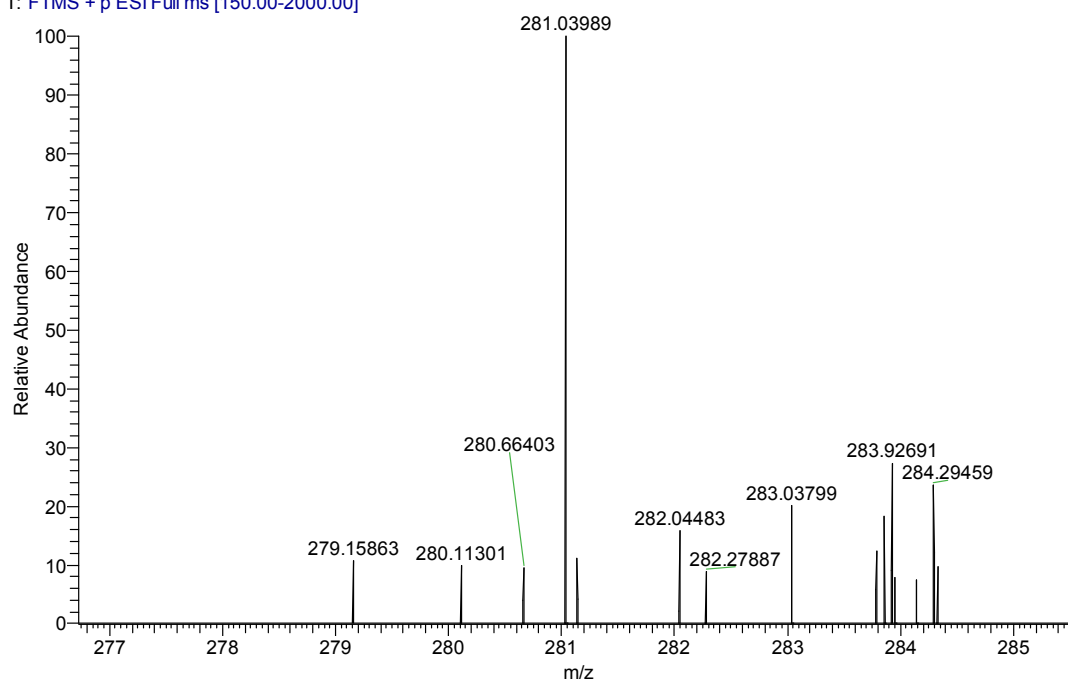


Thermo Scientific LTQ Orbitrap XL

Ion source : ESI

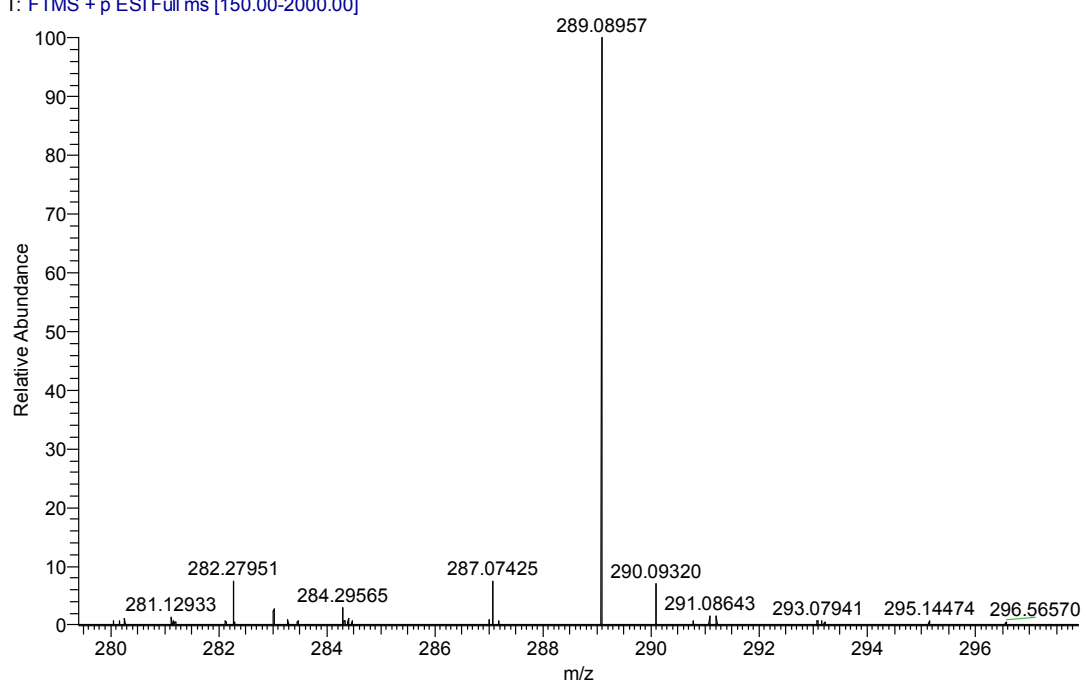
4a HRMS (ESI) m/z calcd for $C_{14}H_{14}ClO_2S^+$ (M+H)⁺ 281.03975, found 281.03989.

99_180906171612 #29 RT: 0.43 AV: 1 NL: 1.87E6
T: FTMS + p ESI Full ms [150.00-2000.00]

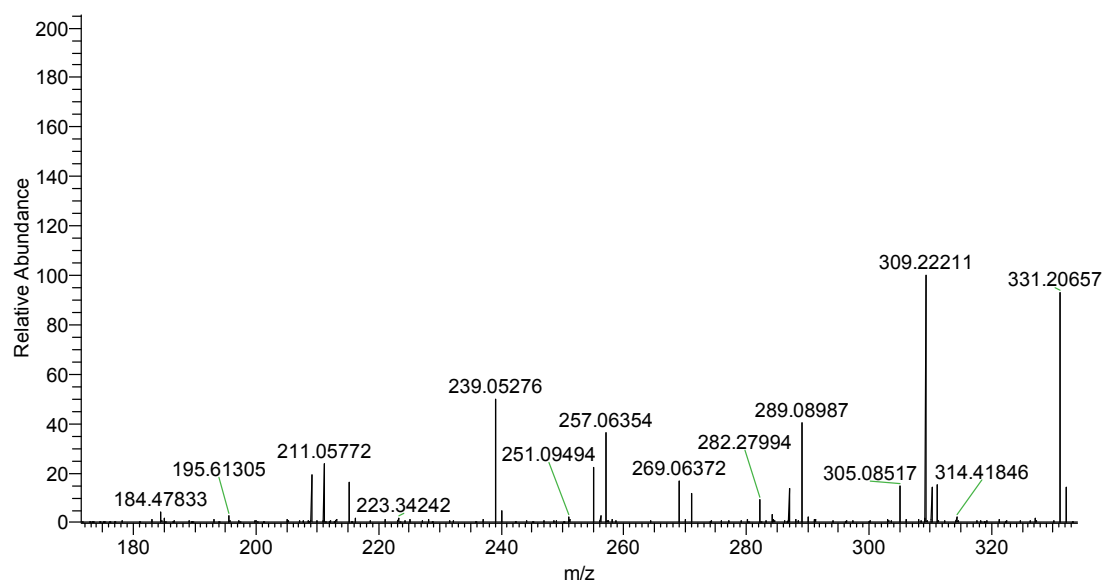


4c. HRMS (ESI) m/z calcd for $C_{16}H_{17}O_3S$ (M+H)⁺ 289.08984, found 289.08957.

