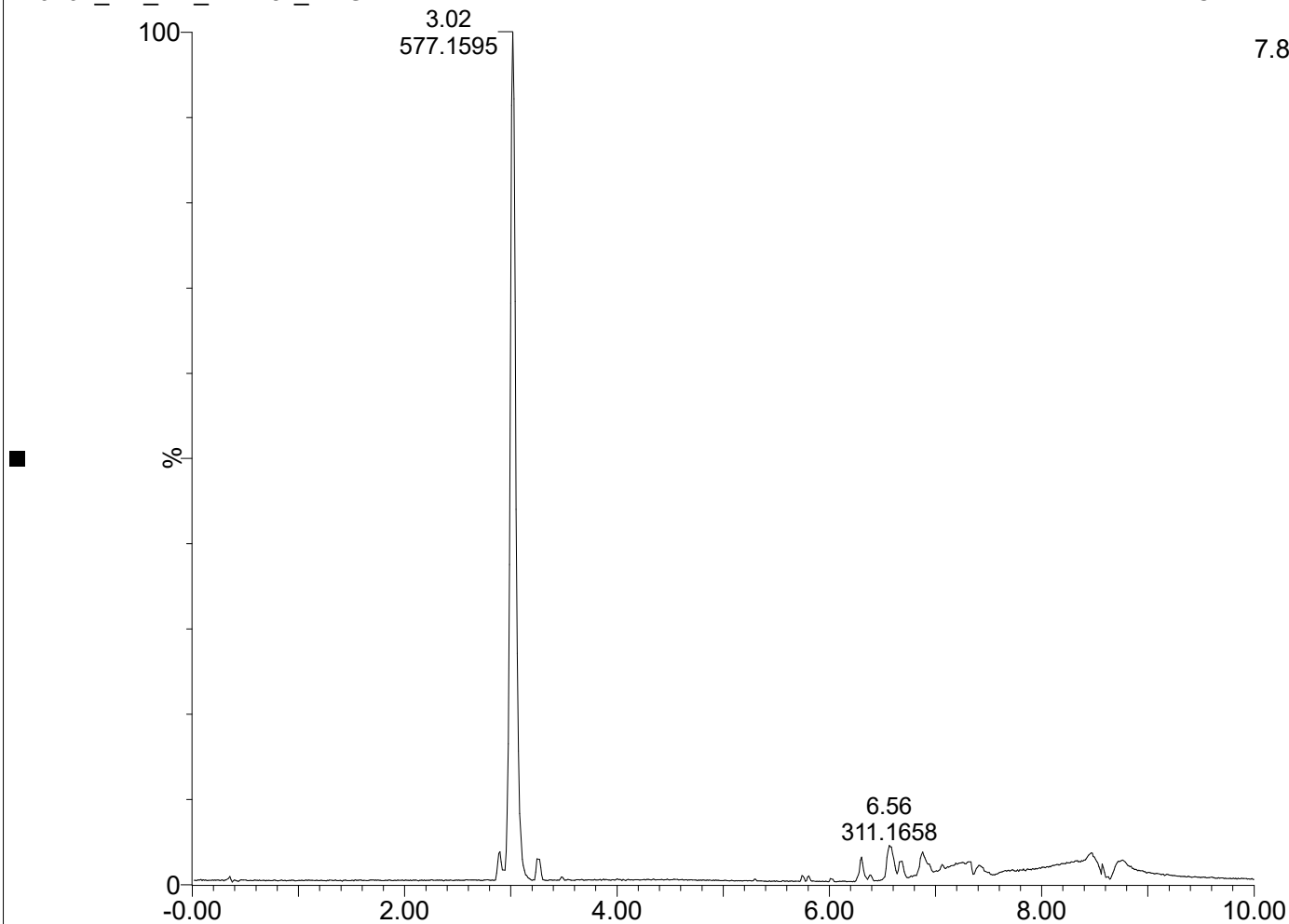


COMPOUND NO. S20 (METHOD A)

