

Supporting Information

**Synthesis of *N*-aryl-2-aminobenzoxazoles from substituted benzoxazole-2-thiol
and 2-chloro-*N*-arylamides in KOH-DMF system**

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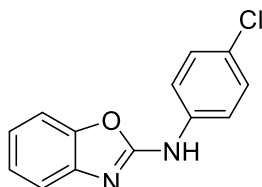
General Information.

All starting materials and reagents were purchased from commercial suppliers. TLC was performed on 0.20 mm Silica Gel 60 F₂₅₄ plates (Qingdao Ocean Chemical Factory, Shandong, China). Nuclear magnetic resonance spectra (NMR) were recorded on a Bruker spectrometer (400 MHz) with TMS as an external reference and reported in parts per million.

General procedures for the reaction of substituted benzoxazole-2-thiol with 2-chloro-N-arylacetamides

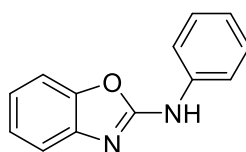
To a solution of substituted benzoxazole-2-thiol (1.0 mmol) and 2-chloro-N-arylacetamides (1.0 mmol) in DMF (10 mL) were added KOH powder (224 mg; 4 mmol) and the reacting mixture was stirred at room temperature for 5 h. After the completion of the reaction, the mixture was poured into 100 mL of water and extracted with CH₂Cl₂ (100 mL×3). The combined organic layers were dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by chromatography to give the desired N-aryl-2-aminobenzoxazoles.

N-(4-Chlorophenyl)benzo[d]oxazol-2-amine (3a)



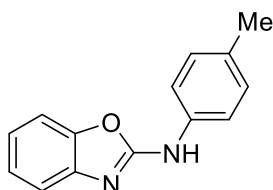
Yellow solid, yield 68 %, m.p. 169-172 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 7.13-7.17 (m, 1H, Benzoxazole-H), 7.23-7.27 (m, 1H, Benzoxazole-H), 7.35-7.37 (m, 3H, Ar-H), 7.48 (d, 1H, *J* = 7.2 Hz, Benzoxazole-H), 7.57-7.60 (m, 2H, Ar-H), 7.67 (s, 1H, NH); ¹³C NMR (DMSO-d₆, 100 MHz) δ: 109.5, 117.2, 119.5, 122.4, 124.6, 126.1, 129.3, 138.2, 142.7, 147.4, 158.1; HRMS (ESI) calcd for [M+H]⁺ C₁₃H₁₀ClN₂O: 245.0476, found: 245.0474.

N-Phenylbenzo[d]oxazol-2-amine (3b)



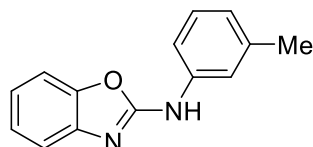
Yellow solid, yield 71 %, m.p. 170-172 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 7.10-7.15 (m, 2H, Ar-H), 7.21-7.26 (m, 1H, Benzoxazole-H), 7.34 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.38-7.42 (m, 2H, Ar-H), 7.48 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.60-7.63 (m, 2H, Ar-H), 7.93 (s, 1H, NH); ¹³C NMR (CDCl₃, 100 MHz) δ: 109.2, 117.0, 118.6, 121.8, 123.4, 124.3, 129.4, 138.0, 142.1, 147.9, 158.7; ; HRMS (ESI) calcd for [M+H]⁺ C₁₃H₁₁N₂O: 211.0866, found: 211.0867.

***N*-(*p*-Tolyl)benzo[*d*]oxazol-2-amine (3c)**



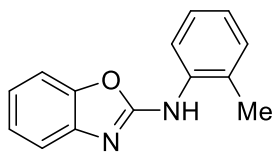
White solid, yield 64 %, m.p. 176-178 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 2.35 (s, 3H, CH₃), 7.11-7.25 (m, 4H, Ar-H), 7.32-7.34 (m, 1H, Ar-H), 7.47-7.49 (m, 3H, Ar-H), 7.92 (s, 1H, NH); ¹³C NMR (CDCl₃, 100 MHz) δ: 20.8, 109.2, 116.8, 119.0, 121.6, 124.3, 129.9, 133.1, 135.4, 142.2, 148.0, 159.1; HRMS (ESI) calcd for [M+H]⁺ C₁₄H₁₃N₂O: 225.1022, found: 225.1021.

***N*-(*m*-Tolyl)benzo[*d*]oxazol-2-amine (3d)**



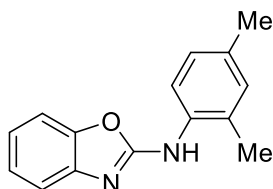
White solid, yield 59 %, m.p. 137-140 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 2.40 (s, 3H, CH₃), 6.92 (d, 1H, *J* = 7.2 Hz, Ar-H), 7.11-7.15 (m, 1H, Benzoxazole-H), 7.22-7.26 (m, 1H, Benzoxazole-H), 7.26-7.30 (m, 1H, Ar-H), 7.34 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.41-7.44 (m, 2H, Ar-H), 7.48 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.90 (s, 1H, NH); ¹³C NMR (CDCl₃, 100 MHz) δ: 21.6, 109.3, 115.9, 116.7, 119.5, 121.6, 124.3, 124.3, 129.2, 138.0, 139.3, 142.0, 148.0, 159.1; HRMS (ESI) calcd for [M+H]⁺ C₁₄H₁₃N₂O: 225.1022, found: 225.1028.

***N*-(*o*-Tolyl)benzo[*d*]oxazol-2-amine (3e)**



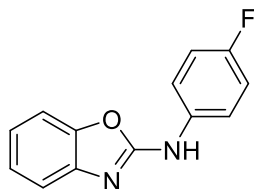
Yellow solid, yield 62 %, m.p. 98-100 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 2.36 (s, 3H, CH₃), 7.06-7.13 (m, 2H, Ar-H), 7.20-7.25 (m, 2H, Ar-H), 7.29-7.33 (m, 2H, Ar-H), 7.45 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 8.06 (d, 1H, *J* = 8.0 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz) δ: 17.8, 109.1, 117.1, 121.1, 121.7, 124.2, 124.5, 127.2, 128.2, 130.8, 136.0, 142.2, 148.0, 159.1; HRMS (ESI) calcd for [M+H]⁺ C₁₄H₁₃N₂O: 225.1022, found: 225.1021.

***N*-(2,4-Dimethylphenyl)benzo[*d*]oxazol-2-amine (3f)**



Brown solid, yield 51 %, m.p. 95-97 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 2.32 (s, 3H, CH₃), 2.33 (s, 3H, CH₃), 7.05-7.11 (m, 3H, Ar-H), 7.20 (t, 1H, *J* = 6.8 Hz, Benzoxazole-H), 7.30 (d, 1H, *J* = 7.6 Hz, Benzoxazole-H), 7.43 (d, 1H, *J* = 7.6 Hz, Benzoxazole-H), 7.82 (d, 1H, *J* = 8.0 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz) δ: 17.8, 20.9, 109.0, 116.8, 121.5, 122.2, 124.1, 127.6, 129.3, 131.5, 133.3, 134.6, 142.5, 148.1, 159.7; HRMS (ESI) calcd for [M+H]⁺ C₁₅H₁₅N₂O: 239.1179, found: 239.1176.

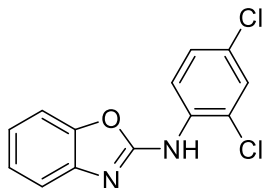
***N*-(4-Fluorophenyl)benzo[*d*]oxazol-2-amine (3g)**



Yellow solid, yield 73 %, m.p. 166-168 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 7.07-7.15 (m, 3H, Ar-H), 7.22-7.26 (m, 1H, Benzoxazole-H), 7.33 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.45 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.56-7.59 (m, 2H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz) δ: 109.2, 115.9 (d, 2C, *J* = 22.6 Hz), 116.8, 120.5 (d, 2C, *J* = 7.9 Hz), 121.9, 124.4, 134.0 (d, 1C, *J* = 2.7 Hz), 141.9, 147.9, 157.9 (d, 1C, *J* =

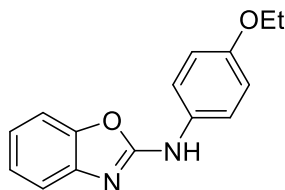
241.1 Hz); HRMS (ESI) calcd for $[M+H]^+$ C₁₃H₁₀FN₂O: 229.0772, found: 229.0771.

***N*-(2,4-Dichlorophenyl)benzo[*d*]oxazol-2-amine (3h)**



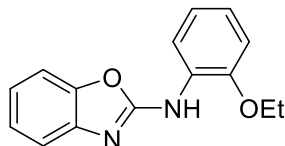
White solid, yield 61 %, m.p. 90-93 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 7.16-7.20 (m, 1H, Benzoxazole-H), 7.25-7.29 (m, 1H, Benzoxazole-H), 7.34-7.38 (m, 2H, Ar-H), 7.42 (d, 1H, *J* = 2.0 Hz, Ar-H), 7.47 (s, 1H, NH), 7.53-7.55 (m, 1H, Benzoxazole-H), 8.57 (d, 1H, *J* = 8.8 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz) δ: 109.2, 117.9, 119.6, 121.9, 122.7, 124.4, 127.8, 128.2, 128.8, 133.3, 142.1, 147.7, 156.6; HRMS (ESI) calcd for $[M+H]^+$ C₁₃H₉Cl₂N₂O: 279.0086, found: 279.0084.

***N*-(4-Ethoxyphenyl)benzo[*d*]oxazol-2-amine (3i)**



Brown solid, yield 52 %, m.p. 123-125 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 1.41 (m, 3H, OCH₂CH₃), 4.03 (m, 2H, OCH₂CH₃), 6.82-6.97 (m, 2H, Ar-H), 7.05-7.13 (m, 1H, Ar-H), 7.19-7.31 (m, 2H, Ar-H), 7.39-7.53 (m, 3H, Ar-H), 7.63 (s, 1H, NH); ¹³C NMR (CDCl₃, 100 MHz) δ: 14.9, 63.9, 109.1, 115.2, 116.6, 121.0, 121.4, 124.2, 131.0, 142.2, 148.0, 155.5, 159.5; HRMS (ESI) calcd for $[M+H]^+$ C₁₅H₁₅N₂O₂: 255.1128, found: 255.1128.

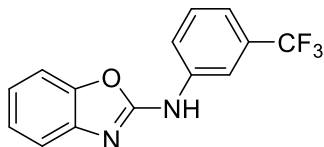
***N*-(2-Ethoxyphenyl)benzo[*d*]oxazol-2-amine (3j)**



Brown solid, yield 63 %, m.p. 40-43 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 1.49 (t, 3H, *J* = 6.8 Hz, OCH₂CH₃), 4.03 (m, 2H, *J* = 6.8 Hz, OCH₂CH₃), 6.88-6.90 (m, 1H, Ar-H), 6.98-7.05 (m, 2H, Ar-H), 7.10-7.14 (m, 1H, Benzoxazole-H), 7.21-7.25 (m, 1H, Benzoxazole-H), 7.33 (d, 1H, *J* = 8.0 Hz, Benzoxazole-H), 7.50 (d, 1H, *J* = 8.0 Hz,

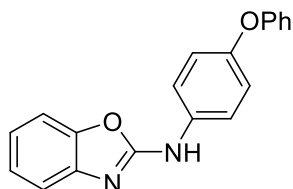
Benzoxazole-H), 7.70 (s, 1H, NH), 8.39 (d, 1H, $J = 7.6$ Hz, Ar-H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 14.9, 64.3, 108.9, 110.9, 117.4, 121.2, 121.9, 122.6, 124.1, 127.5, 142.7, 146.6, 147.8, 157.7; HRMS (ESI) calcd for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2$: 255.1128, found: 255.1123.

***N*-(3-(Trifluoromethyl)phenyl)benzo[*d*]oxazol-2-amine (3k)**



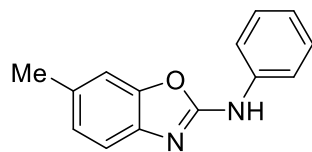
White solid, yield 60 %, m.p. 190-193 °C, ^1H NMR (CDCl_3 , 400 MHz) δ : 7.15-7.19 (m, 1H, Benzoxazole-H), 7.26-7.29 (m, 1H, Ar-H), 7.35-7.40 (m, 2H, Ar-H), 7.50-7.54 (m, 2H, Ar-H), 7.88-7.89 (m, 2H, Ar-H), 8.03 (s, 1H, NH); ^{13}C NMR ($\text{DMSO-}d_6$, 100 MHz) δ : 109.6, 113.9, 117.4, 118.8 (d, 1C, $J = 3.7$ Hz), 121.6, 122.6, 123.3 (d, 1C, $J = 270.8$ Hz), 124.6, 130.1 (d, 1C, $J = 31.5$ Hz), 130.6, 140.0, 142.5, 147.4, 157.9; HRMS (ESI) calcd for $[\text{M}+\text{H}]^+$ $\text{C}_{14}\text{H}_{10}\text{F}_3\text{N}_2\text{O}$: 279.0740, found: 279.0736.

***N*-(4-Phenoxyphenyl)benzo[*d*]oxazol-2-amine (3l)**



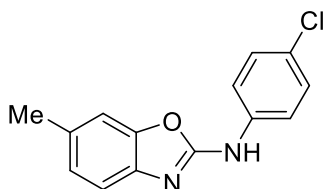
Brown solid, yield 53 %, m.p. 140-143 °C, ^1H NMR (CDCl_3 , 400 MHz) δ : 7.00-7.02 (m, 2H, Ar-H), 7.06-7.10 (m, 3H, Ar-H), 7.11-7.14 (m, 1H, Benzoxazole-H), 7.21-7.26 (m, 1H, Benzoxazole-H), 7.31-7.35 (m, 3H, Ar-H), 7.46 (d, 1H, $J = 8.0$ Hz, Benzoxazole-H), 7.57 (d, 2H, $J = 8.0$ Hz, Ar-H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 109.2, 116.8, 118.4, 120.1, 120.5, 121.7, 123.1, 124.4, 129.8, 133.6, 142.0, 147.9, 153.0, 157.7, 158.9; HRMS (ESI) calcd for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{15}\text{N}_2\text{O}_2$: 303.1128, found: 303.1124.

6-Methyl-*N*-phenylbenzo[*d*]oxazol-2-amine (3m)



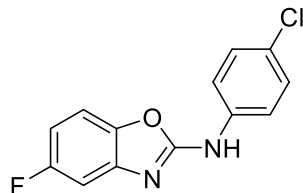
White solid, yield 75 %, m.p. 146-147 °C, ¹H NMR (DMSO-*d*₆, 400 MHz) δ : 2.39 (s, 3H, ArCH₃), 7.00-7.05 (m, 2H, Benzoxazole-H and ArH), 7.32-7.34 (m, 2H, Benzoxazole-H), 7.35-7.39 (m, 2H, ArH), 7.75-7.77 (m, 2H, ArH), 10.55 (s, 1H, NH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ : 21.5, 109.8, 116.6, 117.9, 122.4, 125.1, 129.4, 131.7, 139.3, 140.5, 147.6, 158.0; HRMS (ESI) calcd for [M+H]⁺ C₁₄H₁₃N₂O: 225.1022, found: 225.1017.

N-(4-Chlorophenyl)-6-methylbenzo[*d*]oxazol-2-amine (3n)



White solid, yield 62 %, m.p. 176-178 °C, ¹H NMR (DMSO-*d*₆, 400 MHz) δ : 2.39 (s, 3H, ArCH₃), 7.03 (dd, 1H, *J* = 8.0 Hz, 0.8 Hz, Benzoxazole-H), 7.33-7.35 (m, 2H, Benzoxazole-H), 7.41 (d, 2H, *J* = 8.8 Hz, ArH), 7.77 (d, 2H, *J* = 8.8 Hz, ArH), 10.72 (s, 1H, NH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ : 21.5, 109.9, 116.7, 119.3, 125.2, 126.0, 129.3, 132.0, 138.3, 140.3, 147.6, 157.7; HRMS (ESI) calcd for [M+H]⁺ C₁₄H₁₂ClN₂O: 259.0633, found: 259.0633.

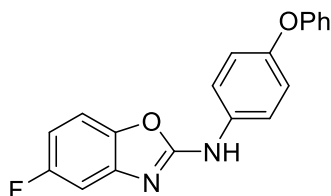
N-(4-Chlorophenyl)-5-fluorobenzo[*d*]oxazol-2-amine (3o)



Yellow solid, yield 55 %, m.p. 203-205 °C, ¹H NMR (DMSO-*d*₆, 400 MHz) δ : 6.93-6.98 (m, 1H, Benzoxazole-H), 7.31 (dd, 1H, *J* = 8.8 Hz, 2.4 Hz, Benzoxazole-H), 7.49 (dd, 1H, *J* = 8.8 Hz, 4.4 Hz, Benzoxazole-H), 7.43 (d, 2H, *J* = 8.8 Hz, ArH), 7.76 (d, 2H, *J* = 8.8 Hz, ArH), 10.91 (s, 1H, NH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ : 104.1 (d, 1C, *J* = 26.4 Hz), 108.6 (d, 1C, *J* = 25.5 Hz), 109.9 (d, 1C, *J* = 10.4 Hz),

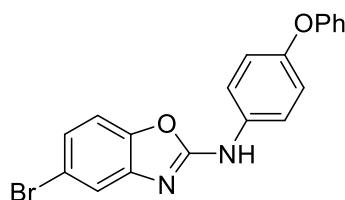
119.7, 126.5, 129.4, 137.9, 143.8 (d, 1C, $J = 5.3$ Hz), 143.9 (d, 1C, $J = 7.4$ Hz), 158.7 (d, 1C, $J = 234$ Hz), 159.6; HRMS (ESI) calcd for $[M+H]^+$ $C_{13}H_9ClFN_2O$: 263.0382, found: 263.0378.

5-Fluoro-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3p)



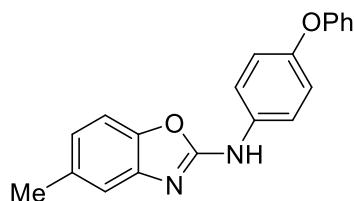
Yellow solid, yield 51 %, m.p. 151-153 °C, 1H NMR (DMSO- d_6 , 400 MHz) δ : 6.91-6.94 (m, 1H, Benzoxazole-H), 6.96 (d, 2H, $J = 8.8$ Hz, ArH), 7.08-7.11 (m, 3H, ArH), 7.29 (dd, 1H, $J = 8.8$ Hz, 2.4 Hz, Benzoxazole-H), 7.35-7.39 (m, 2H, ArH), 7.48 (dd, 1H, $J = 8.8$ Hz, 4.4 Hz, Benzoxazole-H), 7.76 (d, 2H, $J = 8.8$ Hz, ArH), 10.77 (s, 1H, NH); ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 103.9 (d, 1C, $J = 26.3$ Hz), 108.3 (d, 1C, $J = 25.5$ Hz), 109.7 (d, 1C, $J = 10.4$ Hz), 118.0, 119.9, 120.6, 123.3, 130.4, 135.0, 144.0, 144.1 (d, 1C, $J = 13.7$ Hz), 151.5, 158.1, 158.7 (d, 1C, $J = 234.4$ Hz), 160.1; HRMS (ESI) calcd for $[M+H]^+$ $C_{19}H_{14}FN_2O_2$: 321.1034, found: 321.1026.

5-Bromo-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3q)



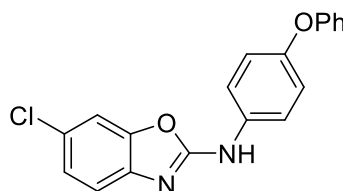
White solid, yield 59 %, m.p. 196-197 °C, 1H NMR ($CDCl_3$, 400 MHz) δ : 7.01-7.04 (m, 2H, ArH), 7.08-7.14 (m, 4H, ArH), 7.20 (d, 1H, $J = 8.4$ Hz, ArH), 7.24 (d, 1H, $J = 1.6$ Hz, ArH), 7.33-7.37 (m, 2H, ArH), 7.57 (d, 2H, $J = 8.4$ Hz, ArH), 7.61 (d, 1H, $J = 2.0$ Hz, ArH); ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 111.1, 116.4, 118.0, 119.5, 120.0, 120.6, 123.3, 124.5, 130.4, 134.8, 145.0, 146.8, 151.6, 158.0, 159.5; HRMS (ESI) calcd for $[M+H]^+$ $C_{19}H_{14}BrN_2O_2$: 381.0233, found: 381.0244.

5-Methyl-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3r)



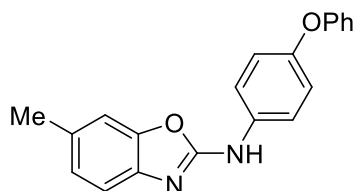
Yellow solid, yield 60 %, m.p. 198-200 °C, ¹H NMR (CDCl₃, 400 MHz) δ: 2.44 (s, 3H, ArCH₃), 6.94 (m, 1H, ArH), 7.01-7.03 (m, 2H, ArH), 7.07-7.12 (m, 3H, ArH), 7.21 (d, 1H, *J* = 8.4 Hz, ArH), 7.26-7.30 (m, 2H, ArH), 7.33-7.37 (m, 2H, ArH), 7.59 (d, 1H, *J* = 8.4 Hz, ArH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ: 108.8, 117.3, 117.9, 119.6, 120.6, 122.7, 123.2, 130.4, 133.6, 135.4, 143.1, 145.7, 151.1, 158.2, 158.7; HRMS (ESI) calcd for [M+H]⁺ C₂₀H₁₇N₂O₂: 317.1285, found: 317.1281.

6-Chloro-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3s)



Yellow solid, yield 42 %, m.p. 191-193 °C, ¹H NMR (DMSO-*d*₆, 400 MHz) δ: 6.96-6.99 (m, 2H, ArH), 7.09-7.11 (m, 3H, ArH), 7.14 (dd, 1H, *J* = 8.4 Hz, 2.4 Hz, ArH), 7.35-7.39 (m, 2H, ArH), 7.50-7.52 (m, 2H, ArH), 7.75 (d, 2H, *J* = 8.8 Hz, ArH), 10.82 (s, 1H, NH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ: 110.5, 116.7, 118.0, 120.0, 120.6, 121.7, 123.3, 128.6, 130.4, 134.9, 144.5, 146.4, 151.6, 158.1, 159.7; HRMS (ESI) calcd for [M+H]⁺ C₁₉H₁₄ClN₂O₂: 337.0738, found: 337.0735.

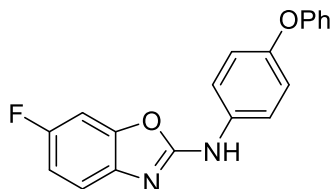
6-Methyl-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3t)



Yellow solid, yield 52 %, m.p. 170-173 °C, ¹H NMR (DMSO-*d*₆, 400 MHz) δ: 2.39 (s, 3H, ArCH₃), 6.96 (m, 2H, ArH), 7.02 (d, 1H, *J* = 8.0 Hz, ArH), 7.07-7.11 (m, 3H, ArH), 7.30-7.32 (m, 2H, ArH), 7.35-7.39 (m, 2H, ArH), 7.77 (d, 2H, *J* = 8.8 Hz, ArH), 10.56 (s, 1H, NH); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ: 21.5, 109.8, 116.5, 117.9,

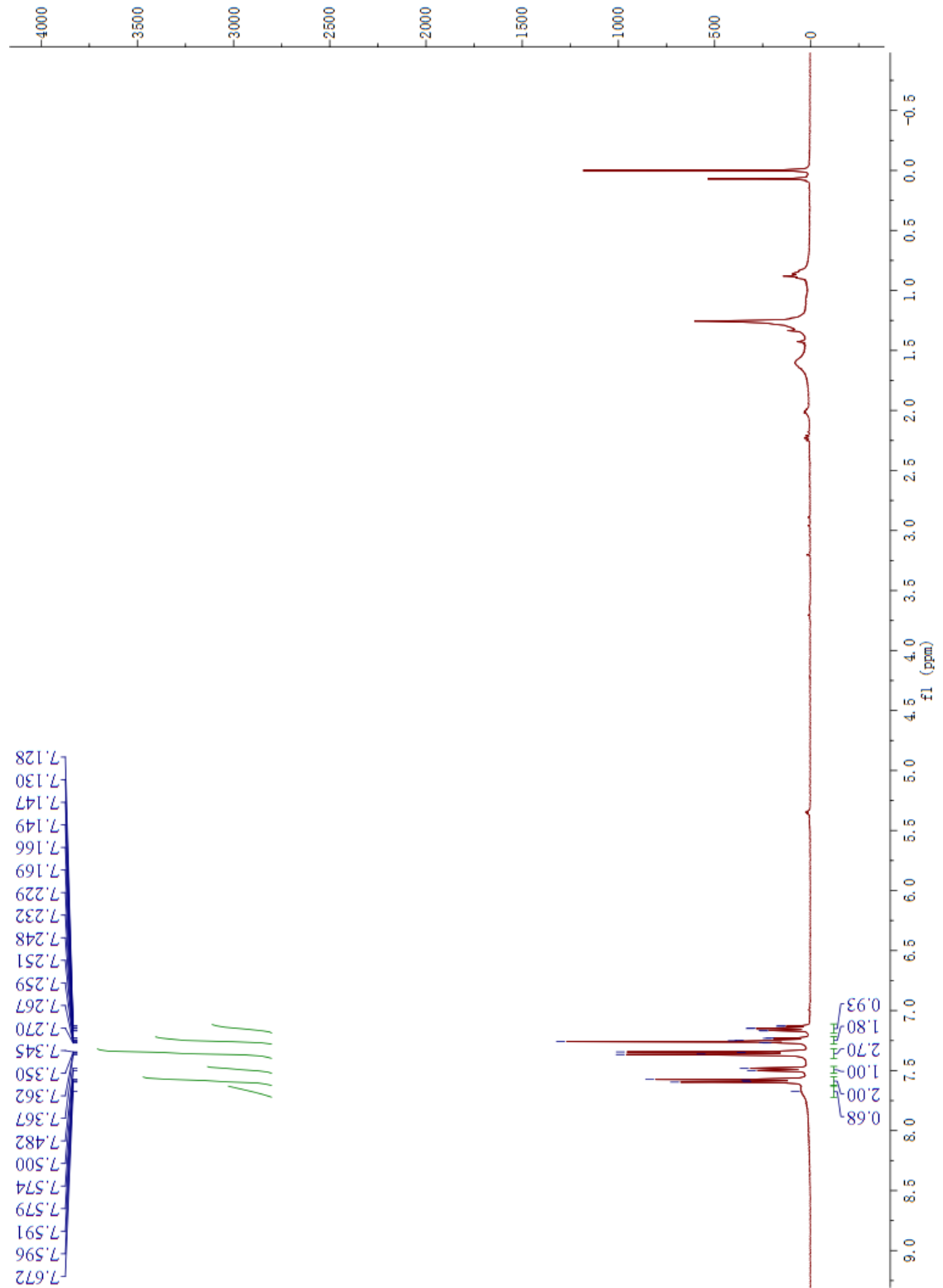
119.5, 120.6, 123.2, 125.1, 130.4, 131.7, 135.4, 140.5, 147.7, 151.0, 158.2, 158.2;
HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{17}N_2O_2$: 317.1285, found: 317.1278.

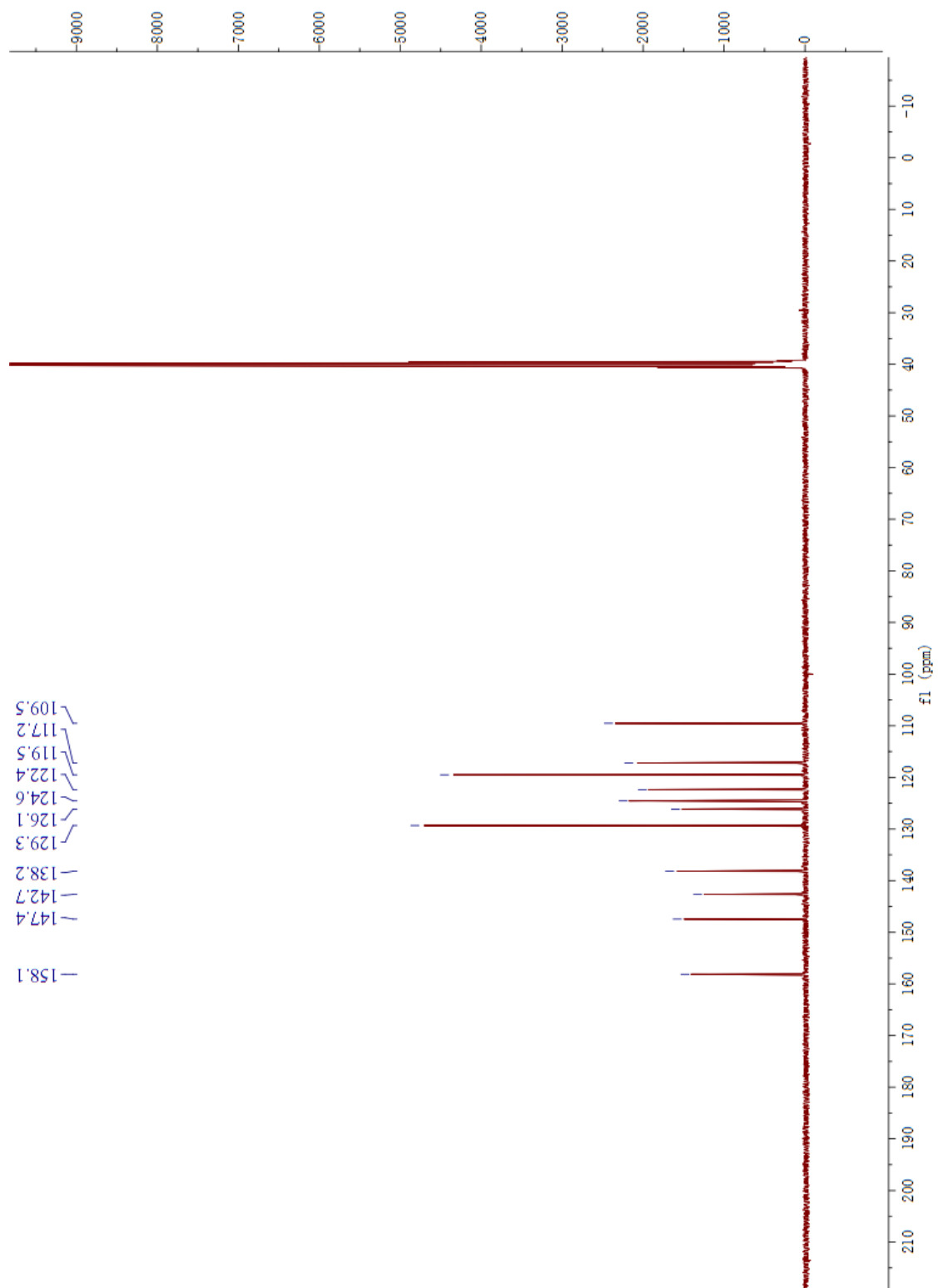
6-Fluoro-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3u)



White solid, yield 53 %, m.p. 168-170 °C, 1H NMR (DMSO- d_6 , 400 MHz) δ : 6.96-6.98 (m, 2H, ArH), 7.08-7.11 (m, 4H, ArH), 7.34-7.39 (m, 2H, ArH), 7.41 (dd, 1H, $J = 8.8$ Hz, 4.8 Hz), 7.51 (dd, 1H, $J = 8.8$ Hz, 2.4 Hz), 7.76 (d, 2H, $J = 8.8$ Hz), 10.69 (s, 1H, NH); ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 98.3 (d, 1C, $J = 28.9$ Hz), 111.1 (d, 1C, $J = 23.6$ Hz), 116.9 (d, 1C, $J = 9.7$ Hz), 118.0, 119.7, 120.6, 123.2, 130.4, 135.1, 139.3, 147.3 (d, 1C, $J = 14.9$ Hz), 151.3, 157.1 (d, 1C, $J = 235.3$ Hz), 158.1, 159.0, 159.0; HRMS (ESI) calcd for $[M+H]^+$ $C_{19}H_{14}FN_2O_2$: 321.1034, found: 321.1033.

