

NO : HRMS180906XT008

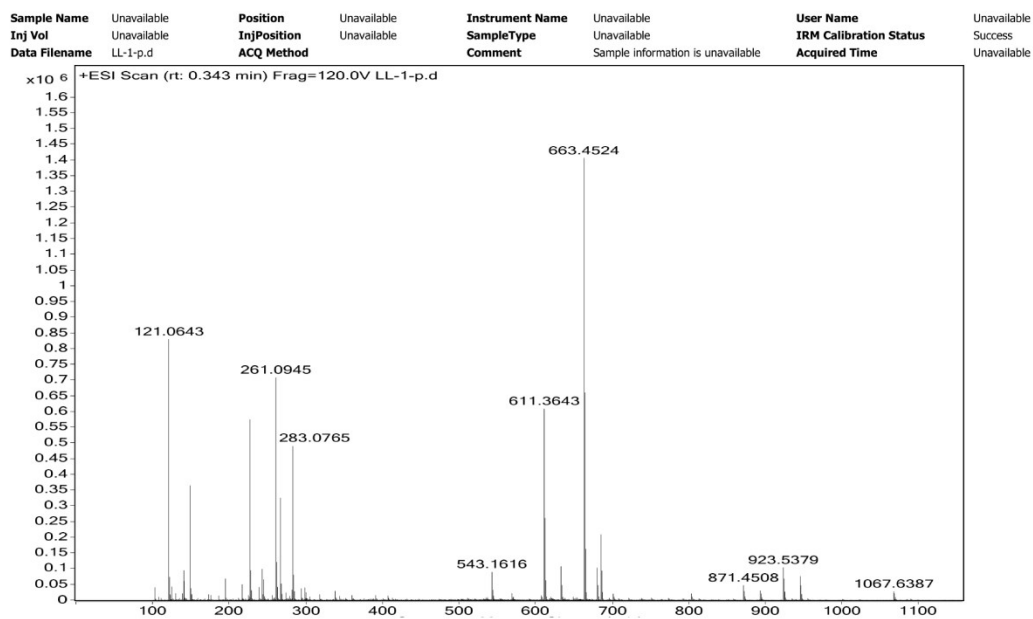
HRMS report

Instrument :

Thermo Scientific LTQ Orbitrap XL

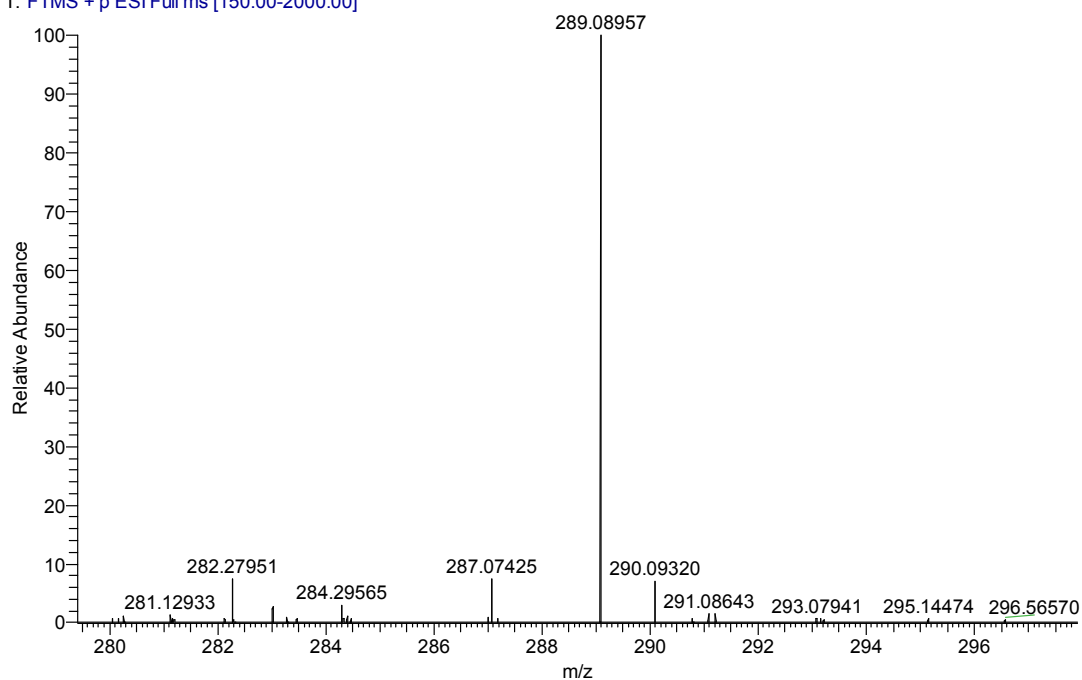
Ionic source : ESI Result :

4b HRMS (ESI) m/z calcd for C₁₅H₁₆O₂Na (M+O+Na)⁺283.0763, found 283.0765.