COL31

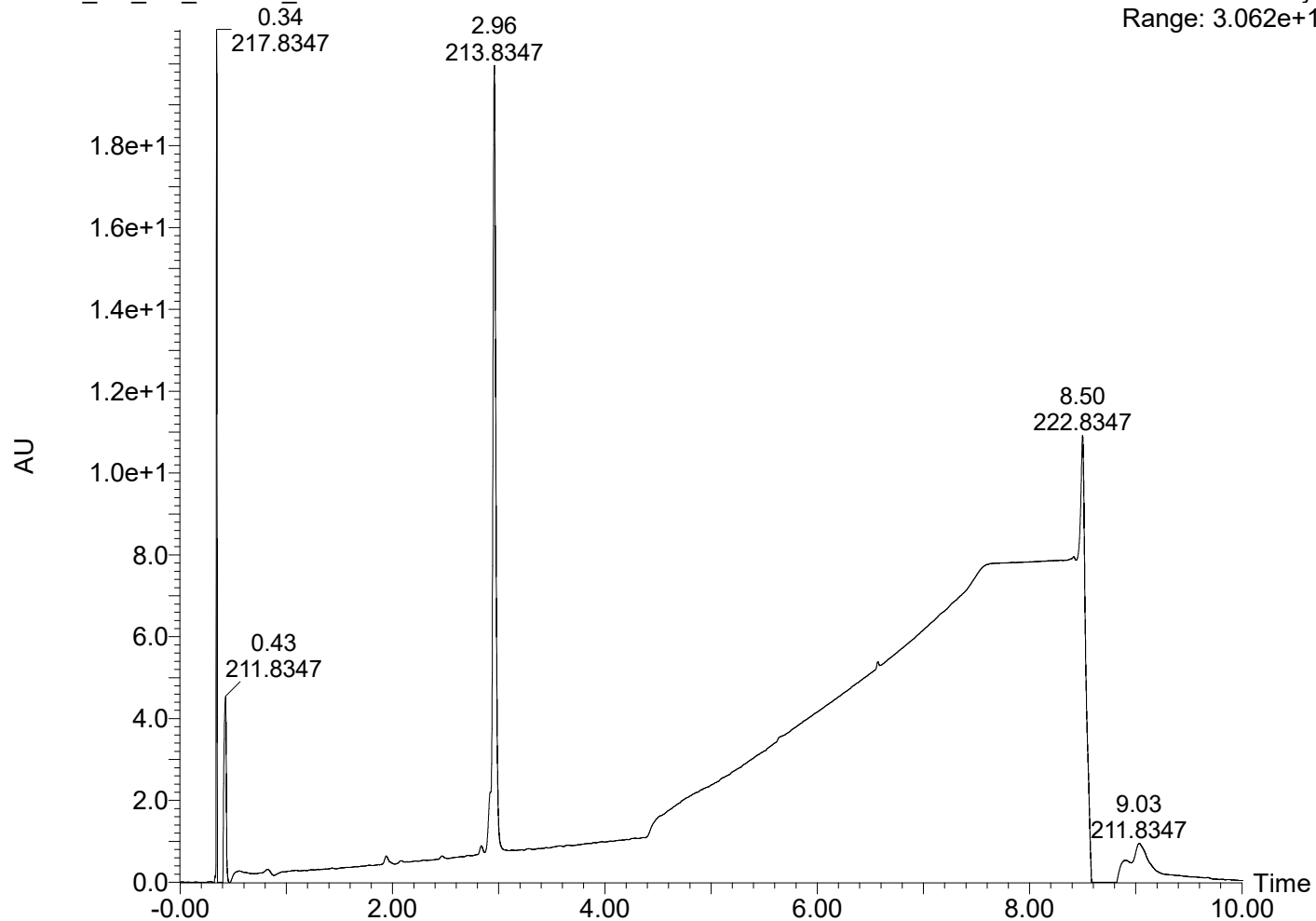
170104\_AA\_NK\_FDK-5ii\_NEG

1: TOF MS ES-  
BPI  
7.89e4



170104\_AA\_NK\_FDK-5ii\_NEG

3: Diode Array  
Range: 3.062e+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