***N*-(4-Chlorophenyl)benzo[*d*]oxazol-2-amine (3a)**





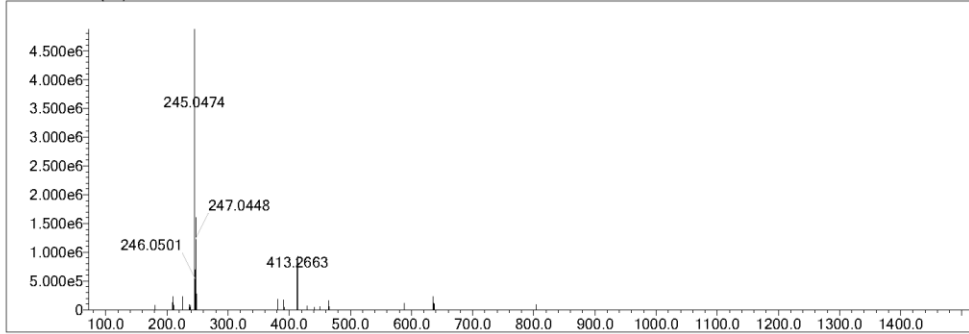
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	¹⁸ O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

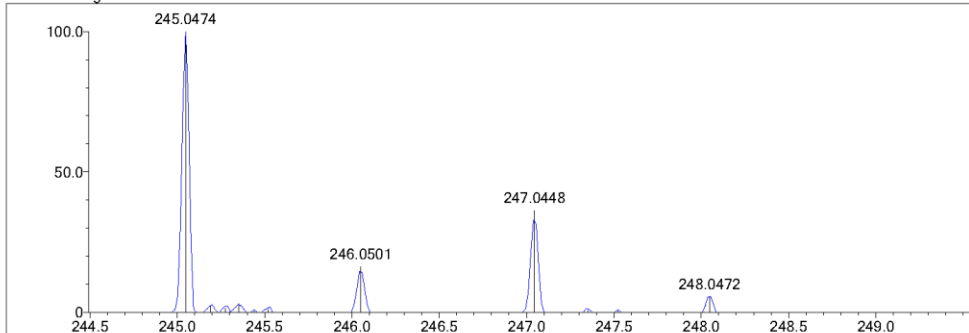
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

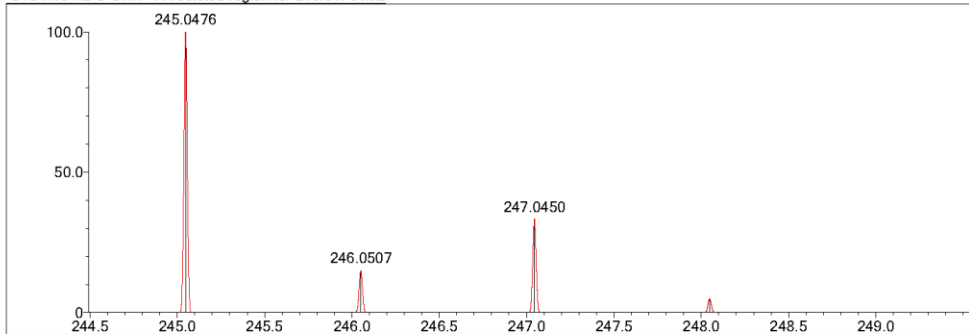
Event#: 1 MS(E+) Ret. Time : 1.187 -> 1.187 Scan#: 238 -> 238



Measured region for 245.0474 m/z

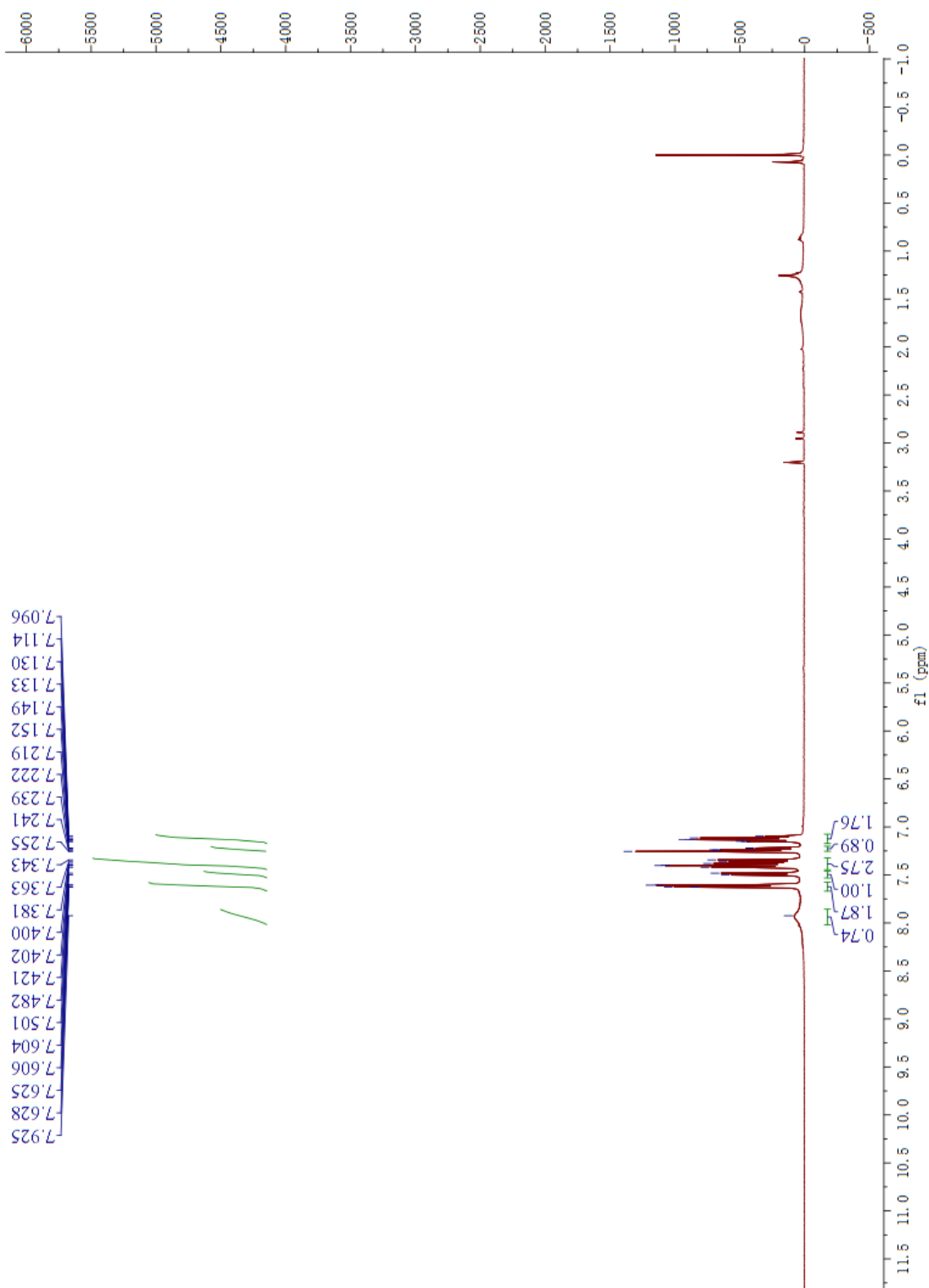


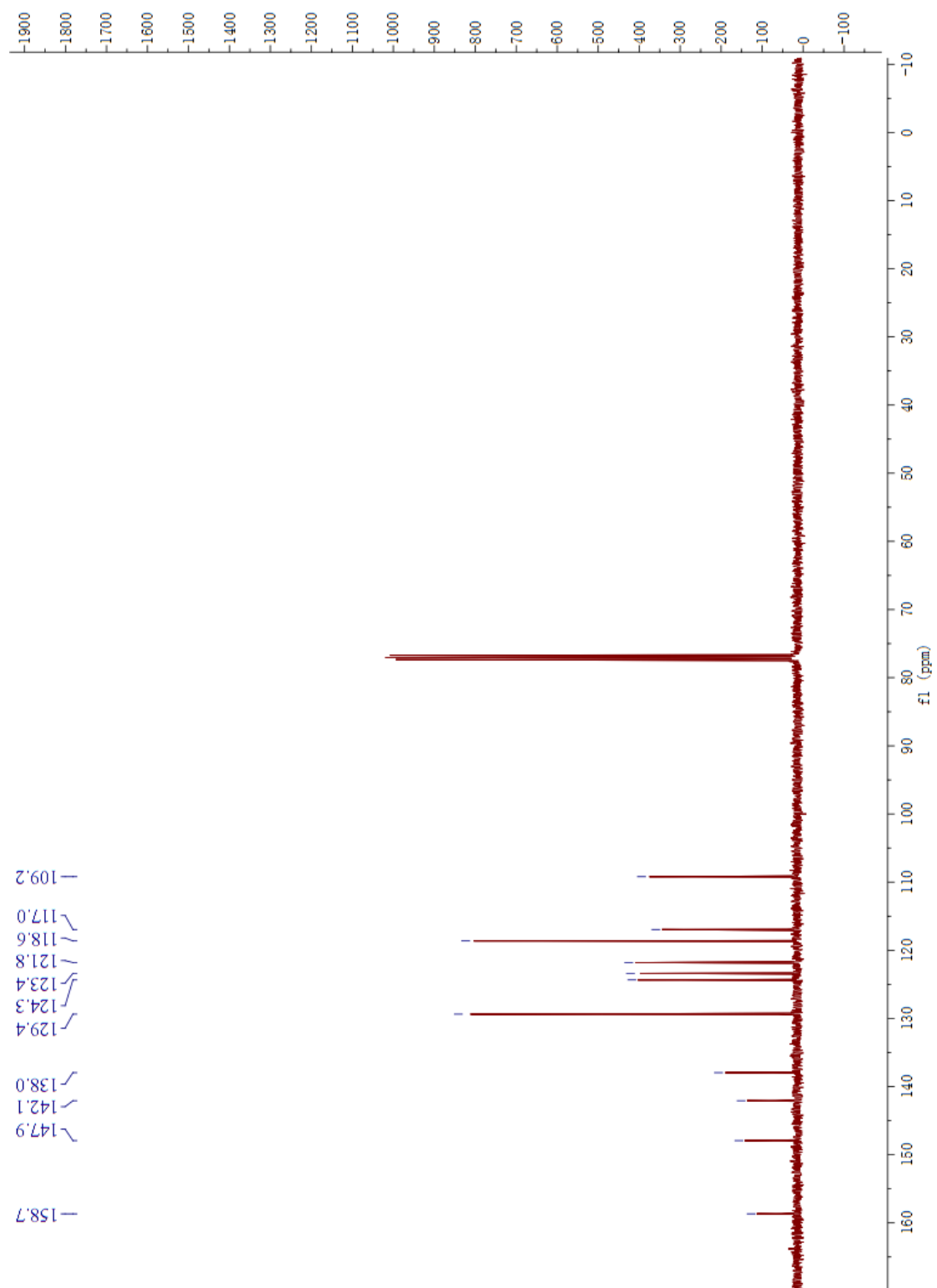
C13 H10 N2 O Cl M+ : Predicted region for 245.0476 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	87.81	C13 H10 N2 O Cl	M+	245.0474	245.0476	-0.2	-0.82	87.81	9.5

N-Phenylbenzo[*d*]oxazol-2-amine (3b)





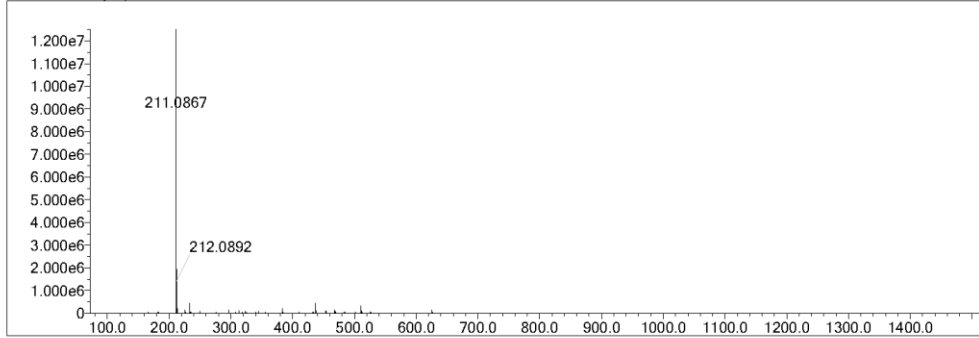
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

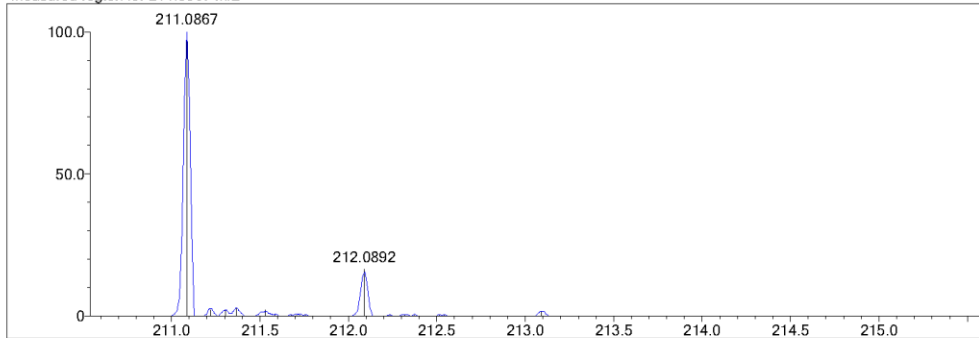
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

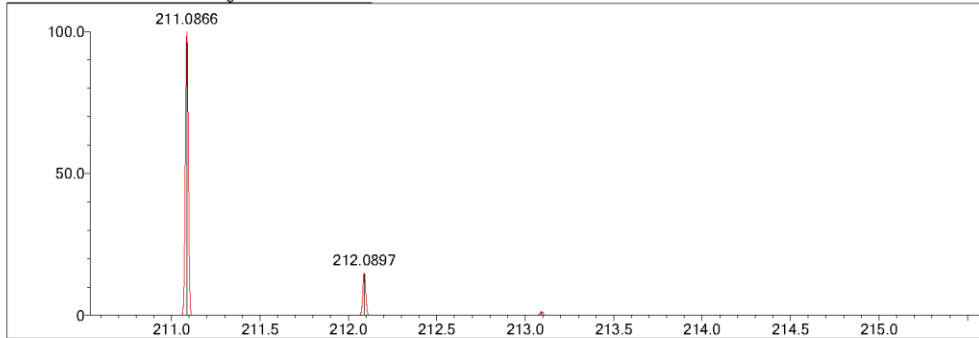
Event#: 1 MS(E+) Ret. Time : 0.997 Scan# : 200



Measured region for 211.0867 m/z

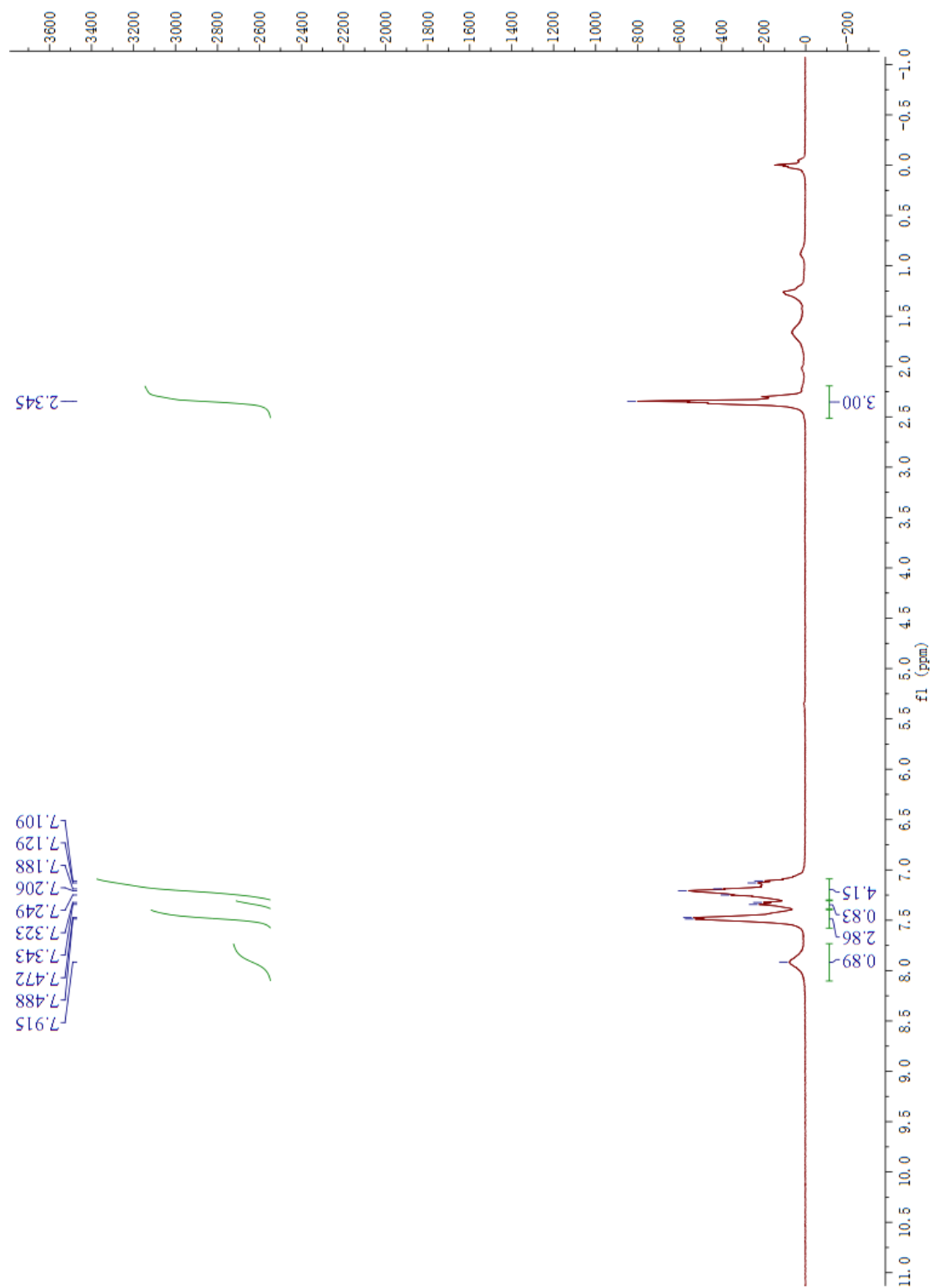


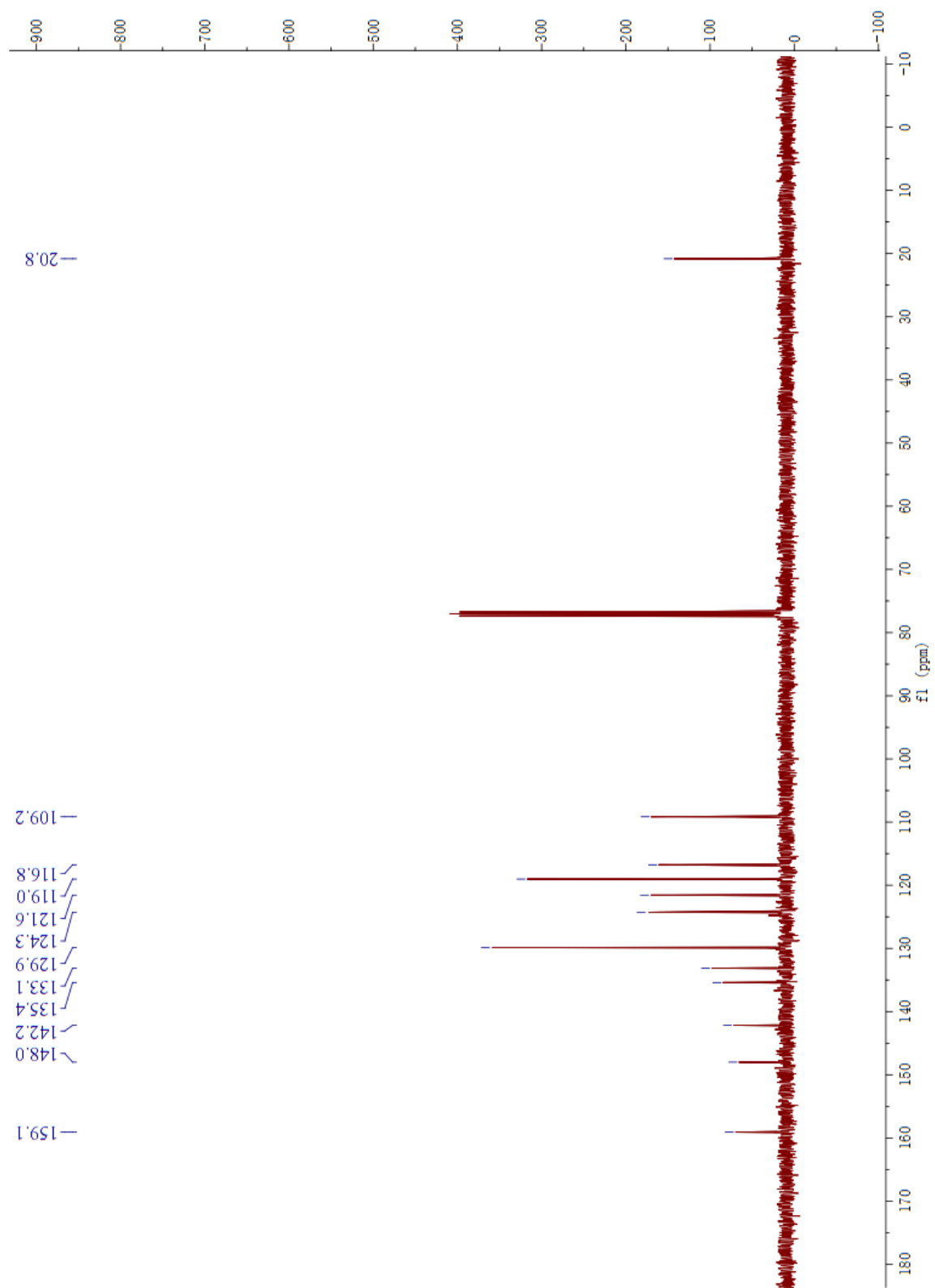
C13 H11 N2 O M+ : Predicted region for 211.0866 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	92.56	C13 H11 N2 O	M+	211.0867	211.0866	0.1	0.47	92.56	9.5

***N*-(*p*-Tolyl)benzo[*d*]oxazol-2-amine (3c)**





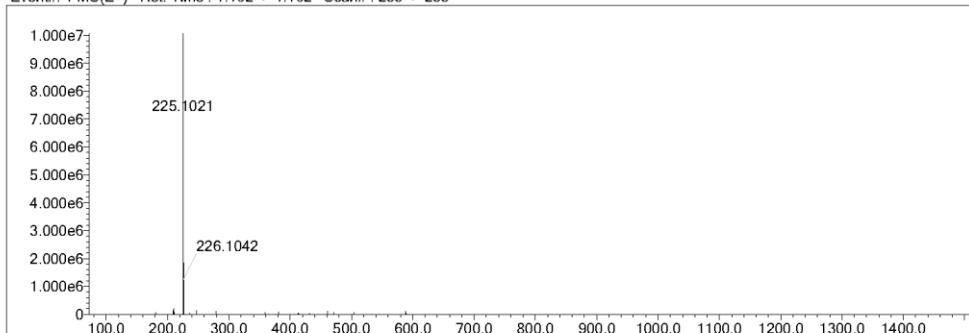
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

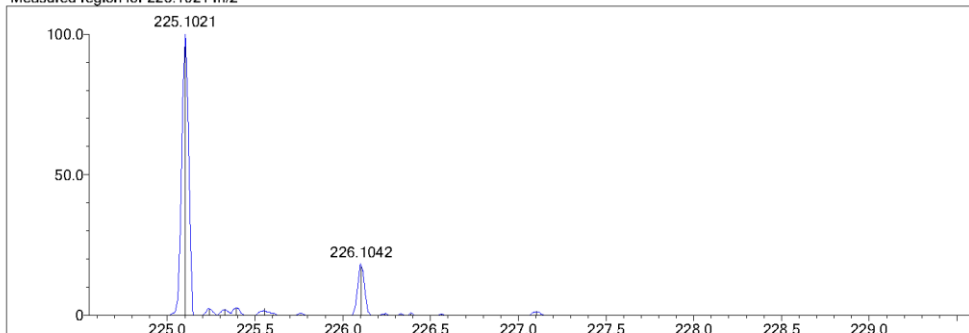
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

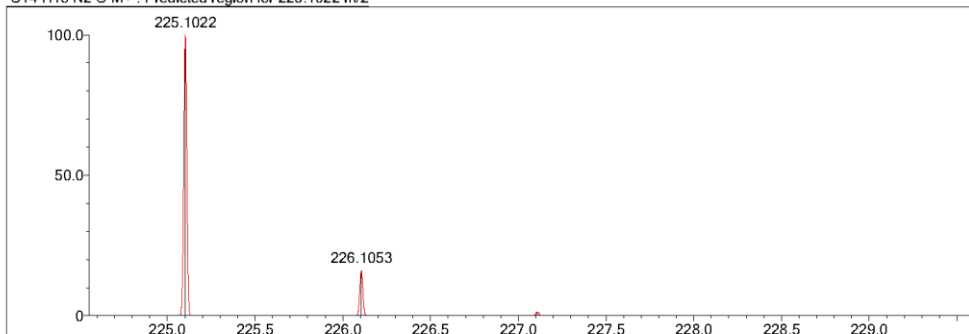
Event#: 1 MS(E+) Ret. Time : 1.162 -> 1.162 Scan#: 233 -> 233



Measured region for 225.1021 m/z

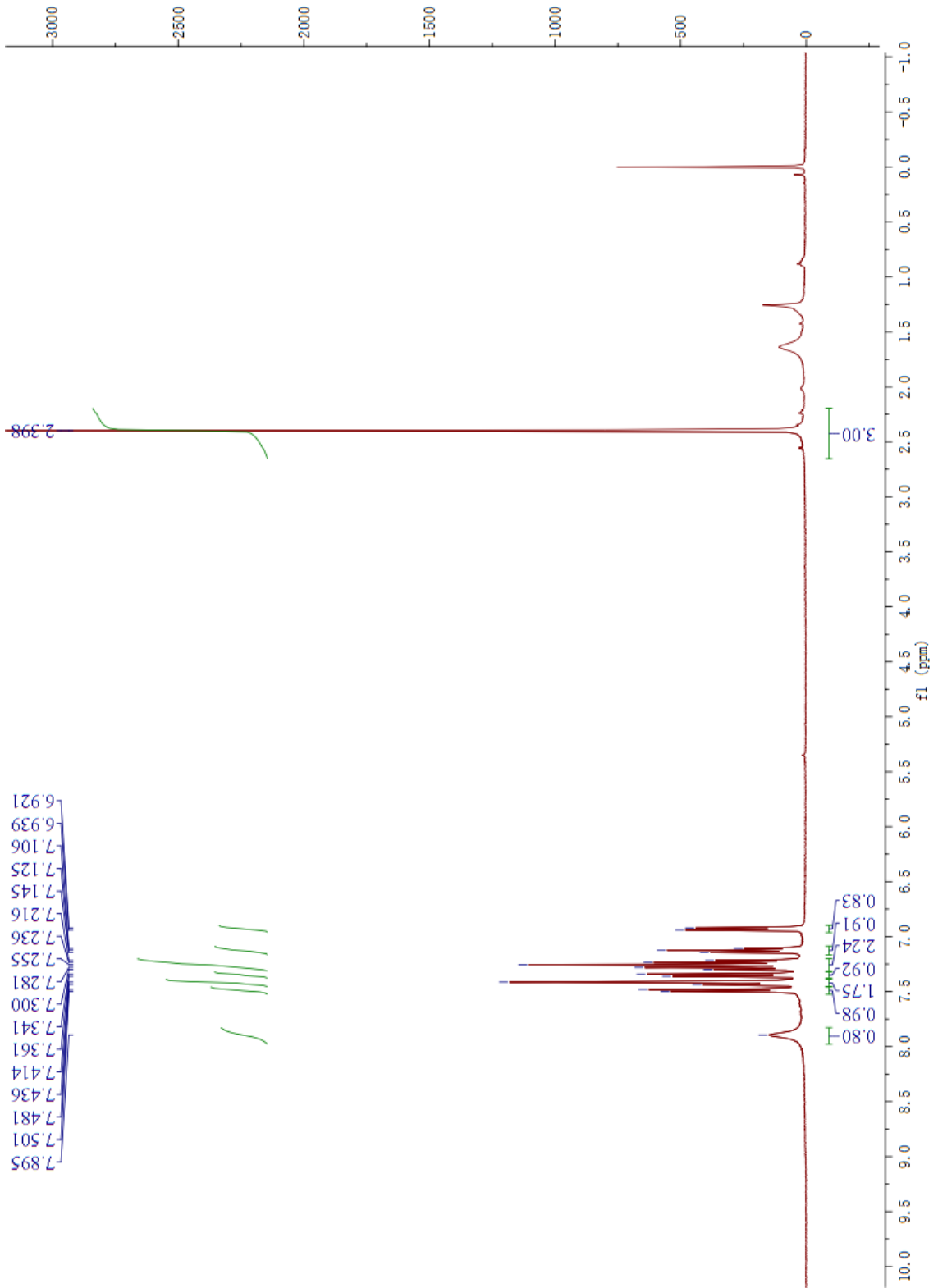


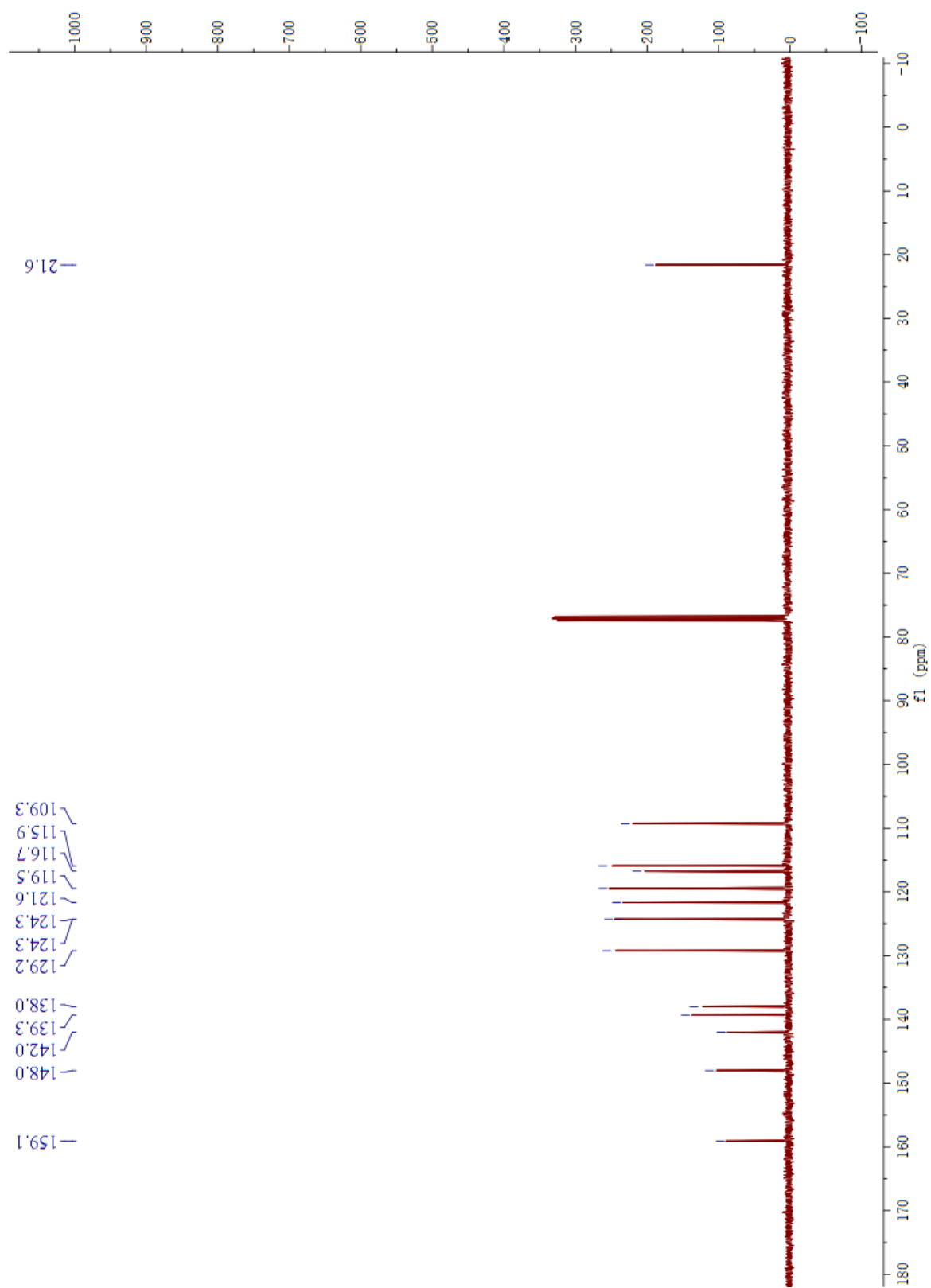
C14 H13 N2 O M+ : Predicted region for 225.1022 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	77.42	C14 H13 N2 O	M+	225.1021	225.1022	-0.1	-0.44	77.42	9.5