98 #26 RT: 0.35 AV: 1 NL: 3.17E6
T: FTMS + p ESI Full ms [150.00-2000.00]

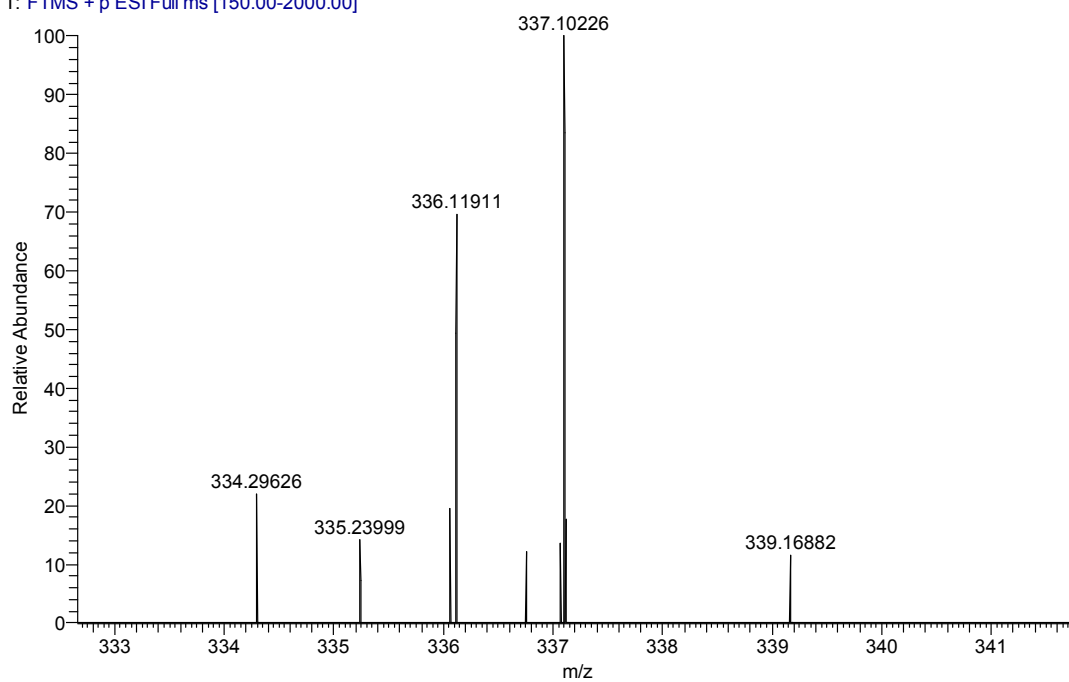


98 #18 RT: 0.24 AV: 1 NL: 1.10E7
T: FTMS + p ESI Full ms [150.00-2000.00]

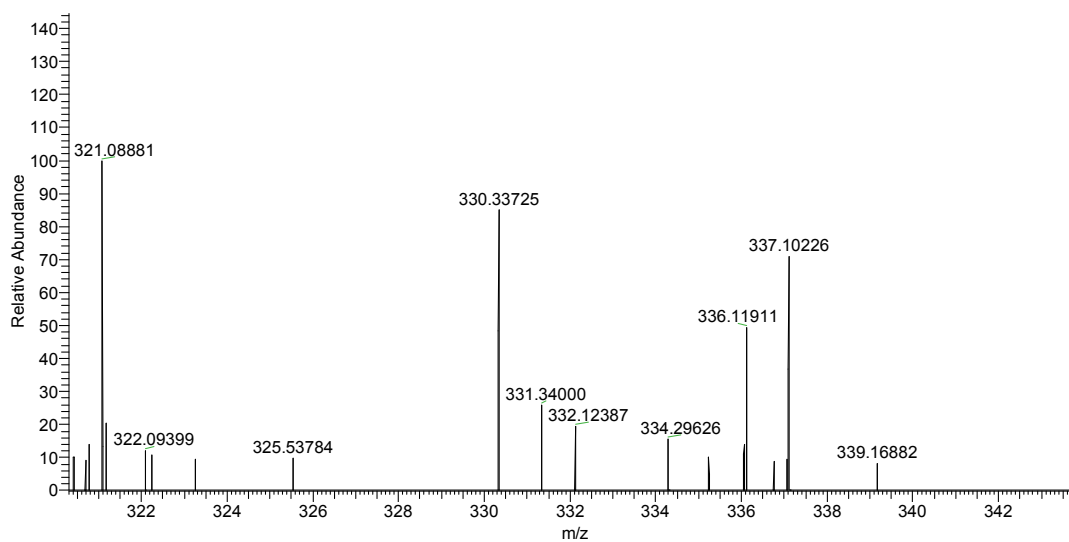


4e HRMS (ESI) m/z calcd for $C_{18}H_{22}ClO_2S^+$ (M+H)⁺ 337.10235, found 337.10226.

123 #24 RT: 0.35 AV: 1 NL: 9.19E5
T: FTMS + p ESI Full ms [150.00-2000.00]

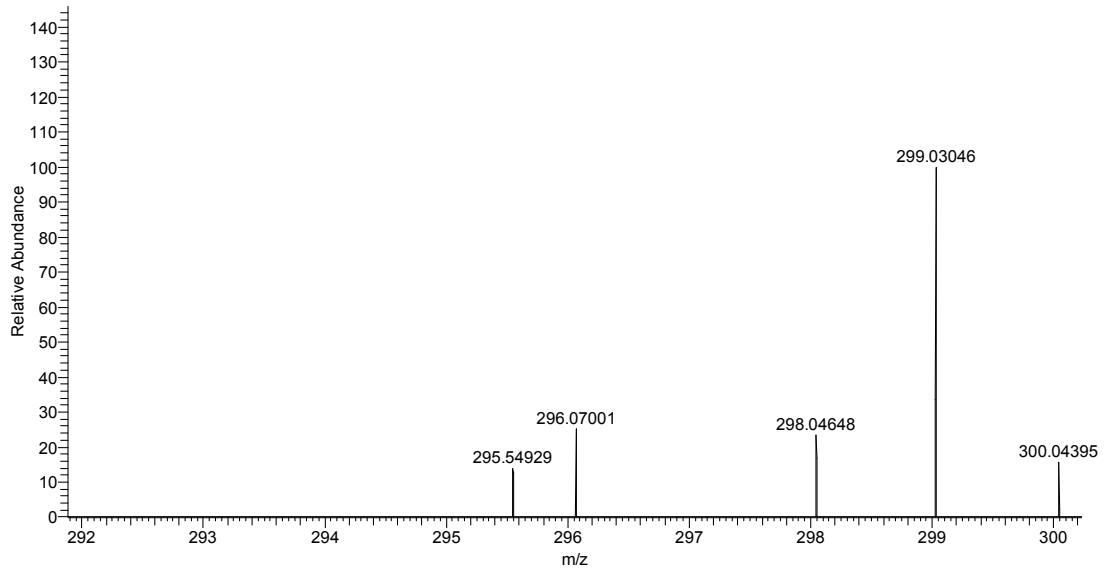


123 #24 RT: 0.35 AV: 1 NL: 1.29E6
T: FTMS + p ESI Full ms [150.00-2000.00]

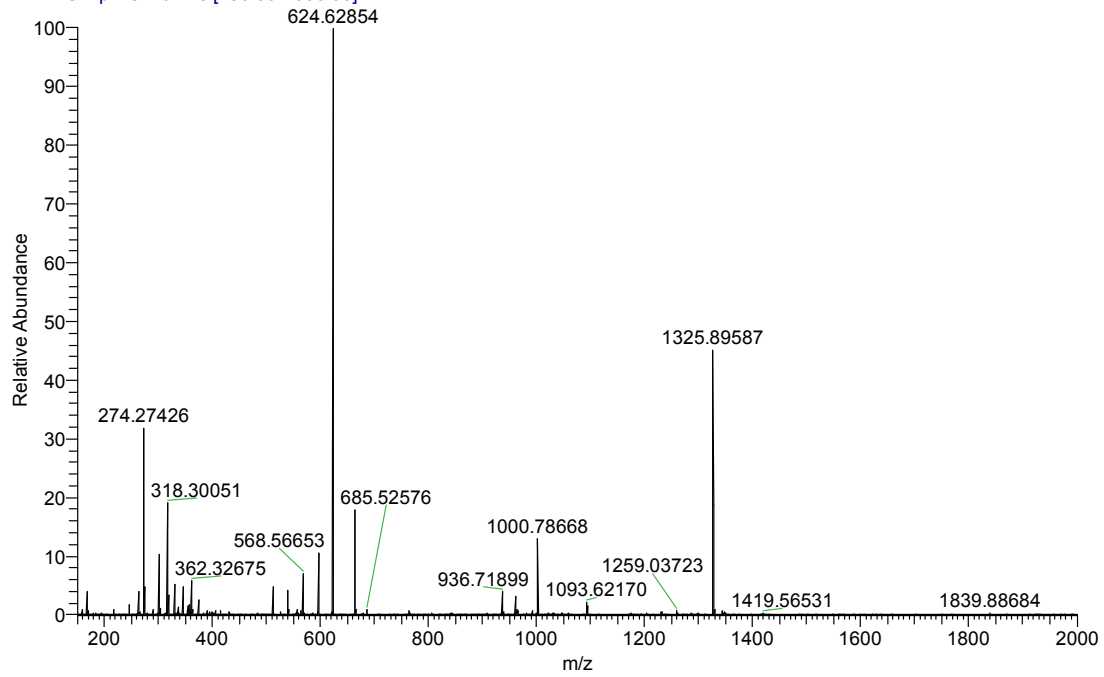


4i HRMS (ESI) m/z calcd for $C_{14}H_{13}ClFO_2S^+$ (M+H)⁺ 299.03033, found 299.03048.

