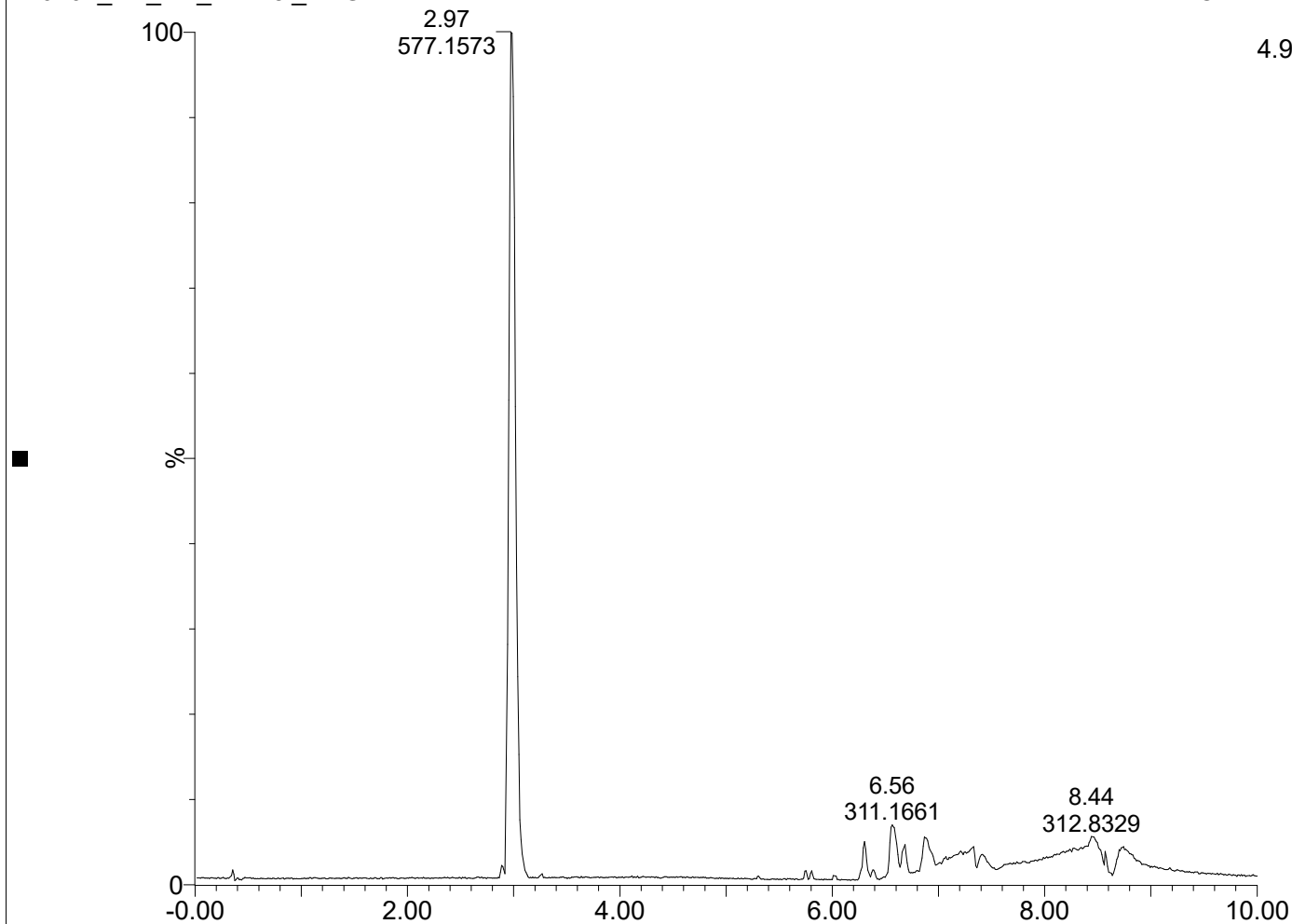


COMPOUND NO. S19 (METHOD A)