***N*-(*m*-Tolyl)benzo[*d*]oxazol-2-amine (3d)**





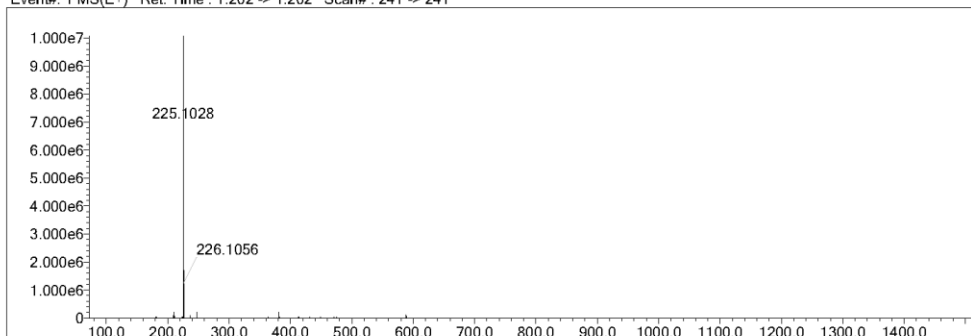
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

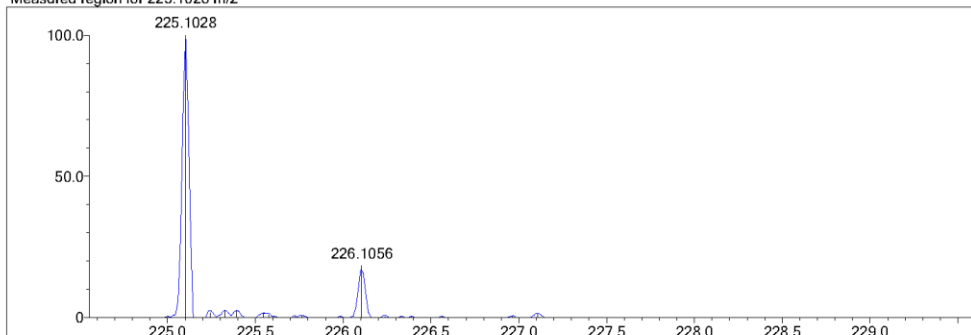
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

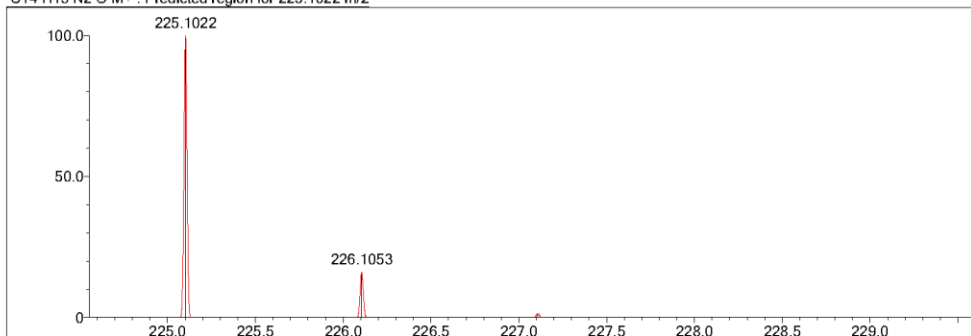
Event#: 1 MS(E+) Ret. Time : 1.202 -> 1.202 Scan#: 241 -> 241



Measured region for 225.1028 m/z

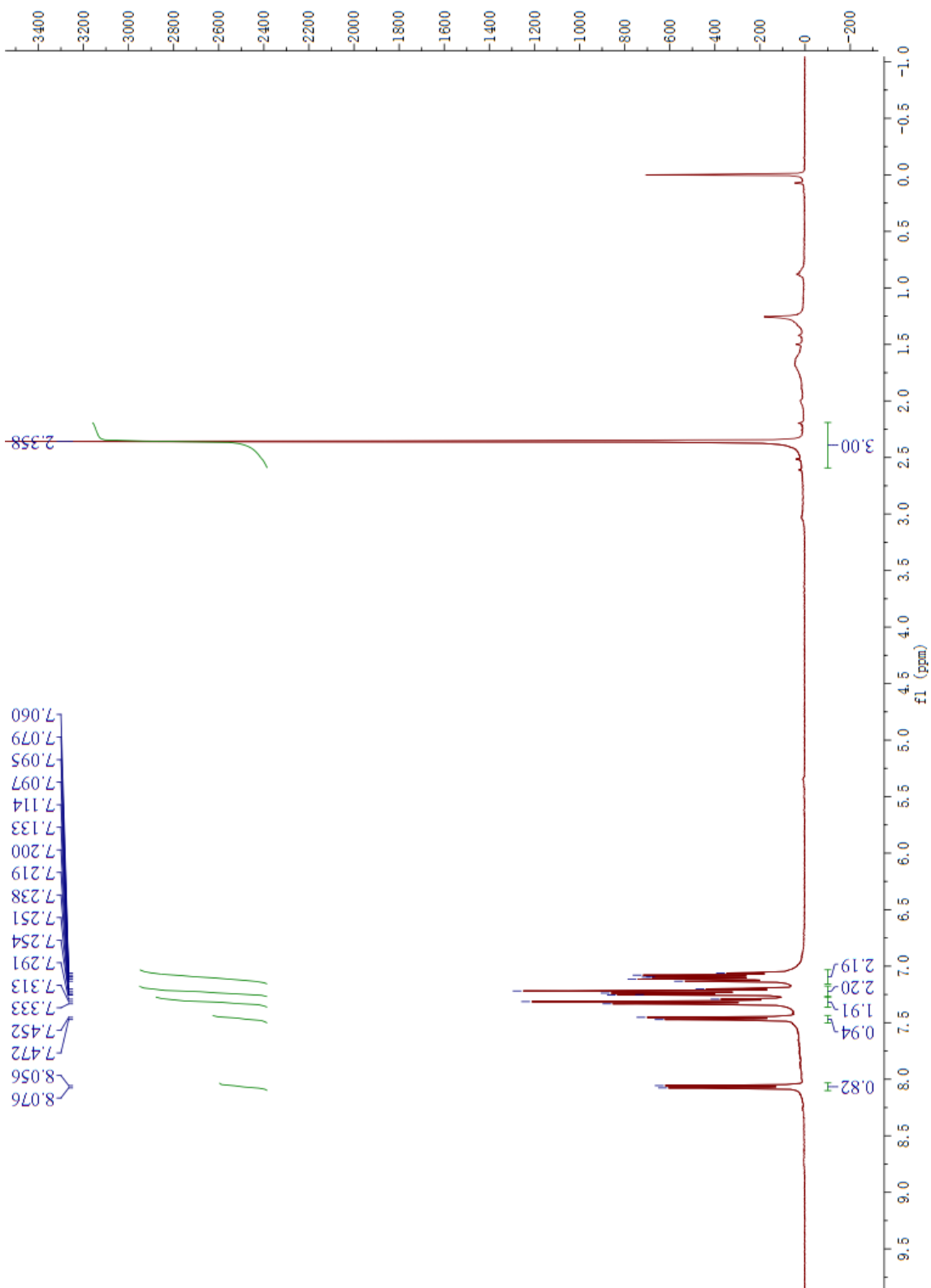


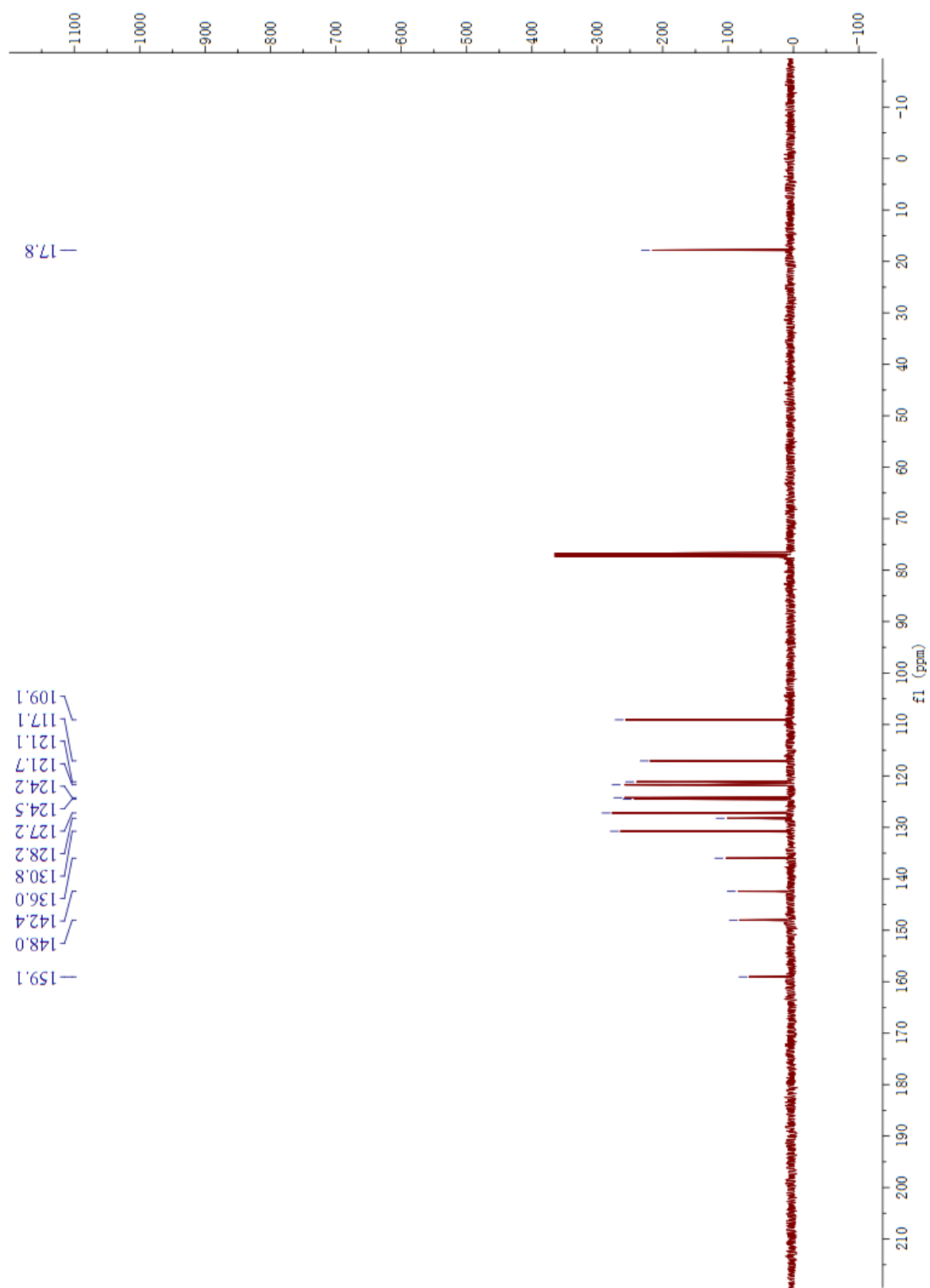
C14 H13 N2 O M+ : Predicted region for 225.1022 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	78.92	C14 H13 N2 O	M+	225.1028	225.1022	0.6	2.67	82.36	9.5

***N*-(*o*-Tolyl)benzo[*d*]oxazol-2-amine (3e)**





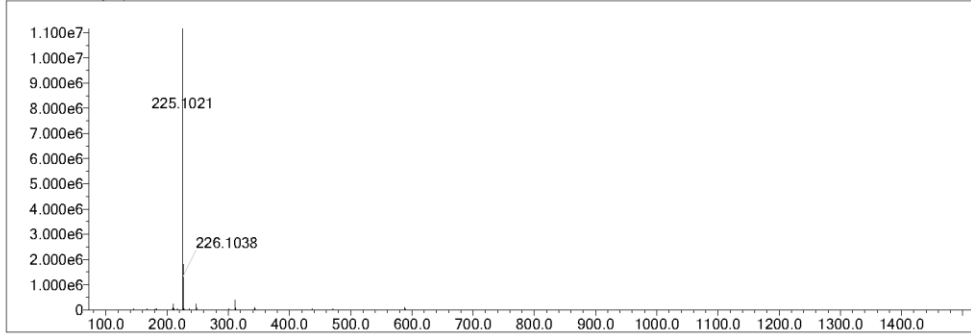
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

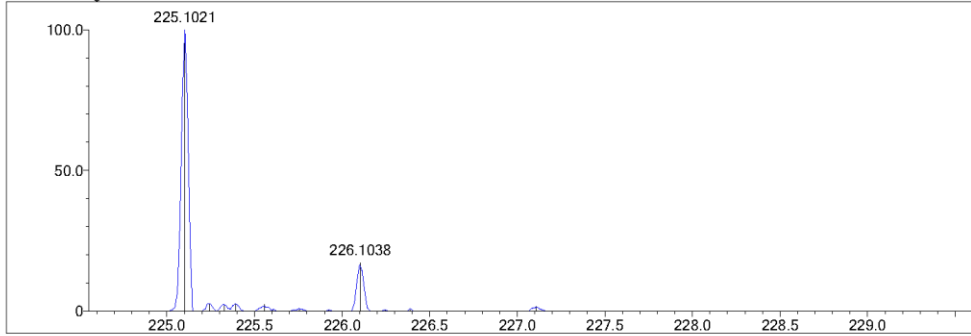
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

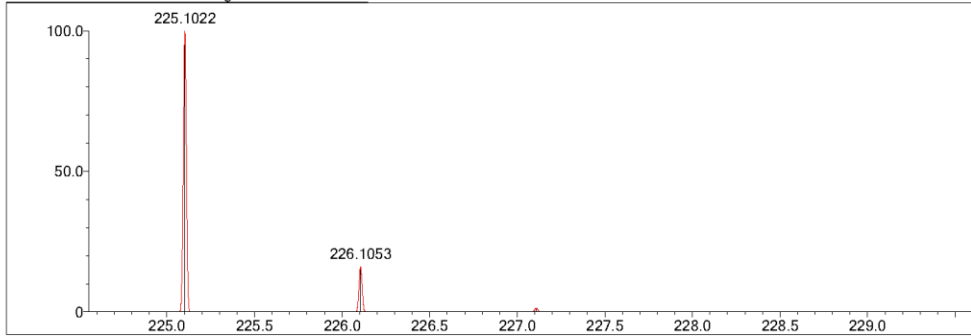
Event#: 1 MS(E+) Ret. Time : 1.452 Scan#: 291



Measured region for 225.1021 m/z

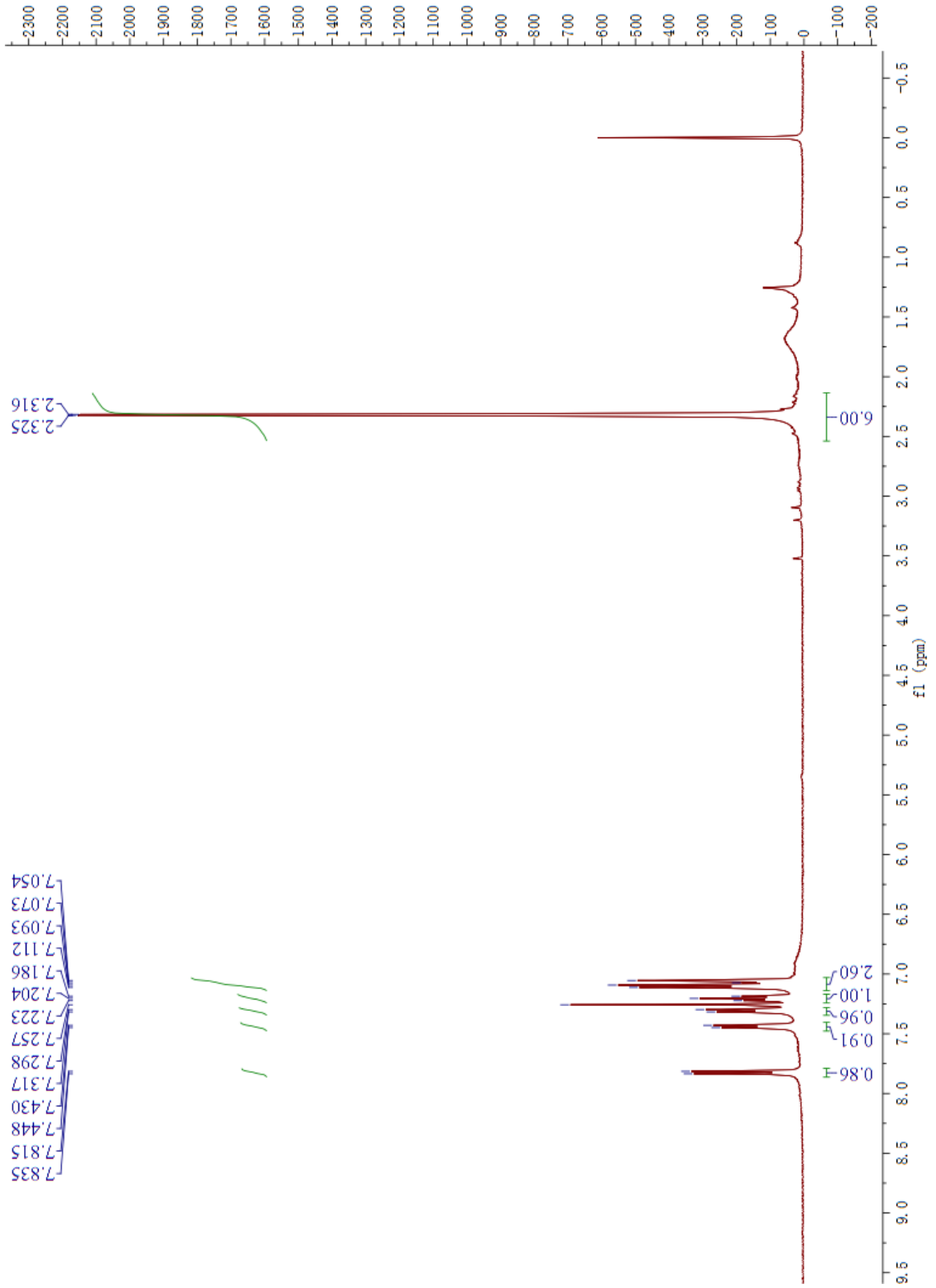


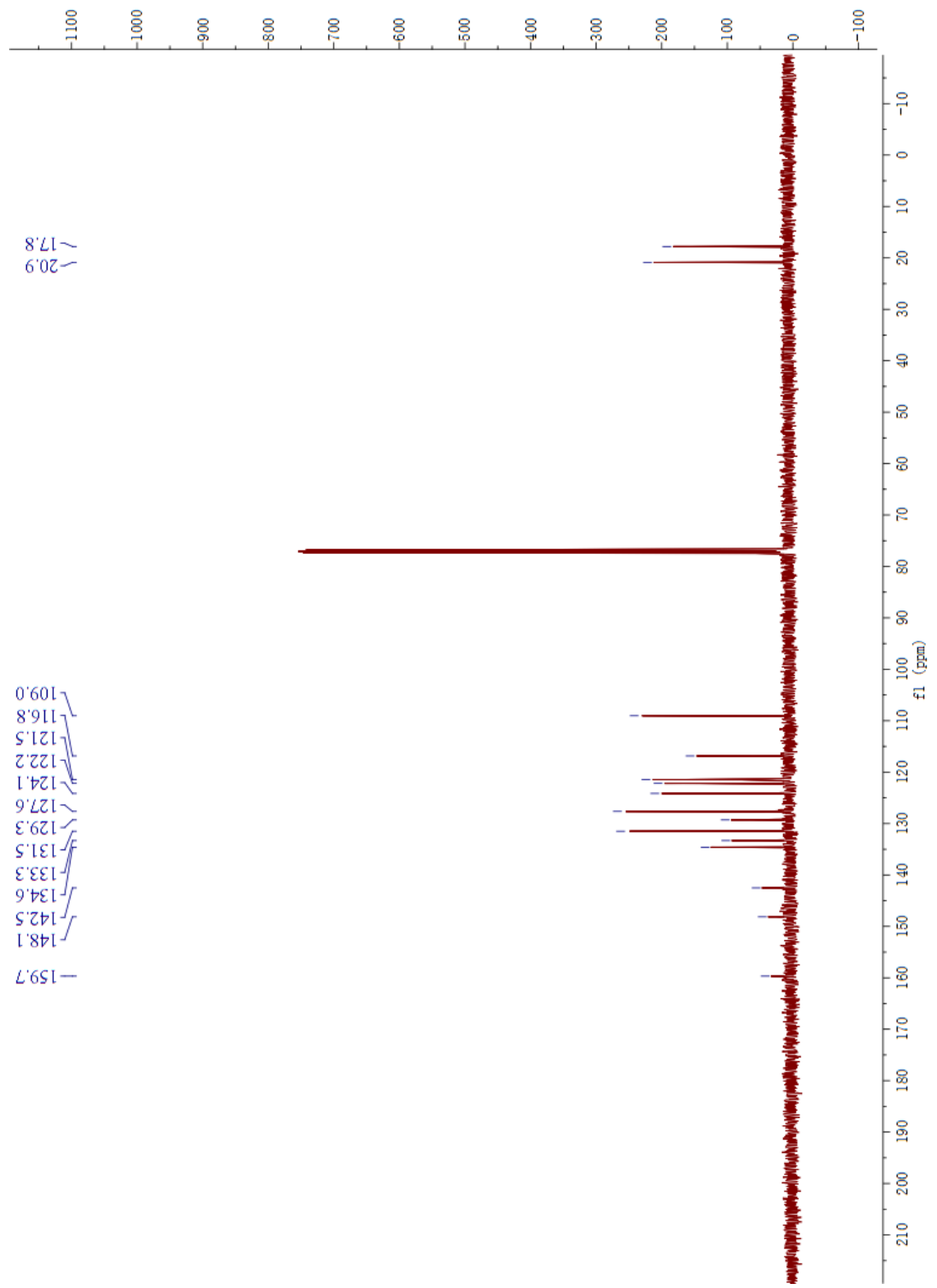
C14 H13 N2 O M+ : Predicted region for 225.1022 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	80.16	C14 H13 N2 O	M+	225.1021	225.1022	-0.1	-0.44	80.16	9.5

***N*-(2,4-Dimethylphenyl)benzo[*d*]oxazol-2-amine (3f)**





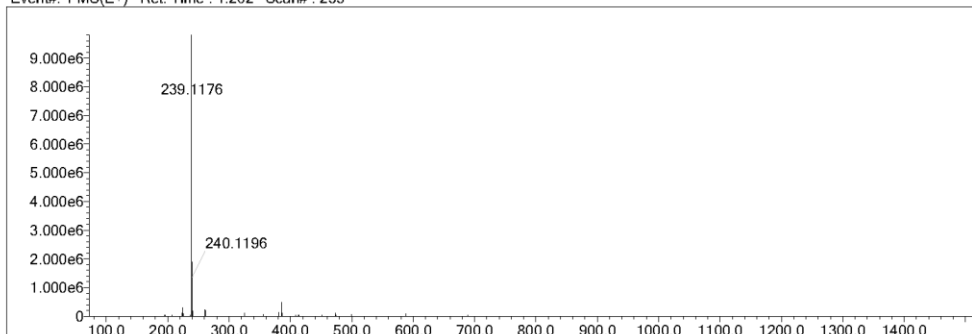
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	¹⁸ O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

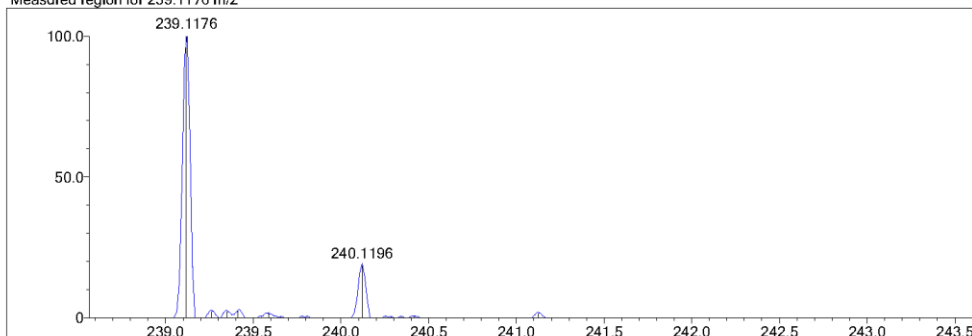
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

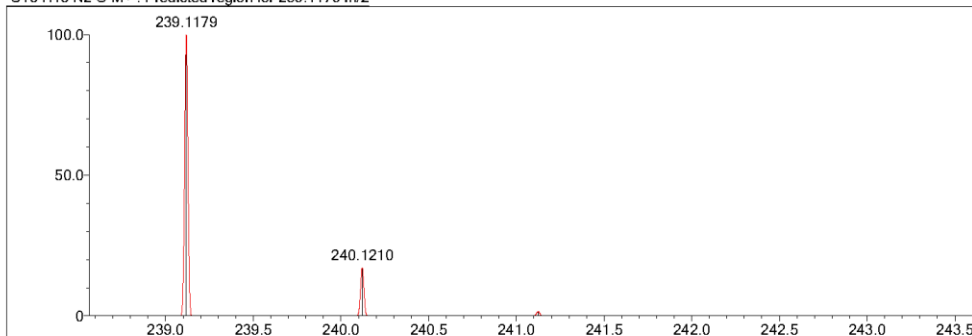
Event#: 1 MS(E+) Ret. Time : 1.262 Scan#: 253



Measured region for 239.1176 m/z

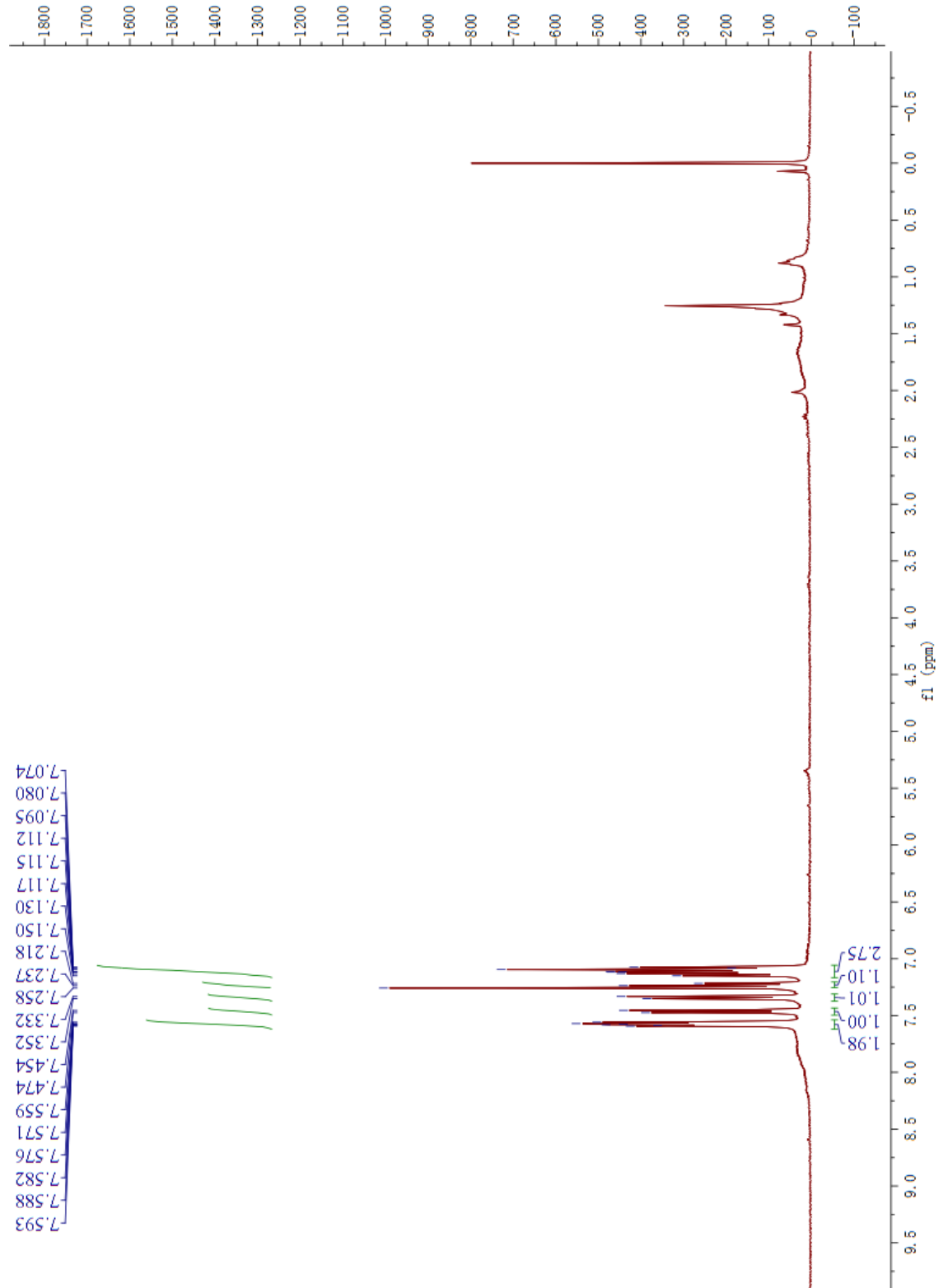


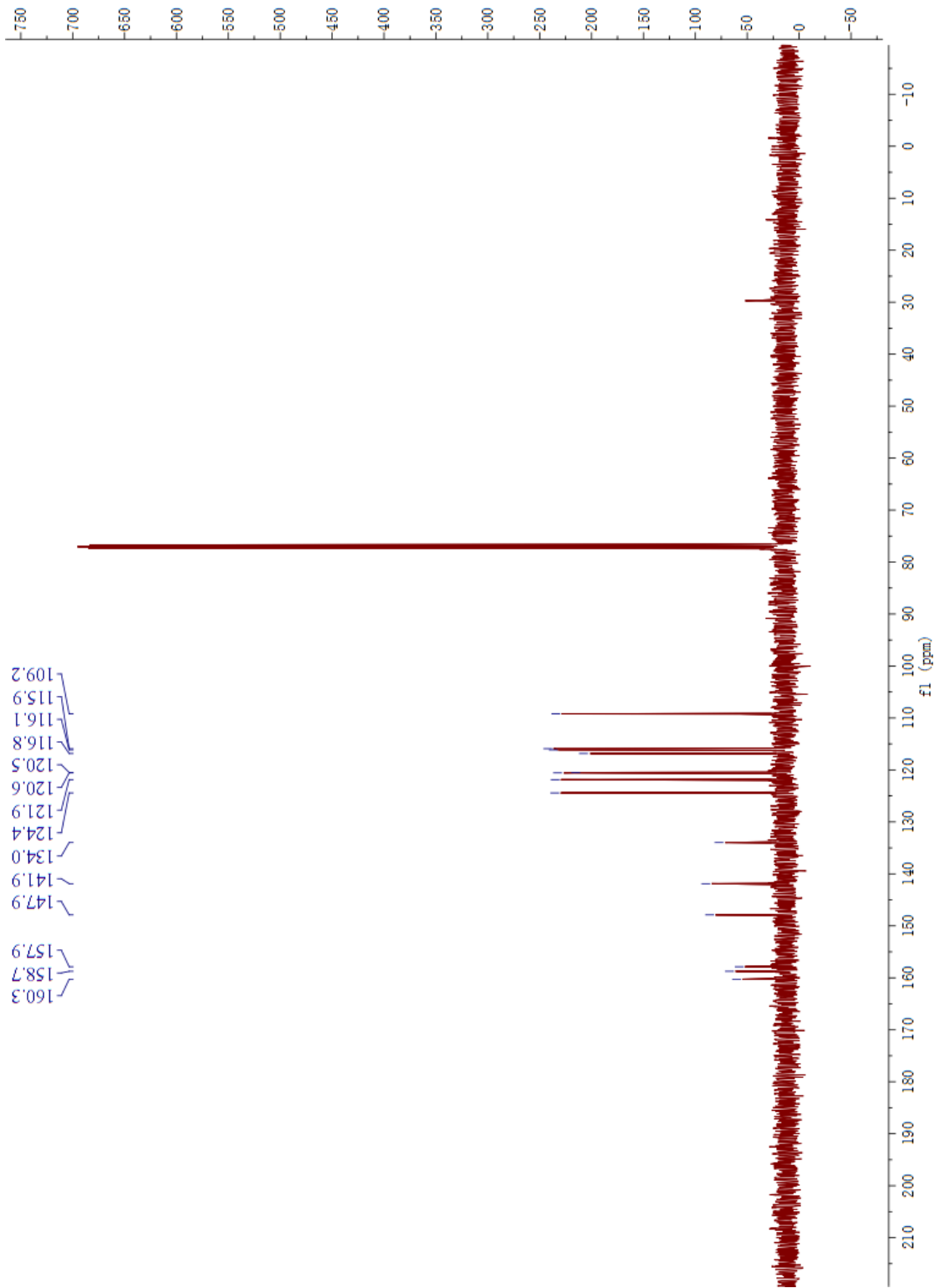
C15 H15 N2 O M+ : Predicted region for 239.1179 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	94.59	C15 H15 N2 O	M+	239.1176	239.1179	-0.3	-1.25	95.18	9.5