122 #30 RT: 0.44 AV: 1 NL: 1.66E6
T: FTMS + p ESI Full ms [150.00-2000.00]

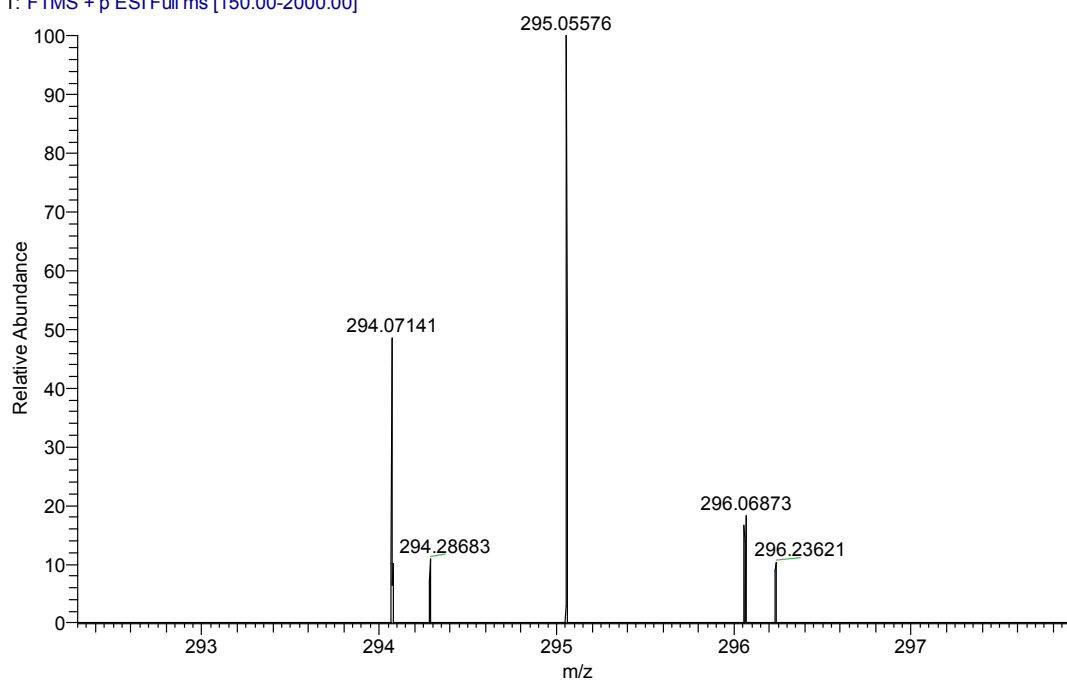


122 #30 RT: 0.44 AV: 1 NL: 4.75E8
T: FTMS + p ESI Full ms [150.00-2000.00]

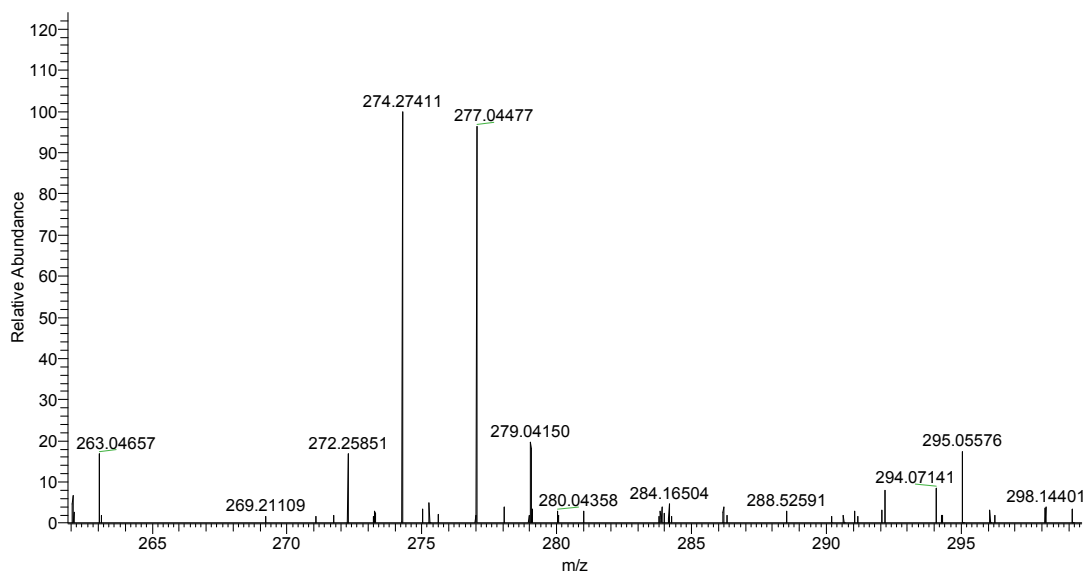


4j HRMS (ESI) m/z calcd for $C_{15}H_{16}ClO_2S^+$ (M+H)⁺ 295.05540, found 295.05576.

124 #12 RT: 0.15 AV: 1 NL: 1.66E6
T: FTMS + p ESI Full ms [150.00-2000.00]

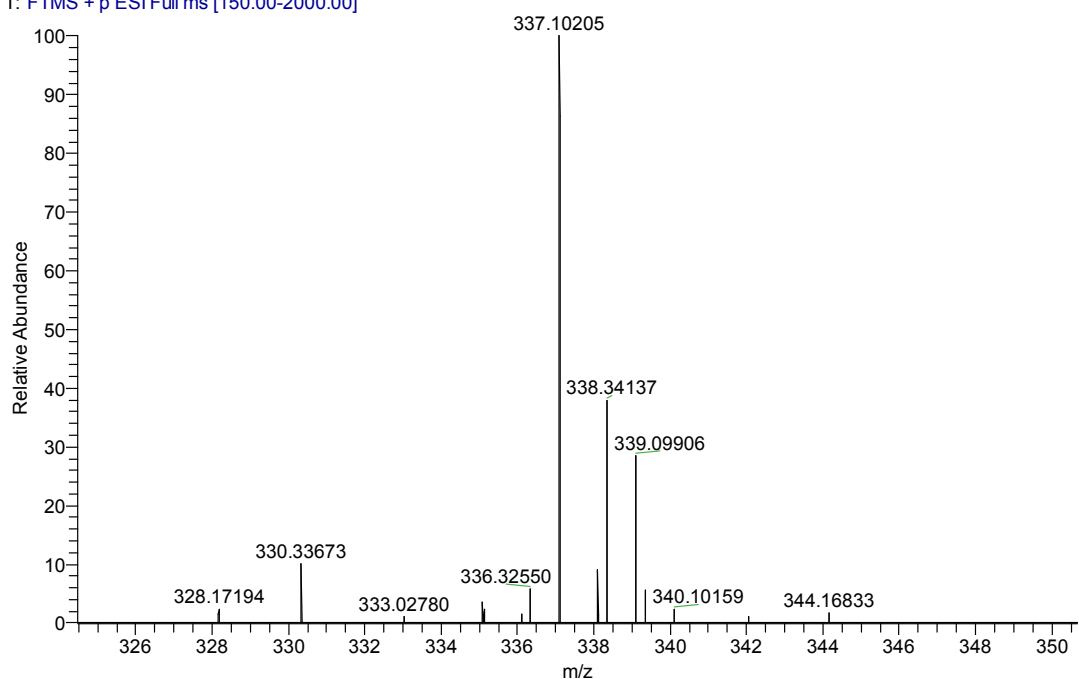


124 #12 RT: 0.15 AV: 1 NL: 9.52E6
T: FTMS + p ESI Full ms [150.00-2000.00]

