

Data File: C:\LabSolutions\Data\1. Chemistry\Evans (CHEM)\Barlow, Sean\SB81-220310-001.lcd

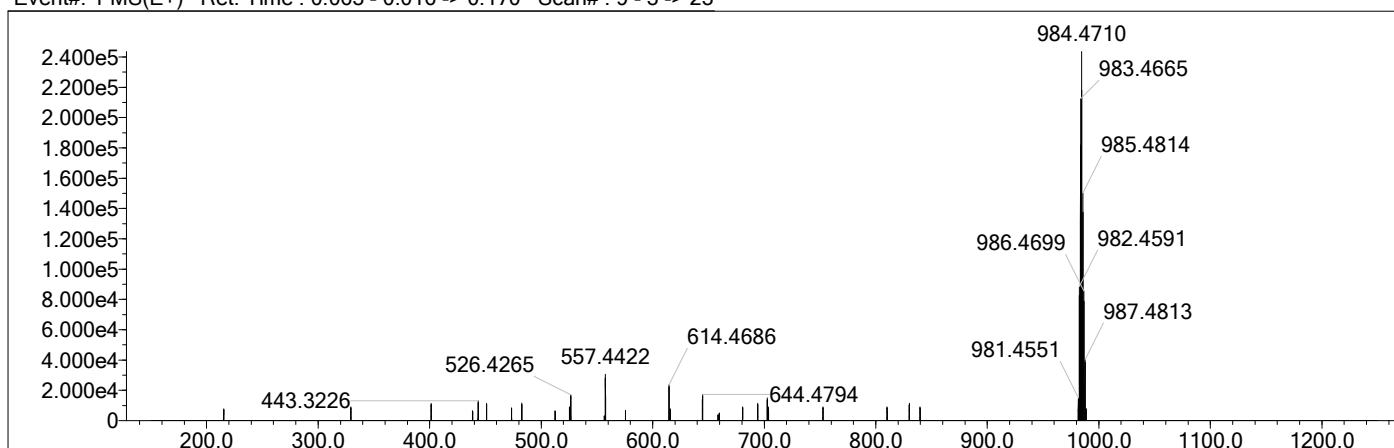
| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 60  | 65  | Na   | 1    | 0   | 0   | Fe   | 2    | 0   | 0   | I    | 3    | 0   | 0   | H          |
| 2H   | 1    | 0   | 0   | Si   | 4    | 0   | 0   | Co   | 2    | 0   | 0   | Re   | 2    | 0   | 0   | Na         |
| B    | 3    | 0   | 0   | P    | 3    | 0   | 0   | Ni   | 2    | 0   | 0   | Ir   | 3    | 0   | 0   | K          |
| C    | 4    | 50  | 55  | S    | 2    | 0   | 0   | Cu   | 2    | 0   | 0   | Pt   | 2    | 0   | 0   | NH4        |
| N    | 3    | 5   | 10  | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |      |      |     |     |            |
| O    | 2    | 10  | 15  | V    | 2    | 0   | 0   | Ru   | 2    | 0   | 0   |      |      |     |     |            |
| F    | 1    | 0   | 0   | Cr   | 2    | 0   | 0   | Ag   | 1    | 0   | 0   |      |      |     |     |            |

Error Margin (ppm): 25  
HC Ratio: unlimited  
Max Isotopes: all  
MSn Iso RI (%): 75.00