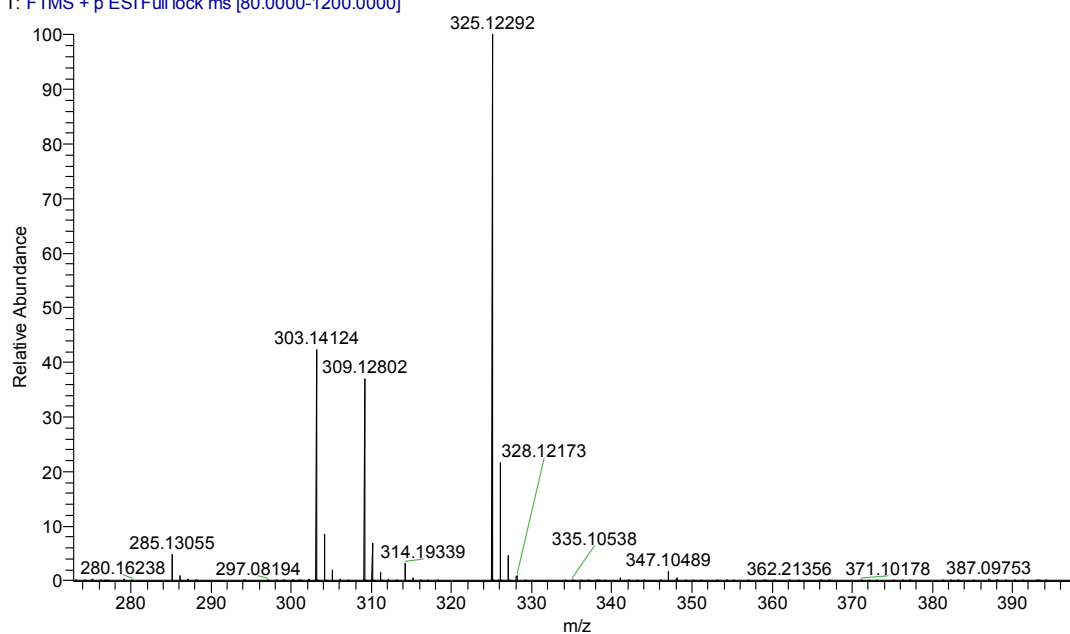
4c. HRMS (ESI) m/z calcd for C₁₆H₁₇O₃S (M+O+H)⁺ 289.08984, found 289.08957.

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



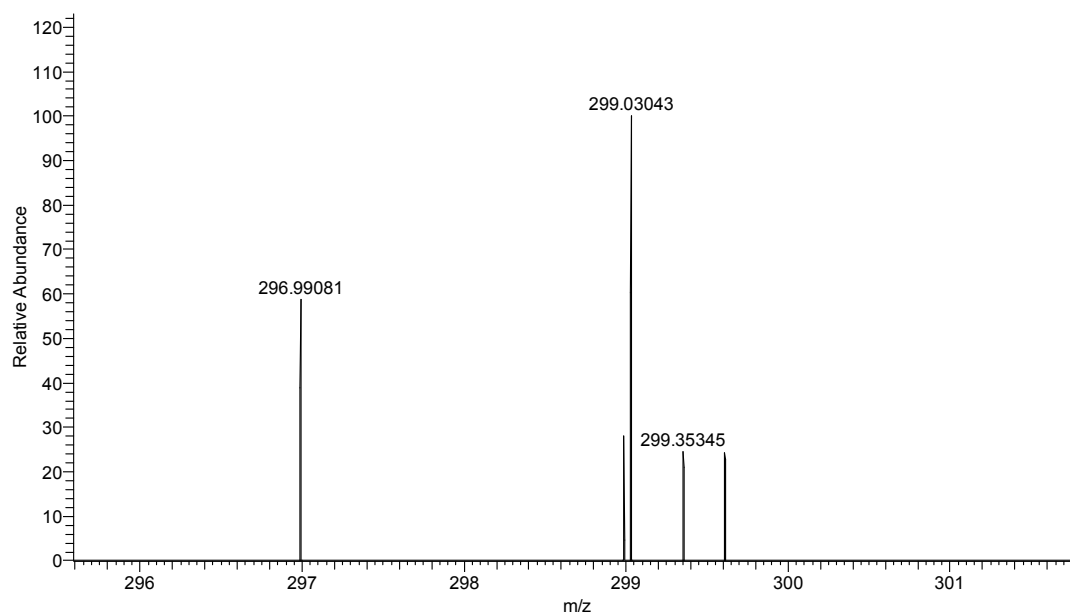
4e HRMS (ESI) m/z calcd for $C_{18}H_{22}OSNa$ ($M+Na$)⁺ 309.1289, found 309.1280;
calcd for $C_{18}H_{22}O_2SNa$ ($M+O+Na$)⁺ 325.1238, found 325.1229; calcd for $C_{18}H_{23}O_2$
($M+O+H$)⁺: 303.1419, found 303.1412.

1-22 #8 RT: 0.07 AV: 1 NL: 9.39E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]



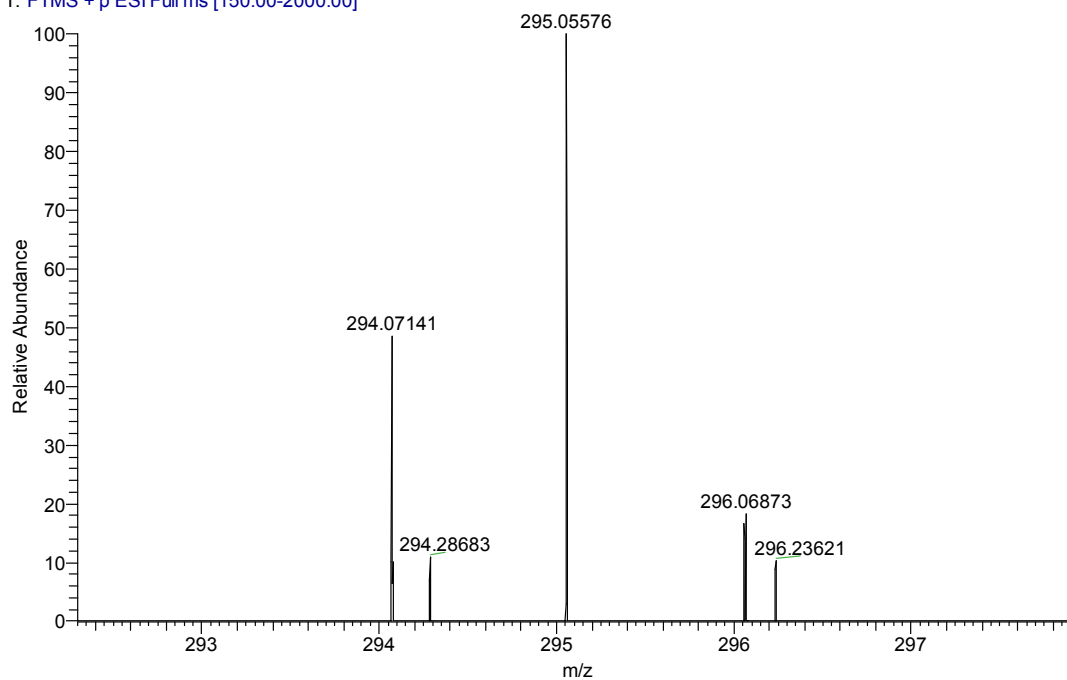
4i HRMS (ESI) m/z calcd for $C_{14}H_{13}ClFO_2S^+$ ($M+O+H$)⁺ 299.03033, found 299.03043.