***N*-(4-Fluorophenyl)benzo[*d*]oxazol-2-amine (3g)**





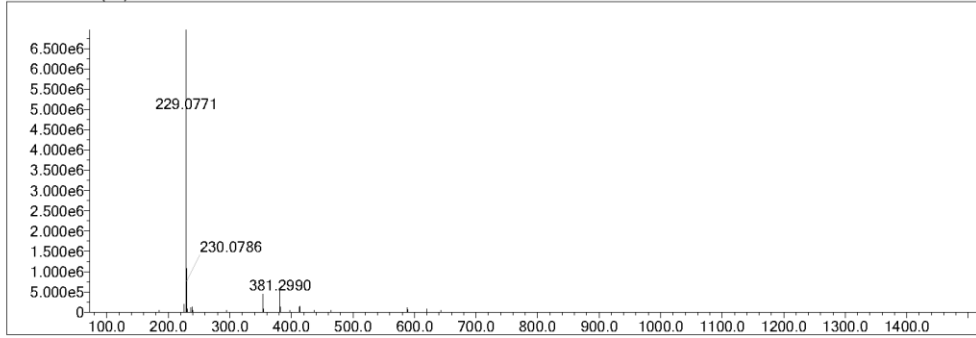
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	1	0	1	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

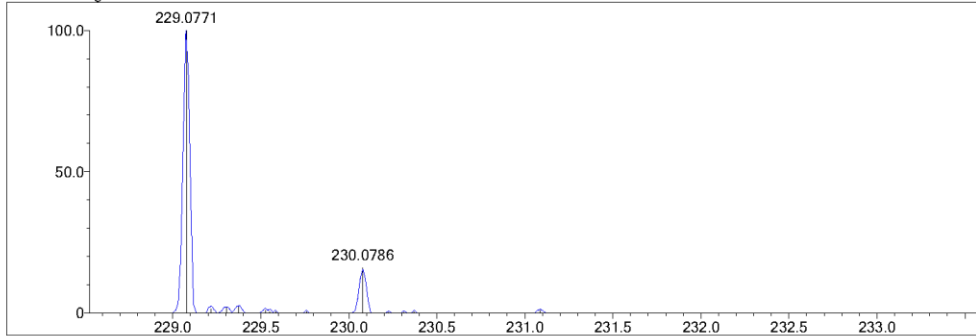
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

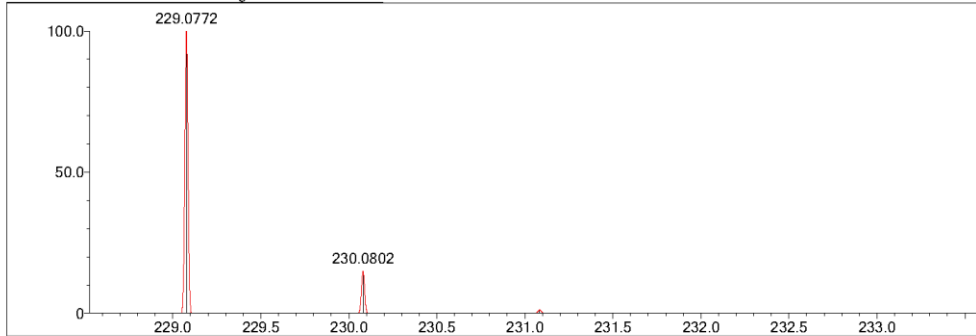
Event#: 1 MS(E+) Ret. Time : 1.117 Scan#: 224



Measured region for 229.0771 m/z

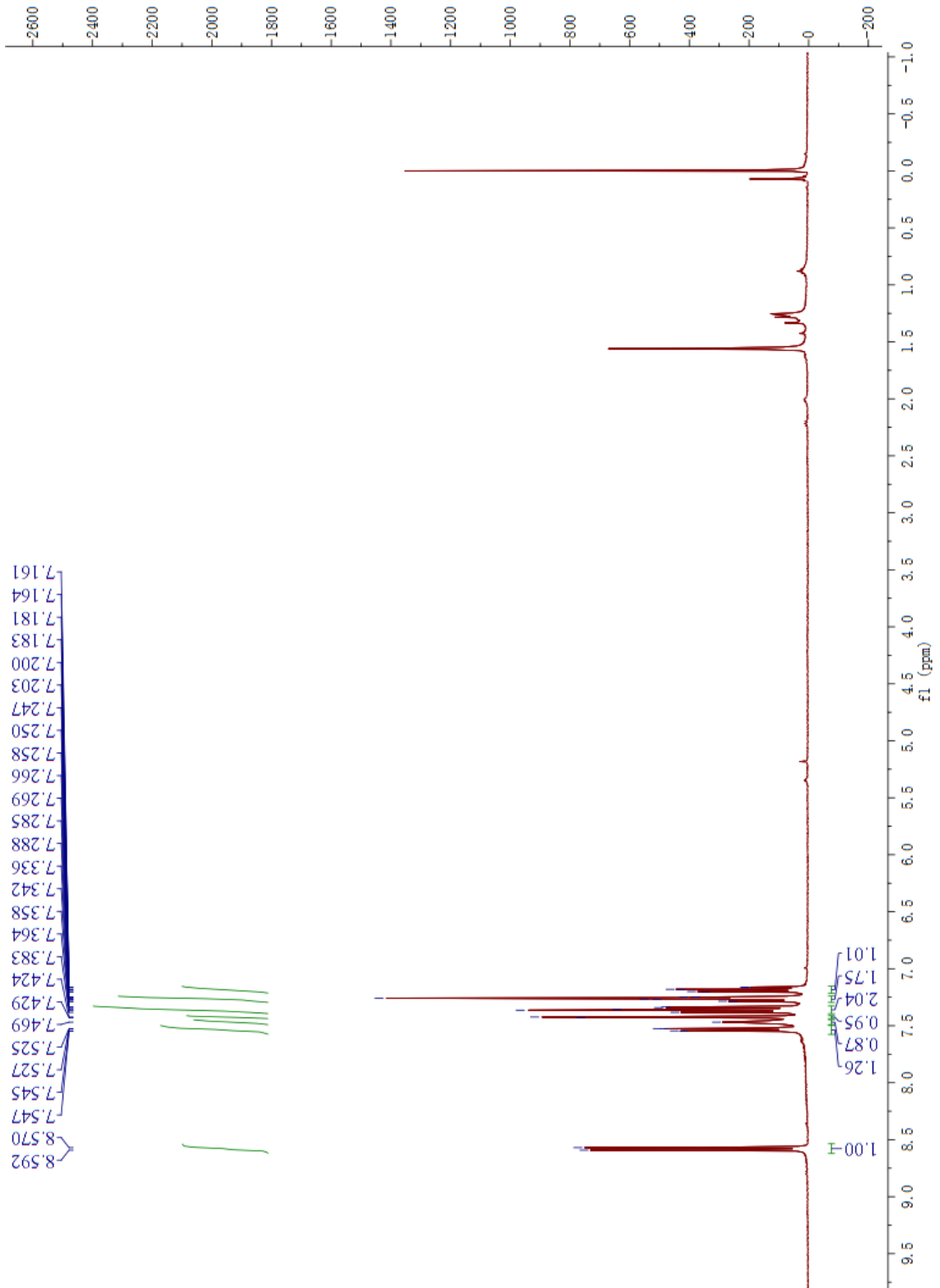


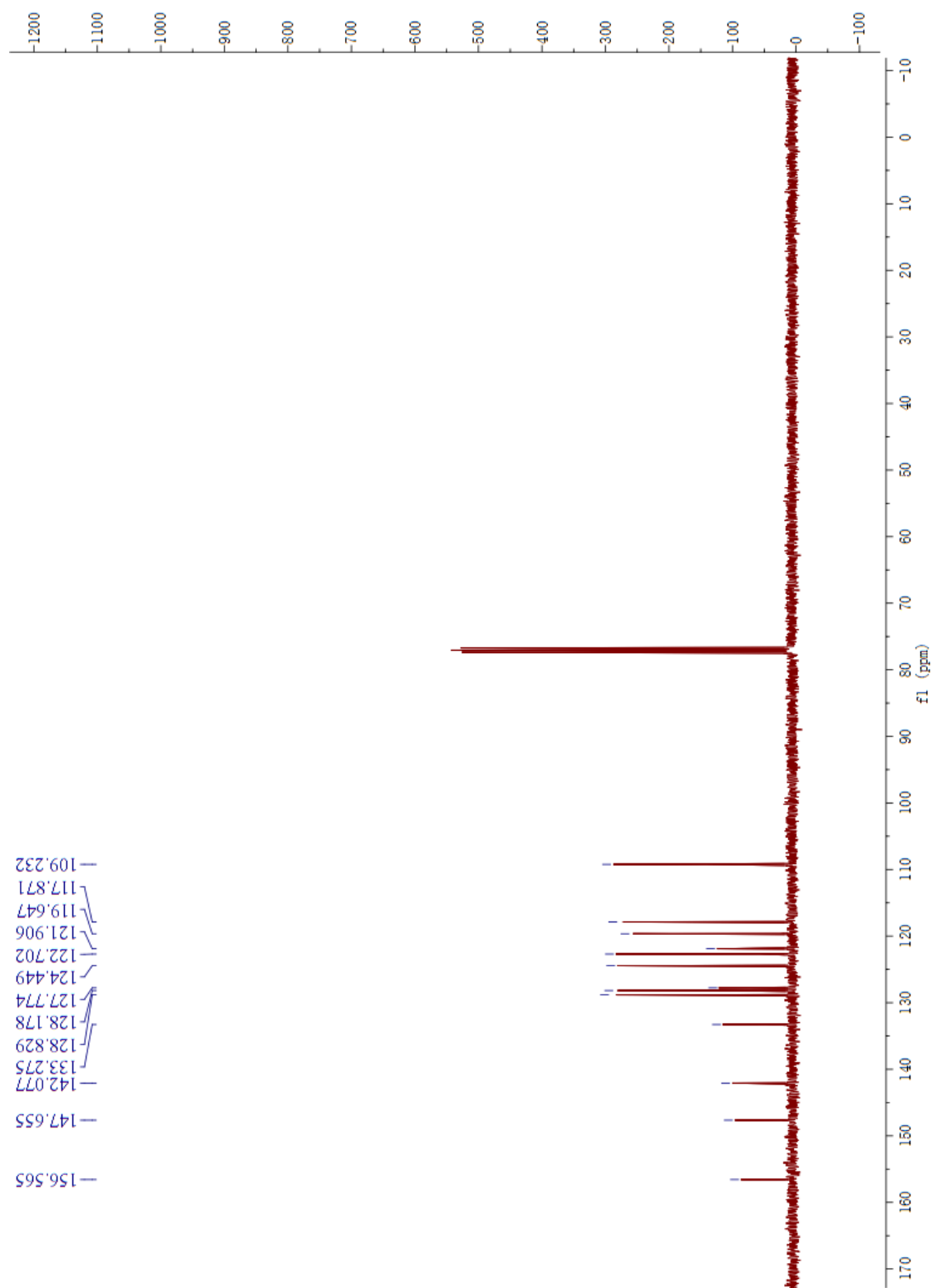
C13 H10 N2 O F M+ : Predicted region for 229.0772 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	89.48	C13 H10 N2 O F	M+	229.0771	229.0772	-0.1	-0.44	89.48	9.5

***N*-(2,4-Dichlorophenyl)benzo[*d*]oxazol-2-amine (3h)**





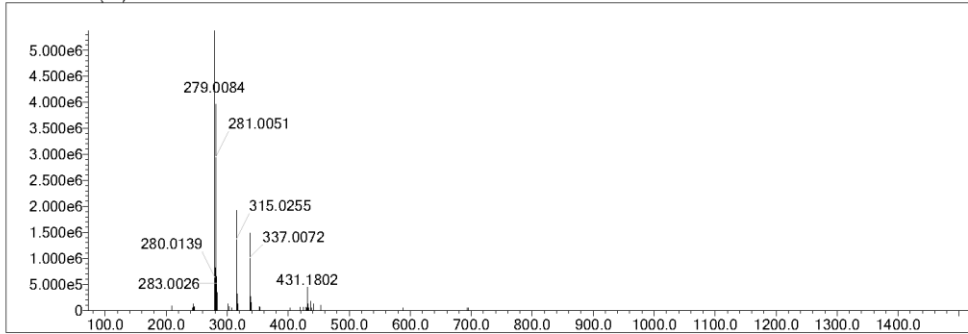
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	1	Cl	1	0	2	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

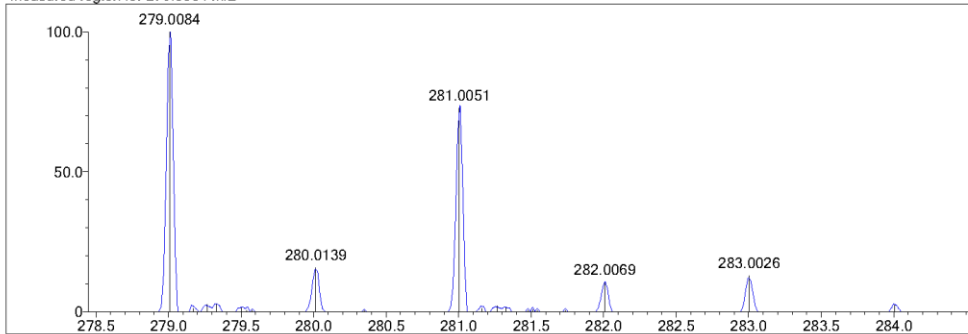
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

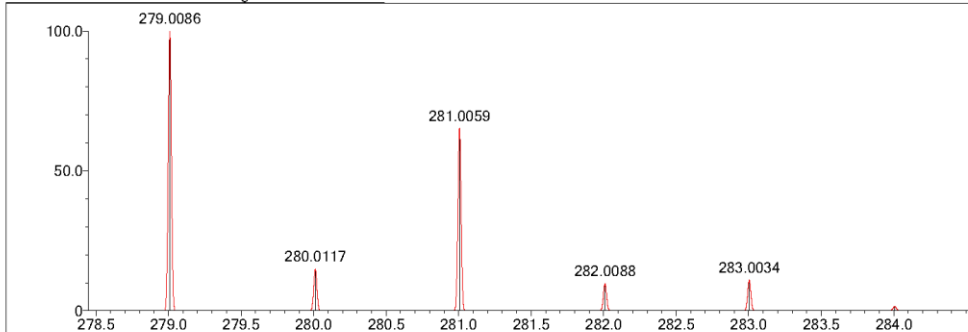
Event#: 1 MS(E+) Ret. Time : 1.007 -> 1.007 Scan#: 202 -> 202



Measured region for 279.0084 m/z

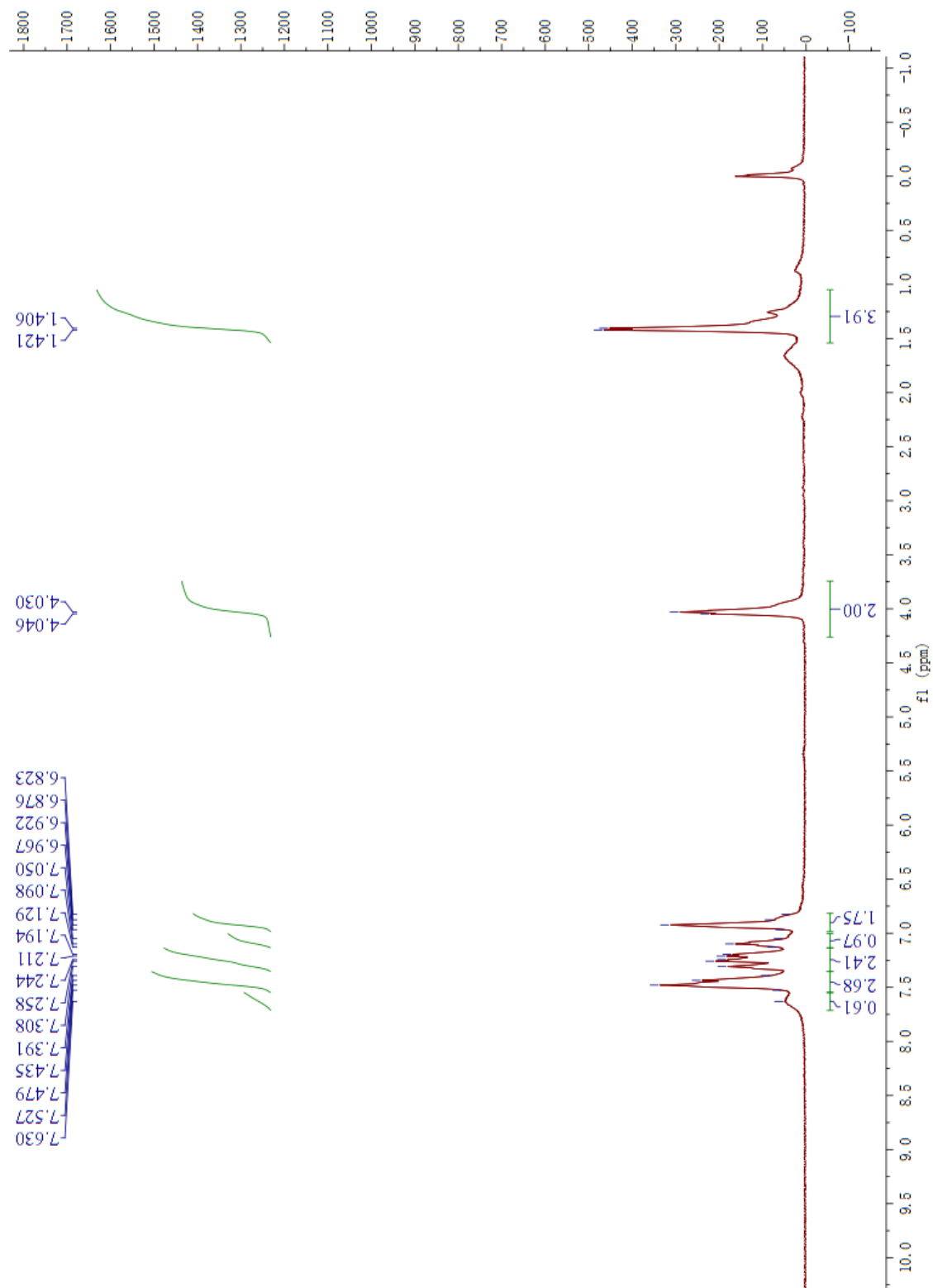


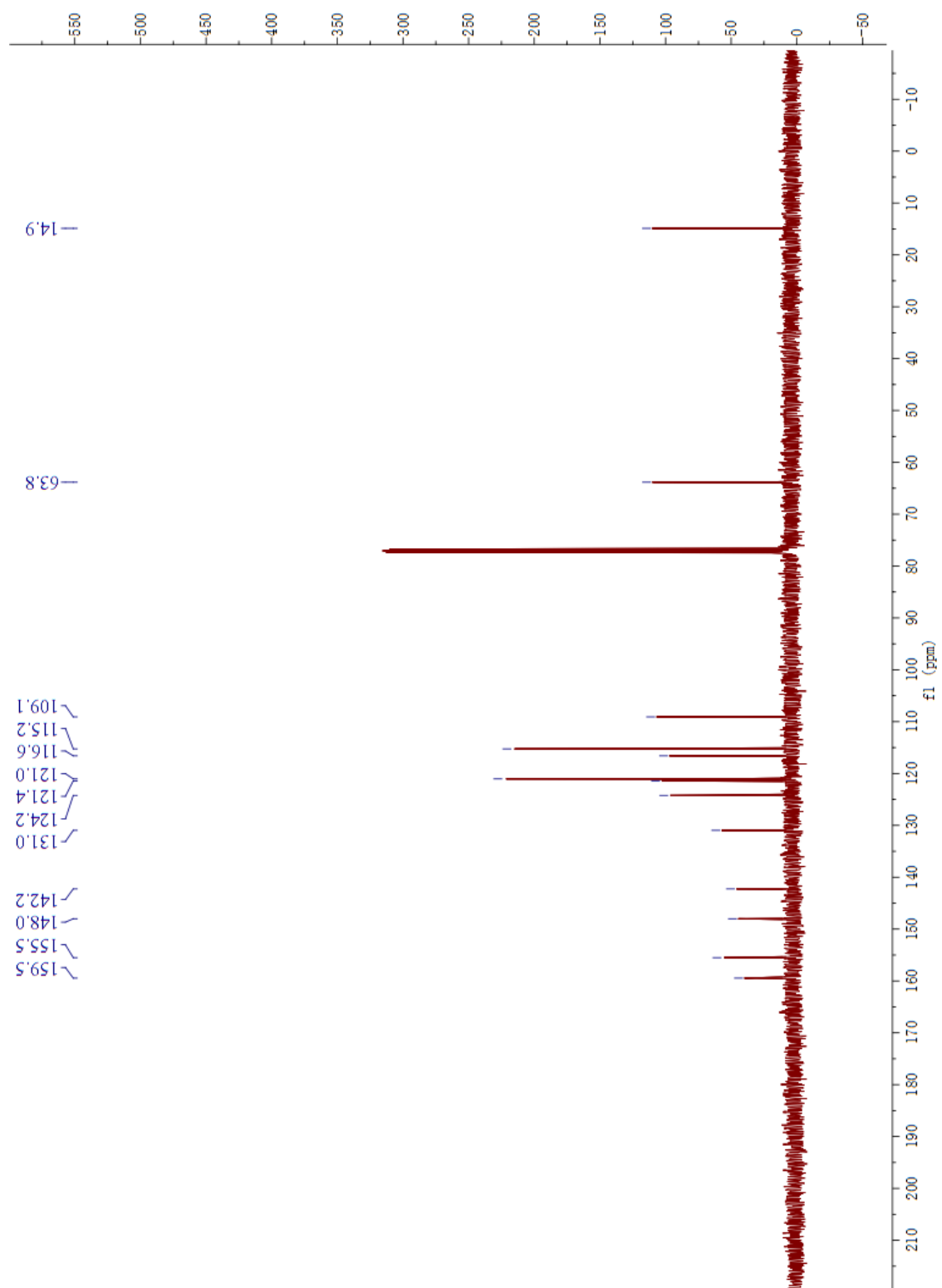
C13 H9 N2 O Cl2 M+ : Predicted region for 279.0086 m/z



Rank	Score	Formula (M)	Ion	Mees. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
5	91.35	C13 H9 N2 O Cl2	M+	279.0084	279.0086	-0.2	-0.72	91.35	9.5

***N*-(4-Ethoxyphenyl)benzo[*d*]oxazol-2-amine (3i)**





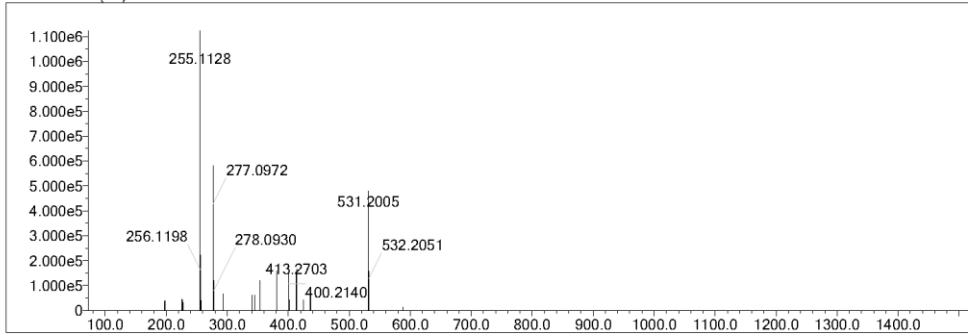
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	1	Cl	1	0	2	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

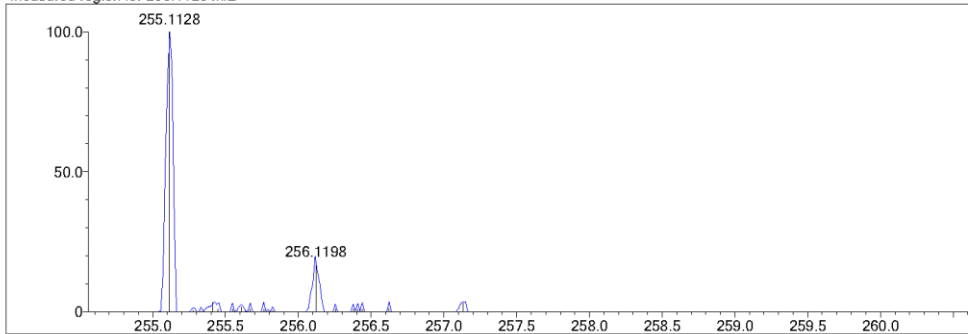
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

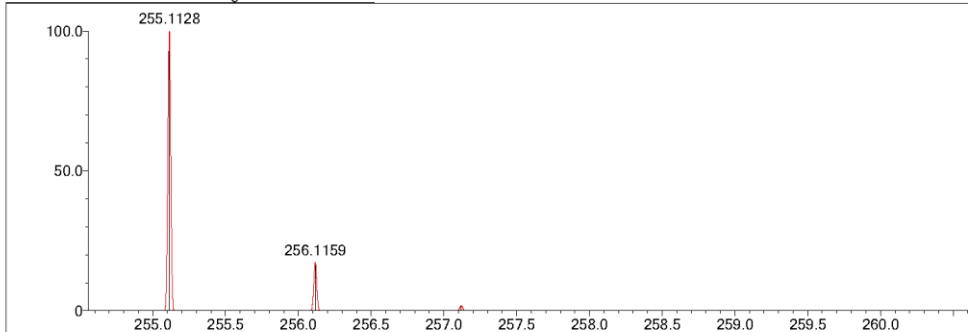
Event#: 1 MS(E+) Ret. Time : 1.107 - 1.537 -> 1.900 Scan#: 222 - 308 -> 381



Measured region for 255.1128 m/z

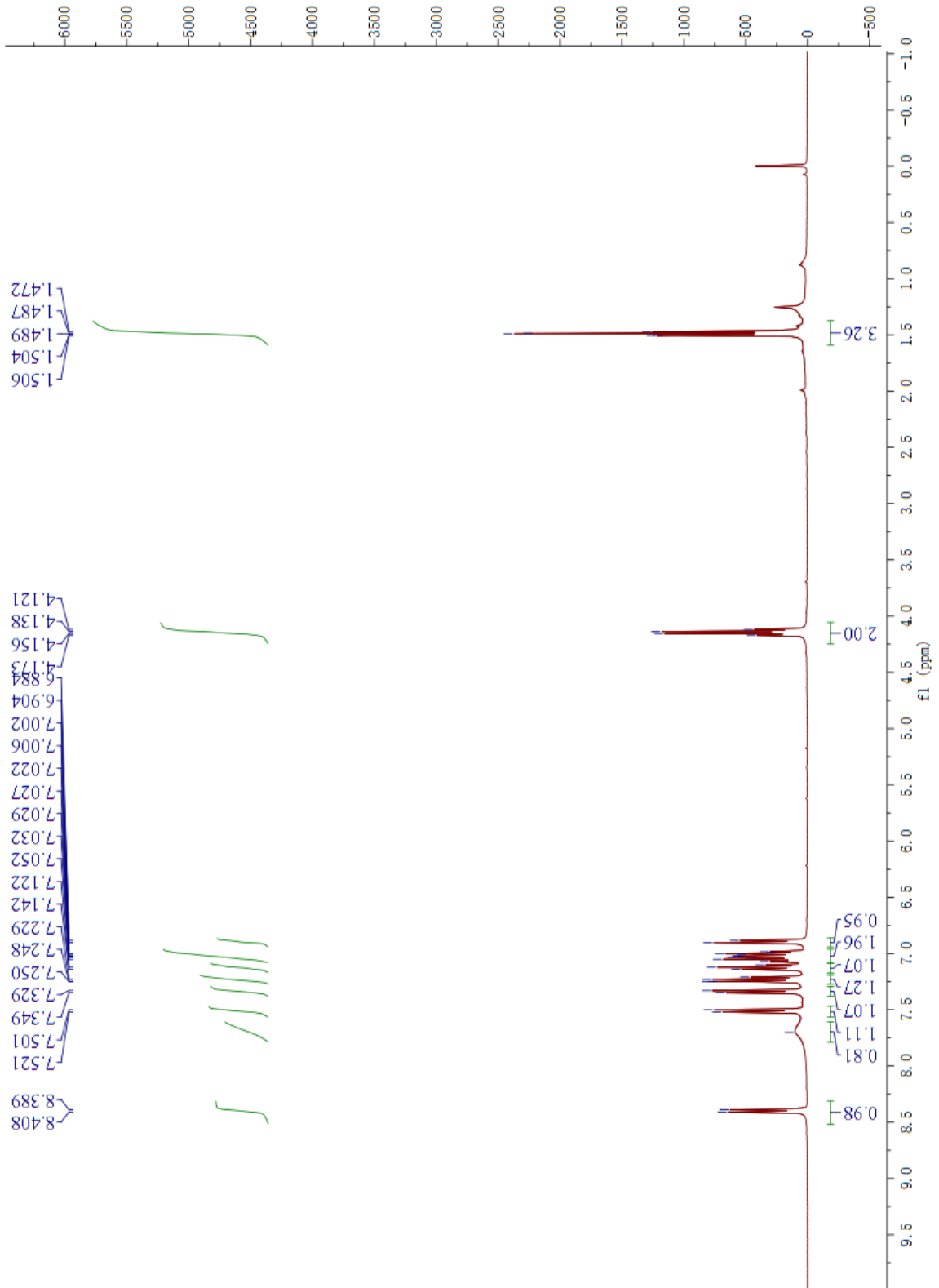


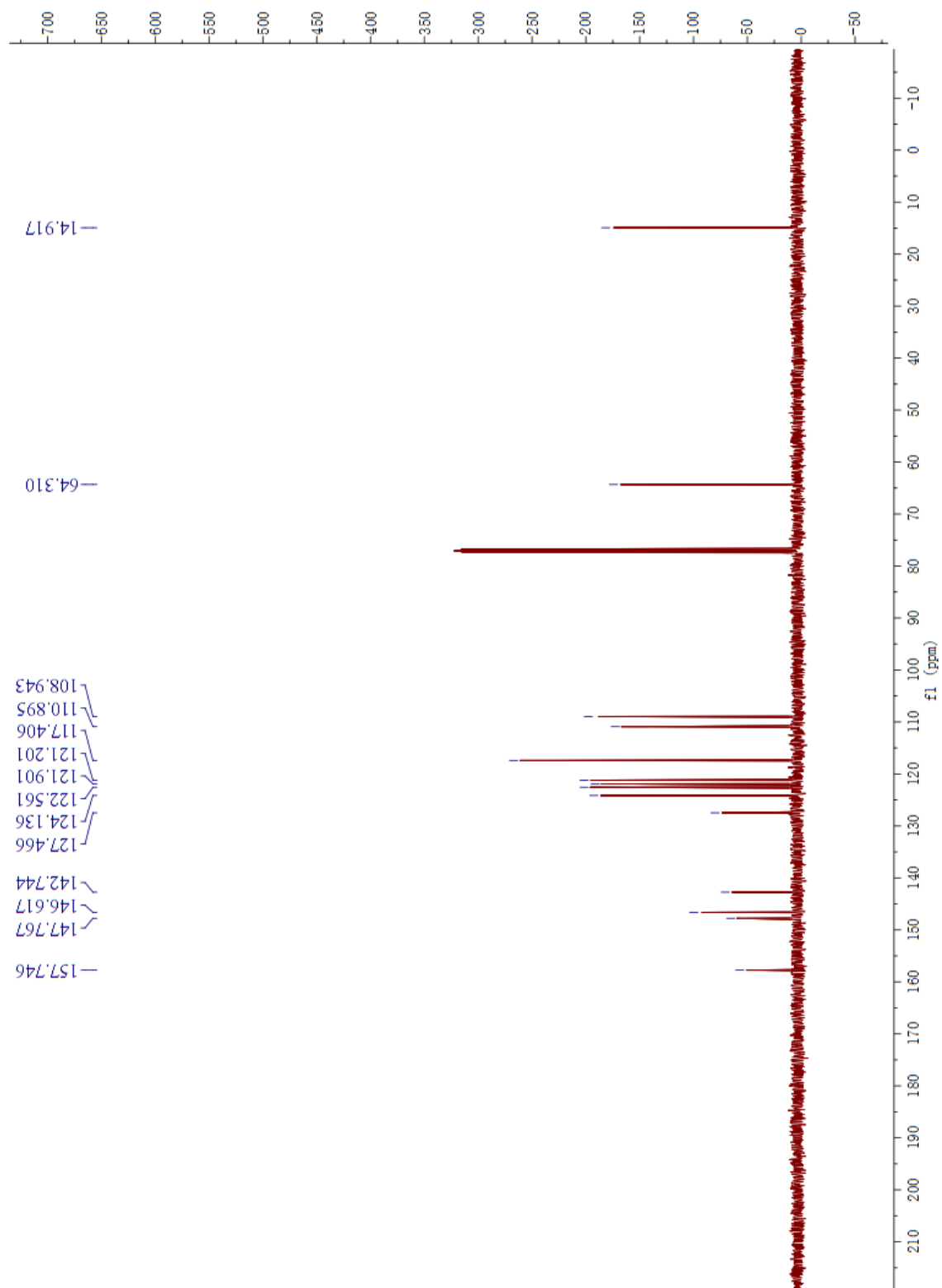
C15 H15 N2 O2 M+ : Predicted region for 255.1128 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	63.36	C15 H15 N2 O2	M+	255.1128	255.1128	-0.0	0.00	63.36	9.5