COL31

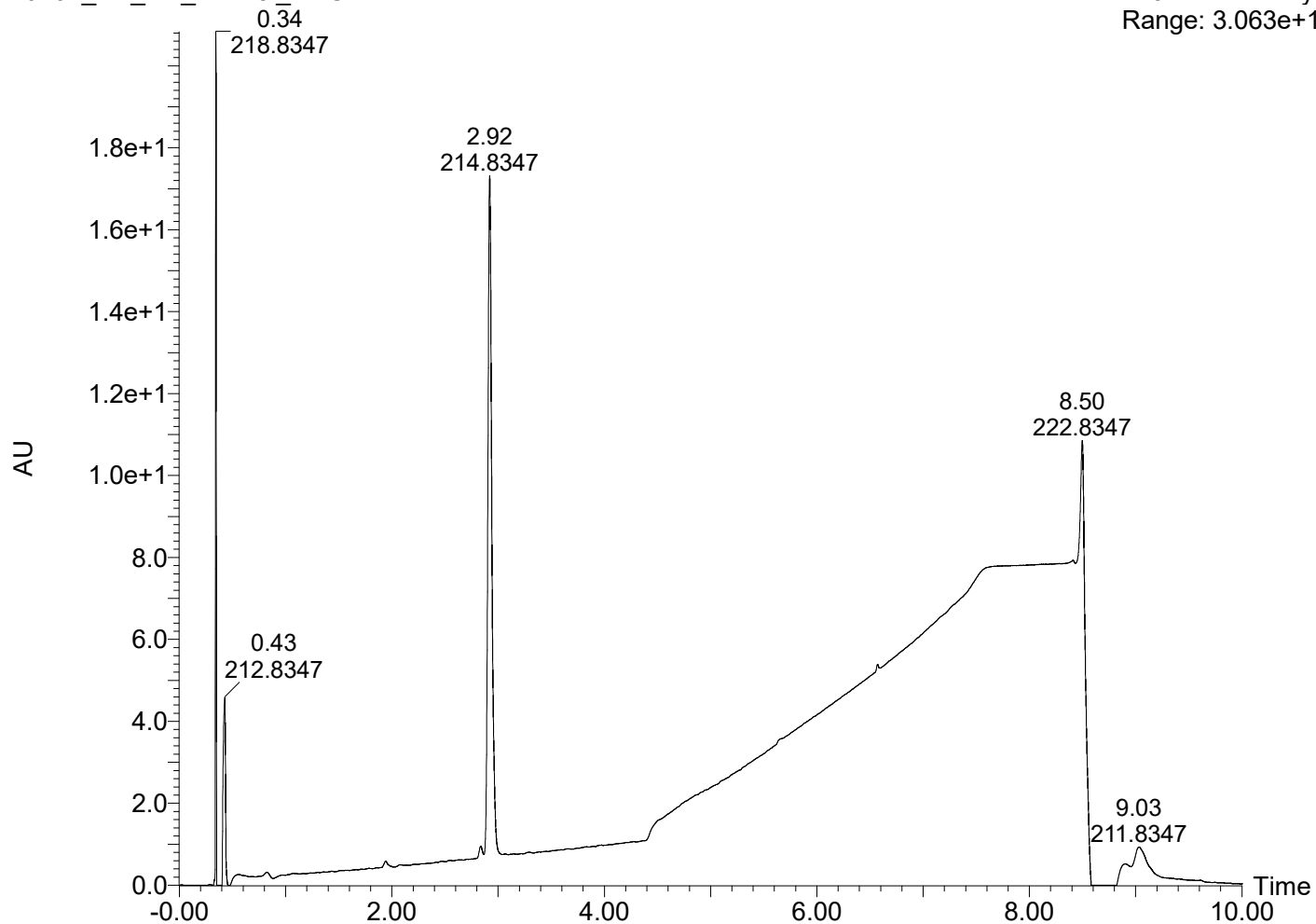
170104\_AA\_NK\_FDK-5i\_NEG

1: TOF MS ES-  
BPI  
4.95e4



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

3: Diode Array  
Range: 3.063e+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