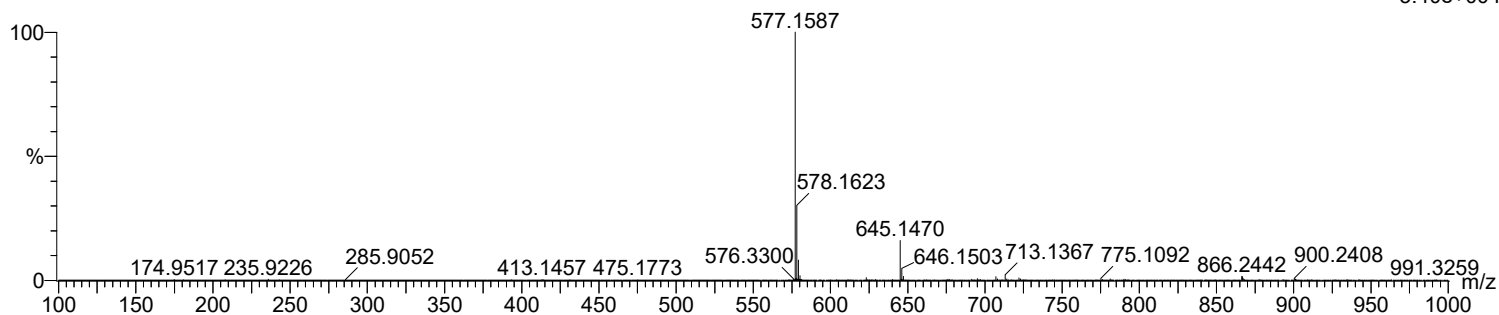
162 formula(e) evaluated with 4 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104\_AA\_NK\_FDK-5ii\_NEG 262 (3.039)

1: TOF MS ES-  
5.40e+004

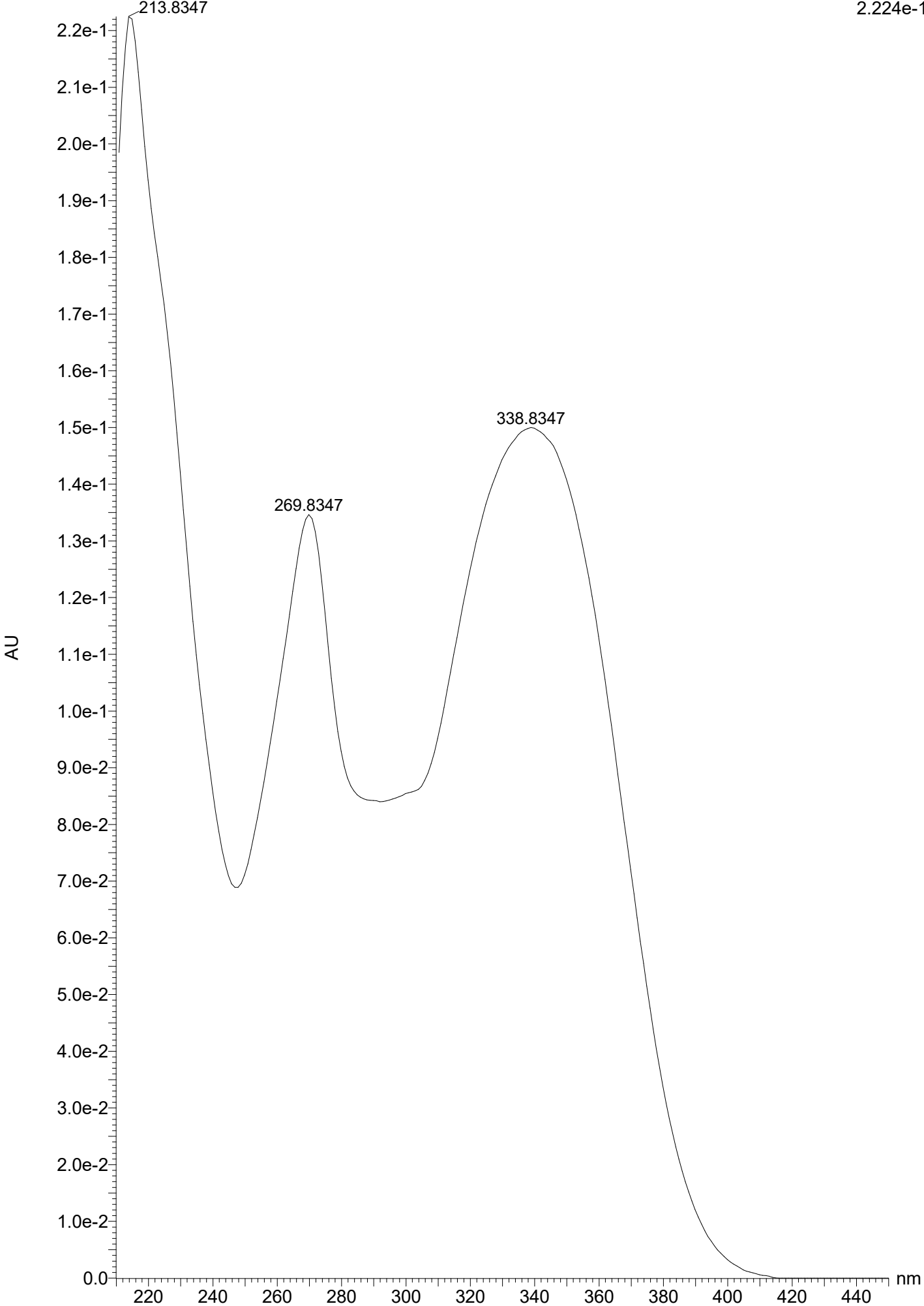
Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1587	577.1557	3.0	5.2	13.5	181.5	0.004	99.65	C27 H29 O14
577.1616		-2.9	-5.0	4.5	188.1	6.555	0.14	C20 H33 O19
577.1592		-0.5	-0.9	35.5	188.2	6.672	0.13	C45 H21 O
577.1651		-6.4	-11.1	26.5	188.7	7.106	0.08	C38 H25 O6