***N*-(2-Ethoxyphenyl)benzo[*d*]oxazol-2-amine (3j)**

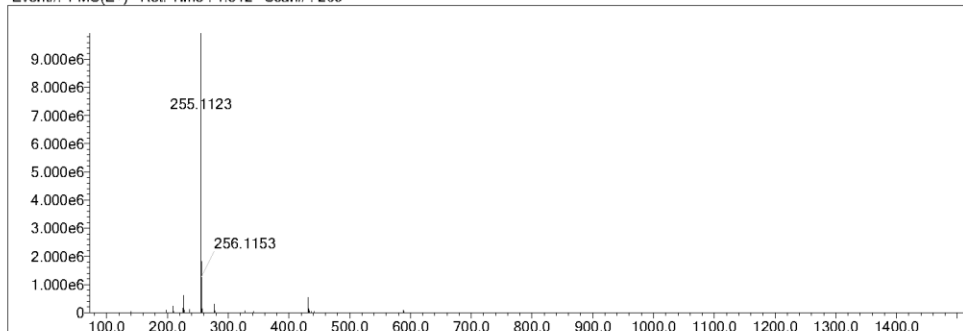




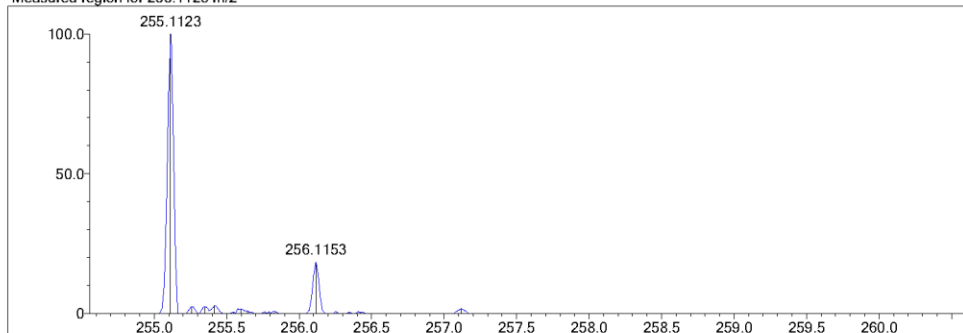
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	¹⁸ O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	1	Cl	1	0	2	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100 DBE Range: -2.0 - 1000.0 Electron Ions: both
 HC Ratio: unlimited Apply N Rule: no Use MSn Info: no
 Max Isotopes: all Isotope RI (%): 1.00 Isotope Res: 10000
 MSn Iso RI (%): 75.00 MSn Logic Mode: AND Max Results: 500

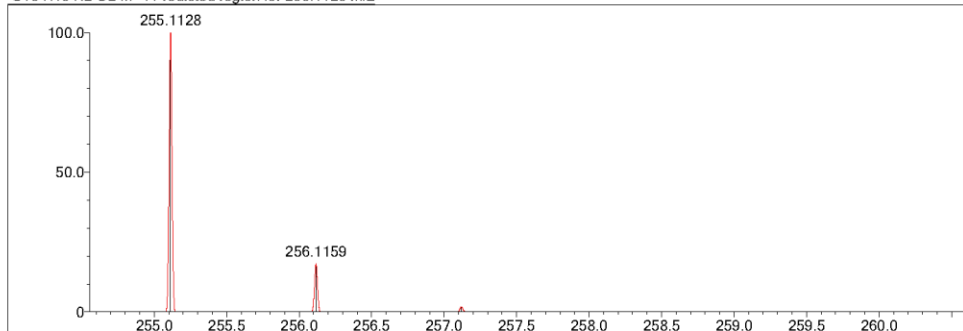
Event#: 1 MS(E+) Ret. Time : 1.342 Scan#: 269



Measured region for 255.1123 m/z

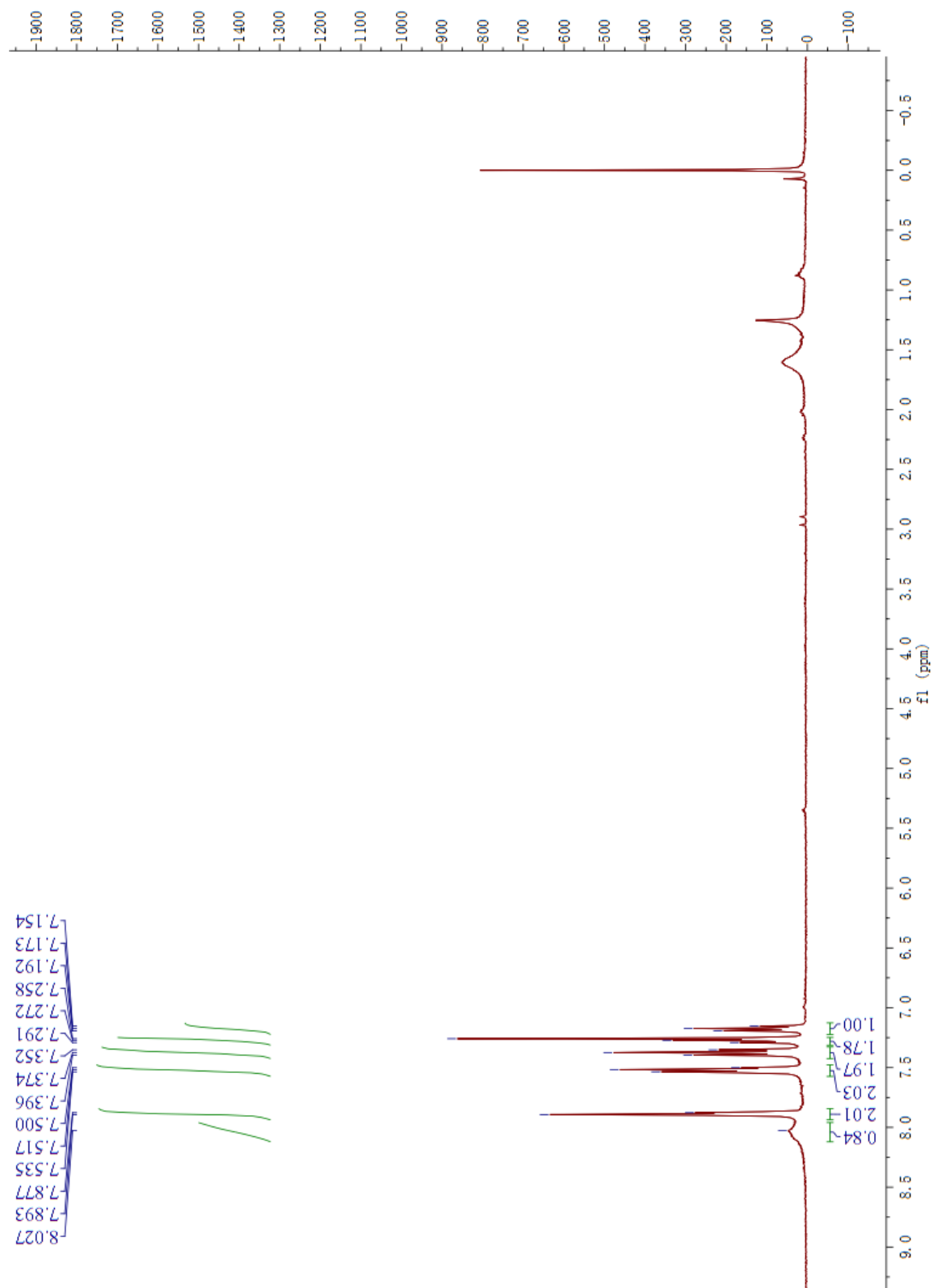


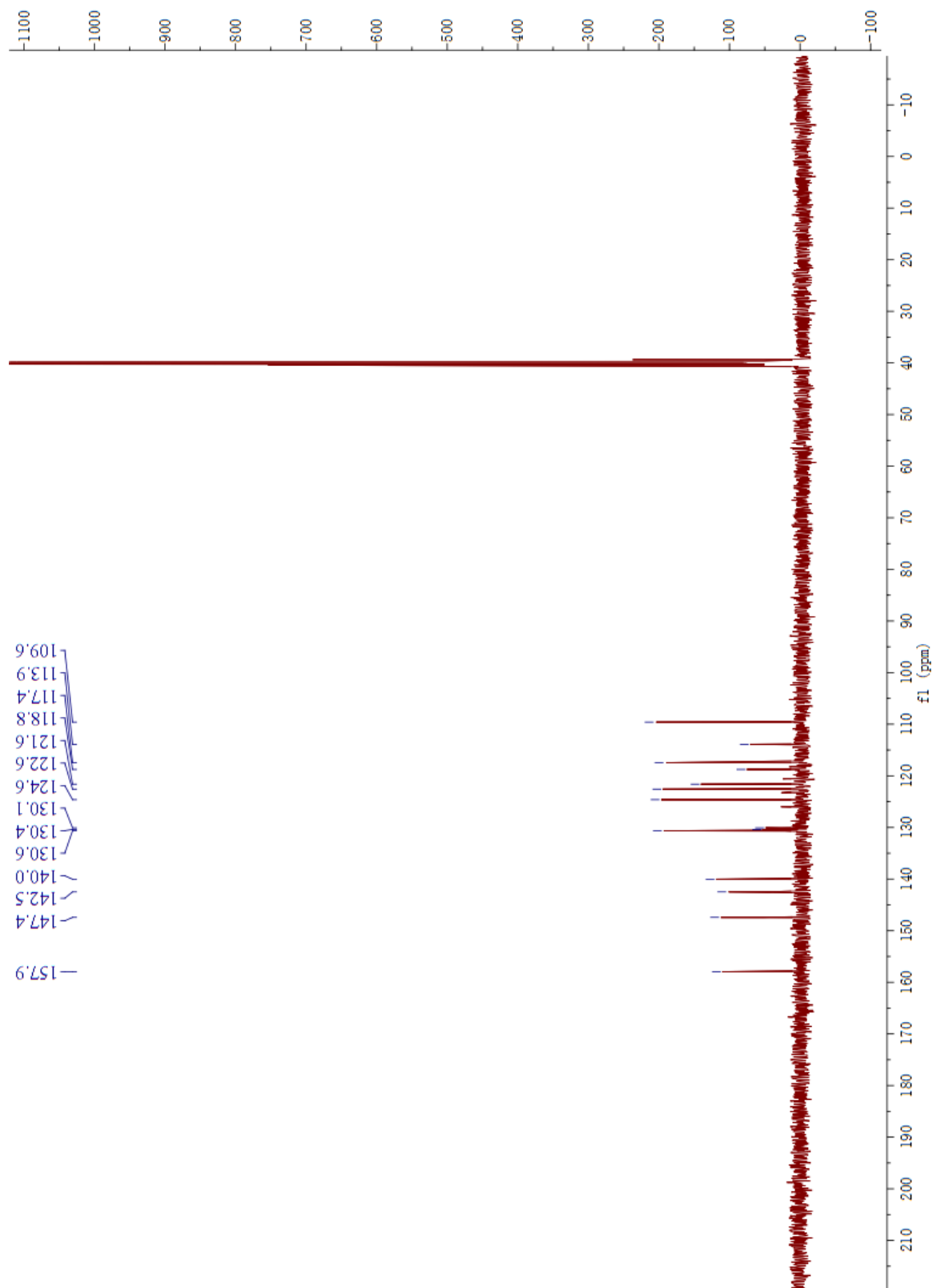
C15 H15 N2 O2 M+ : Predicted region for 255.1128 m/z



Rank	Score	Formula (M)	Ion	Mees. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	86.92	C15 H15 N2 O2	M+	255.1123	255.1128	-0.5	-1.96	89.06	9.5

***N*-3-(Trifluoromethyl)phenylbenzo[*d*]oxazol-2-amine (3k)**





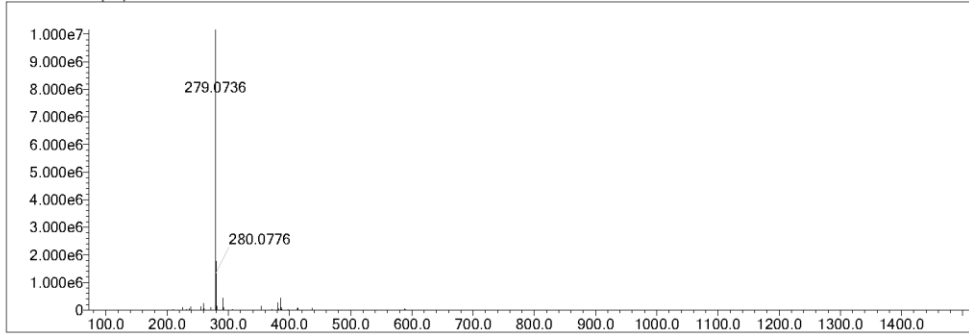
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	3	Cl	1	0	2	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

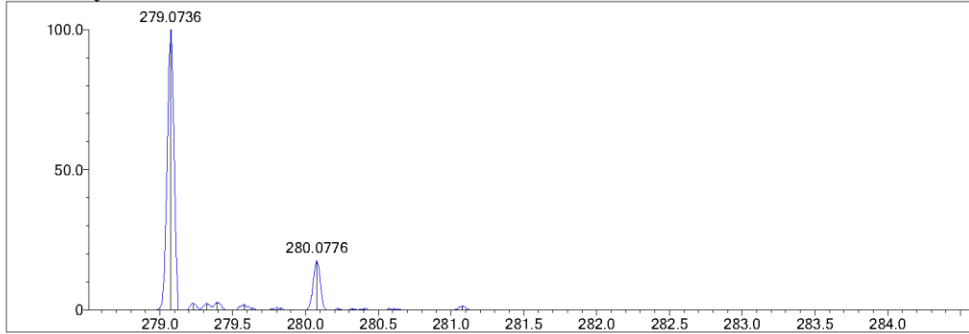
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

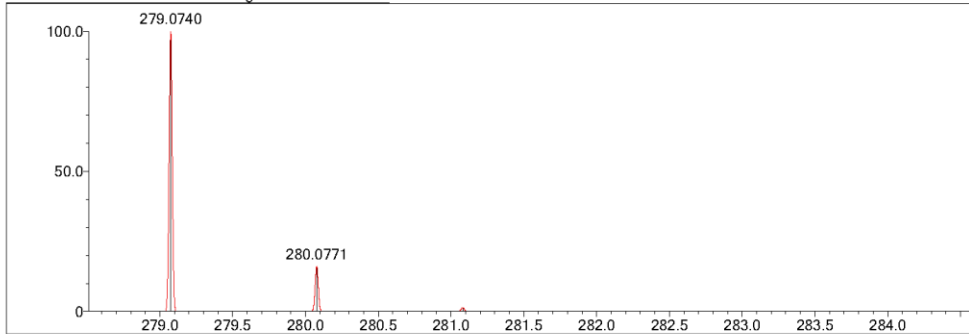
Event#: 1 MS(E+) Ret. Time : 1.127 -> 1.137 Scan#: 226 -> 228



Measured region for 279.0736 m/z

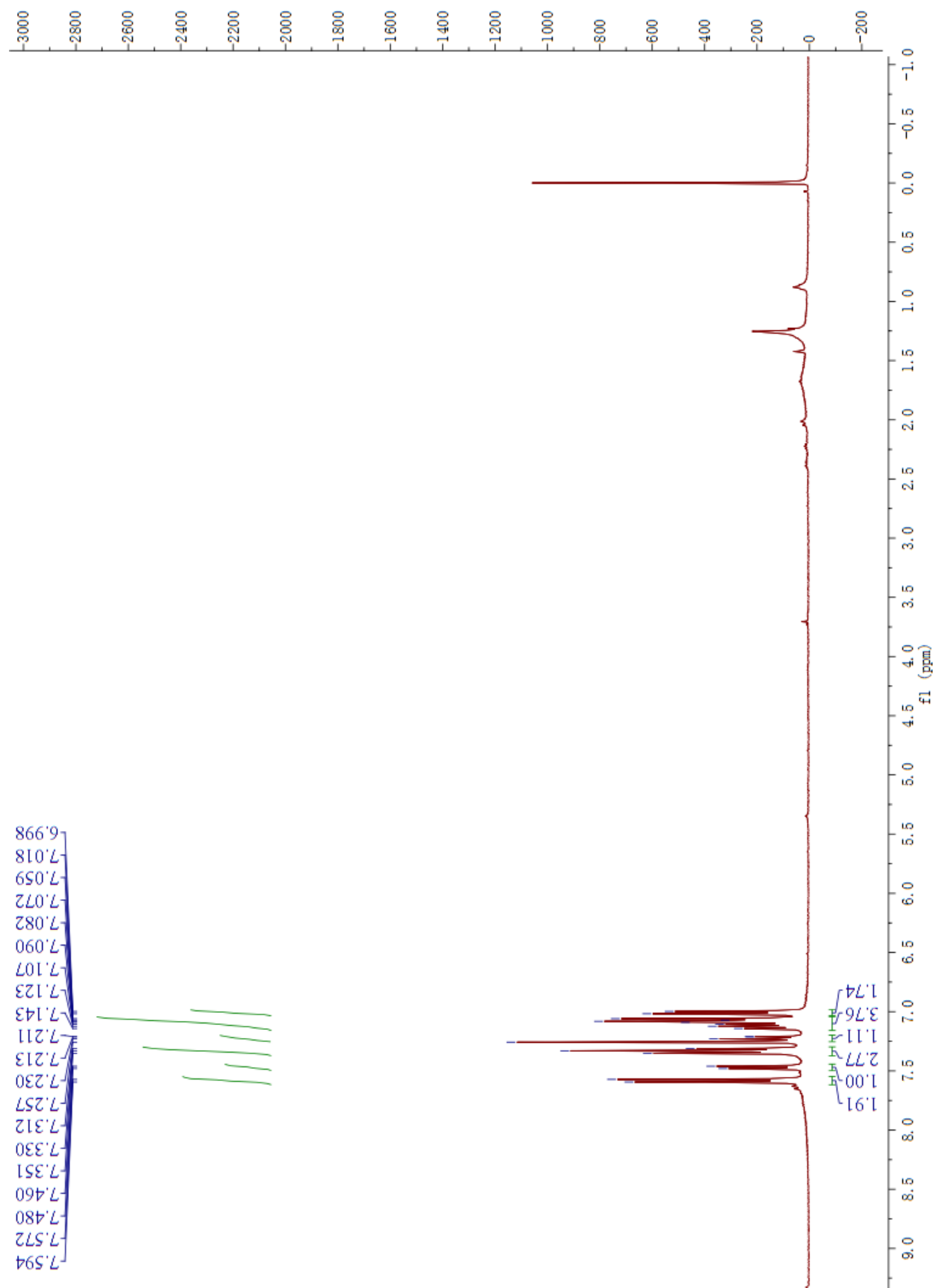


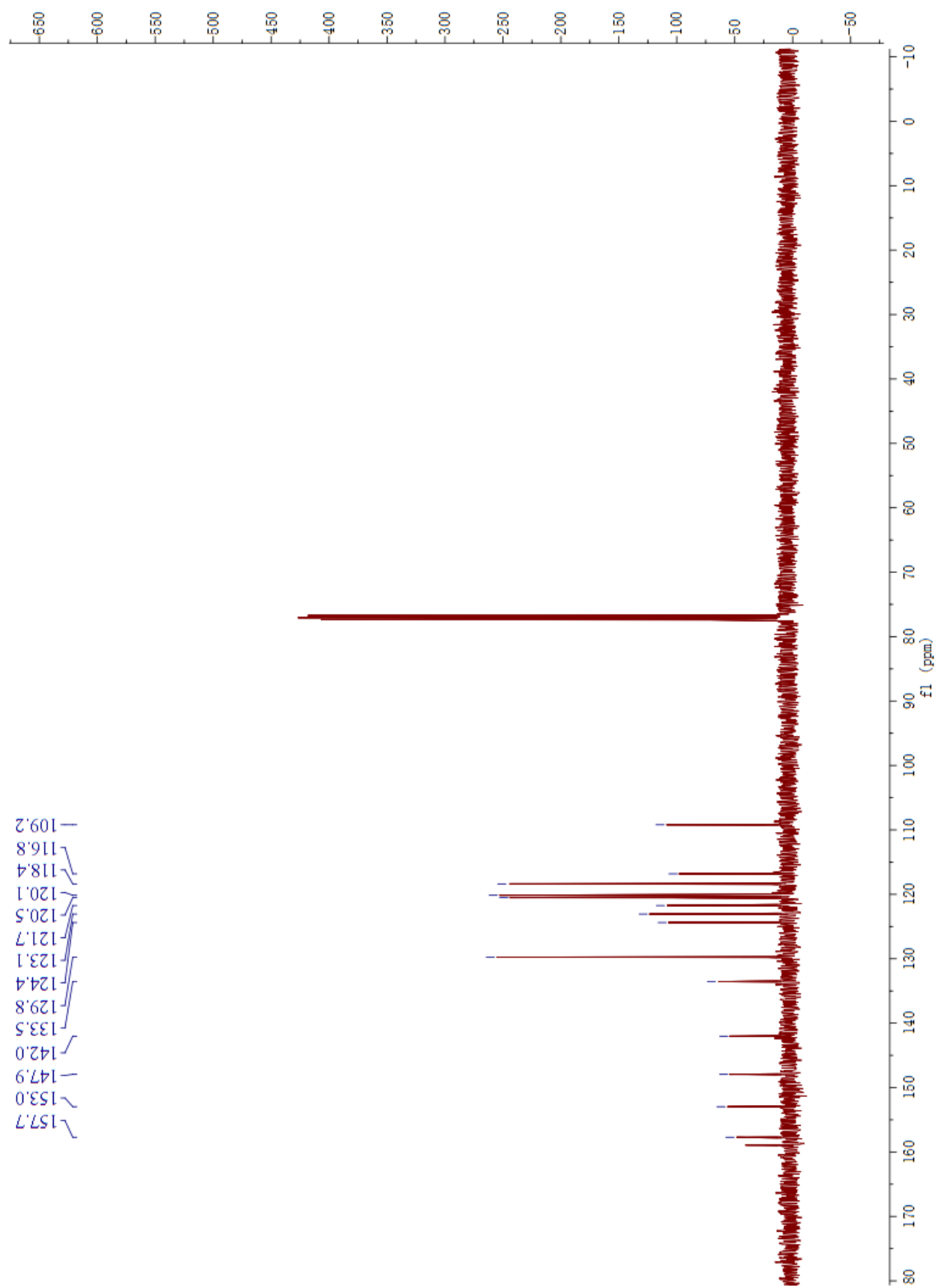
C14 H10 N2 O F3 M+ : Predicted region for 279.0740 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	88.10	C14 H10 N2 O F3	M+	279.0736	279.0740	-0.4	-1.43	89.05	9.5

***N*-(4-Phenoxyphenyl)benzo[*d*]oxazol-2-amine (3l)**





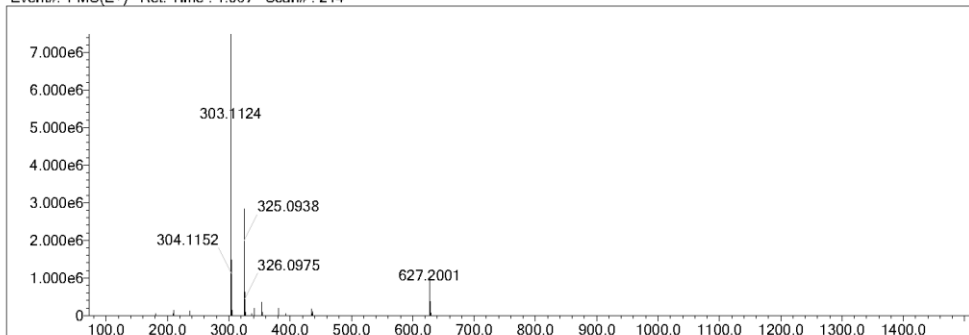
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	1	Br	1	0	0	Na
C	4	0	38	F	1	0	3	Cl	1	0	2	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

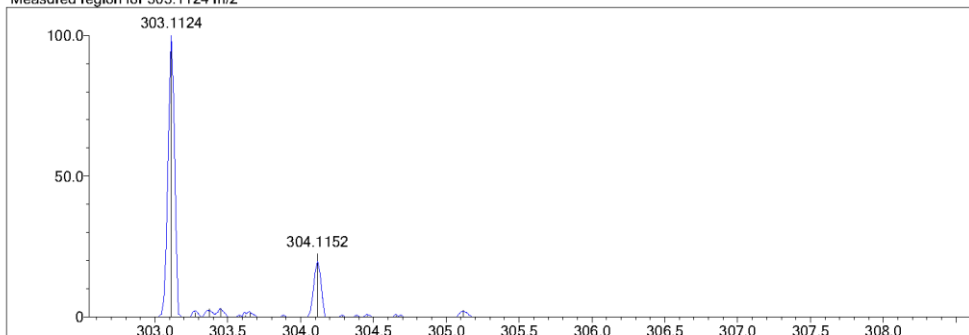
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

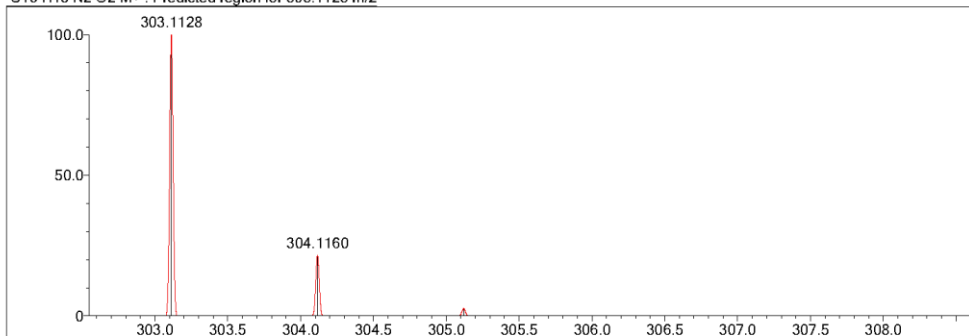
Event#: 1 MS(E+) Ret. Time : 1.067 Scan#: 214