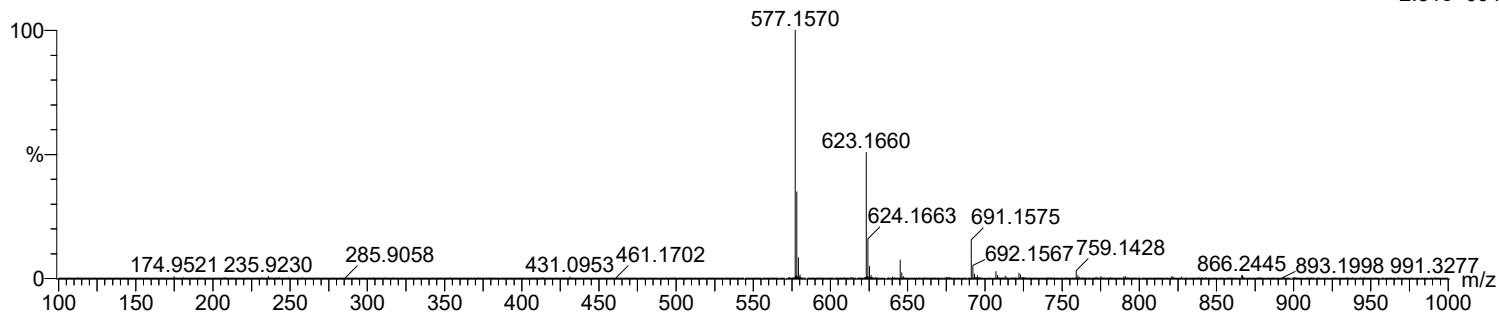
162 formula(e) evaluated with 5 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

COL31

170104\_AA\_NK\_FDK-5i\_NEG 254 (2.954)