COL31

170104\_AA\_NK\_FDK-5ii\_NEG 3550 (2.958)

3: Diode Array  
2.224e-1

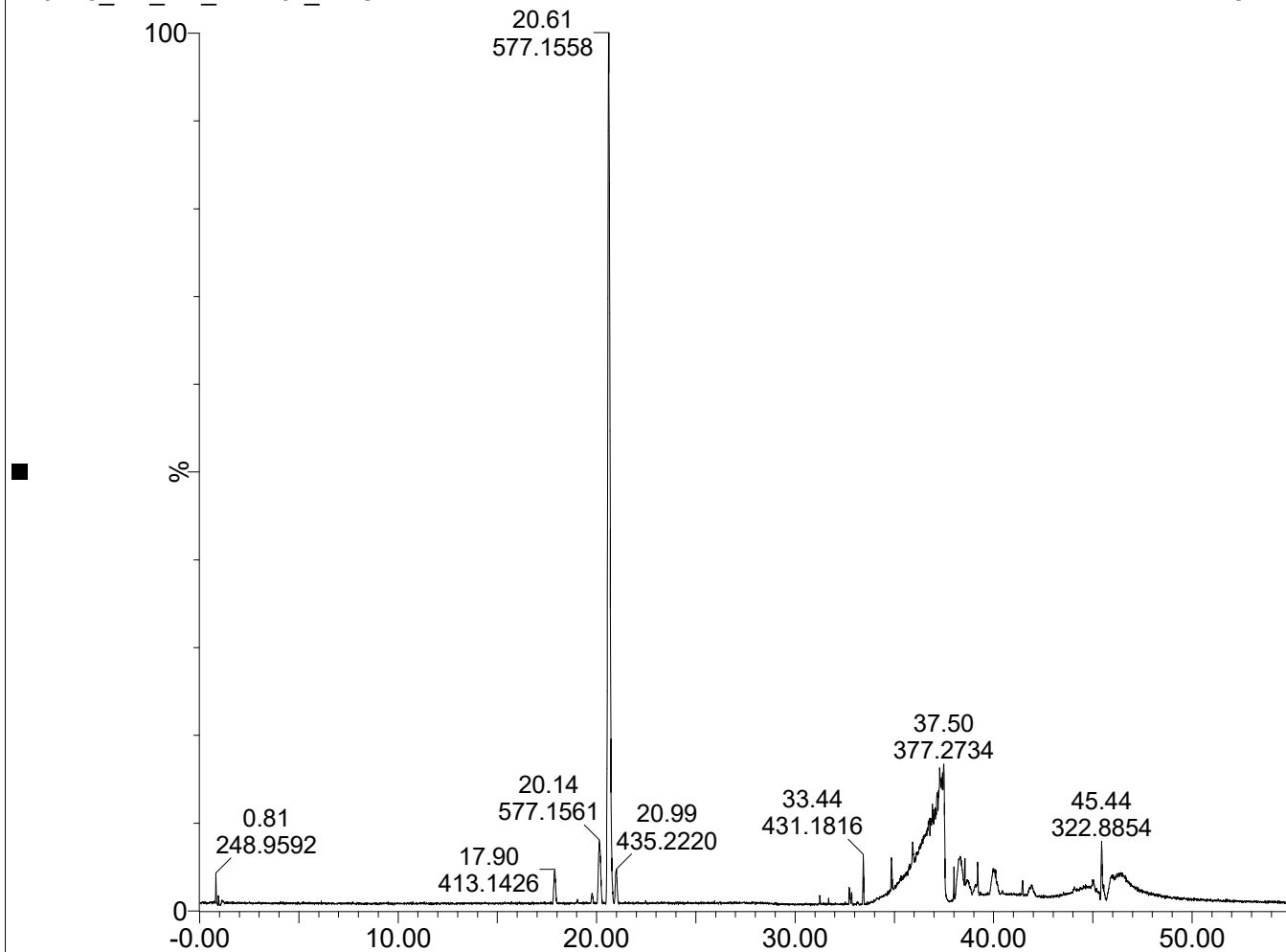


# COMPOUND NO. S20 (METHOD B)

Col 32

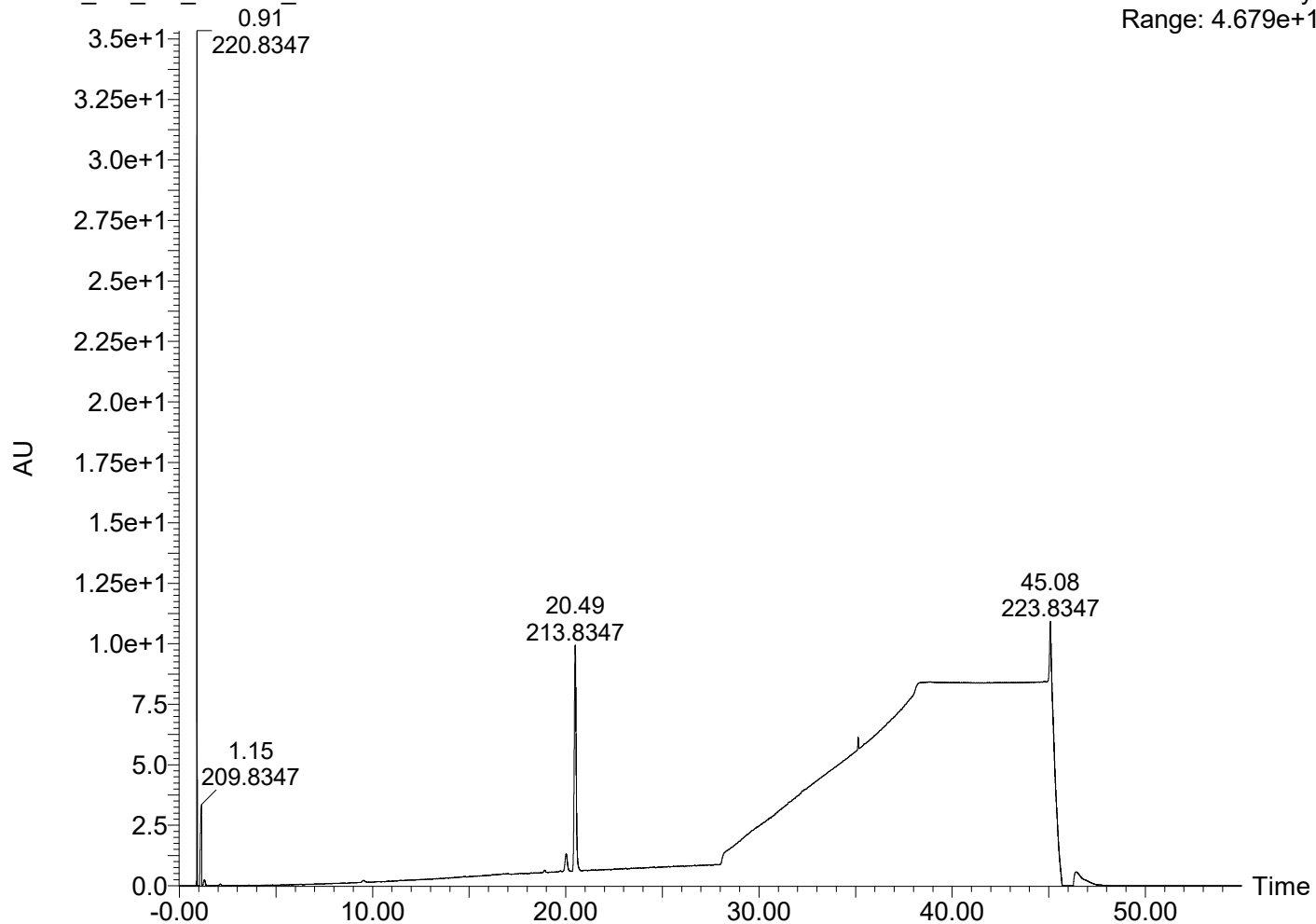
170123\_AA\_NK\_FDK-5ii\_NEG

1: TOF MS ES-  
BPI  
2.99e4



170123\_AA\_NK\_FDK-5ii\_NEG