125 #5 RT: 0.05 AV: 1 NL: 2.13E5
T: FTMS + p ESI Full ms [150.00-2000.00]



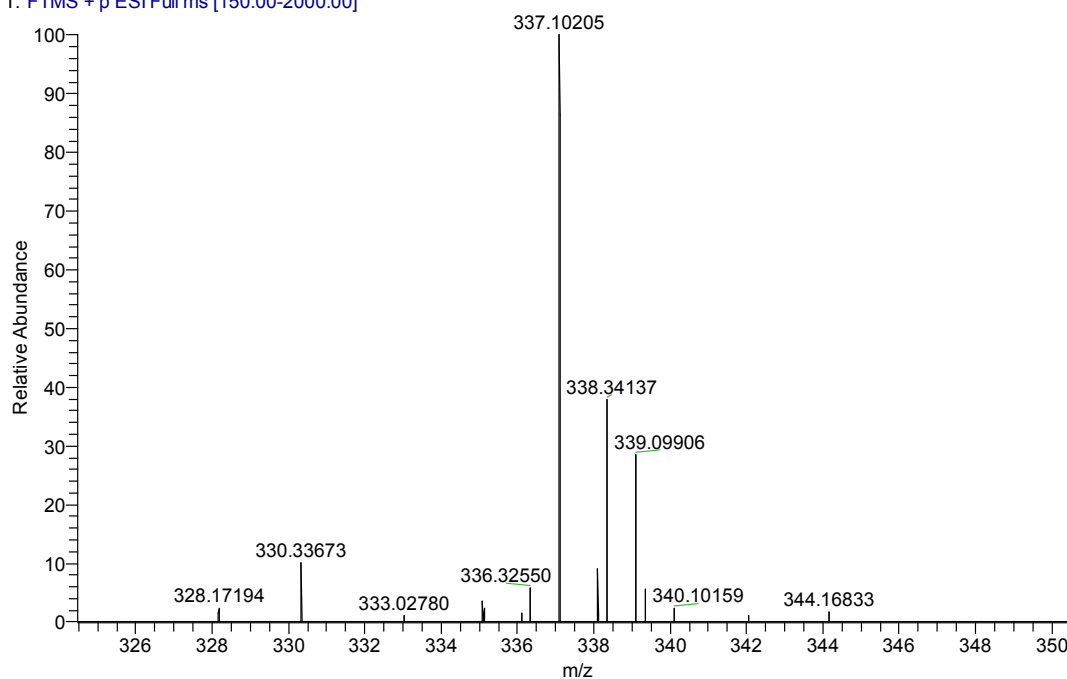
4j HRMS (ESI) m/z calcd for $C_{15}H_{16}ClO_2S^+$ (M+O+H)⁺ 295.05540, found 295.05576.

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



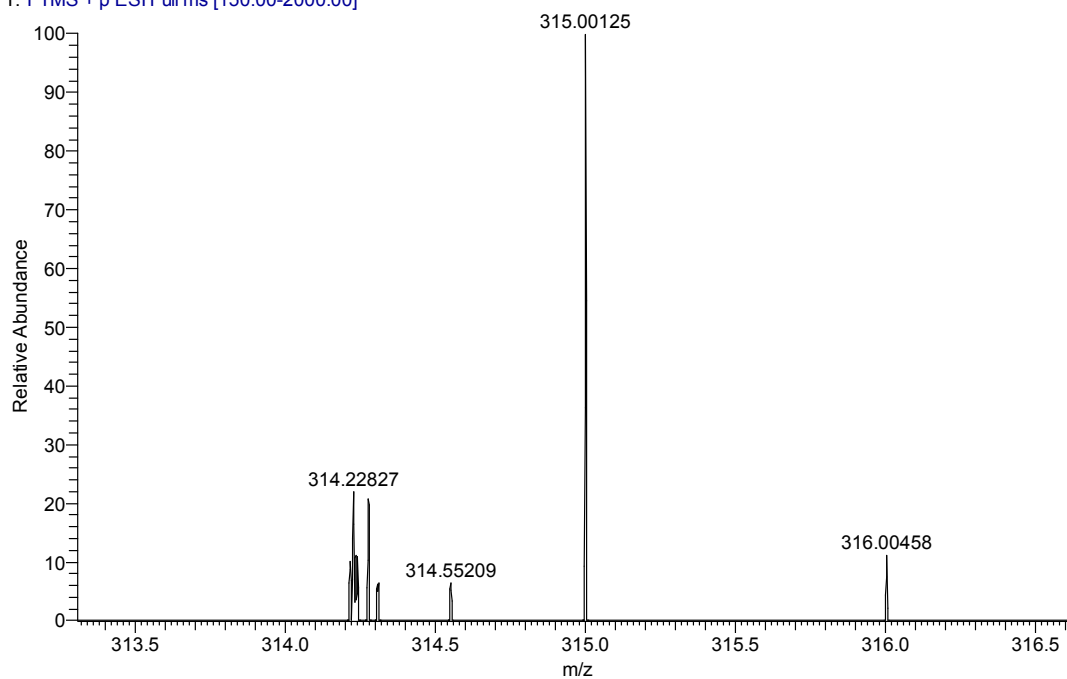
4k. HRMS (ESI) m/z calcd for $C_{18}H_{22}ClO_2S^+$ (M+O+H)⁺ 337.10235, found 337.10205.