1: TOF MS ES-  
2.81e+004

Minimum: -1.5

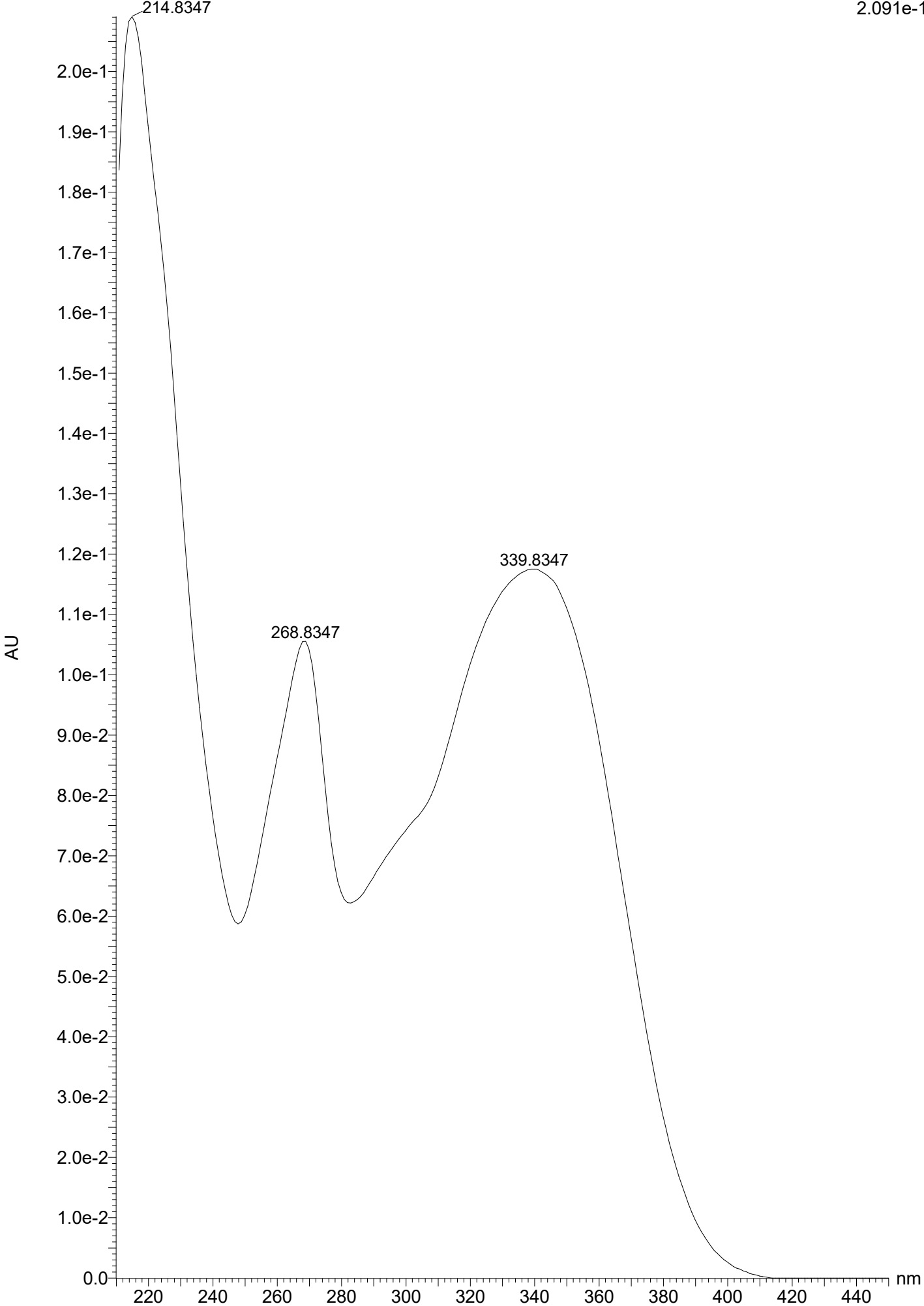
Maximum: 5.0 15.0 50.0

| Mass     | Calc. Mass | mDa  | PPM   | DBE  | i-FIT | Norm  | Conf (%) | Formula     |
|----------|------------|------|-------|------|-------|-------|----------|-------------|
| 577.1570 | 577.1557   | 1.3  | 2.3   | 13.5 | 166.6 | 1.589 | 20.42    | C27 H29 O14 |
| 577.1592 |            | -2.2 | -3.8  | 35.5 | 171.4 | 6.344 | 0.18     | C45 H21 O   |
| 577.1616 |            | -4.6 | -8.0  | 4.5  | 170.5 | 5.462 | 0.42     | C20 H33 O19 |
| 577.1499 |            | 7.1  | 12.3  | 22.5 | 165.3 | 0.254 | 77.57    | C34 H25 O9  |
| 577.1651 |            | -8.1 | -14.0 | 26.5 | 169.3 | 4.260 | 1.41     | C38 H25 O6  |

COL31

170104\_AA\_NK\_FDK-5i\_NEG 3500 (2.916)

