Supporting Information

Iodine-catalyzed oxidative annulation of 3-cyanoacetylindoles with benzylamines : facile access to 5-(3-indolyl)oxazoles

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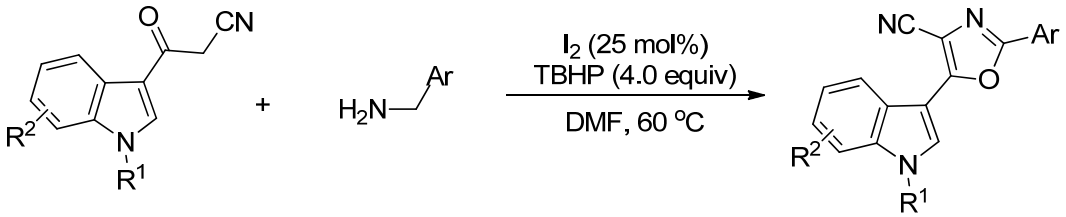
Table of Contents

1. General information

Unless otherwise noted, all commercial materials and solvents were used without further purification. Commercially available chemicals were obtained from Energy Chemical, TCI, Alfa Aesar and J&K. Thin layer chromatography (TLC) was carried out on GF254 plates (0.25 mm layer thickness) and visualized under UV light (254 nm). The silica gel (200-300 meshes) was used for column chromatography. ^{1}H NMR and ^{13}C NMR were recorded on Agilent 400 MHz spectrometer using TMS as internal standard. Spin multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), td (triplet of doublet), as well as brs (broad). Coupling constants (*J*) are given in hertz (Hz). High resolution mass spectra were obtained on Agilent 6210 ESI/TOF spectrometer.

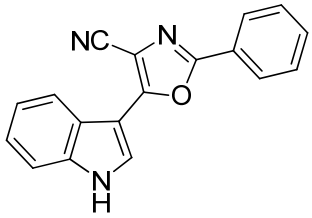
2. General procedure for the oxidative annulation of 3-cyanoacetylindoles with benzylamines



1 **2** **3**

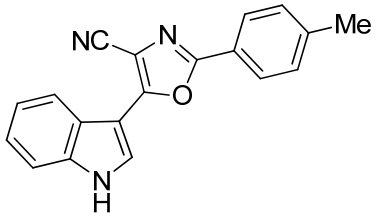
A 25 mL Schlenk tube was charged with a stir bar, 3-cyanoacetylindole **1**[1] (0.5 mmol), and DMF (3 mL) under air at room temperature. Then to the tube, benzylamine **2** (1.0 mmol, 2 equiv), TBHP (0.28 mL, 70% aqueous solution, 2.0 mmol, 4 equiv) and I_2 (32 mg, 25 mol%) were added. The resulting mixture was stirred at 60 ℃ for 7 hours. After that, the reaction mixture was cooled to room temperature, and concentrated under reduced pressure. The residue was purified by silica gel chromatography (Petroleum ether/EtOAc) to give the desired product.

3. Characterization data of products



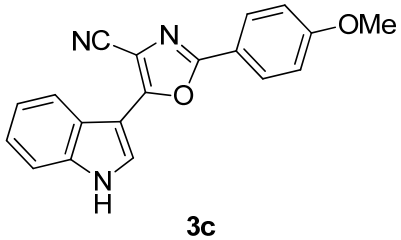
3a

5-(1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3a): Brown solid, 110 mg, 77% yield, mp 224.8-226.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.16 (d, J = 1.8 Hz, 1H), 8.08 (ddd, J = 9.1, 4.1, 1.9 Hz, 3H), 7.61 – 7.53 (m, 4H), 7.31 – 7.22 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.80, 157.48, 136.64, 131.77, 129.75, 127.98, 126.60, 125.87, 123.90, 123.56, 121.98, 120.41, 115.21, 113.14, 104.45, 101.49. HRMS-ESI (m/z): calcd for $C_{18}H_{12}N_3O$ $[M + H]^+$: 286.0975, found 286.0979.



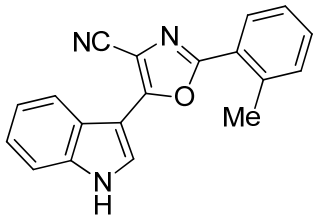
3b

5-(1*H*-indol-3-yl)-2-(*p*-tolyl)oxazole-4-carbonitrile (3b): Brown solid, 116 mg, 78% yield, mp 261.6-262.6 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.23 – 12.11 (m, 1H), 8.19 (d, J = 2.9 Hz, 1H), 8.14 – 8.06 (m, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.64 – 7.51 (m, 1H), 7.42 (d, J = 8.0 Hz, 2H), 7.36 – 7.22 (m, 2H), 2.40 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.16, 157.27, 141.99, 136.70, 130.40, 128.00, 126.68, 123.96, 123.61, 123.26, 122.02, 120.45, 115.30, 113.20, 104.48, 101.55, 21.62. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1129.