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



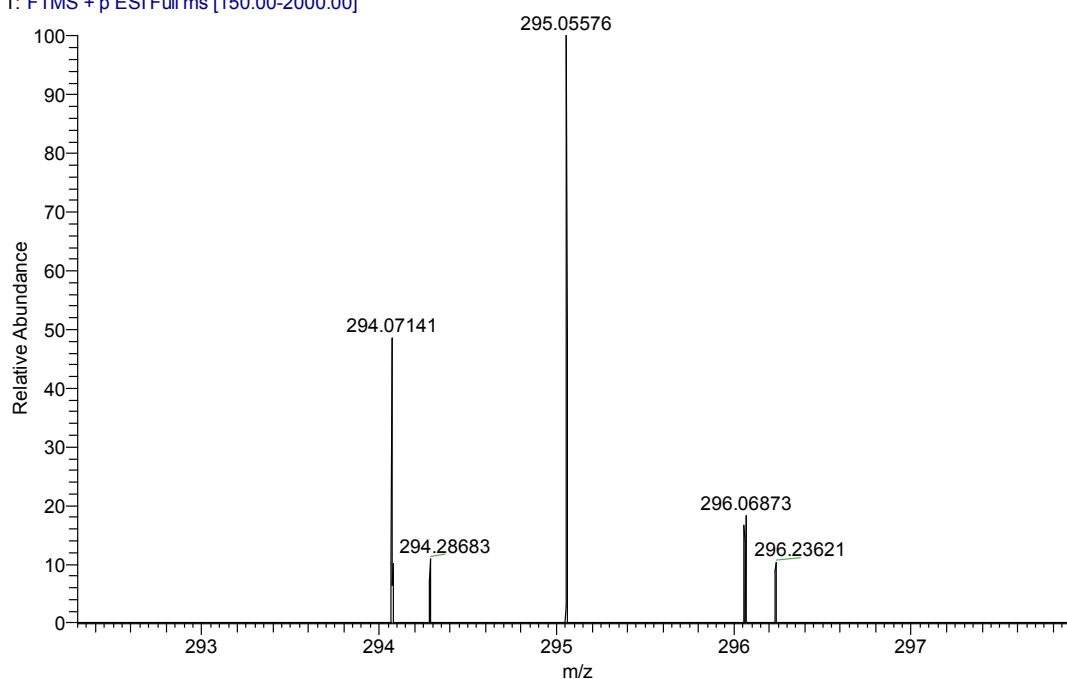
4l. HRMS (ESI) m/z calcd for $C_{14}H_{13}Cl_2O_2S^+$ (M+O+H)⁺ 315.00078, found 315.00125.

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



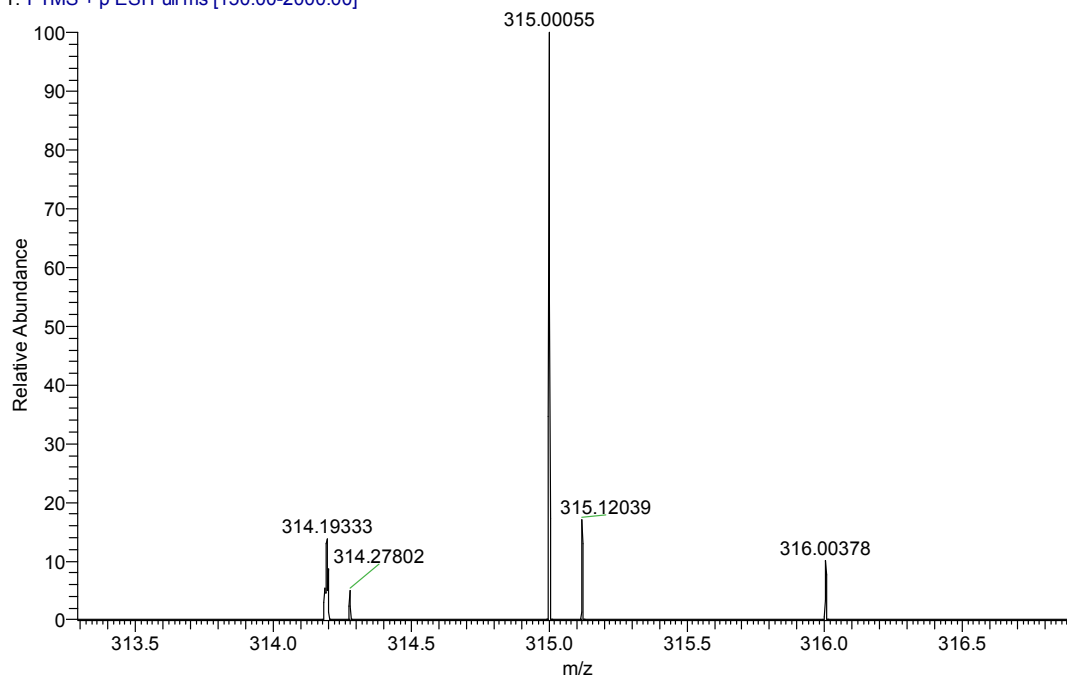
4m HRMS (ESI) m/z calcd for $C_{15}H_{16}ClO_2S^+$ (M+O+H)⁺ 295.05540, found 295.05576.

