O9
	563.1460	-5.3	-9.4	4.5	192.9	9.968	0.00	C19 H31 O19
	563.1436	-2.9	-5.1	35.5	194.7	11.847	0.00	C44 H19 O

Col 32

170123_AA_NK_PLC5-FA_NEG 20080 (16.735)

3: Diode Array
1.539e-1