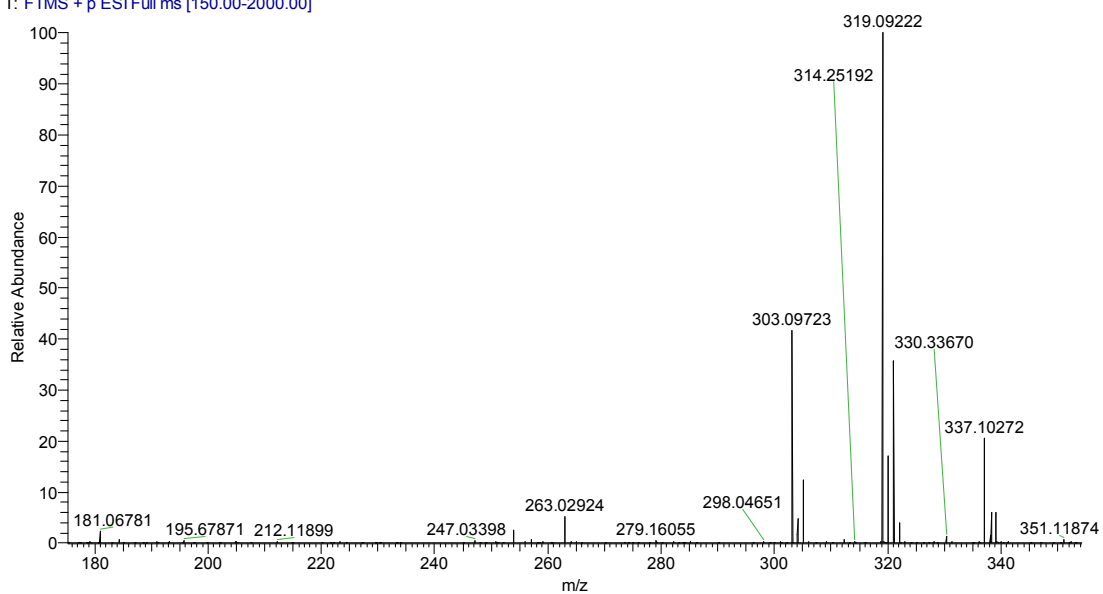


4k. HRMS (ESI) m/z calcd for $C_{18}H_{22}ClO_2^+$ (M+H)⁺ 337.10235, found 337.10205.

100_180906171755 #33 RT: 0.50 AV: 1 NL: 1.12E7
T: FTMS + p ESI Full ms [150.00-2000.00]

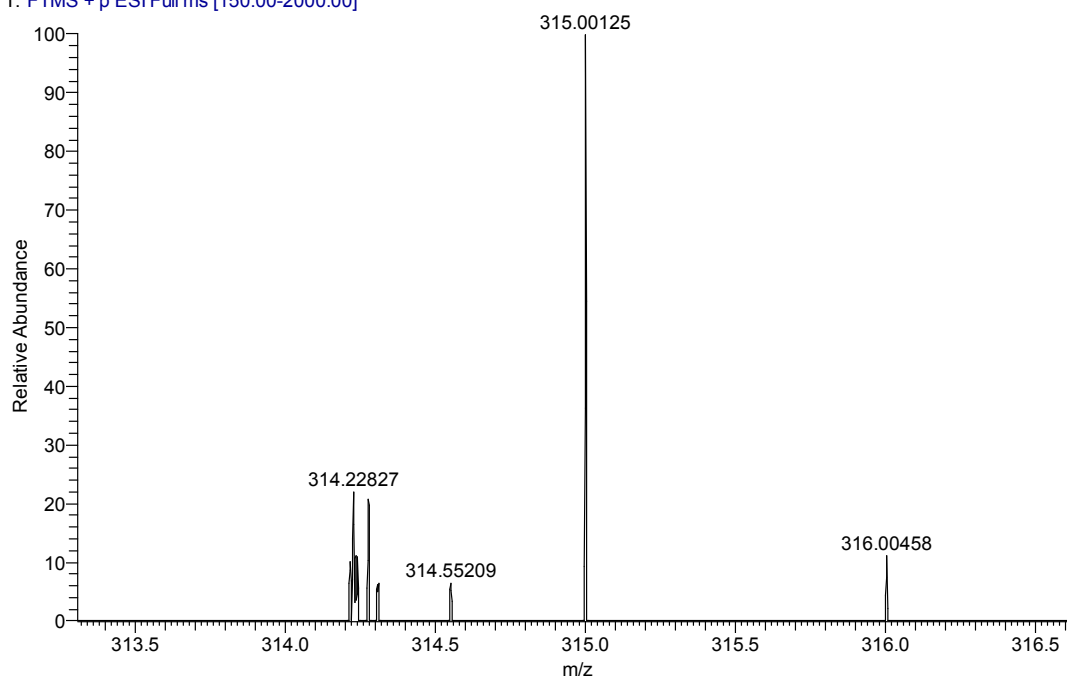


100 #8 RT: 0.09 AV: 1 NL: 8.83E7
T: FTMS + p ESI Full ms [150.00-2000.00]

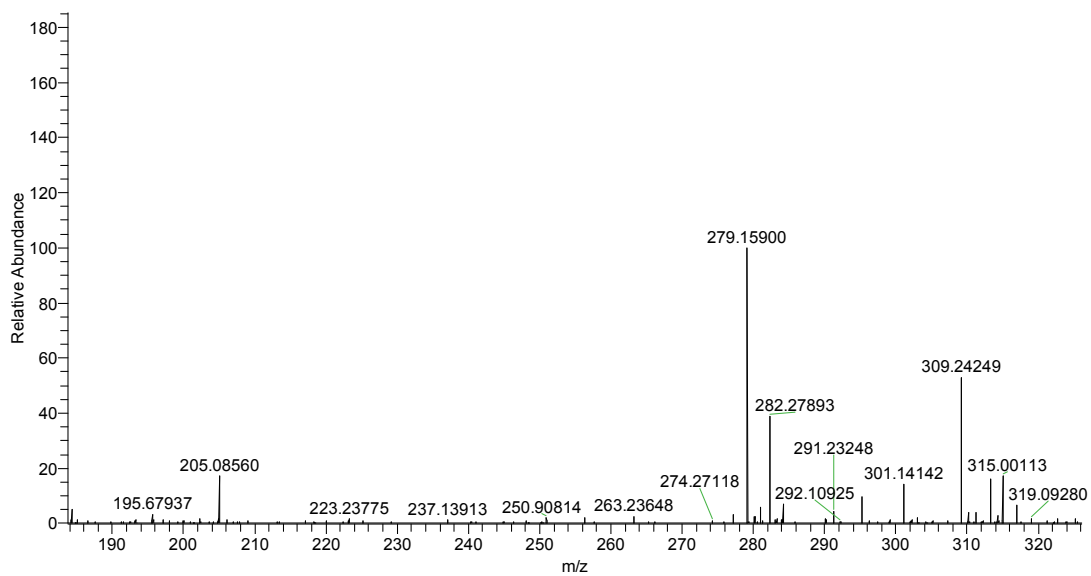


4I. HRMS (ESI) m/z calcd for $C_{14}H_{13}Cl_2O_2S^+$ (M+H)⁺ 315.00078, found 315.00125.

101_180906171913 #35 RT: 0.52 AV: 1 NL: 1.89E6
T: FTMS + p ESI Full ms [150.00-2000.00]

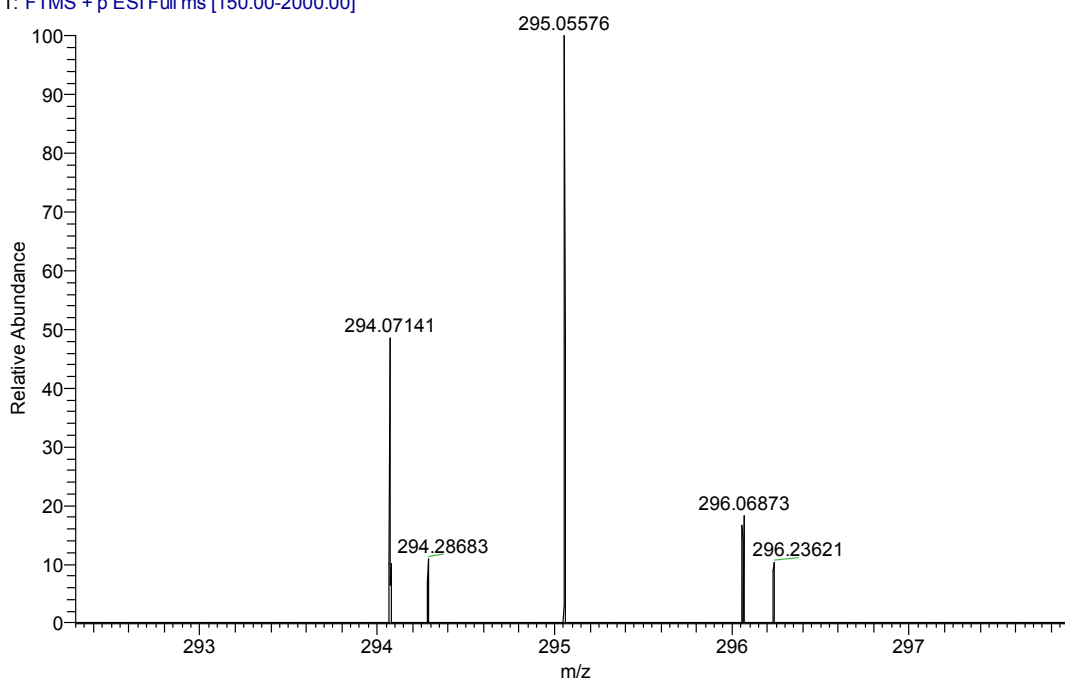


101 #7 RT: 0.08 AV: 1 NL: 1.52E7
T: FTMS + p ESI Full ms [150.00-2000.00]