Measured region for 303.1124 m/z

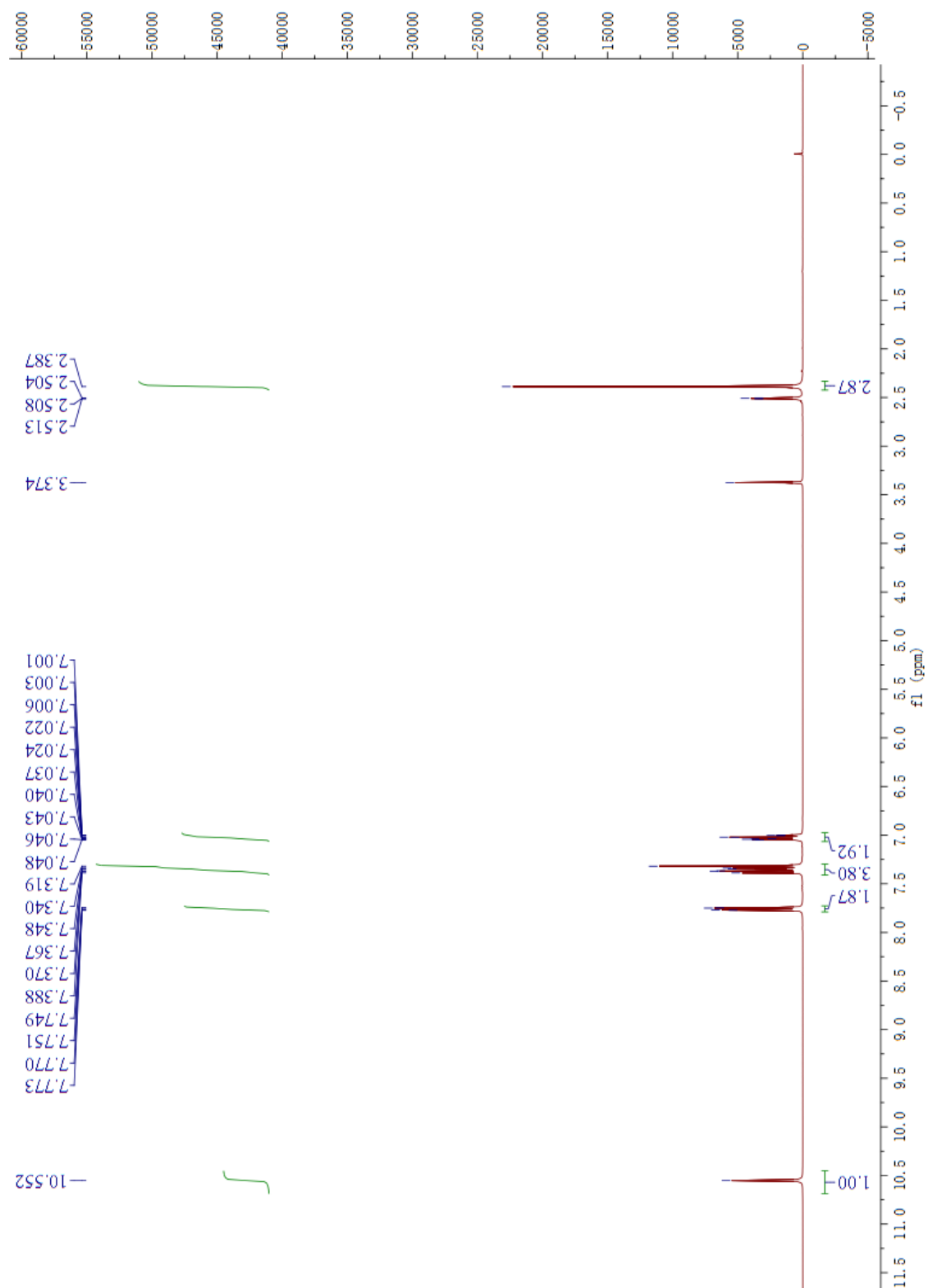


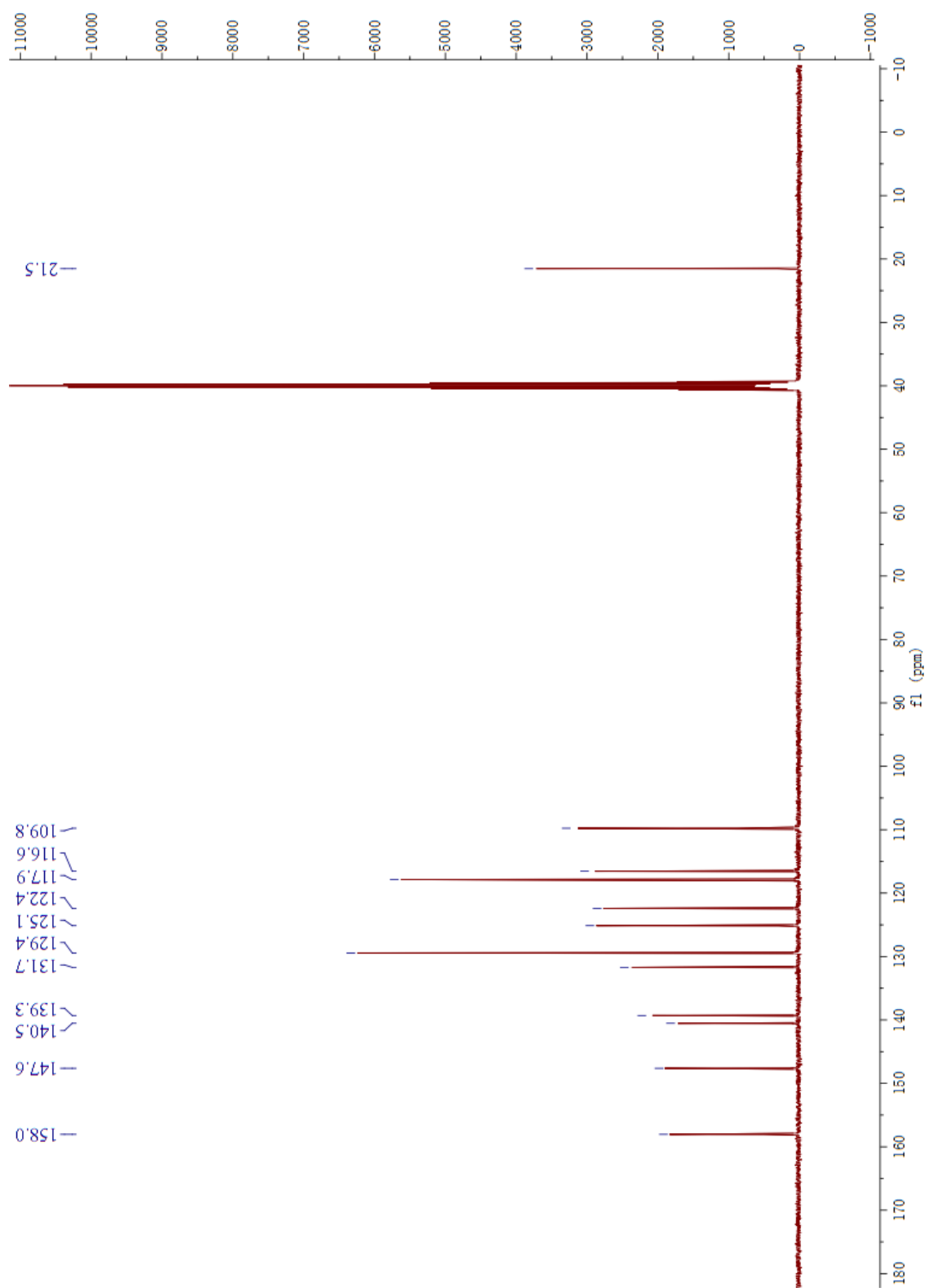
C19H15N2O2 M+ : Predicted region for 303.1128 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
5	79.75	C19H15N2O2	M+	303.1124	303.1128	-0.4	-1.32	80.39	13.5

6-Methyl-N-phenylbenzo[d]oxazol-2-amine (3m)





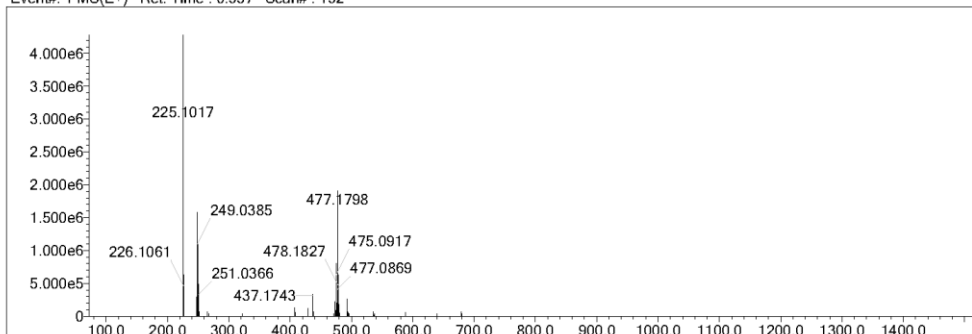
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

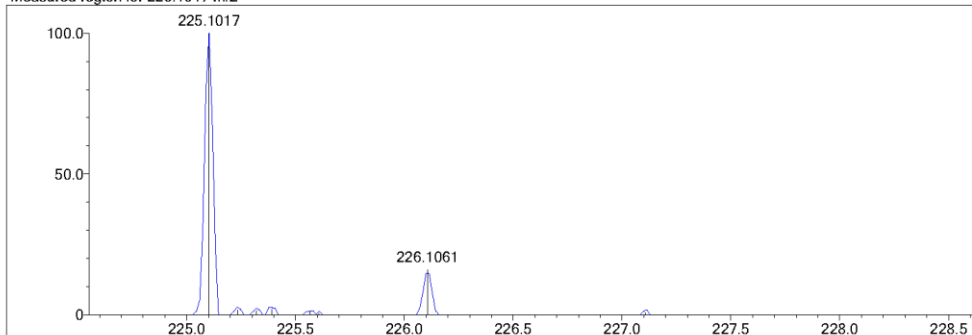
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

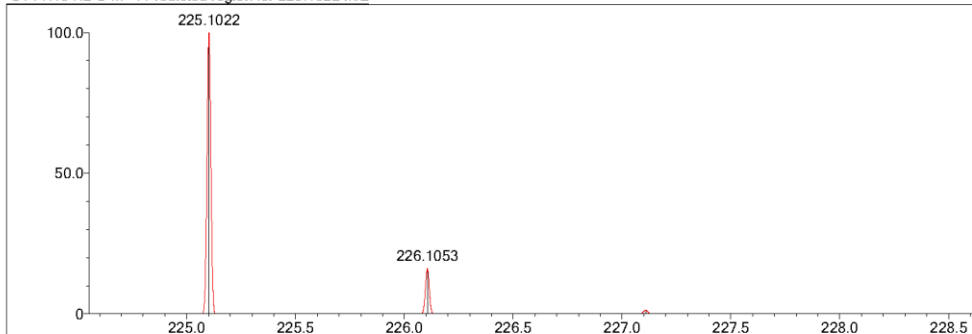
Event#: 1 MS(E+) Ret. Time : 0.957 Scan#: 192



Measured region for 225.1017 m/z

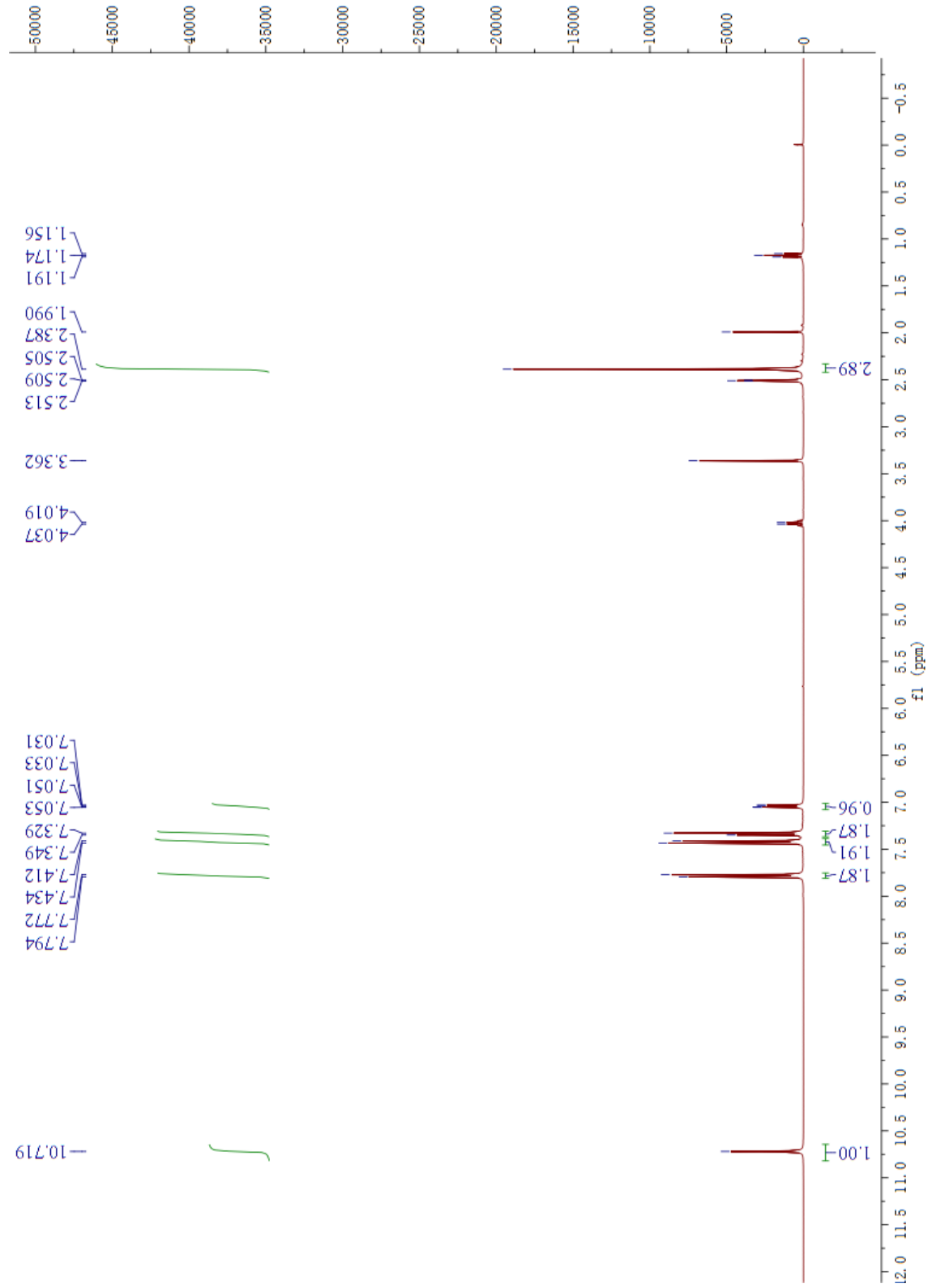


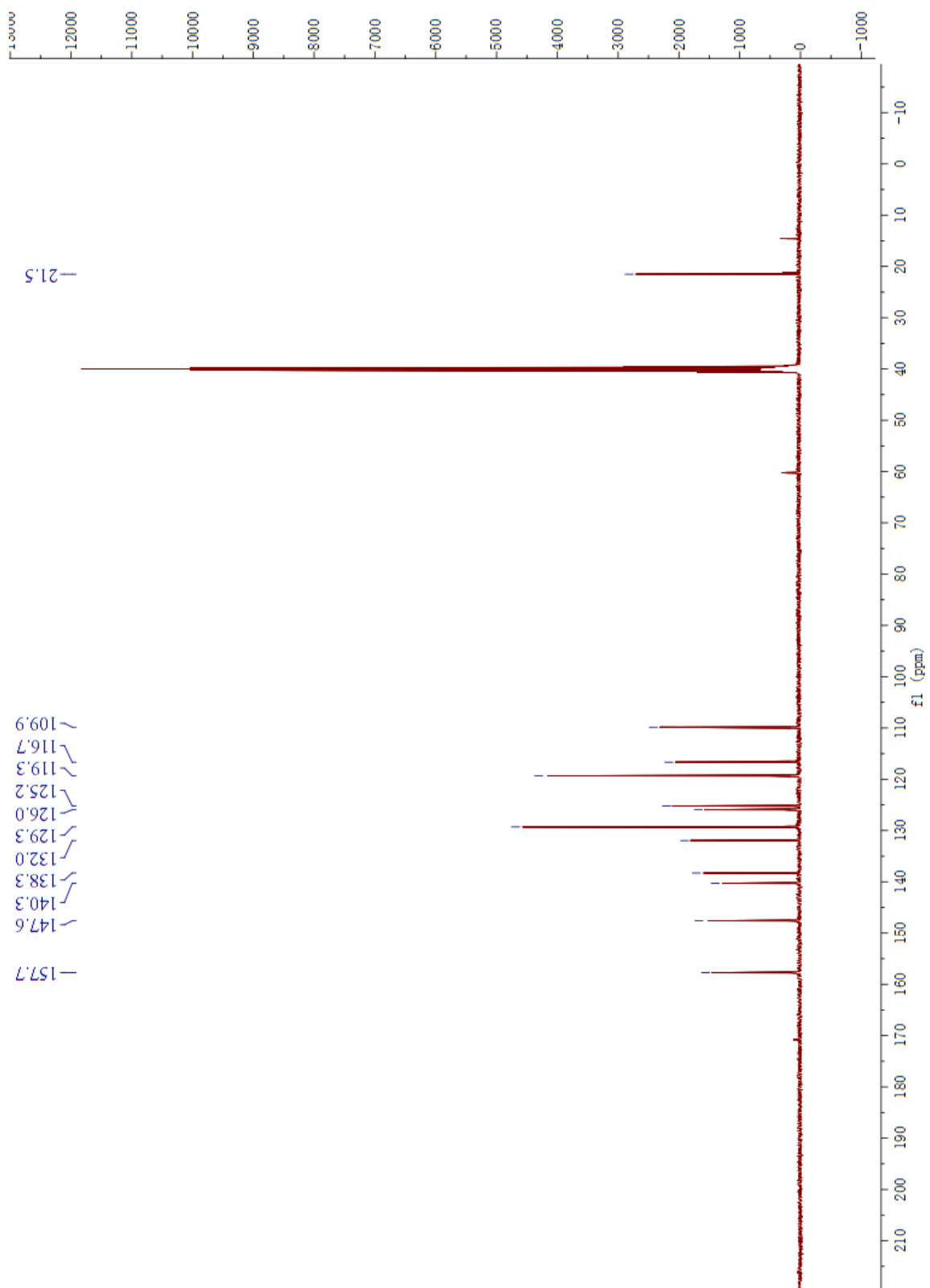
C14 H13 N2 O M+ : Predicted region for 225.1022 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	88.86	C14 H13 N2 O	M+	225.1017	225.1022	-0.5	-2.22	91.65	9.5

***N*-(4-Chlorophenyl)-6-methylbenzo[*d*]oxazol-2-amine (3n)**

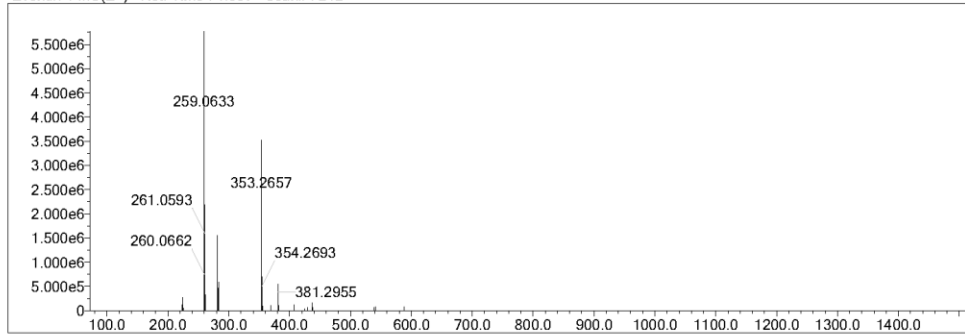




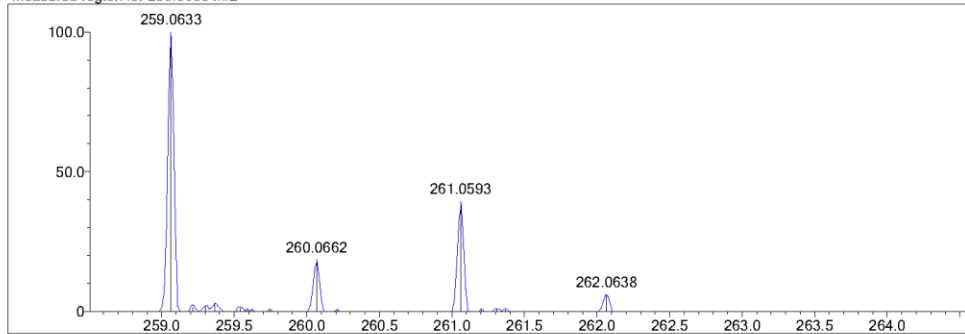
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100 DBE Range: -2.0 - 1000.0 Electron Ions: both
 HC Ratio: unlimited Apply N Rule: no Use MSn Info: no
 Max Isotopes: all Isotope RI (%): 1.00 Isotope Res: 10000
 MSn Iso RI (%): 75.00 MSn Logic Mode: AND Max Results: 500

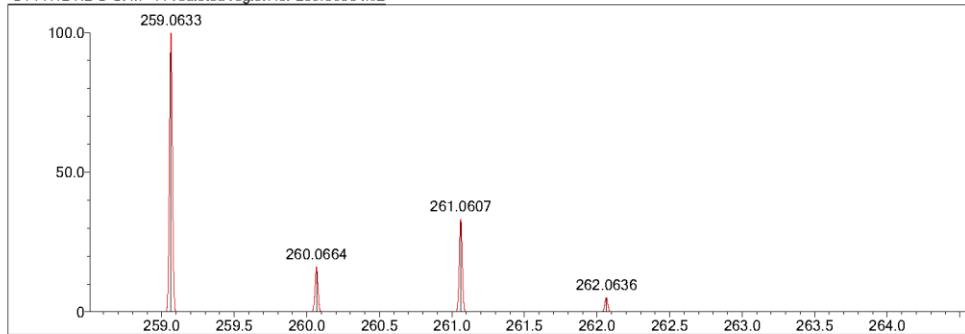
Event#: 1 MS(E+) Ret. Time : 1.057 Scan# : 212



Measured region for 259.0633 m/z

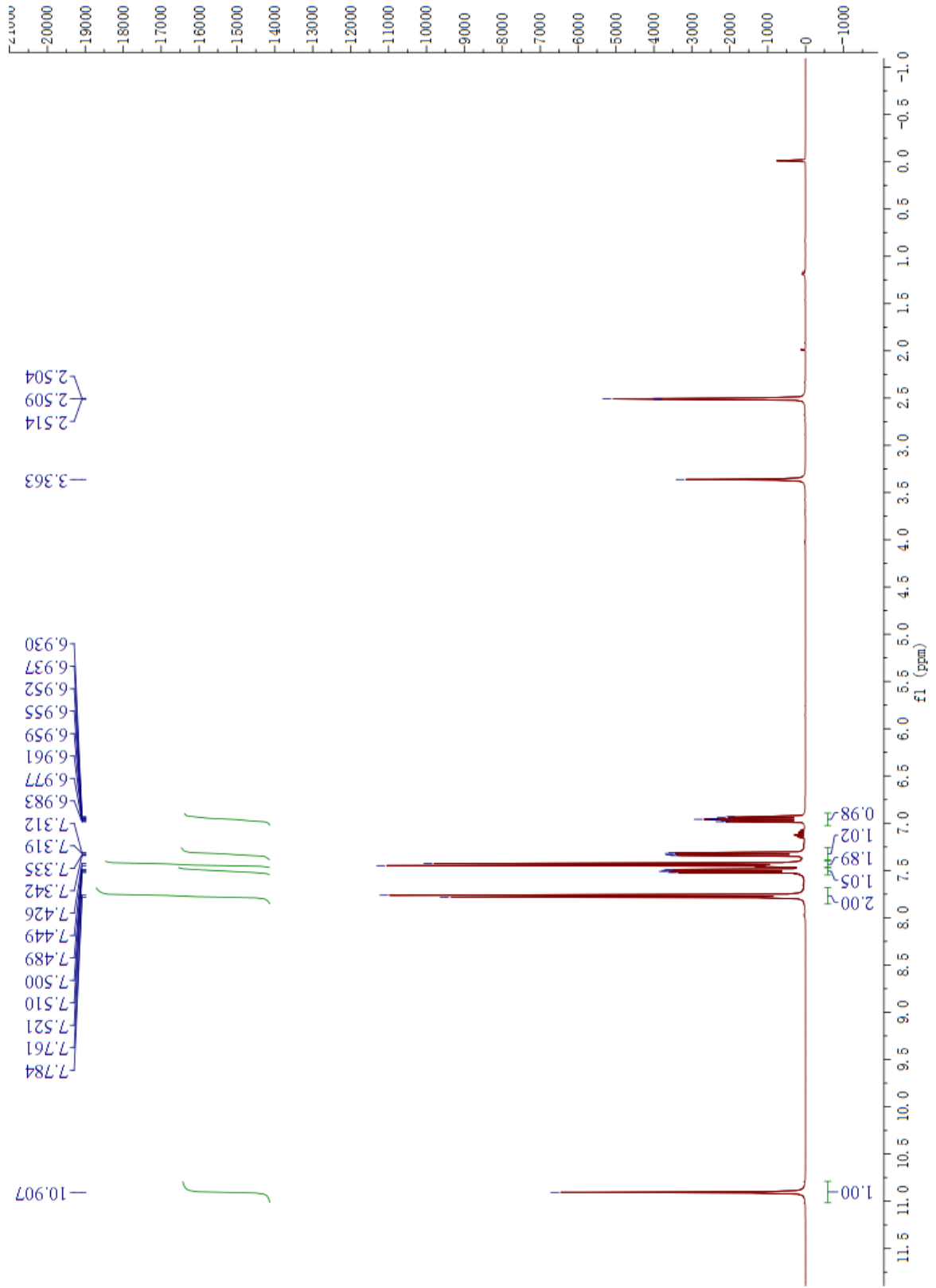


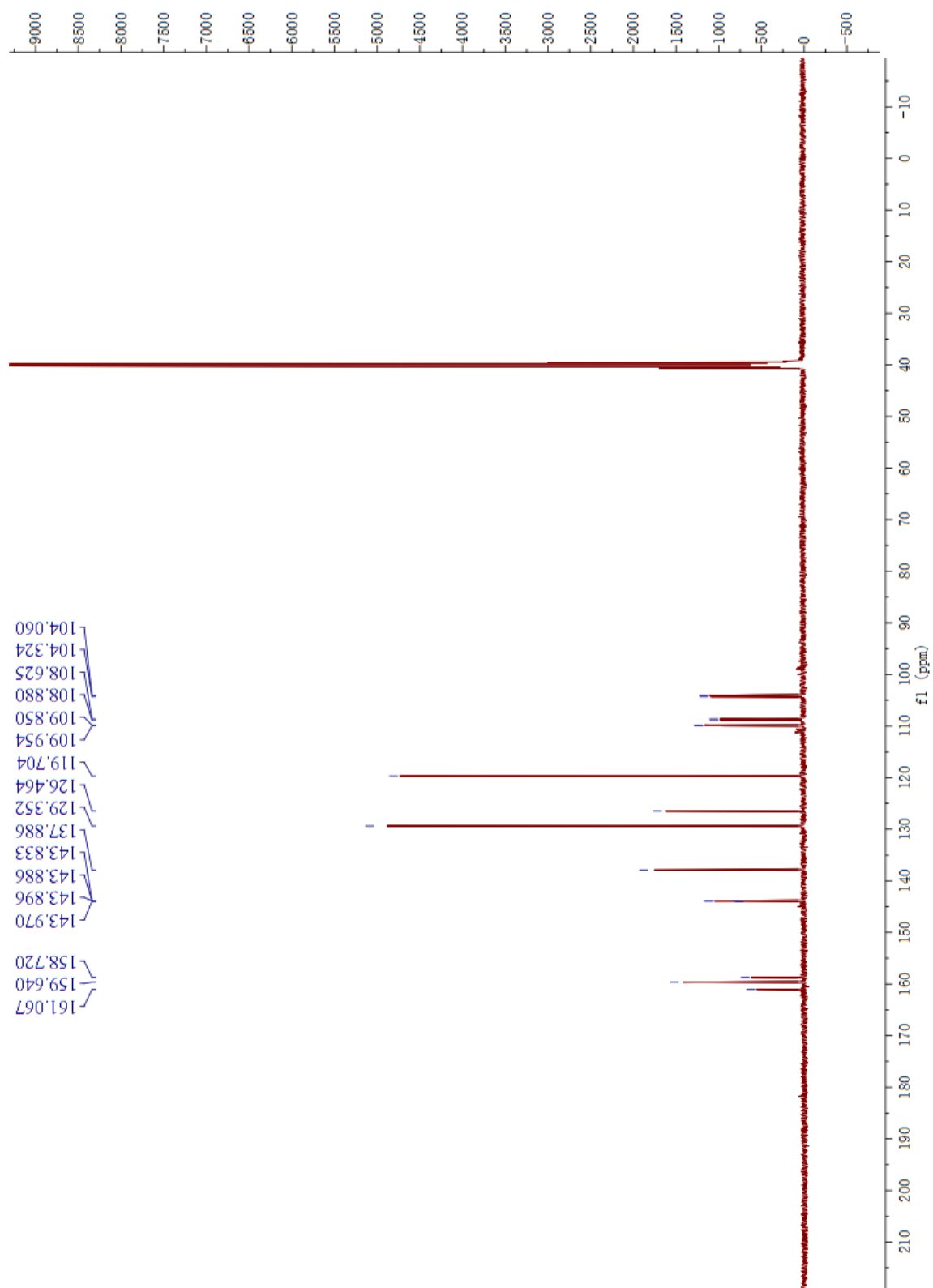
C14 H12 N2 O Cl M+ : Predicted region for 259.0633 m/z



Rank	Score	Formula (M)	Ion	Mees. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	92.48	C14 H12 N2 O Cl	M+	259.0633	259.0633	0.0	0.00	92.48	9.5

***N*-(4-Chlorophenyl)-5-fluorobenzo[*d*]oxazol-2-amine (3o)**





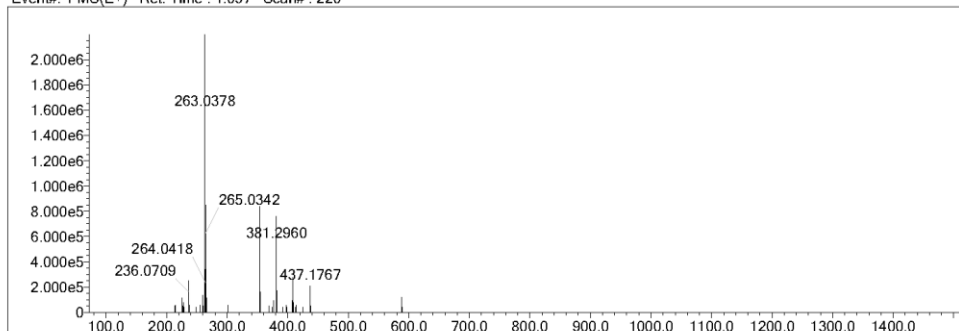
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	¹⁸ O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

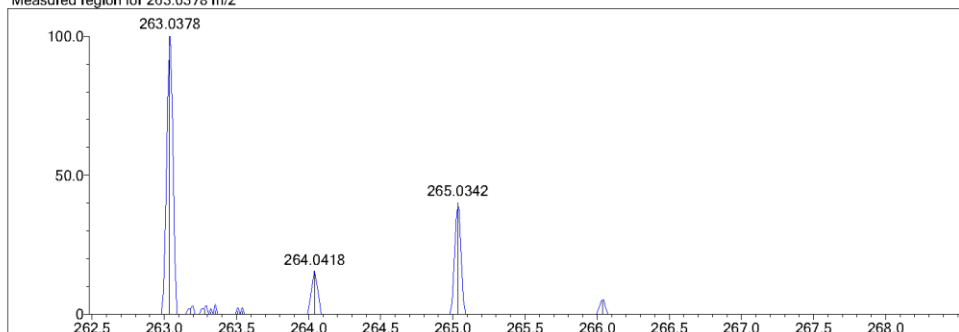
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

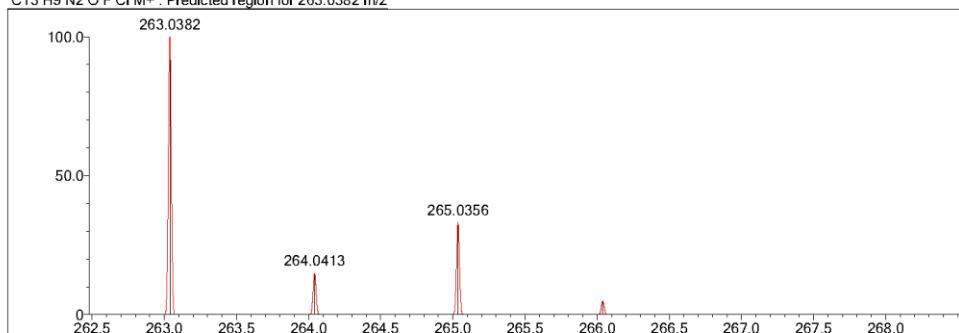
Event#: 1 MS(E+) Ret. Time : 1.097 Scan#: 220