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



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

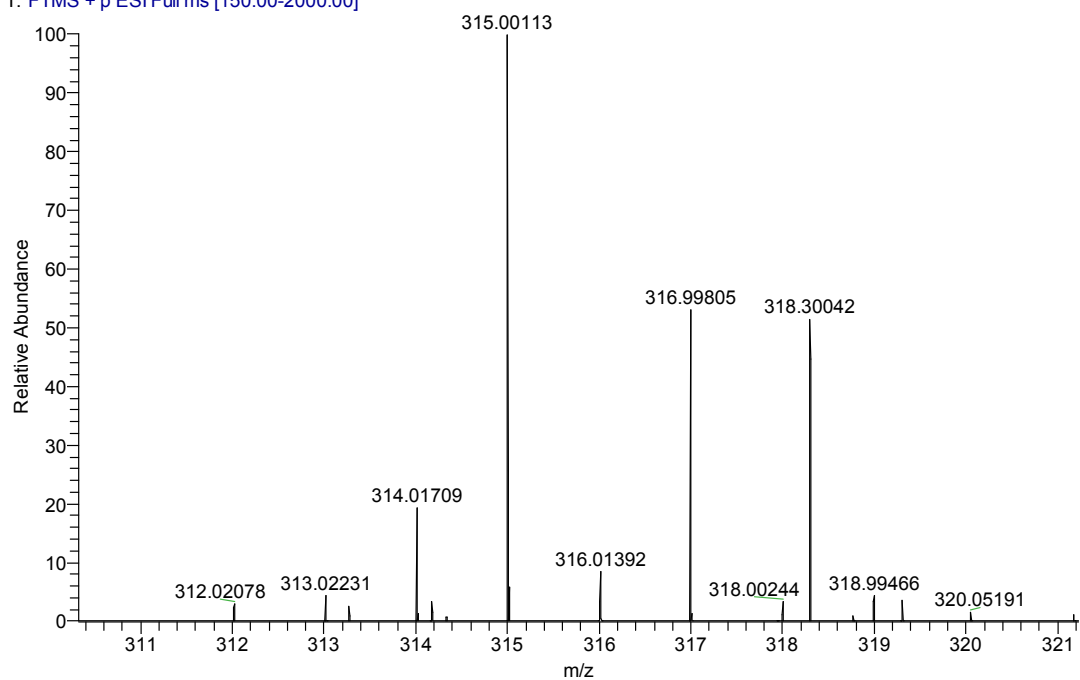
103_180906172141 #2 RT: 0.01 AV: 1 NL: 7.88E5
T: FTMS + p ESI Full ms [150.00-2000.00]



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

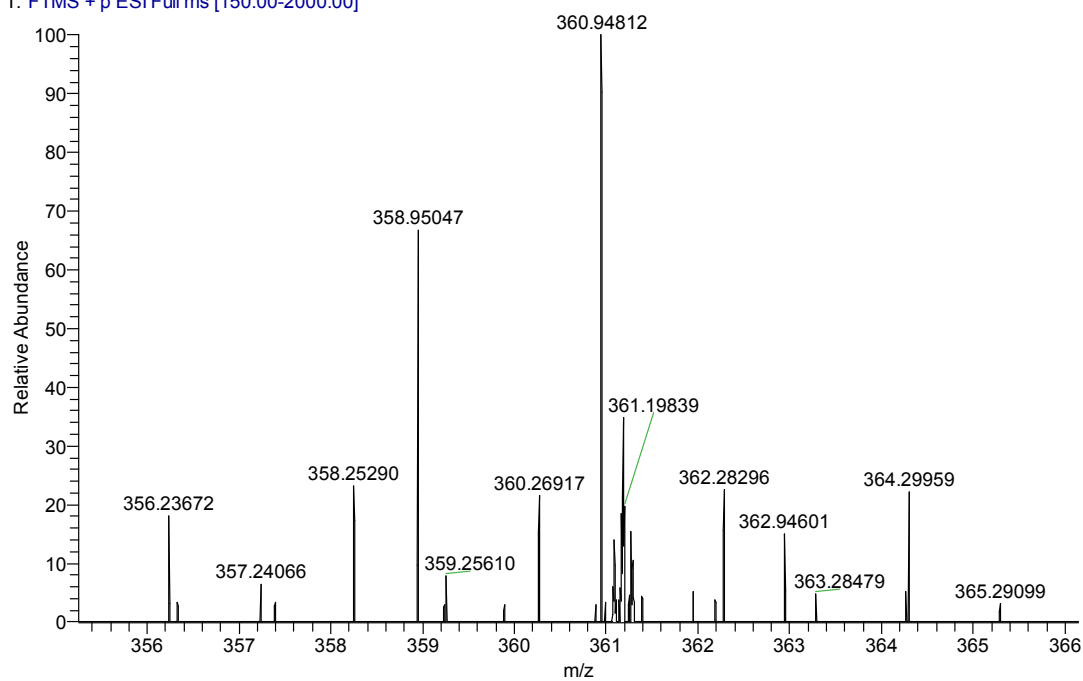
315.00113.