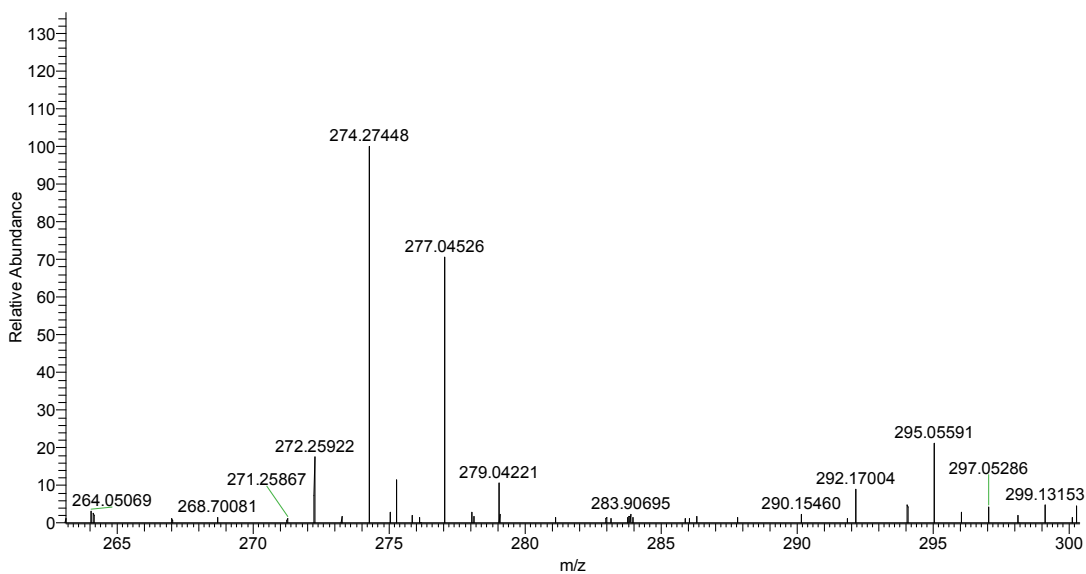


4m HRMS (ESI) m/z calcd for $C_{15}H_{16}ClO_2S^+$ (M+H)⁺ 295.05540, found 295.05576.

124 #12 RT: 0.15 AV: 1 NL: 1.66E6
T: FTMS + p ESI Full ms [150.00-2000.00]

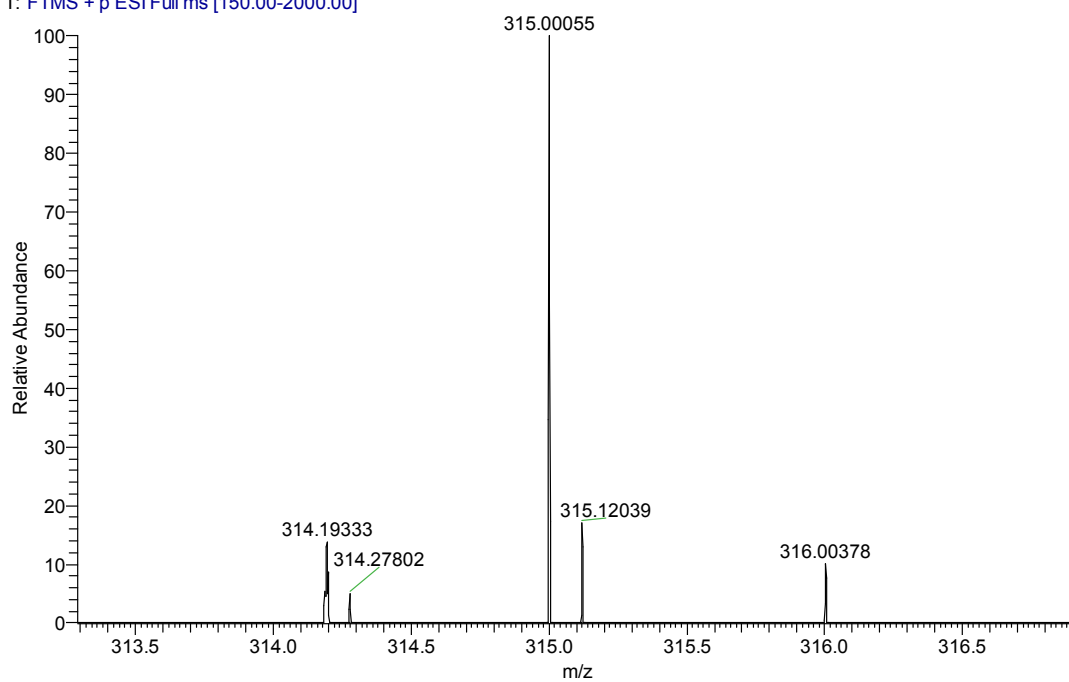


124 #13 RT: 0.17 AV: 1 NL: 1.61E7
T: FTMS + p ESI Full ms [150.00-2000.00]

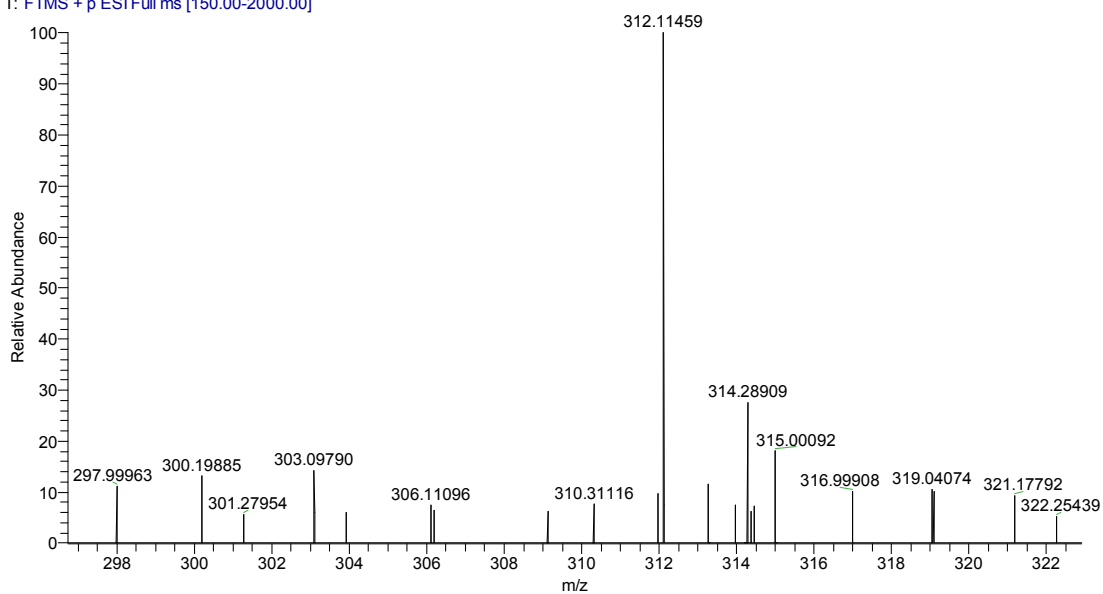


4n. HRMS (ESI) m/z calcd for $C_{14}H_{13}Cl_2O_2S^+$ (M+H)⁺ 315.00078, found 315.00055.