3: Diode Array  
2.091e-1

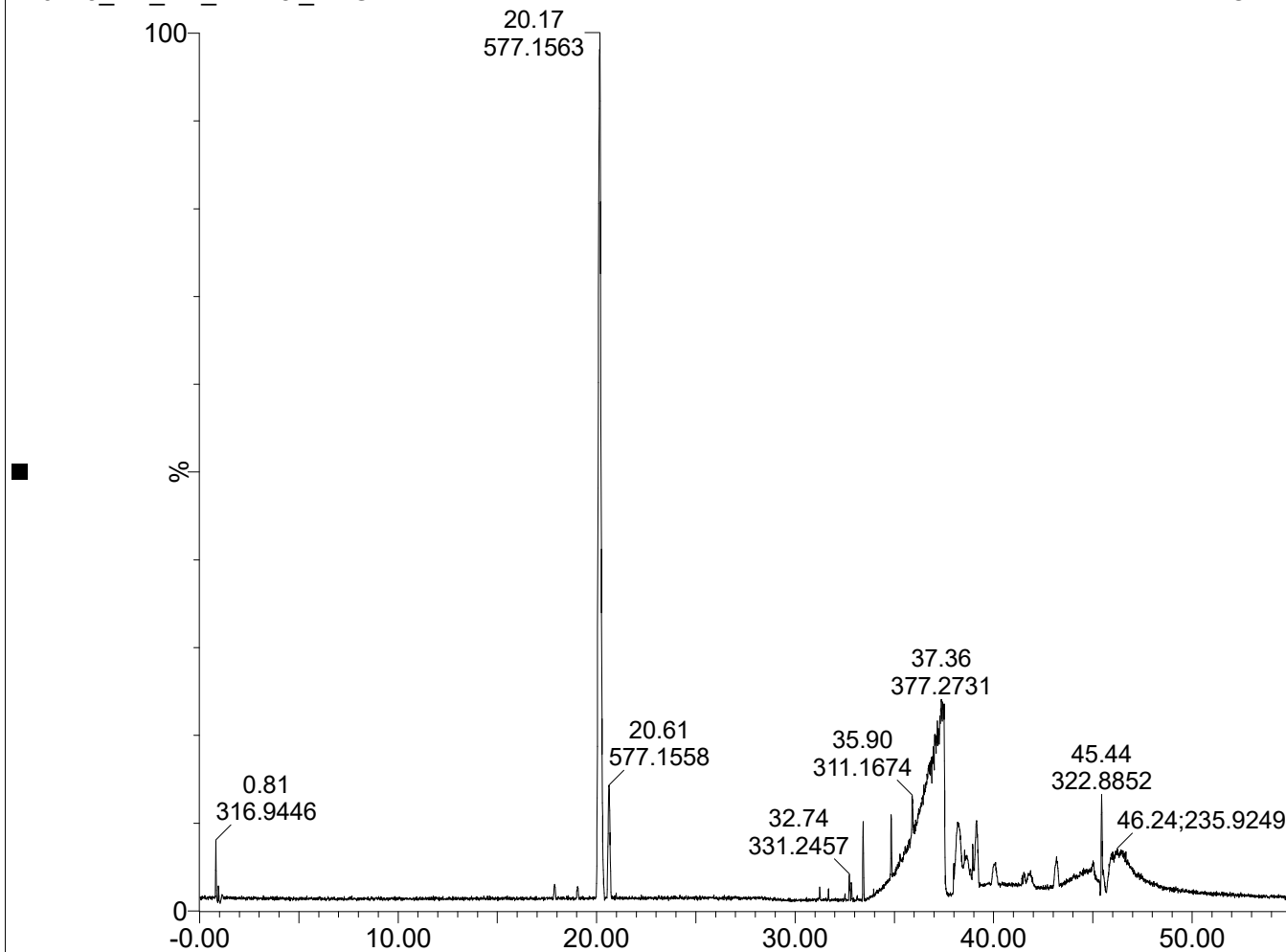


# COMPOUND NO. S19 (METHOD B)

Col 32

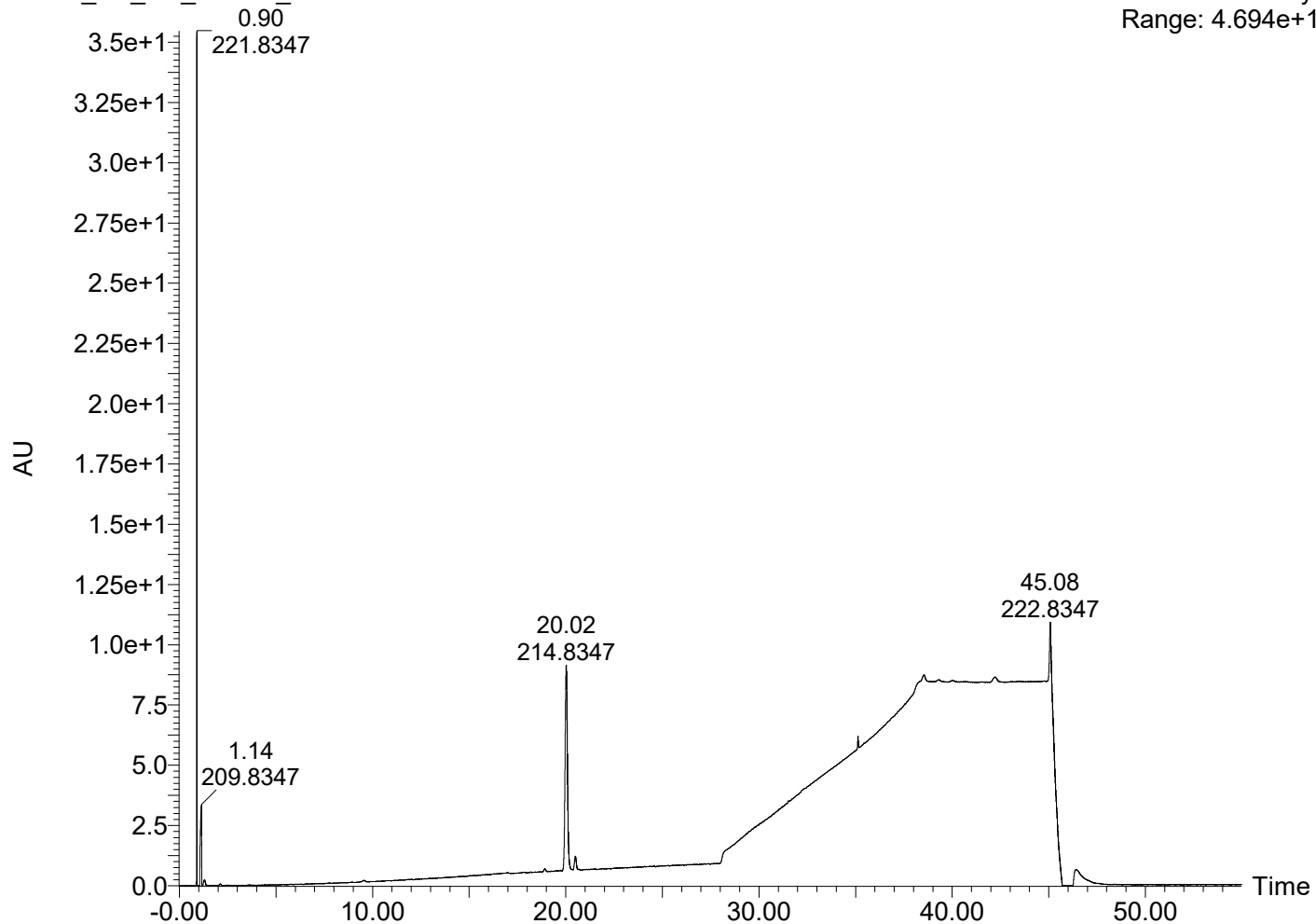
170123\_AA\_NK\_FDK-5i\_NEG

1: TOF MS ES-  
BPI  
1.88e4



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

3: Diode Array  
Range: 4.694e+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

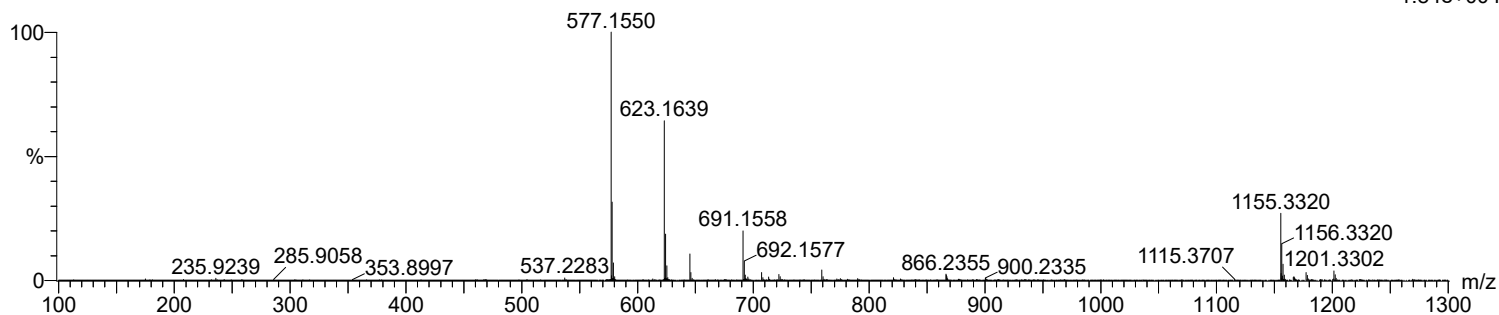
162 formula(e) evaluated with 5 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

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

Col 32

170123\_AA\_NK\_FDK-5i\_NEG 1716 (20.150)

1: TOF MS ES-  
1.84e+004

Minimum: -1.5  
Maximum: 5.0 15.0 50.0

| Mass     | Calc. Mass | mDa  | PPM   | DBE  | i-FIT | Norm  | Conf (%) | Formula     |
|----------|------------|------|-------|------|-------|-------|----------|-------------|
| 577.1550 | 577.1557   | -0.7 | -1.2  | 13.5 | 179.8 | 0.006 | 99.36    | C27 H29 O14 |
| 577.1499 |            | 5.1  | 8.8   | 22.5 | 185.0 | 5.236 | 0.53     | C34 H25 O9  |
| 577.1616 |            | -6.6 | -11.4 | 4.5  | 186.9 | 7.175 | 0.08     | C20 H33 O19 |
| 577.1592 |            | -4.2 | -7.3  | 35.5 | 188.4 | 8.666 | 0.02     | C45 H21 O   |
| 577.1463 |            | 8.7  | 15.1  | 0.5  | 189.0 | 9.243 | 0.01     | C16 H33 O22 |

Col 32

170123\_AA\_NK\_FDK-5i\_NEG 24019 (20.018)

3: Diode Array  
1.225e-1