Measured region for 263.0378 m/z

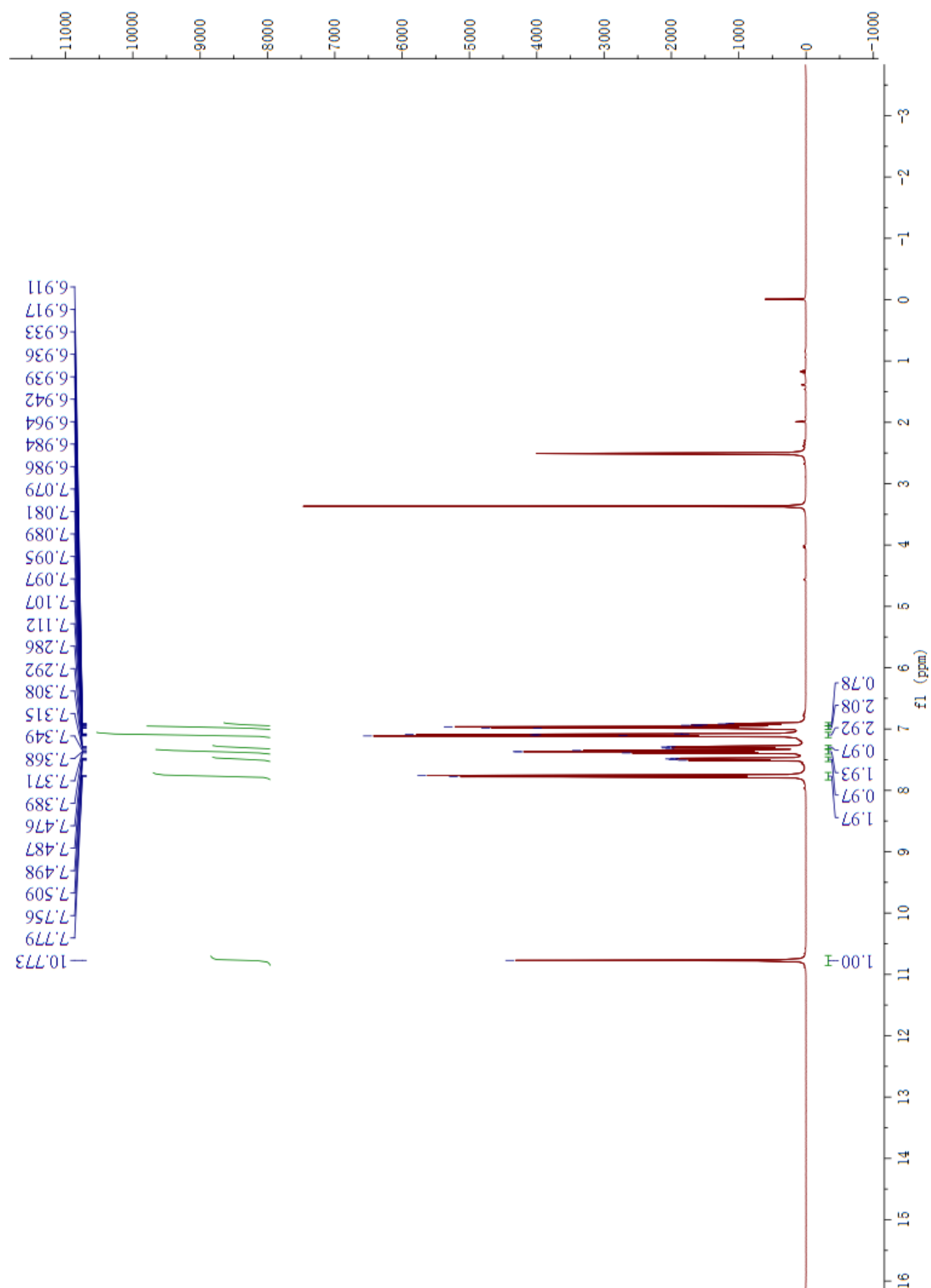


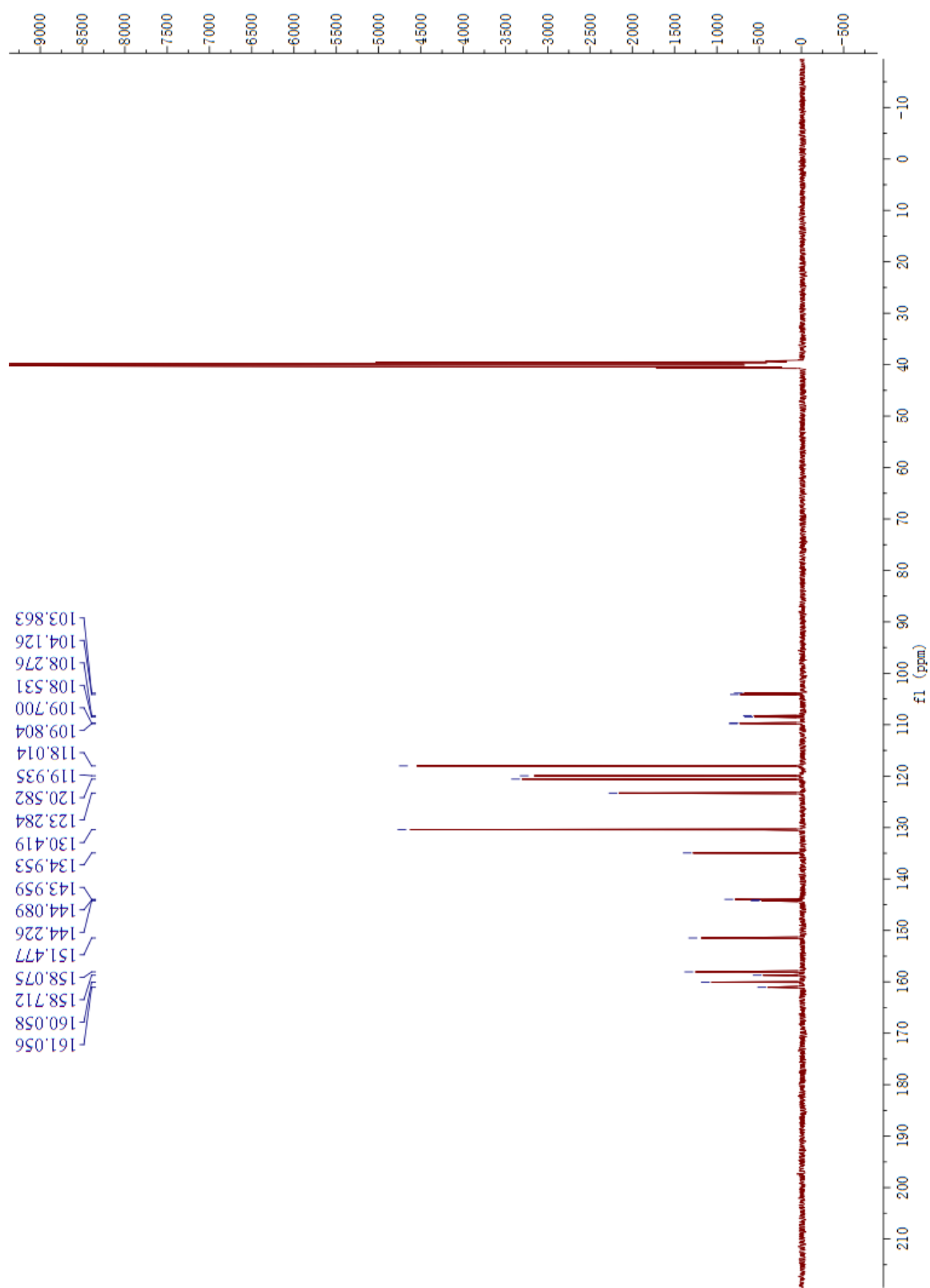
C13 H9 N2 O F Cl M+ : Predicted region for 263.0382 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	80.15	C13 H9 N2 O F Cl	M+	263.0378	263.0382	-0.4	-1.52	81.20	9.5

5-Fluoro-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3p)





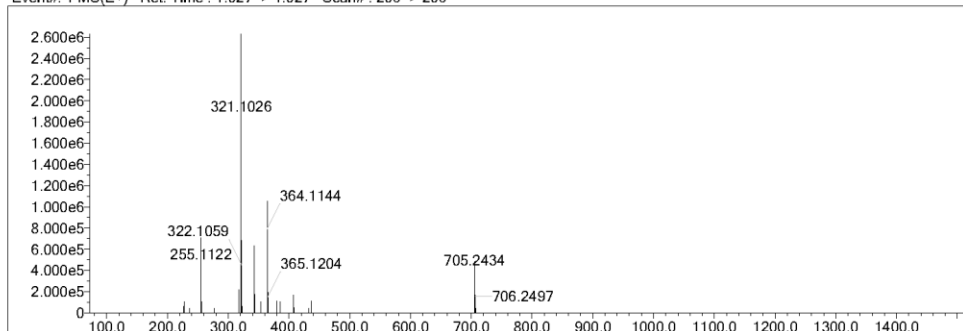
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

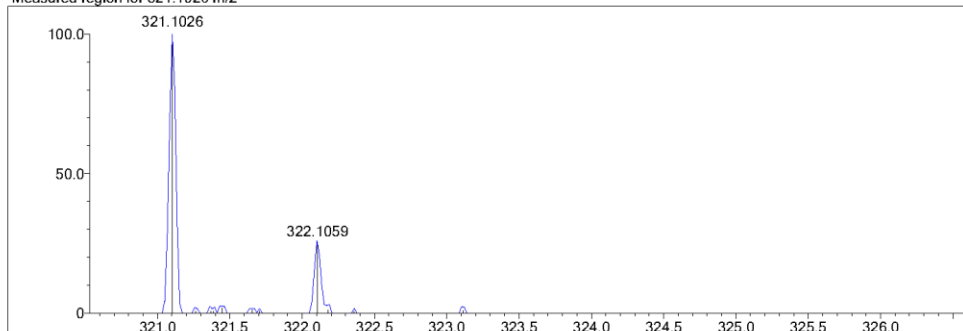
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

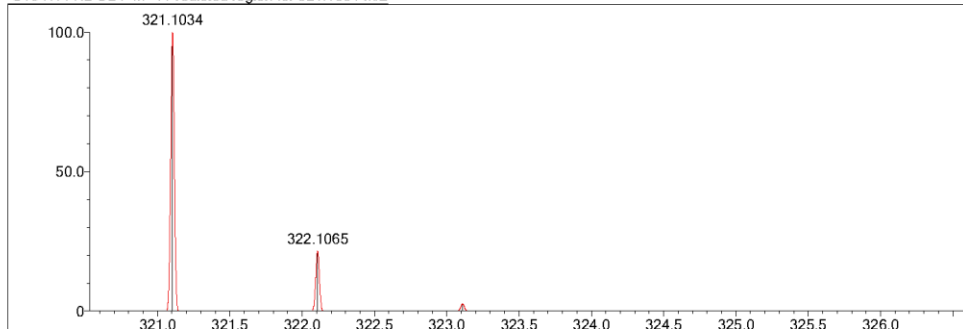
Event#: 1 MS(E+) Ret. Time : 1.027 -> 1.027 Scan#: 206 -> 206



Measured region for 321.1026 m/z

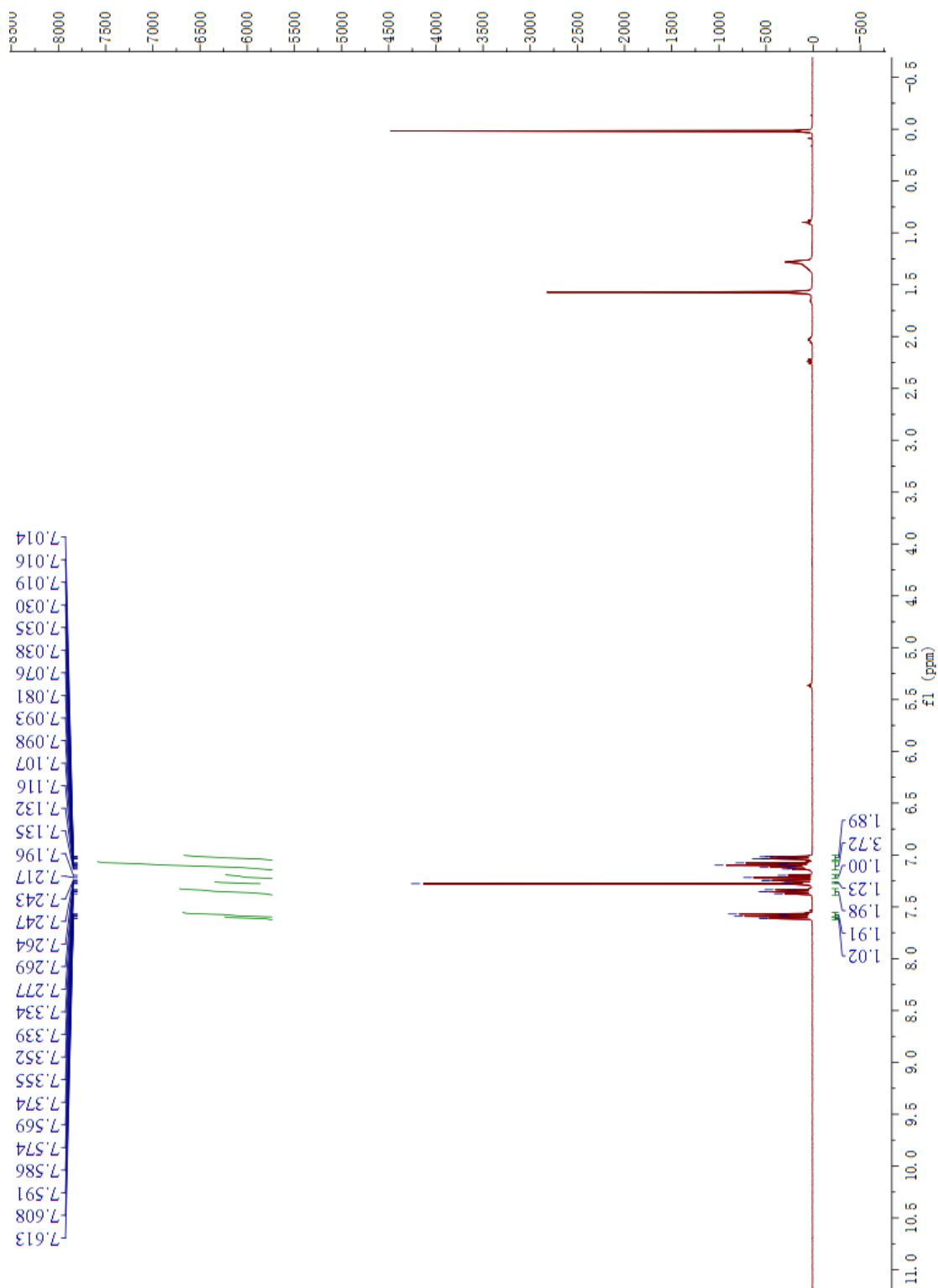


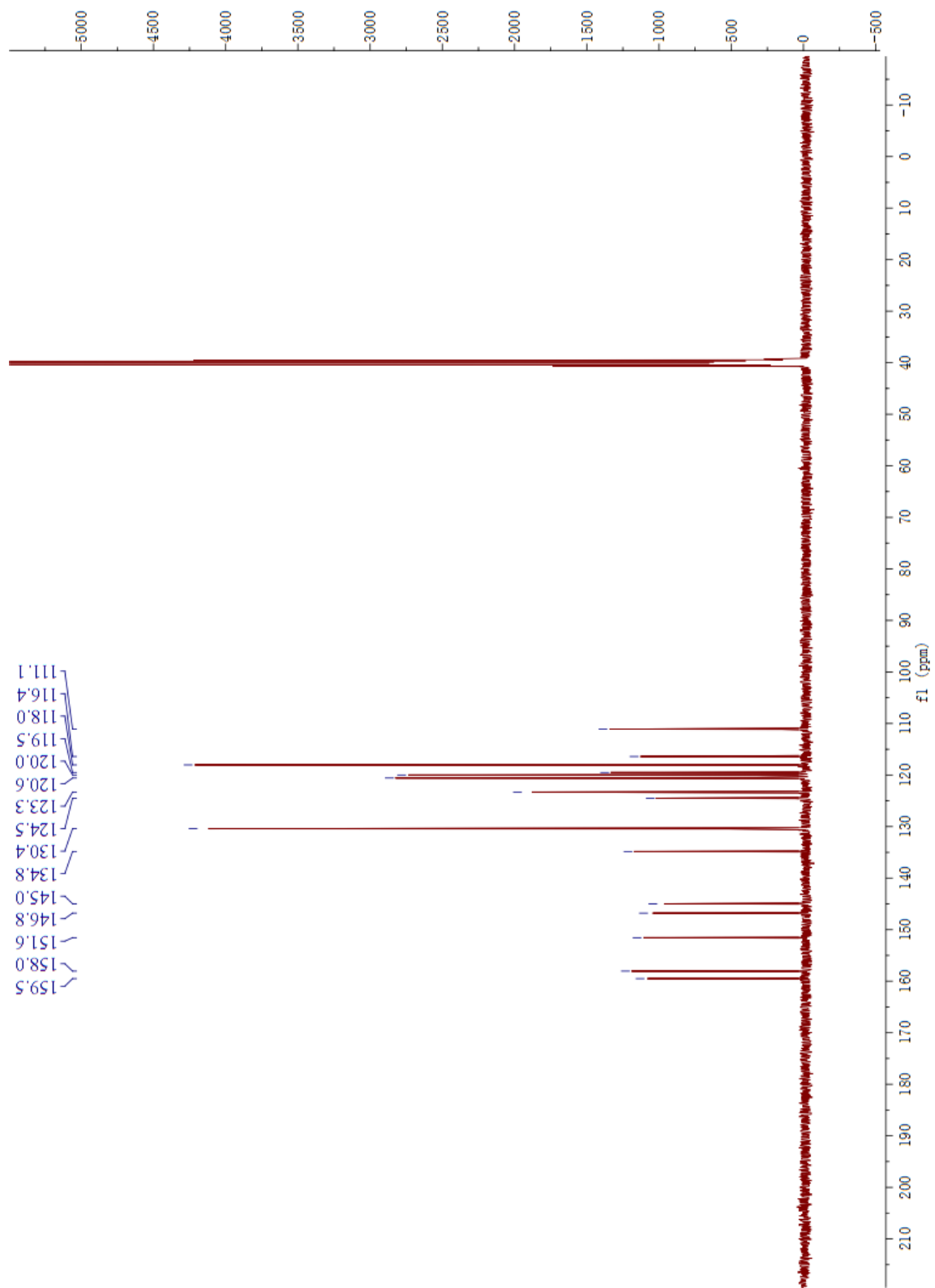
C19 H14 N2 O2 F M+ : Predicted region for 321.1034 m/z



Rank	Score	Formula (M)	Ion	Mees. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	94.76	C19 H14 N2 O2 F	M+	321.1026	321.1034	-0.8	-2.49	98.43	13.5

5-Bromo-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3q)





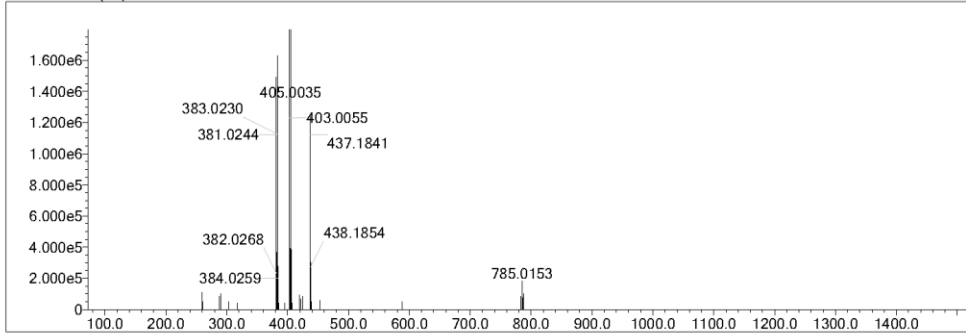
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	0	Cl	1	0	0	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

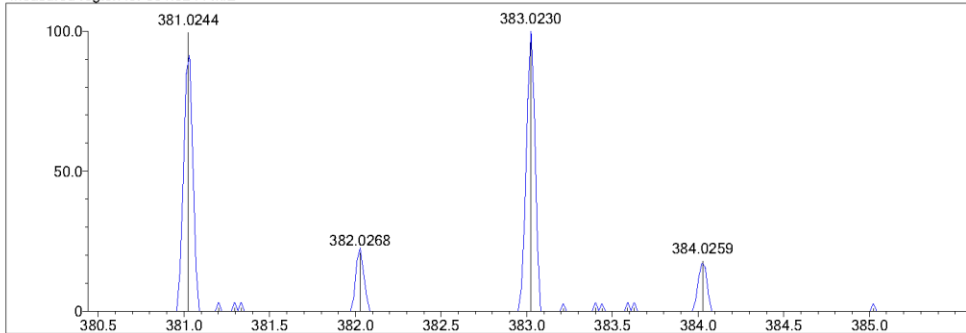
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

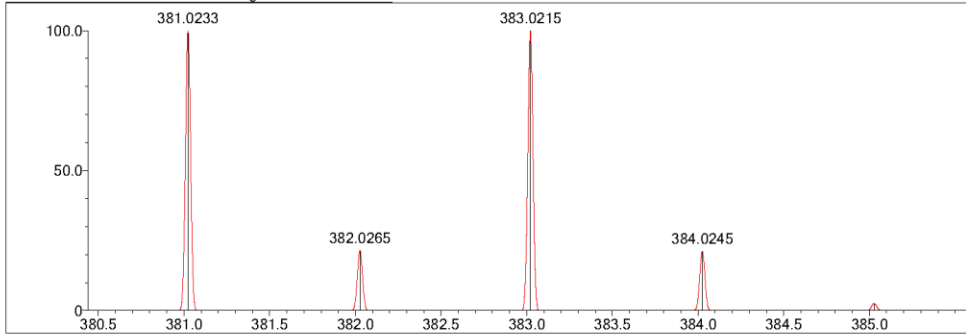
Event#: 1 MS(E+) Ret. Time : 0.942 Scan#: 189



Measured region for 381.0244 m/z

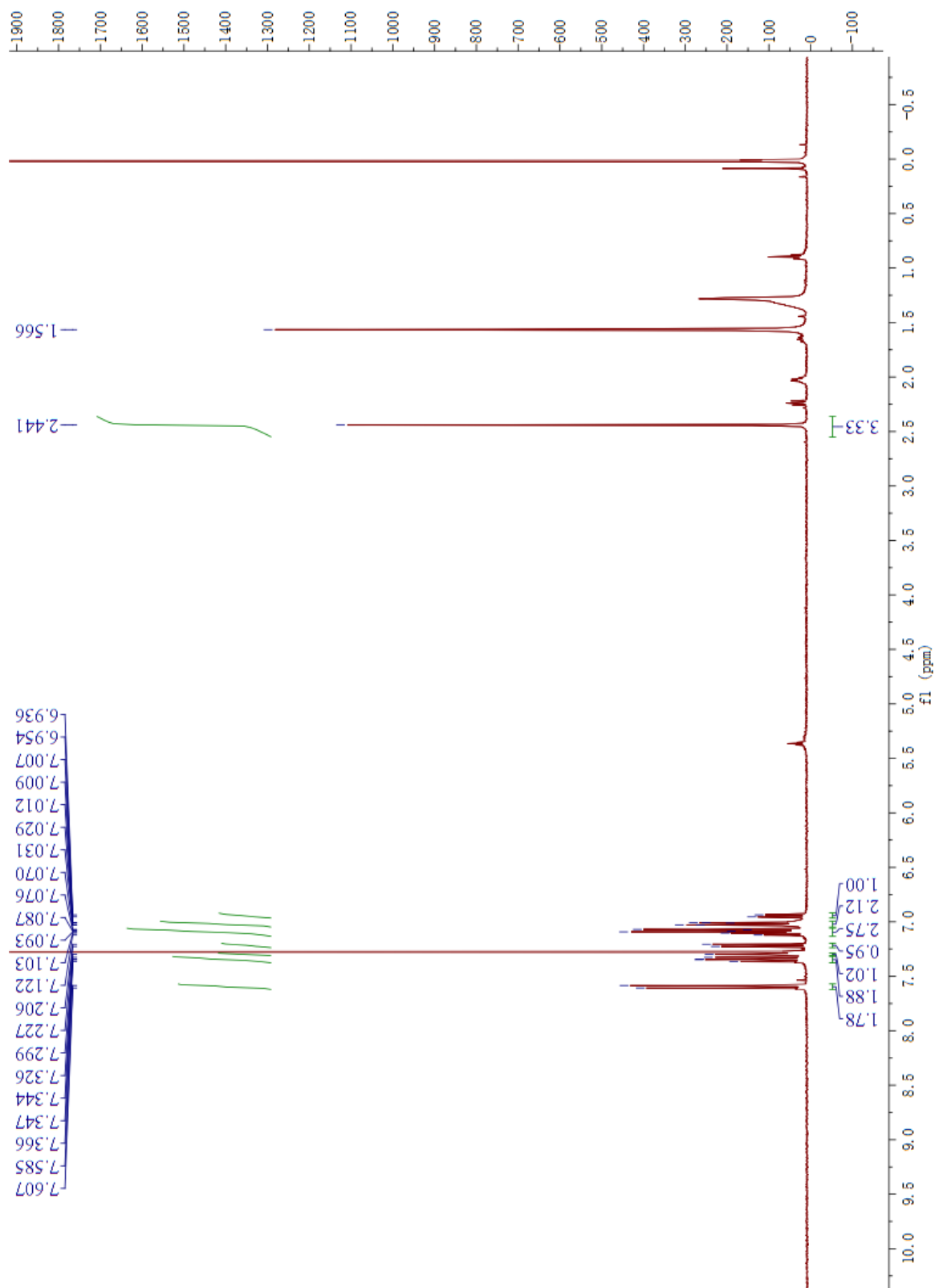


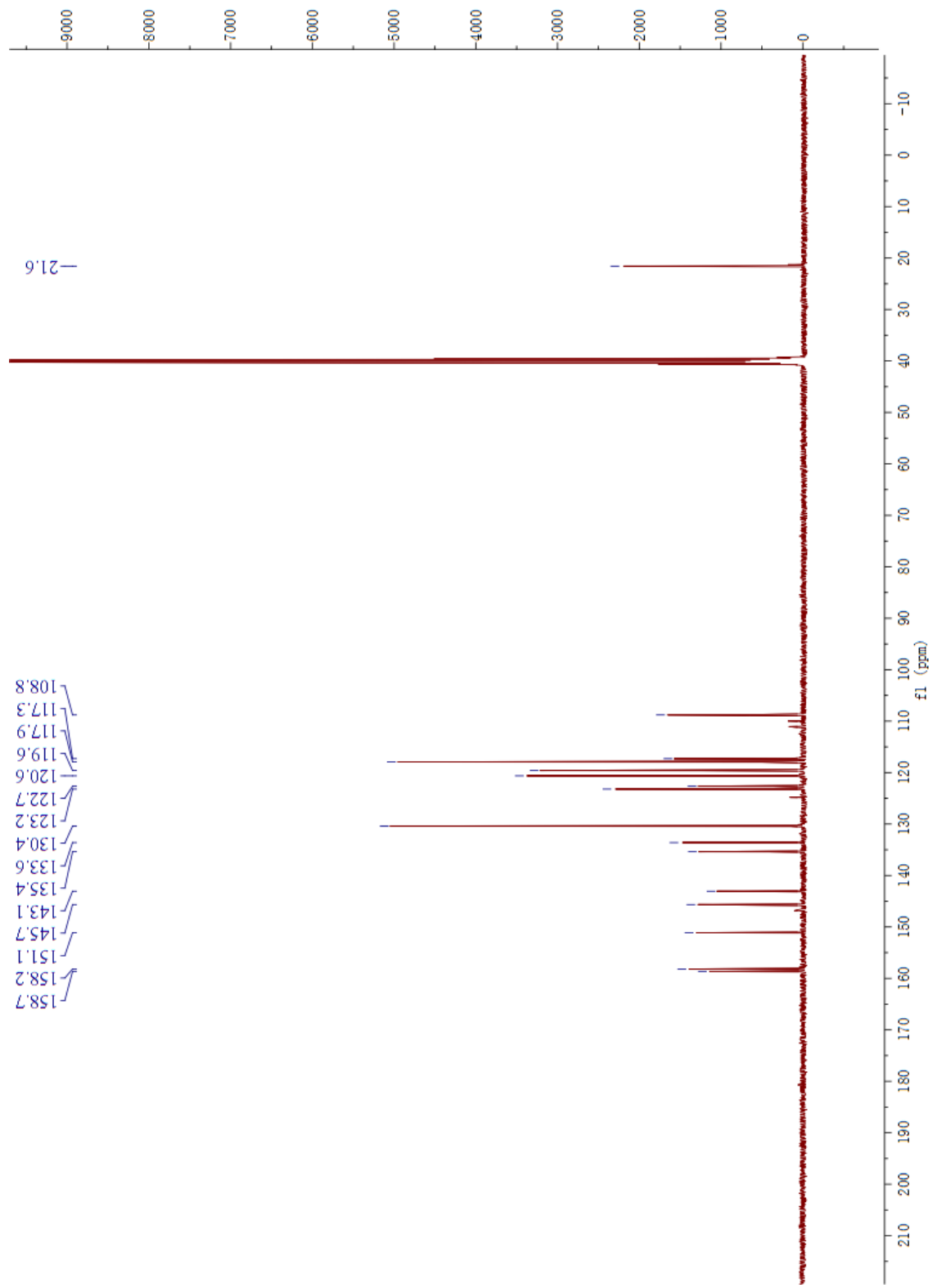
C19 H14 N2 O2 Br M+ : Predicted region for 381.0233 m/z



Rank	Score	Formula (M)	Ion	Mees. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	66.31	C19 H14 N2 O2 Br	M+	381.0244	381.0233	1.1	2.89	69.60	13.5

5-Methyl-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3r)

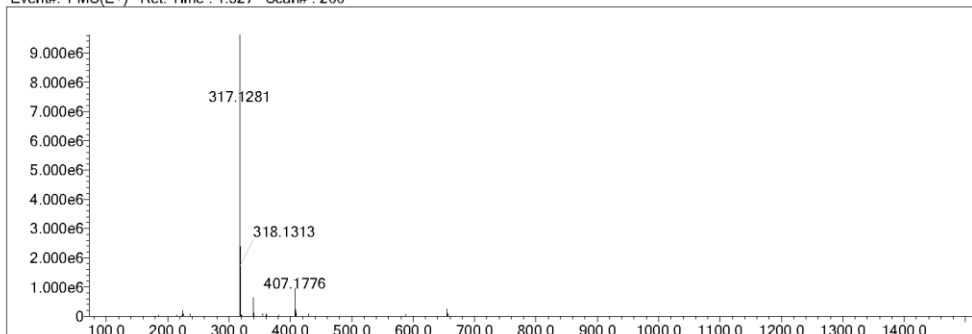




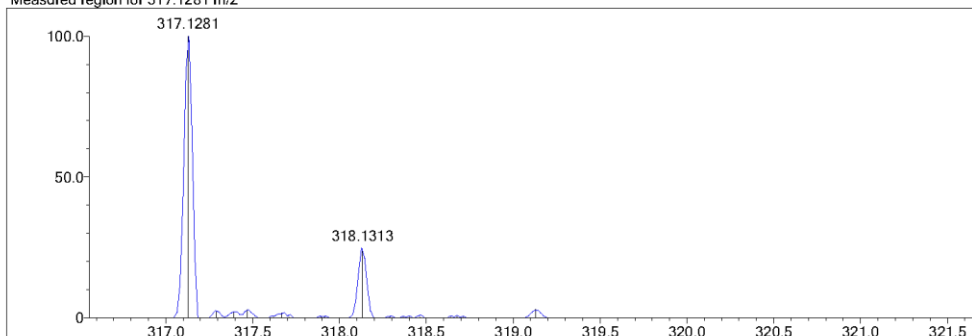
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	0	Cl	1	0	0	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100 DBE Range: -2.0 - 1000.0 Electron Ions: both
 HC Ratio: unlimited Apply N Rule: no Use MSn Info: no
 Max Isotopes: all Isotope RI (%): 1.00 Isotope Res: 10000
 MSn Iso RI (%): 75.00 MSn Logic Mode: AND Max Results: 500

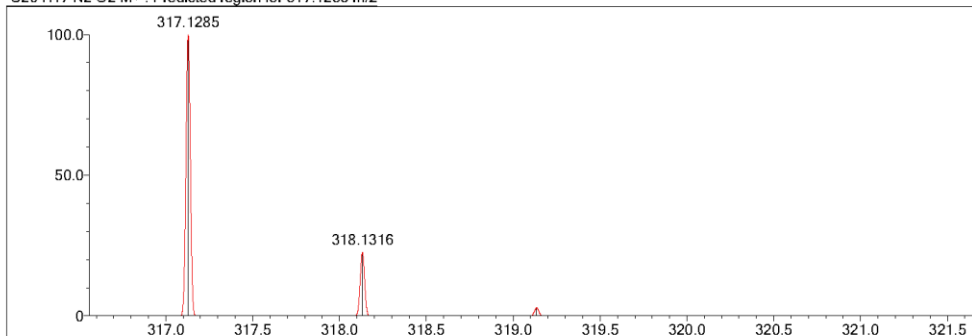
Event#: 1 MS(E+) Ret. Time : 1.327 Scan#: 266