103_180906172141 #2 RT: 0.01 AV: 1 NL: 7.88E5
T: FTMS + p ESI Full ms [150.00-2000.00]

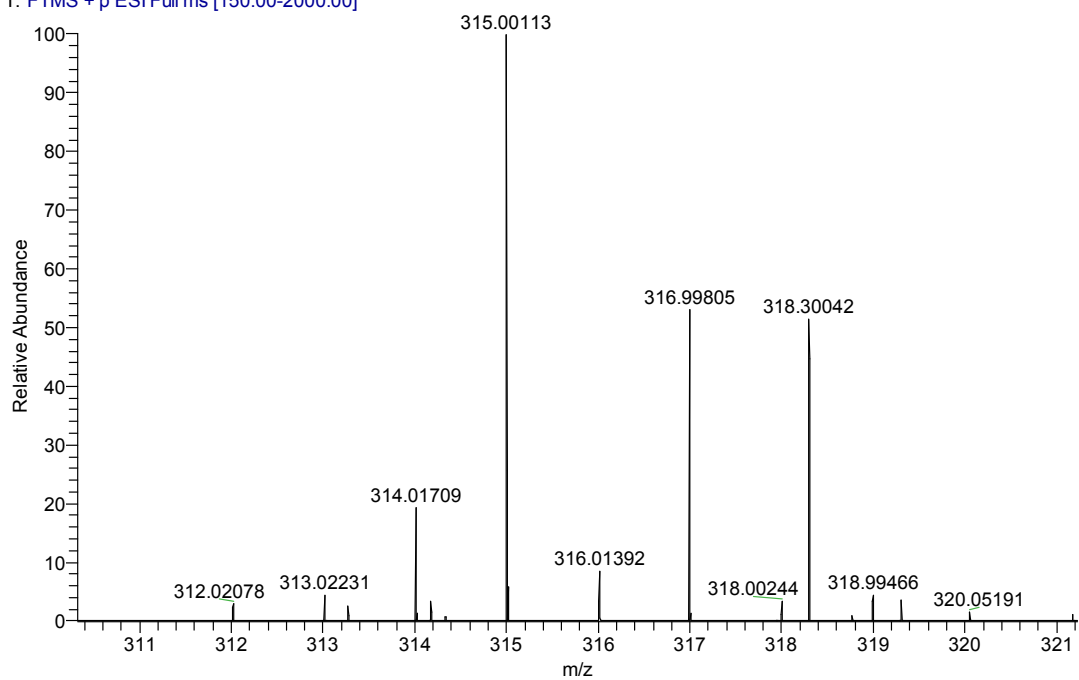


103 #2 RT: 0.01 AV: 1 NL: 1.81E5
T: FTMS + p ESI Full ms [150.00-2000.00]

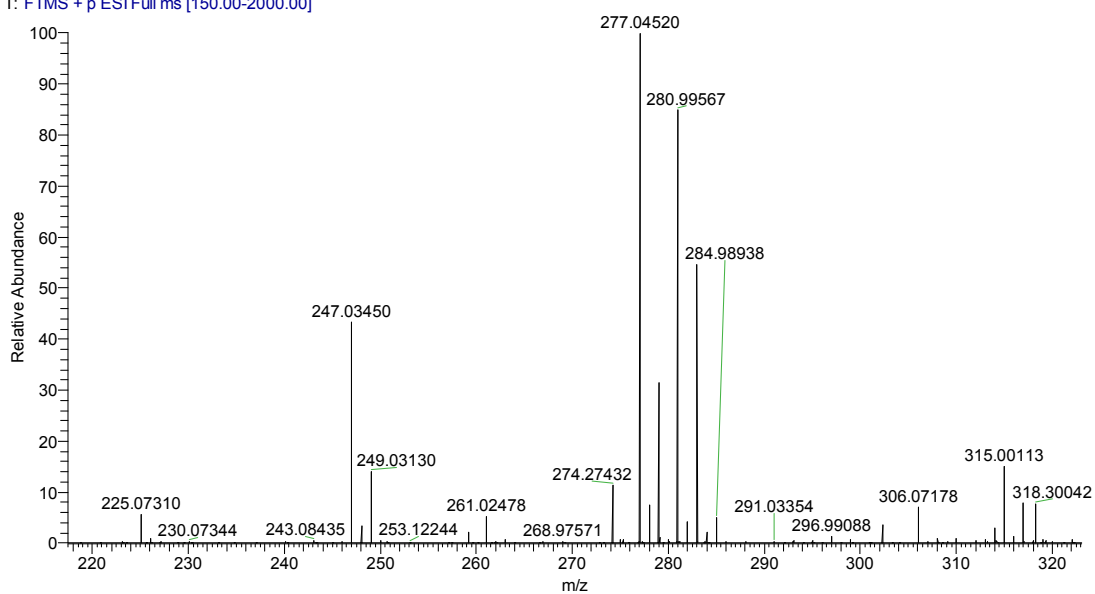


4o HRMS (ESI) m/z calcd for $C_{14}H_{13}Cl_2O_2S^+$ (M+H)⁺ 315.00078, found 315.00113.

119 #6 RT: 0.06 AV: 1 NL: 3.92E6
T: FTMS + p ESI Full ms [150.00-2000.00]

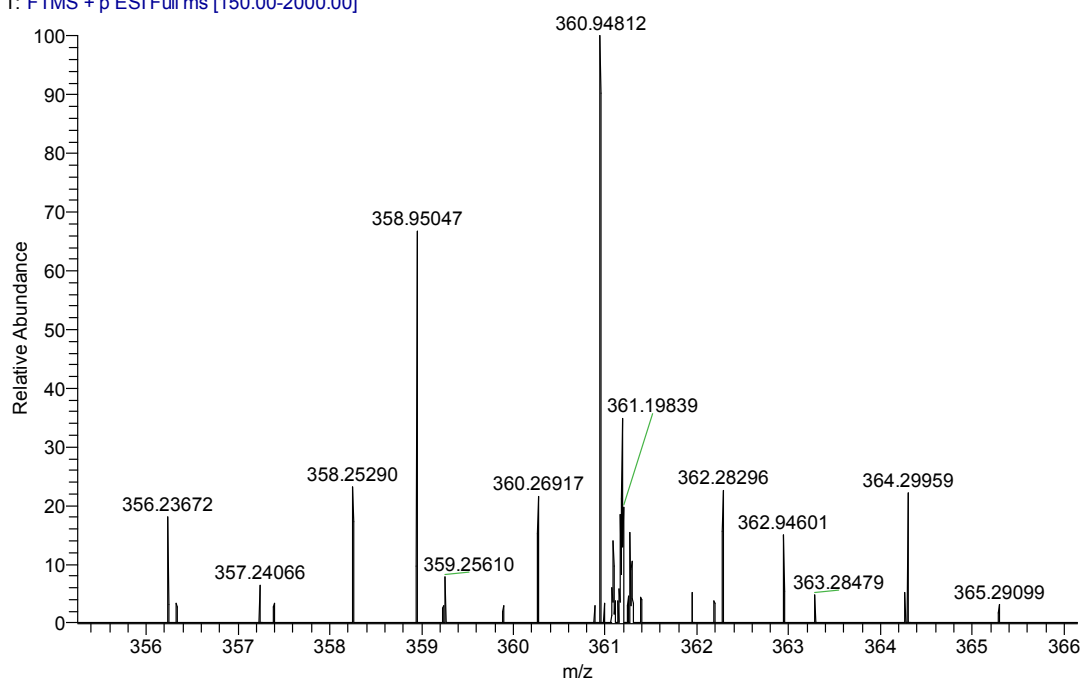


119 #6 RT: 0.06 AV: 1 NL: 2.61E7
T: FTMS + p ESI Full ms [150.00-2000.00]



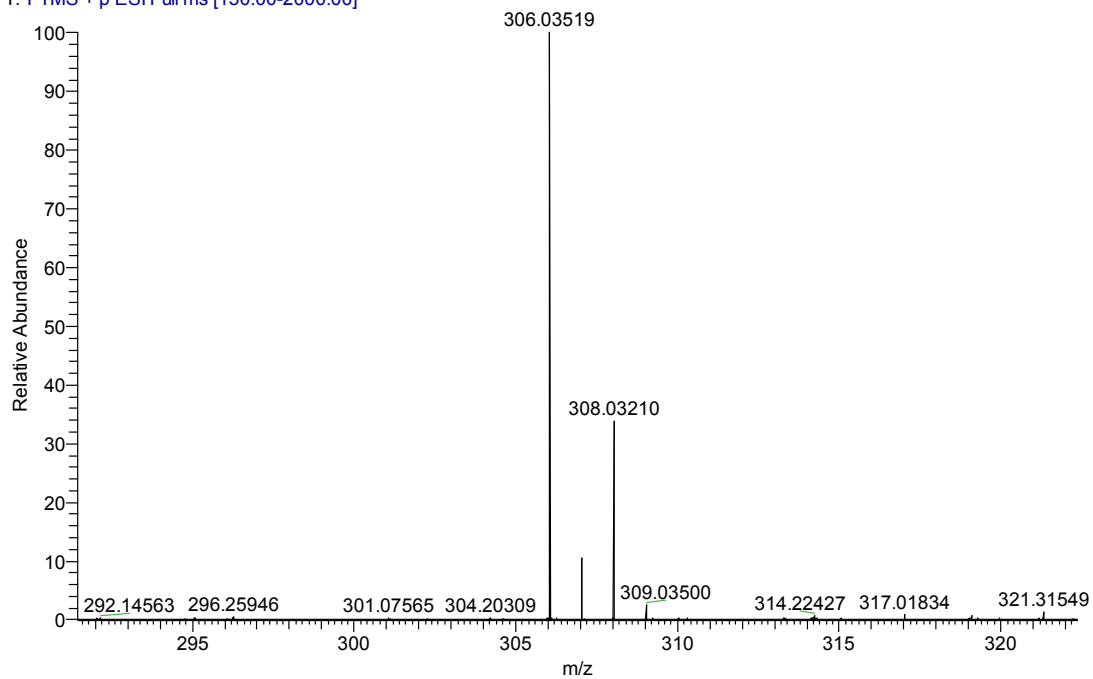
4q. HRMS (ESI) m/z calcd for $C_{14}H_{13}ClBrO_2S^+$ (M+H)⁺ 358.95027, found 358.95047.