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



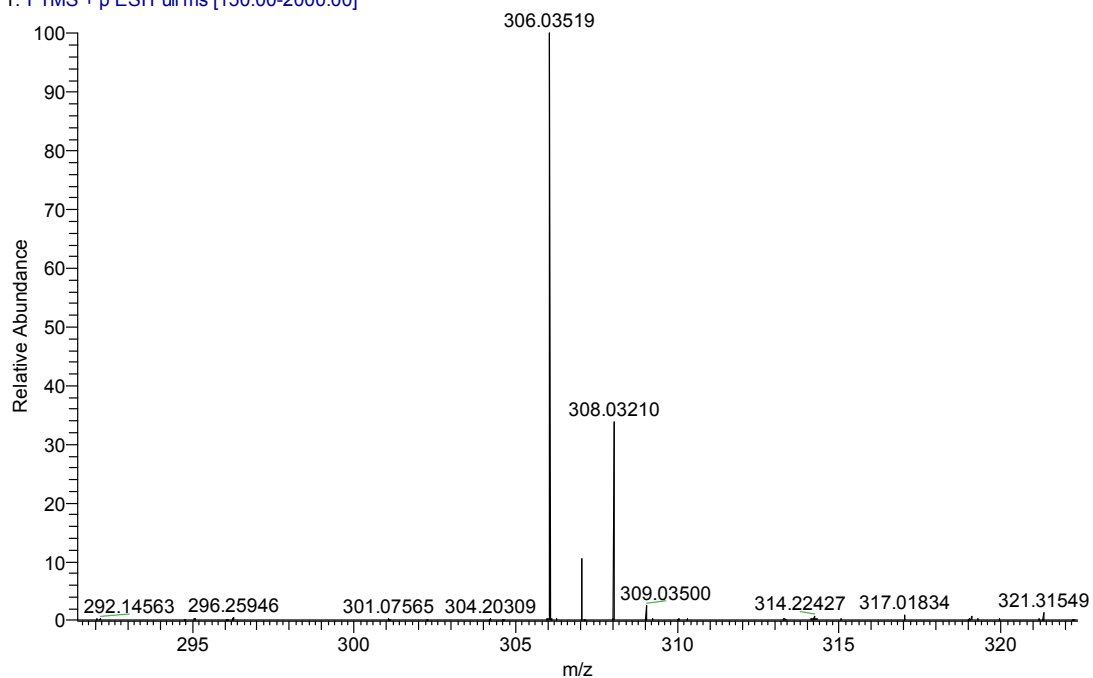
4p. HRMS (ESI) m/z calcd for $C_{14}H_{13}ClBrO_2S^+$ (M+O+H)⁺ 358.95027, found 358.95047.

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



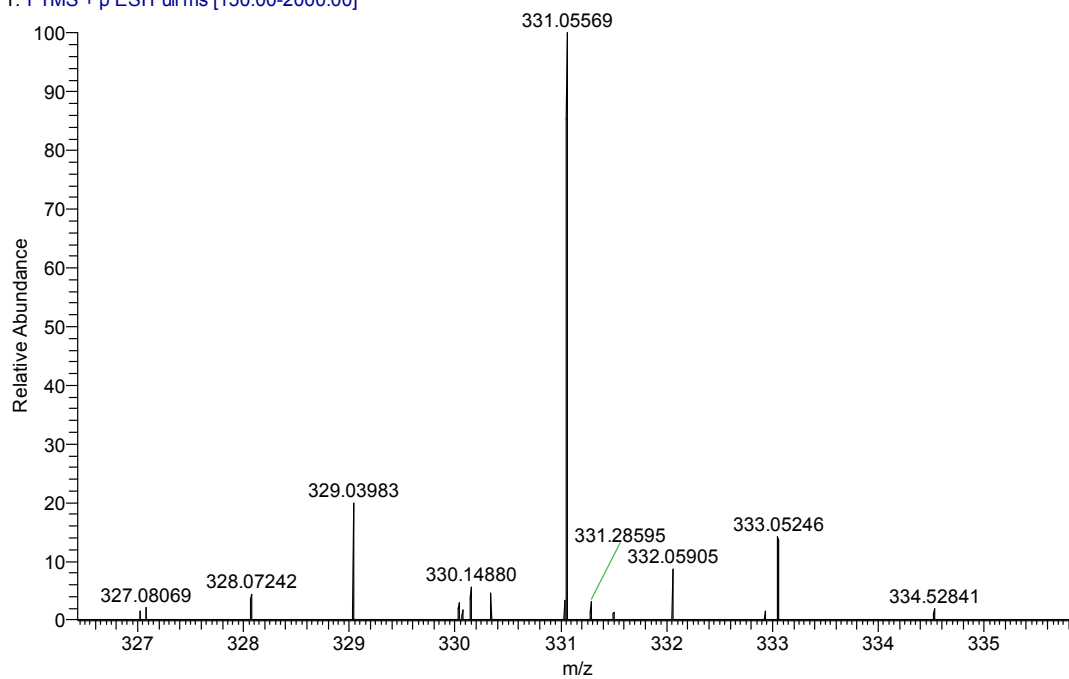
4q. HRMS (ESI) m/z calcd for $C_{15}H_{13}ClNO_2S^+$ (M+O+H)⁺ 306.03500, found 306.03519.