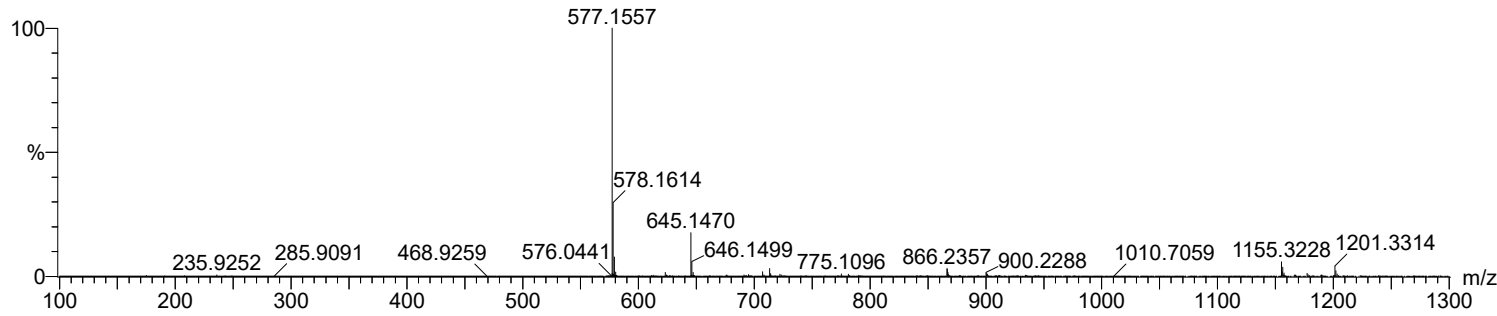
3: Diode Array  
Range: 4.679e+1



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 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\_FDK-5ii\_NEG 1753 (20.612)

1: TOF MS ES-  
2.99e+004



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
577.1557	577.1557	0.0	0.0	13.5	175.6	0.001	99.92	C27 H29 O14
577.1616		-5.9	-10.2	4.5	183.5	7.893	0.04	C20 H33 O19
577.1499		5.8	10.0	22.5	183.6	7.947	0.04	C34 H25 O9
577.1592		-3.5	-6.1	35.5	186.0	10.409	0.00	C45 H21 O

Col 32

170123\_AA\_NK\_FDK-5ii\_NEG 24575 (20.482)

3: Diode Array  
1.197e-1