104_180906172255 #43 RT: 0.63 AV: 1 NL: 2.91E6
T: FTMS + p ESI Full ms [150.00-2000.00]

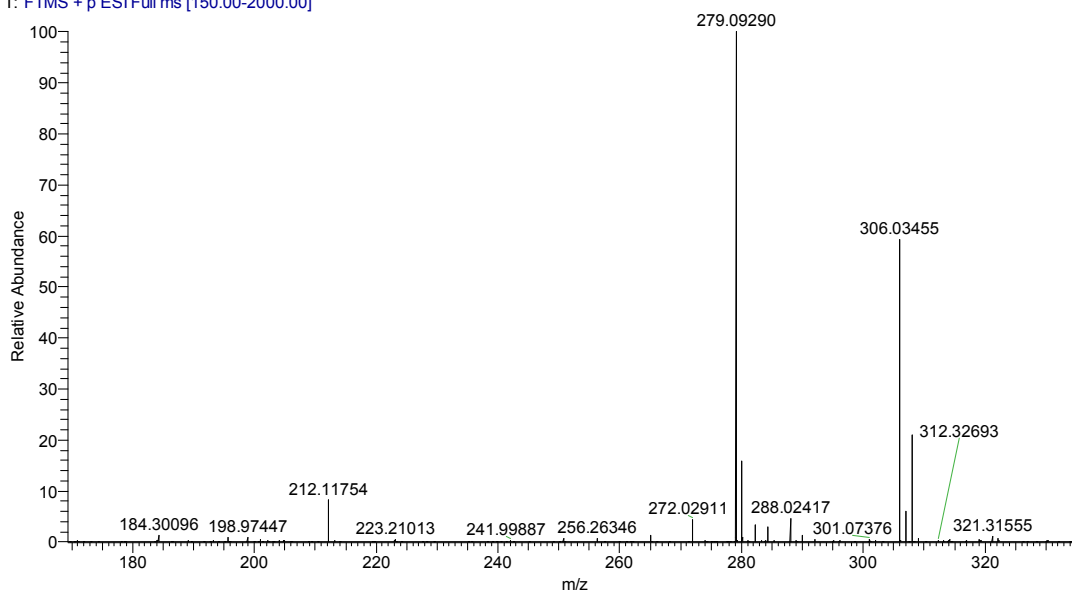


4r. HRMS (ESI) m/z calcd for $C_{15}H_{13}ClNO_2S^+$ (M+H)⁺ 306.03500, found 306.03519.

105 #40 RT: 0.60 AV: 1 NL: 4.64E7
T: FTMS + p ESI Full ms [150.00-2000.00]

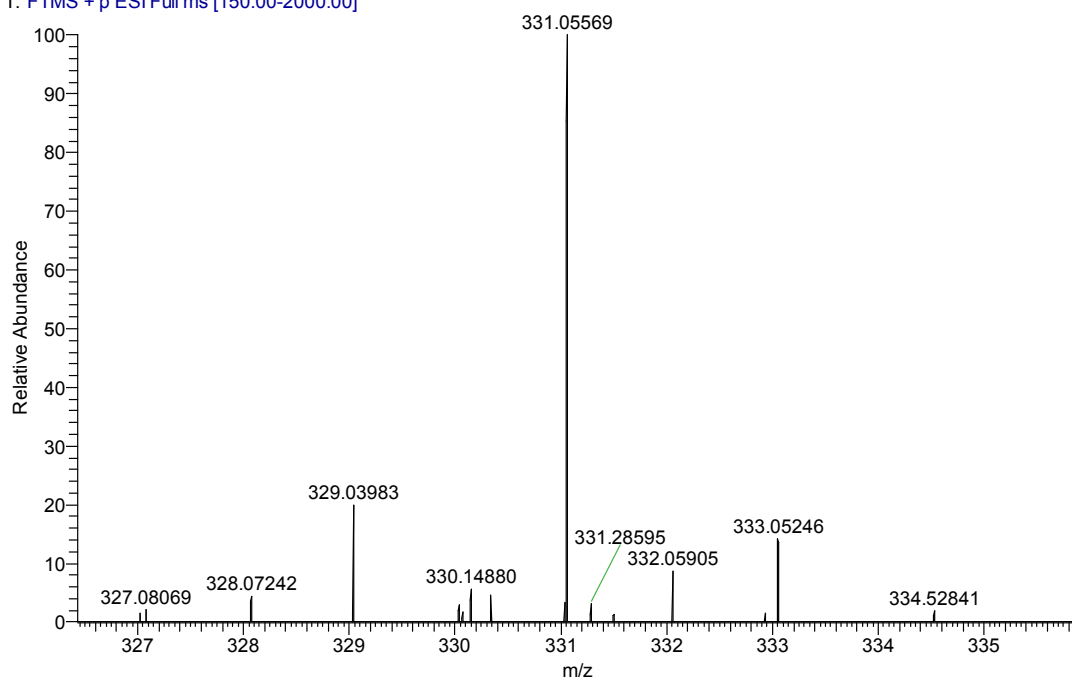


105 #34 RT: 0.51 AV: 1 NL: 6.25E7
T: FTMS + p ESI Full ms [150.00-2000.00]



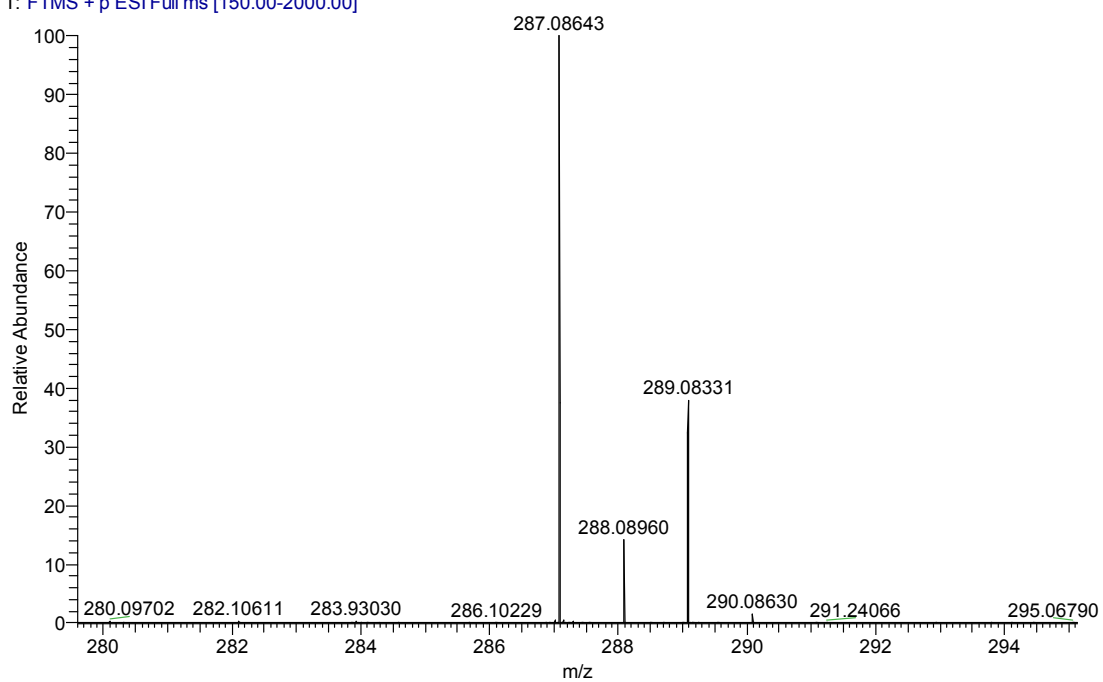
4s. HRMS (ESI) m/z calcd for $C_{18}H_{16}ClO_2S^+$ (M+H)⁺ 331.05540, found 331.05569.