Measured region for 317.1281 m/z

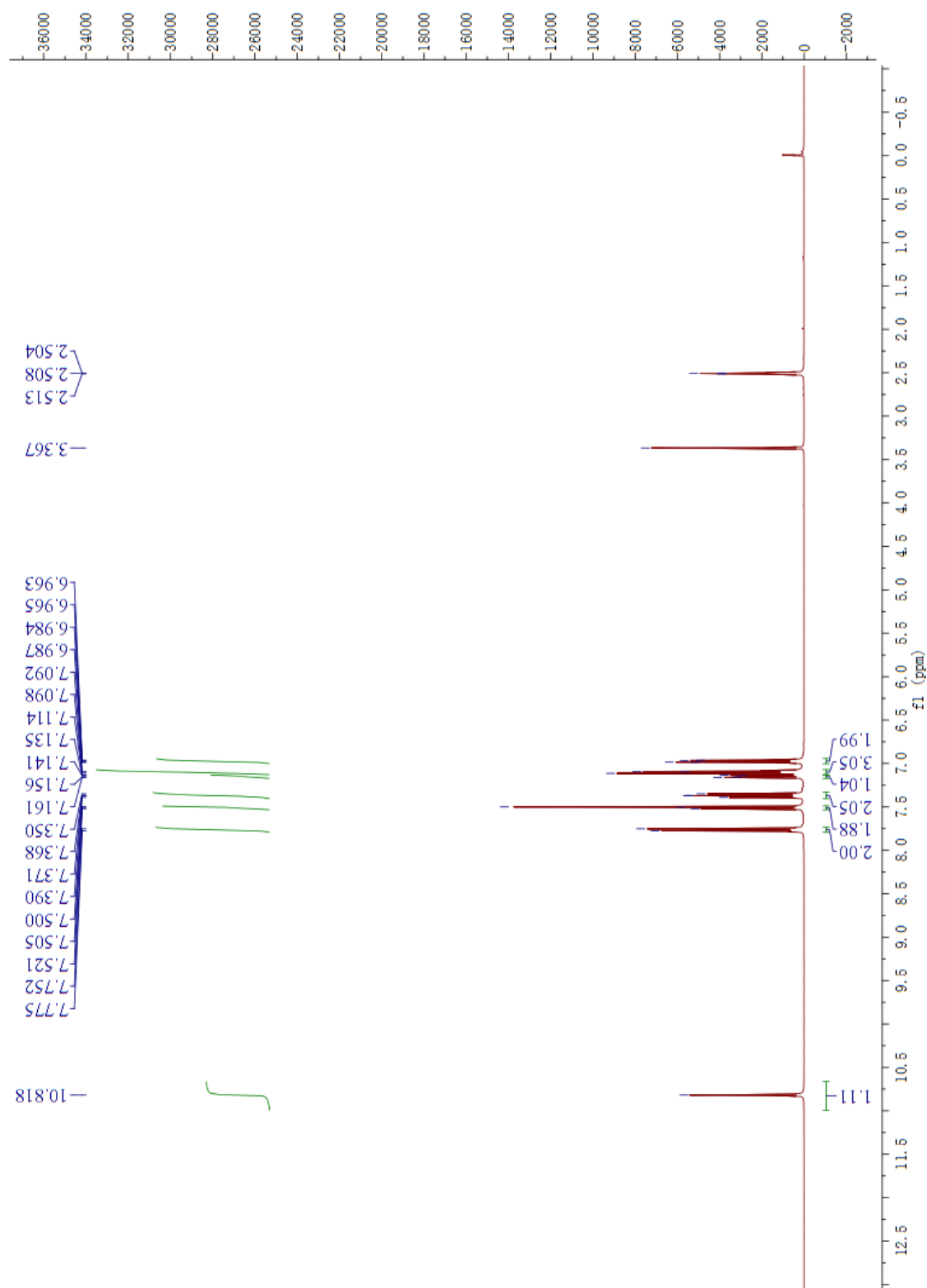


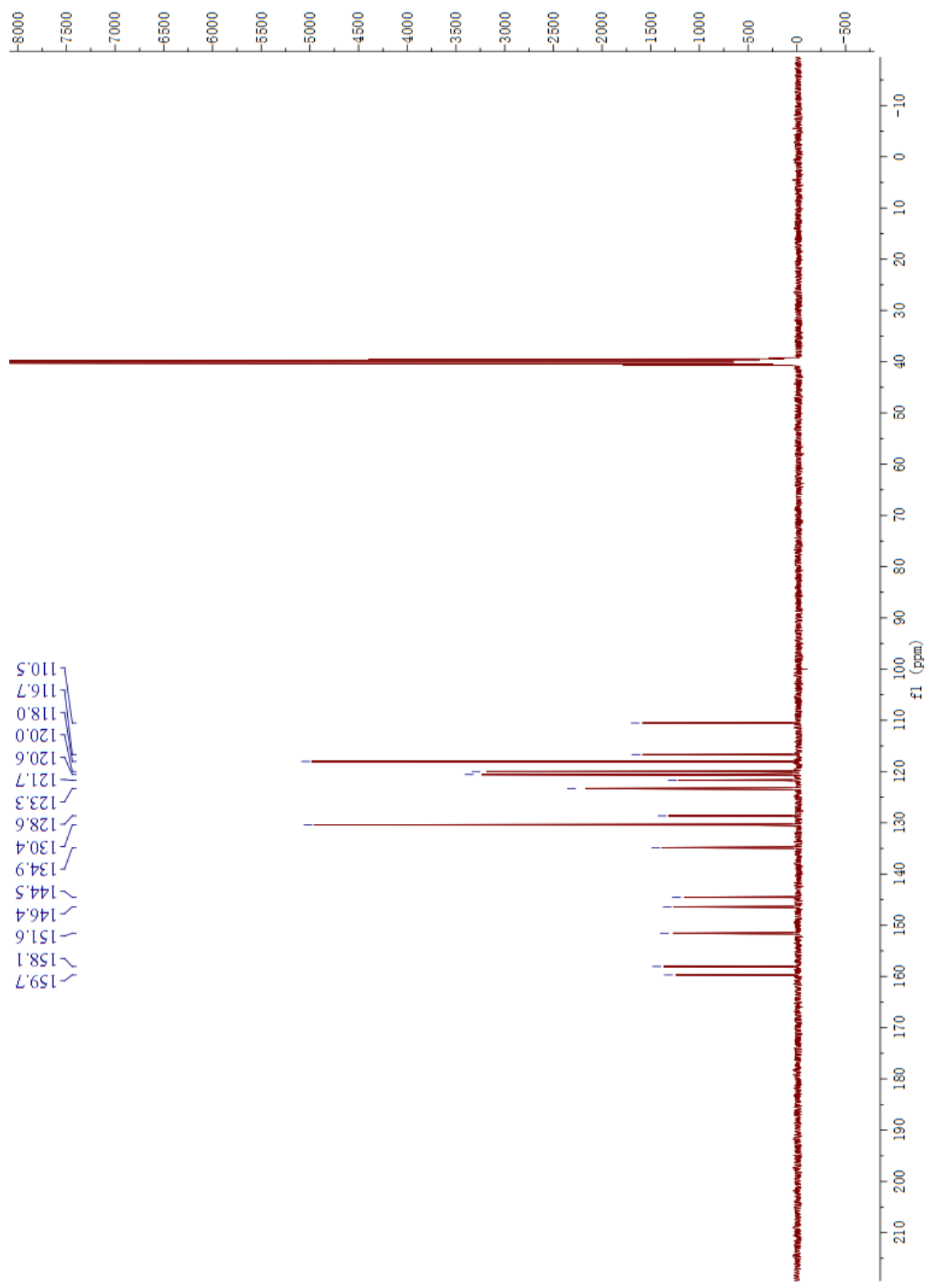
C20 H17 N2 O2 M+ : Predicted region for 317.1285 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	91.25	C20 H17 N2 O2	M+	317.1281	317.1285	-0.4	-1.26	91.85	13.5

6-Chloro-*N*-(4-phenoxyphenyl)benzo[*d*]oxazol-2-amine (3s)





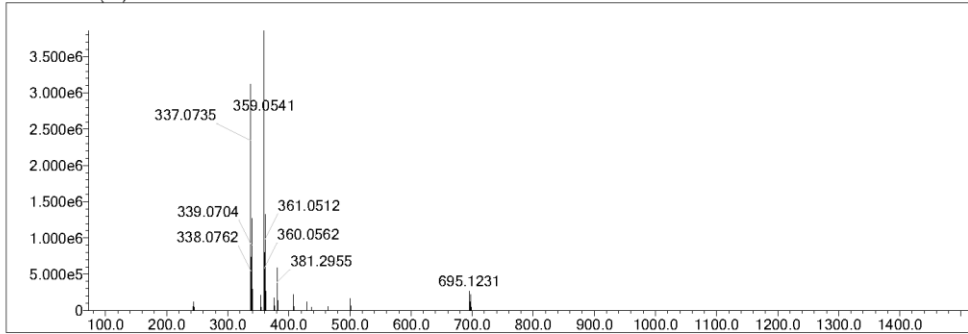
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

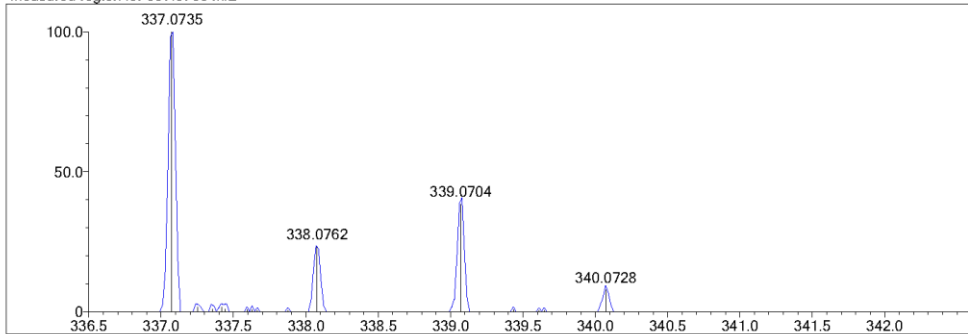
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

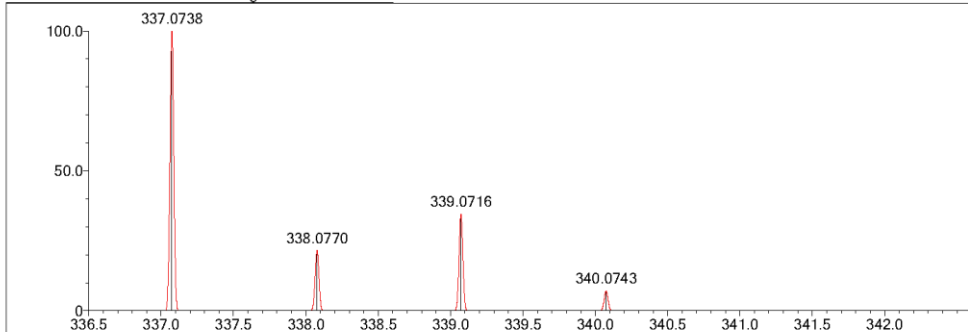
Event#: 1 MS(E+) Ret. Time : 1.112 -> 1.112 Scan#: 223 -> 223



Measured region for 337.0735 m/z

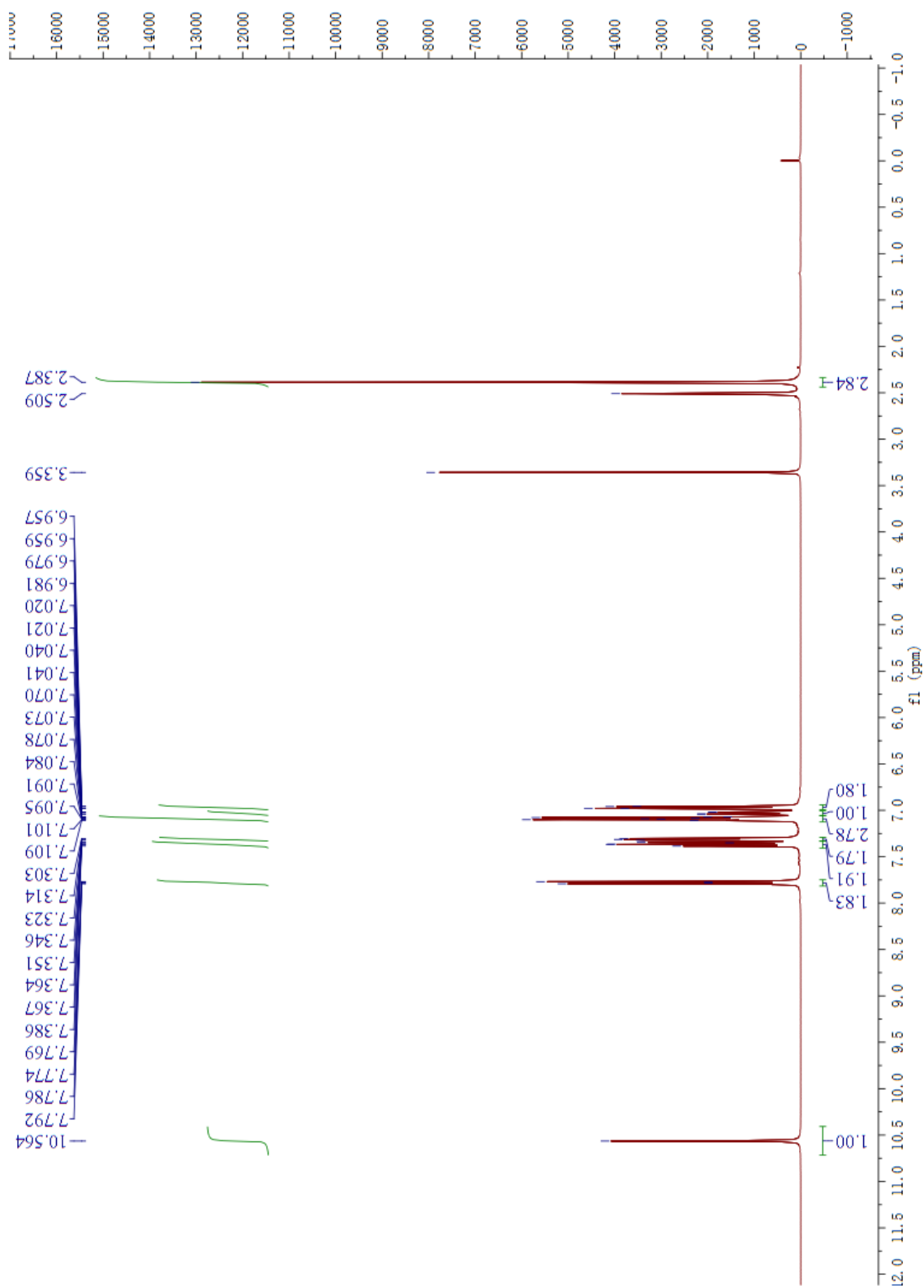


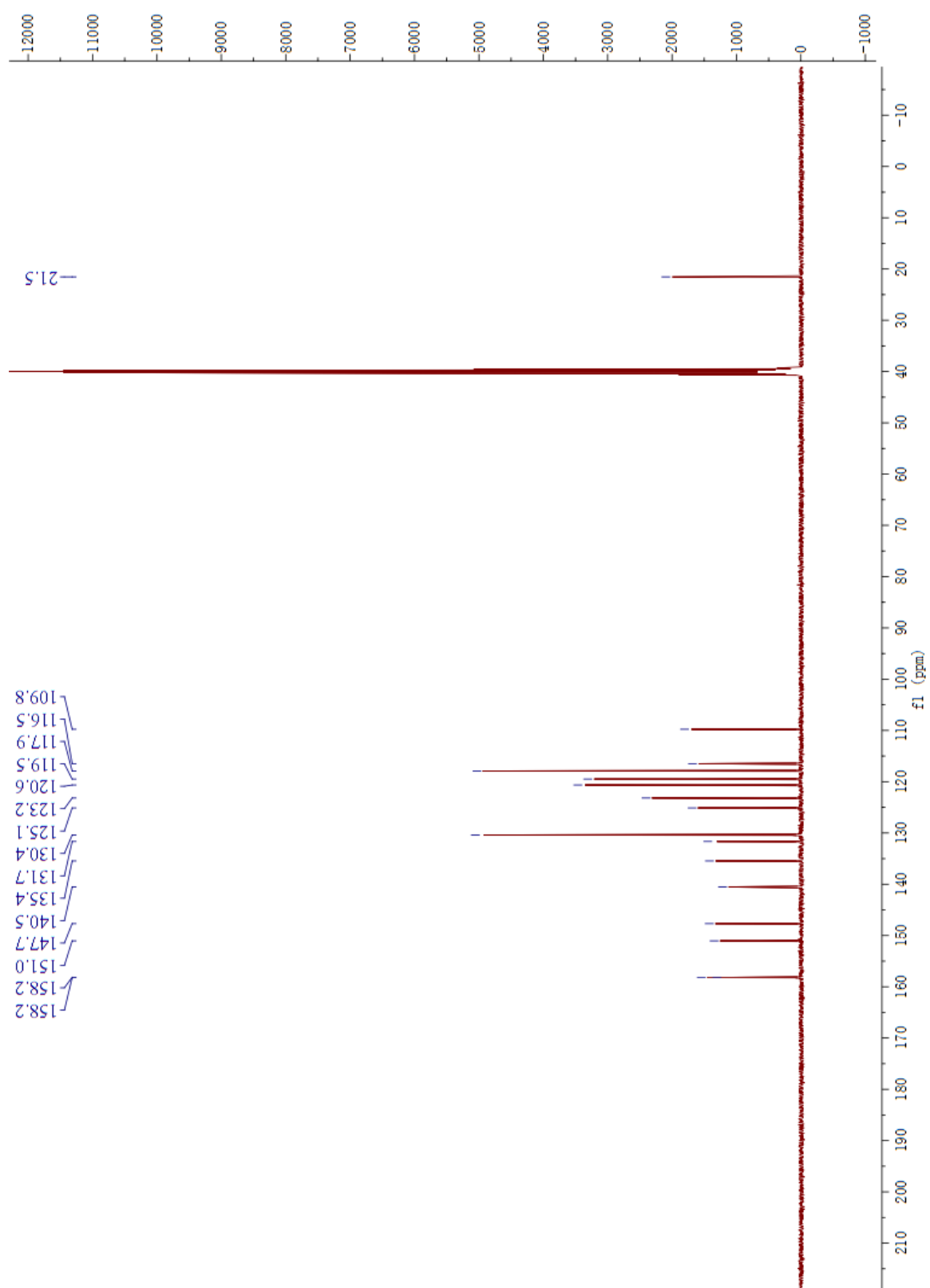
C19 H14 N2 O2 Cl M+ : Predicted region for 337.0738 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	85.89	C19 H14 N2 O2 Cl	M+	337.0735	337.0738	-0.3	-0.89	85.89	13.5

6-Methyl-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3t)





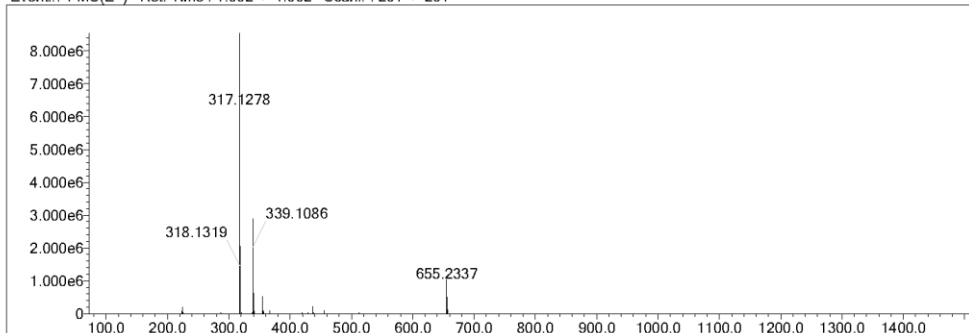
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

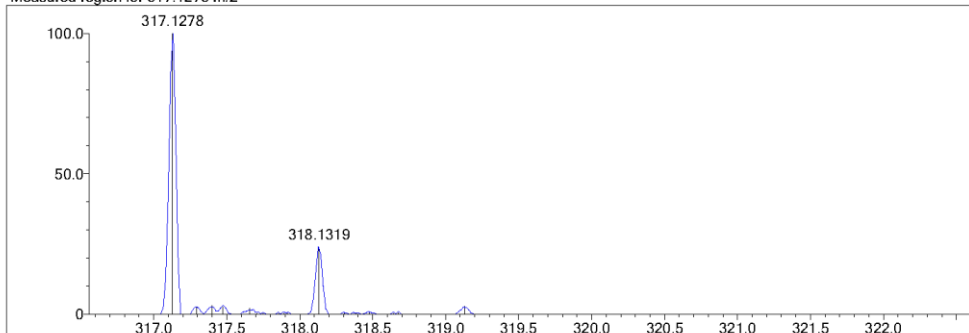
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

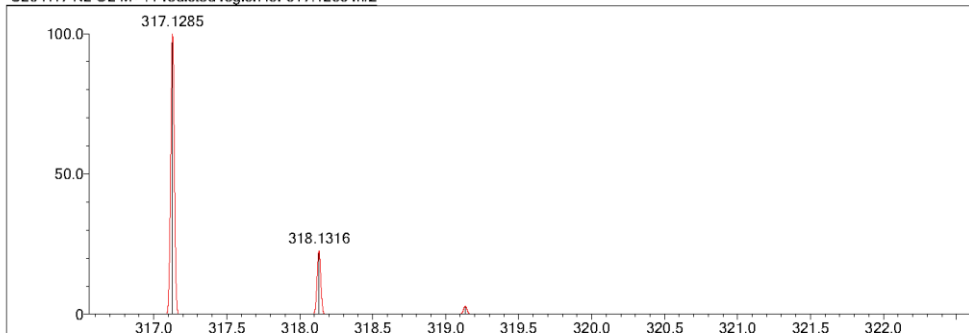
Event#: 1 MS(E+) Ret. Time : 1.002 -> 1.002 Scan#: 201 -> 201



Measured region for 317.1278 m/z

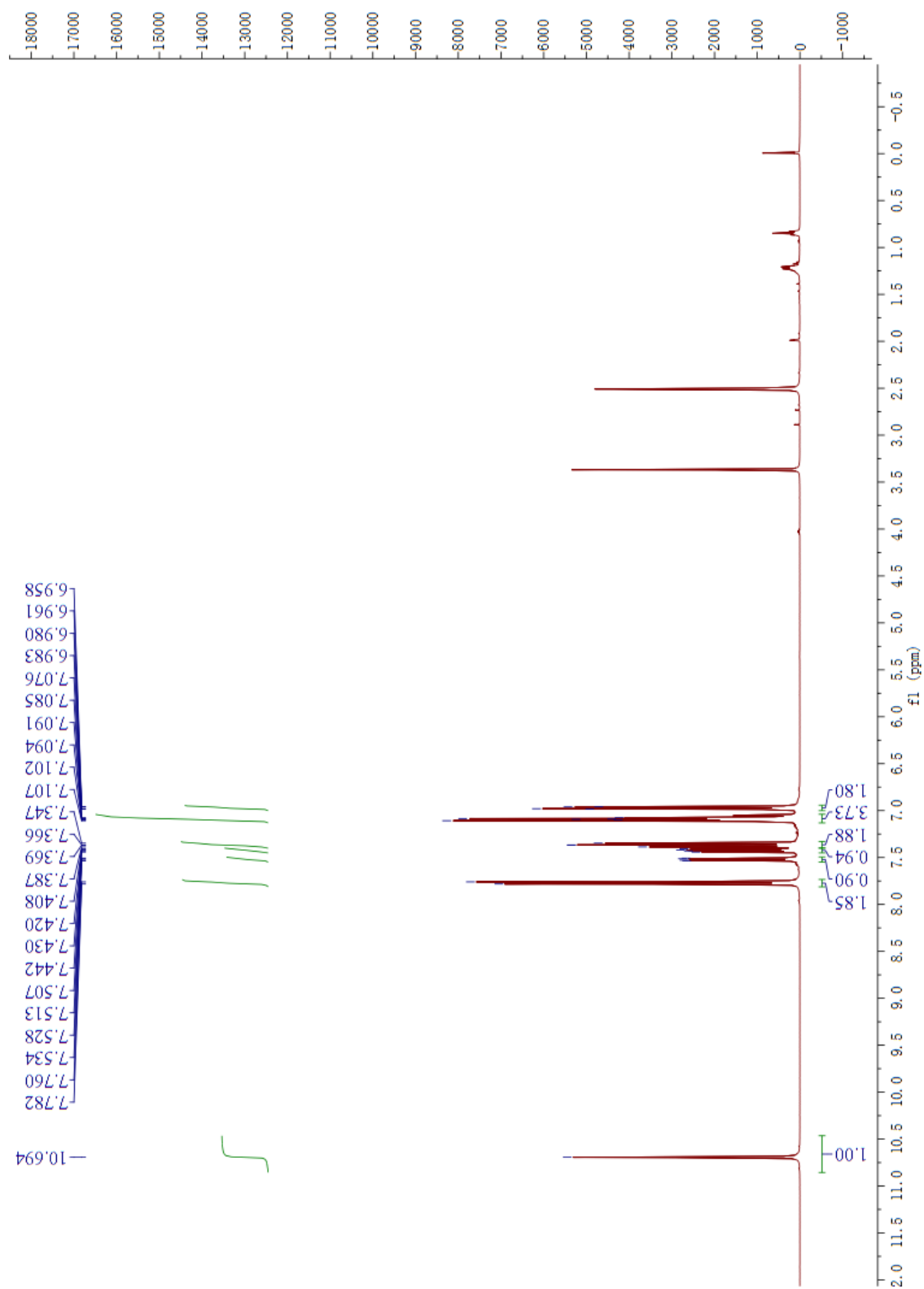


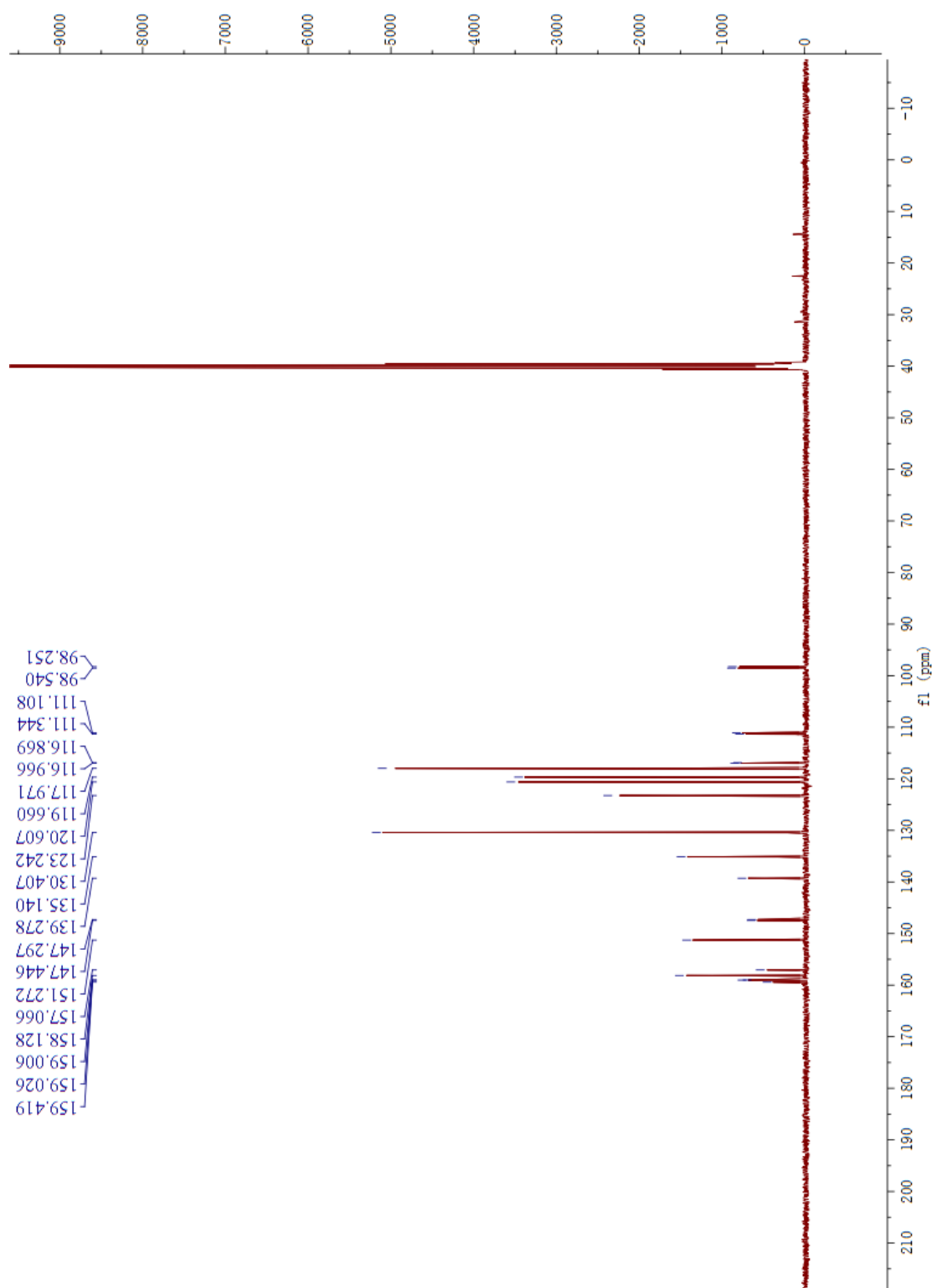
C20 H17 N2 O2 M+ : Predicted region for 317.1285 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.28	C20 H17 N2 O2	M+	317.1278	317.1285	-0.7	-2.21	91.03	13.5

6-Fluoro-N-(4-phenoxyphenyl)benzo[d]oxazol-2-amine (3u)





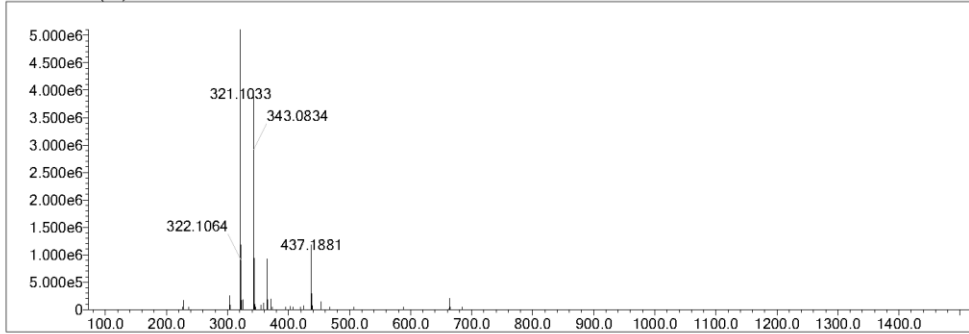
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	7	P	3	0	0	Cu	2	0	0	H
B	3	0	0	18O	2	0	0	S	2	0	0	Br	1	0	1	Na
C	4	0	38	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	3	Si	4	0	0	Ni	2	0	0					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

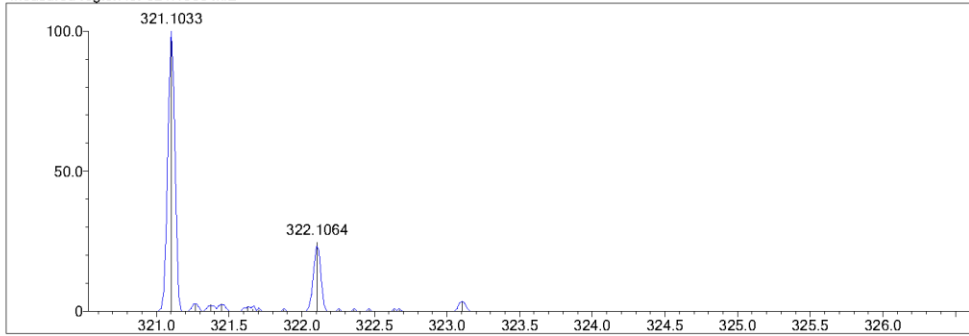
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

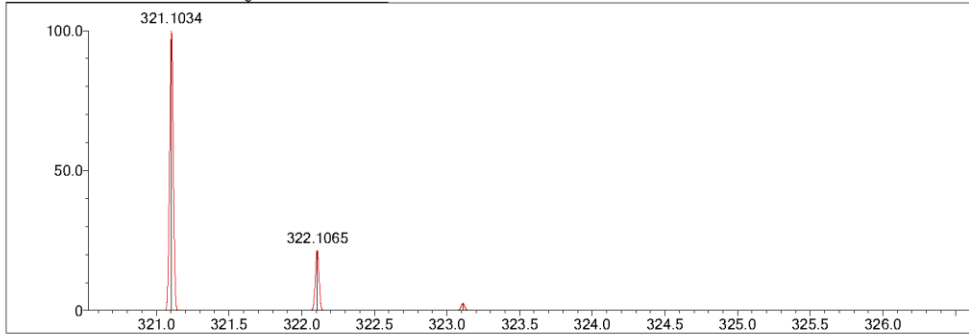
Event#: 1 MS(E+) Ret. Time : 0.952 Scan#: 191



Measured region for 321.1033 m/z



C19 H14 N2 O2 F M+ : Predicted region for 321.1034 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	83.32	C19 H14 N2 O2 F	M+	321.1033	321.1034	-0.1	-0.31	83.32	13.5