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



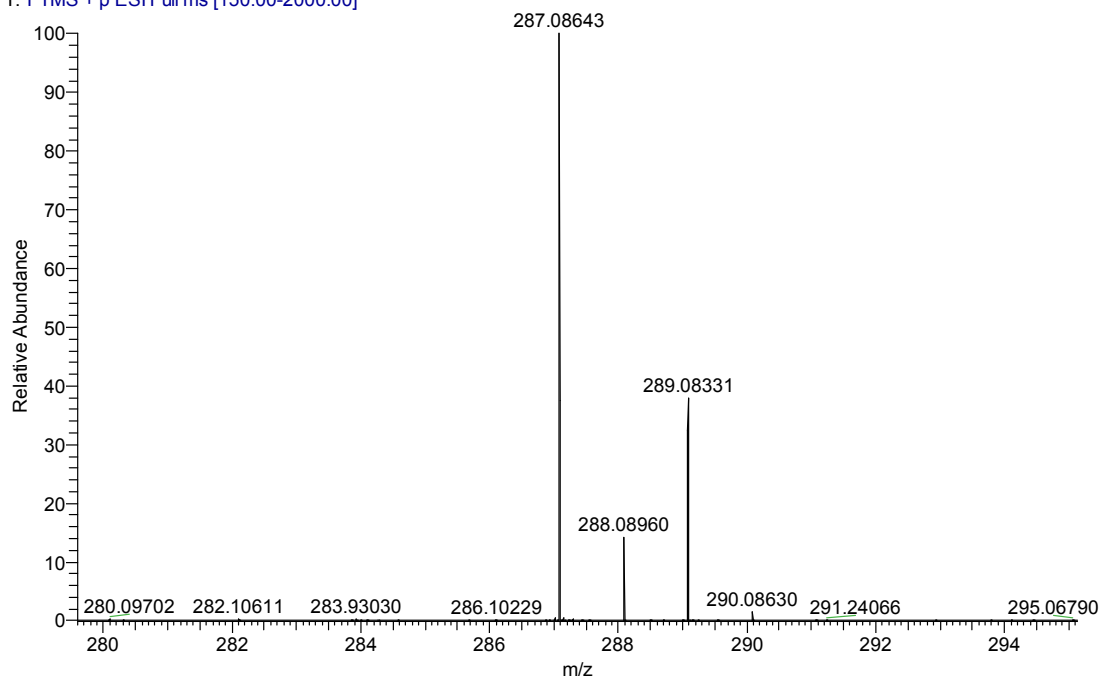
4r. HRMS (ESI) m/z calcd for $C_{18}H_{16}ClO_2S^+$ (M+O+H)⁺ 331.05540, found 331.05569.

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



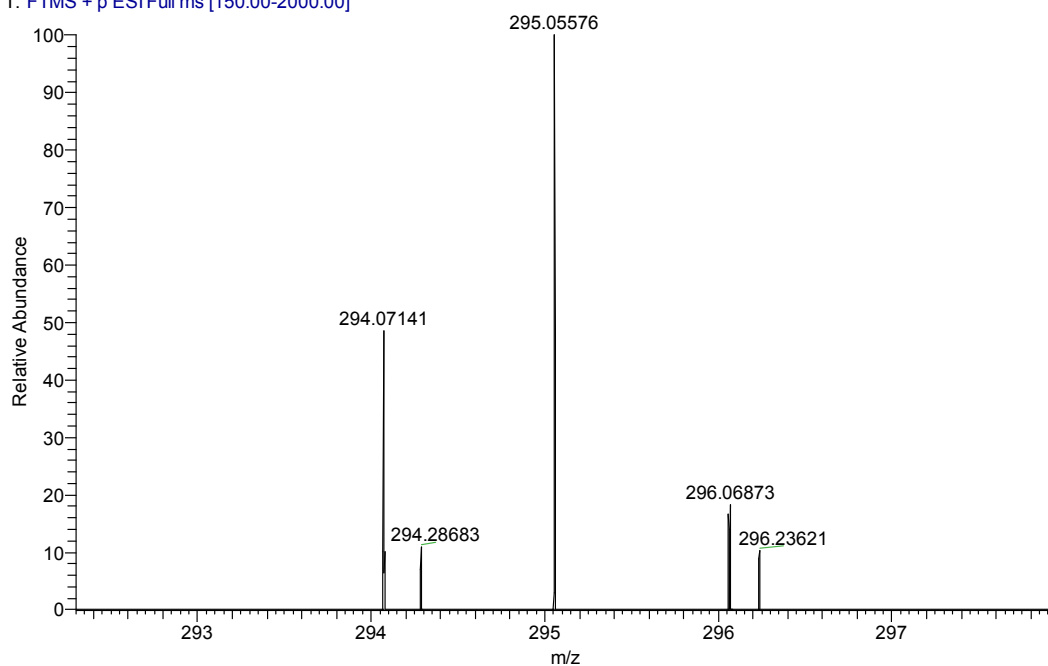
4t. HRMS (ESI) m/z calcd for $C_{14}H_{20}ClO_2S^+$ (M+O+H)⁺ 287.08670, found 287.08643.