106 #36 RT: 0.55 AV: 1 NL: 4.45E6
T: FTMS + p ESI Full ms [150.00-2000.00]

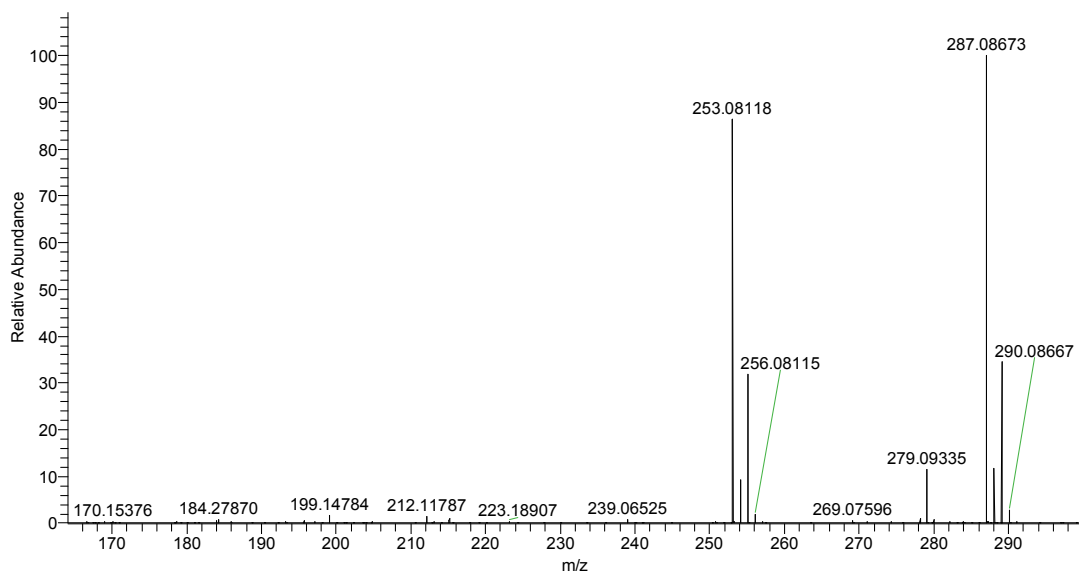


4t. HRMS (ESI) m/z calcd for $C_{14}H_{20}ClO_2S^+$ (M+H)⁺ 287.08670, found 287.08643.

107 #35 RT: 0.53 AV: 1 NL: 1.04E8
T: FTMS + p ESI Full ms [150.00-2000.00]

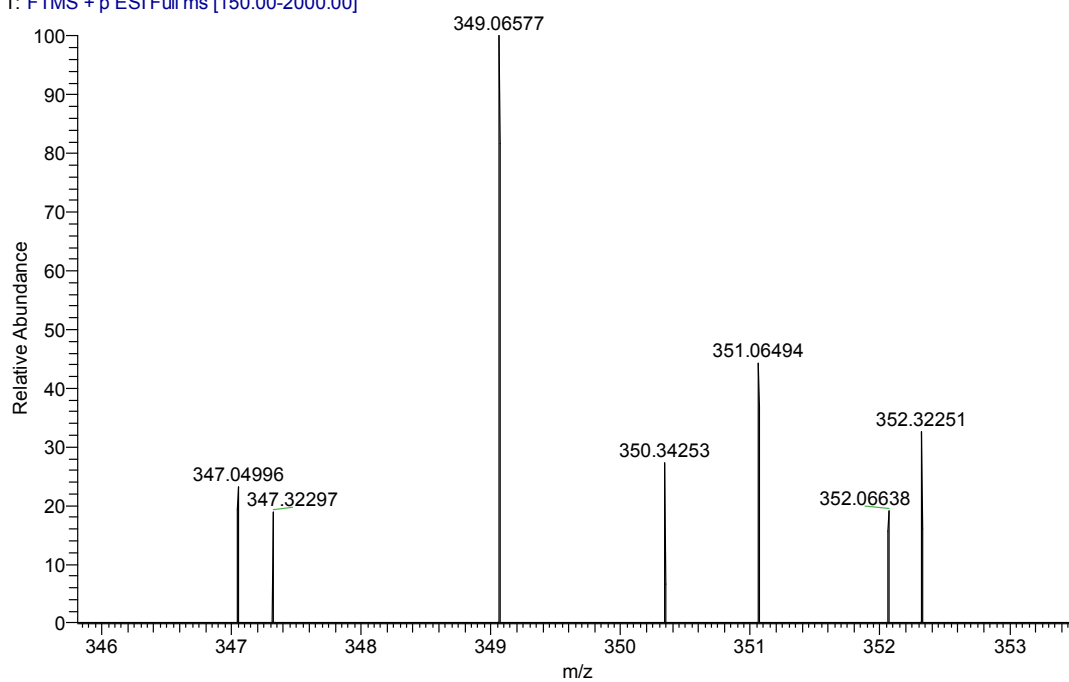


107 #30 RT: 0.45 AV: 1 NL: 9.64E7
T: FTMS + p ESI Full ms [150.00-2000.00]



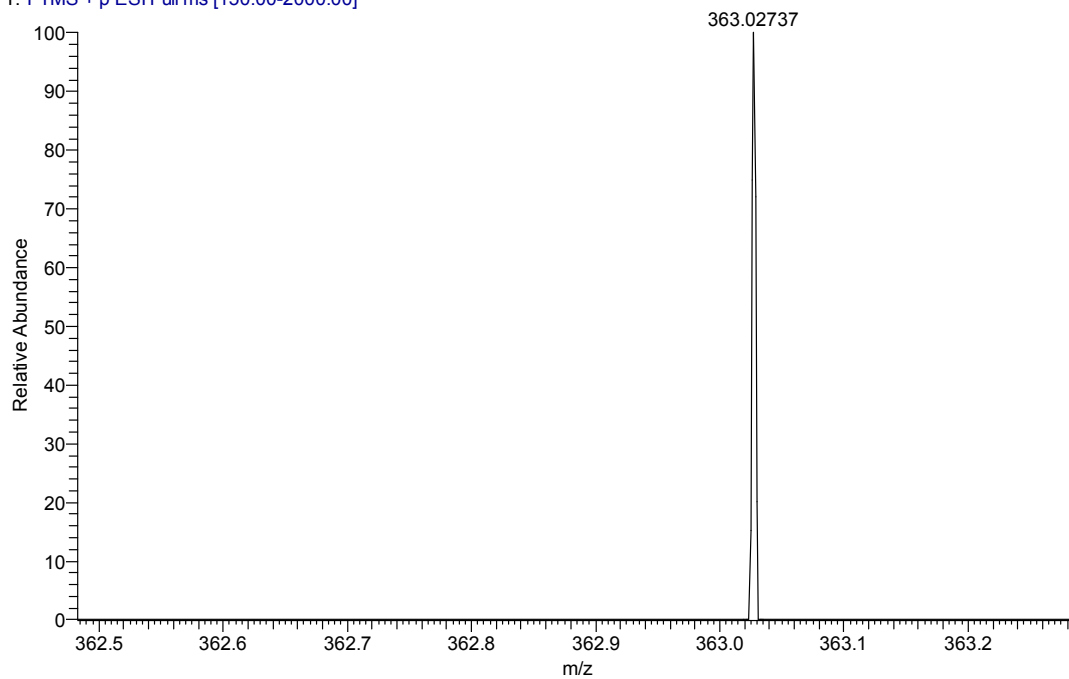
7. HRMS (ESI) m/z calcd for $C_{18}H_{18}ClO_3S^+$ (M+H)⁺ 349.06597, found 349.06577.

108 #44 RT: 0.68 AV: 1 NL: 2.57E5
T: FTMS + p ESI Full ms [150.00-2000.00]



10. HRMS (ESI) m/z calcd for $C_{18}H_{16}ClO_2S^+$ (M+H)⁺ 363.02748, found 363.02737.

109 #32 RT: 0.49 AV: 1 NL: 8.00E4
T: FTMS + p ESI Full ms [150.00-2000.00]



109#32 RT: 0.49 AV: 1 NL: 1.17E6
T: FTMS + p ESI Full ms [150.00-2000.00]