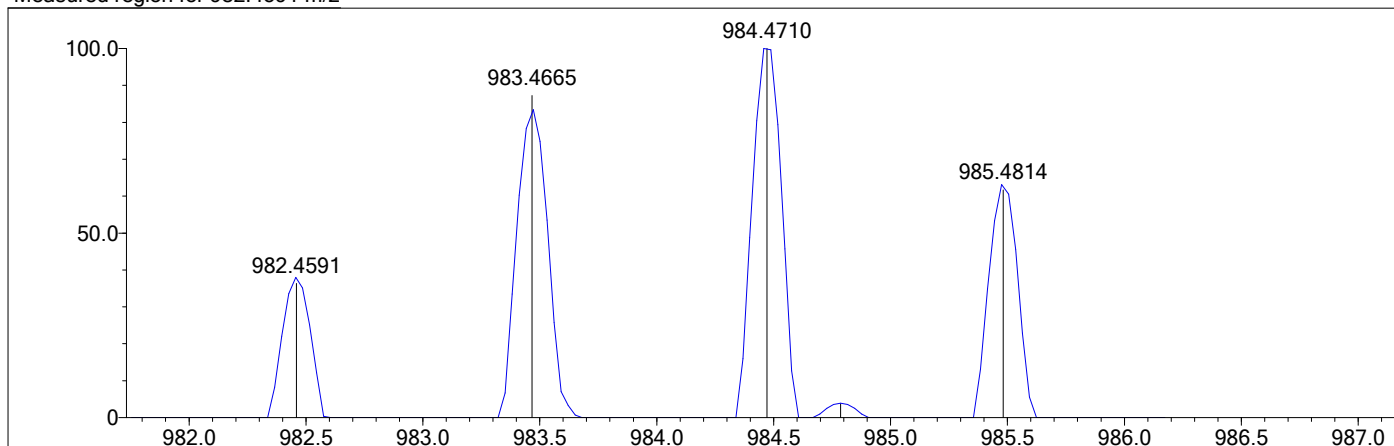
DBE Range: -2.0 - 1000.0  
Apply N Rule: no  
Isotope RI (%): 1.00  
MSn Logic Mode: AND

Electron Ions: both  
Use MSn Info: yes  
Isotope Res: 6000  
Max Results: 500

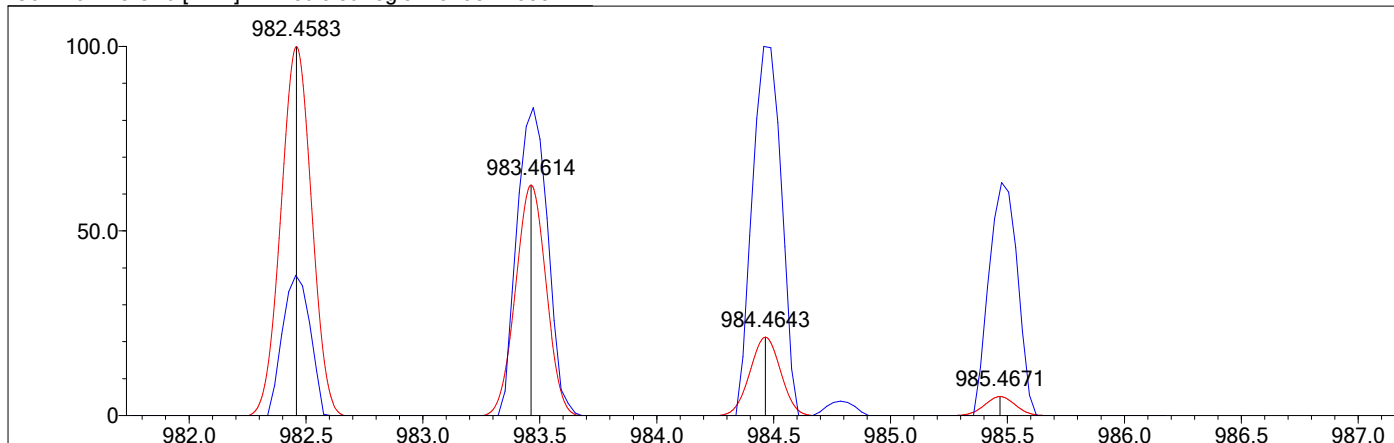
Event#: 1 MS(E+) Ret. Time : 0.063 - 0.016 -&gt; 0.170 Scan#: 9 - 3 -&gt; 23



Measured region for 982.4591 m/z



C54 H61 N8 O10 [M+H]+ : Predicted region for 982.4583 m/z



| Rank | Score | Formula (M)    | Ion    | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso   | DBE  |
|------|-------|----------------|--------|-----------|-----------|-----------|-----------|-------|------|
| 1    | 47.06 | C54 H61 N8 O10 | [M+H]+ | 982.4591  | 982.4583  | 0.8       | 0.81      | 47.06 | 28.5 |