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



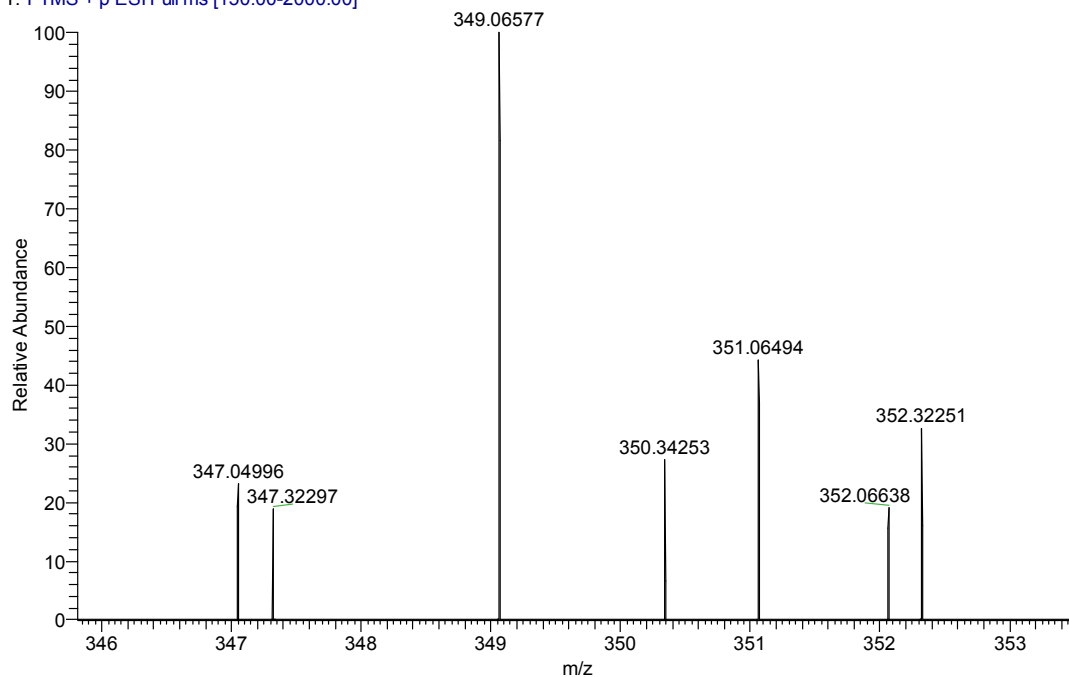
6 HRMS (ESI) m/z calcd for $C_{15}H_{16}ClO_2S^+$ (M+O+H)⁺ 295.05540, found 295.05576.

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

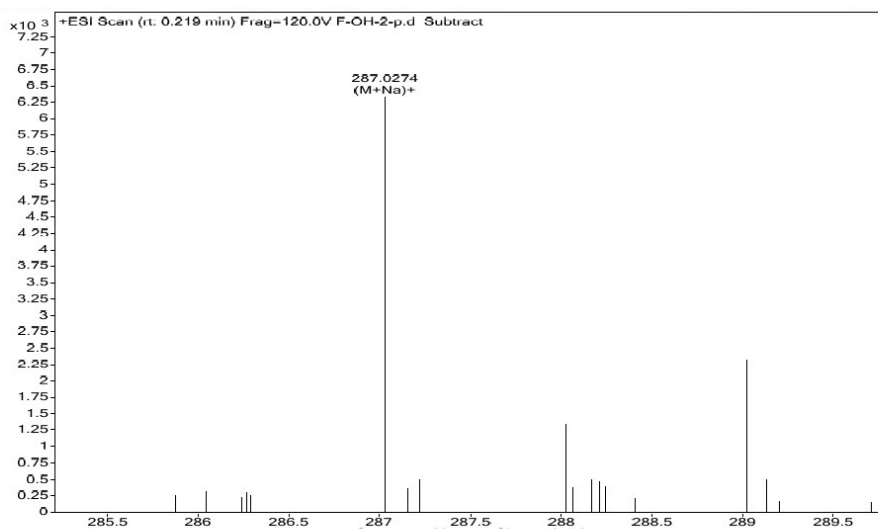


7. HRMS (ESI) m/z calcd for $C_{18}H_{18}ClO_3S^+$ (M+O+H)⁺ 349.06597, found 349.06577.

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

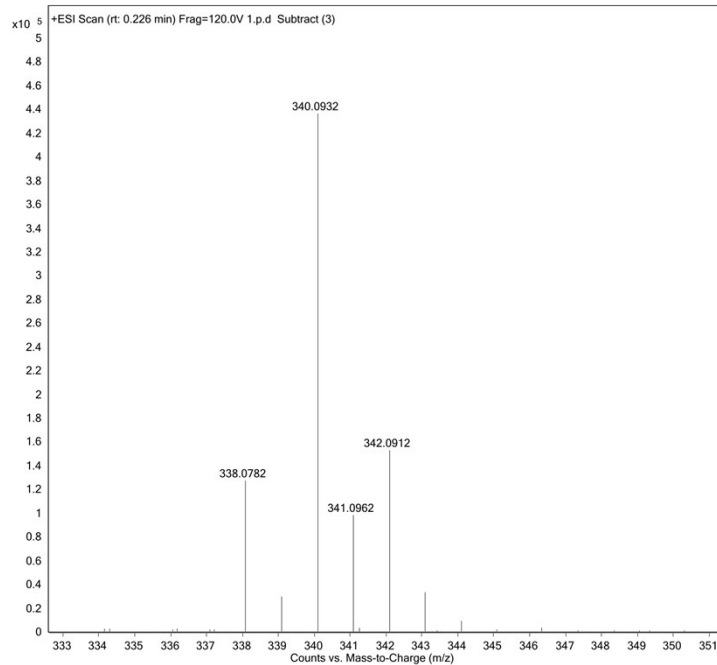


8 HRMS (ESI) m/z calcd for $C_{14}H_{13}ClOSNa^+$ (M+Na)⁺ 287.0268, found 287.0274



9 HRMS (ESI) m/z M+H⁺ calcd for C₂₀H₁₉ClNS⁺ 340.0921, found 349.0932

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable
User Name	Unavailable	Inj Vol	Unavailable	InjPosition	Unavailable
Sample Type	Unavailable	IRM Calibration Status	Success	Data Filename	1.p.d
ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



10. HRMS (ESI) m/z calcd for C₁₈H₁₆ClO₂S⁺ (M+O+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]