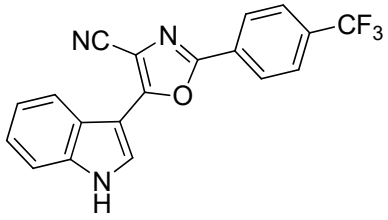
3c

5-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)oxazole-4-carbonitrile (3c): Pale yellow solid, 106 mg, 67% yield, mp 250.9-252.3 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.12 (d, J = 3.0 Hz, 1H), 8.11 (d, J = 2.9 Hz, 1H), 8.08 – 8.02 (m, 1H), 8.01 – 7.93 (m, 2H), 7.60 – 7.49 (m, 1H), 7.33 – 7.19 (m, 2H), 7.09 (d, J = 8.9 Hz, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.04, 159.00, 156.93, 136.64, 128.42, 127.65, 123.92, 123.49, 121.86, 120.39, 118.39, 115.34, 115.14, 113.10, 104.32, 101.61, 55.86. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O_2$ $[M + H]^+$: 316.1081, found 316.1079.



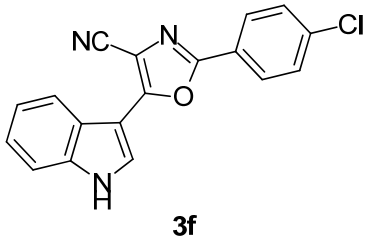
3d

5-(1*H*-indol-3-yl)-2-(*o*-tolyl)oxazole-4-carbonitrile (3d): Pale yellow solid, 97 mg, 65% yield, mp 252.0-253.6 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.23 – 8.10 (m, 1H), 8.08 – 7.92 (m, 2H), 7.62 – 7.50 (m, 1H), 7.41 (dq, J = 12.6, 7.6, 7.1 Hz, 3H), 7.32 – 7.13 (m, 2H), 2.65 (d, J = 3.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.99, 156.85, 137.63, 136.68, 132.23, 131.23, 128.89, 127.94, 126.90, 124.79, 123.92, 123.49, 121.89, 120.23, 115.35, 113.14, 104.50, 101.47, 22.20. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1130.



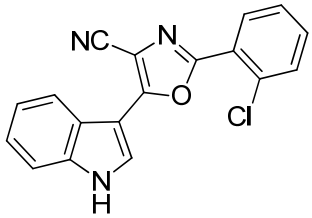
3e

5-(1*H*-indol-3-yl)-2-(4-(trifluoromethyl)phenyl)oxazole-4-carbonitrile (3e): Brown solid, 92 mg, 52% yield, mp 300.7-301.3 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.21 (s, 1H), 8.22 (d, J = 8.1 Hz, 2H), 8.17 (s, 1H), 8.10 – 8.04 (m, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.54 (dd, J = 6.1, 3.1 Hz, 1H), 7.26 (dd, J = 6.3, 2.7 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.10, 157.37, 136.67, 131.20 (q, J = 32.1 Hz), 129.43 (d, J = 1.5 Hz), 128.38, 127.30, 126.67 (q, J = 3.8 Hz), 124.27(q, J = 271 Hz), 123.87, 123.65, 122.07, 120.41, 114.94, 113.20, 104.76, 101.32. HRMS-ESI (m/z): calcd for $C_{19}H_{11}F_3N_3O$ $[M + H]^+$: 354.0849, found 354.0851.



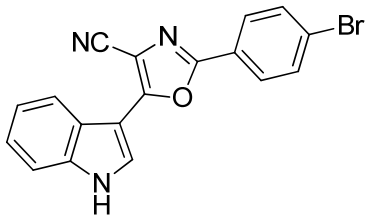
3f

2-(4-chlorophenyl)-5-(1H-indol-3-yl)oxazole-4-carbonitrile (3f): Brown solid, 99 mg, 62% yield, mp 286.2-287.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.15 (s, 1H), 8.05 (dd, J = 8.5, 6.9 Hz, 3H), 7.66 – 7.59 (m, 2H), 7.57 – 7.50 (m, 1H), 7.25 (qd, J = 7.2, 6.8, 3.4 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.90, 157.67, 136.66, 136.46, 129.88, 128.34, 128.15, 124.70, 123.88, 123.60, 122.00, 120.43, 115.09, 113.16, 104.55, 101.41. HRMS-ESI (m/z): calcd for $C_{18}H_{11}ClN_3O$ $[M + H]^+$: 320.0585, found 320.0586.



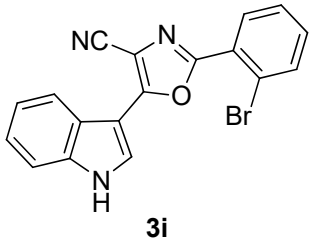
3g

2-(2-chlorophenyl)-5-(1*H*-indol-3-yl)oxazole-4-carbonitrile (3g): Brown solid, 126 mg, 79% yield, mp 217.9-219.7 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.23 (s, 1H), 8.22 (s, 1H), 8.19 – 8.04 (m, 2H), 7.79 – 7.68 (m, 1H), 7.60 (tdd, J = 7.2, 5.8, 4.3 Hz, 3H), 7.36 – 7.21 (m, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 157.72, 156.71, 136.74, 133.10, 131.82, 131.75, 131.64, 128.40, 128.34, 124.70, 123.94, 123.67, 122.08, 120.34, 115.08, 113.27, 104.58, 101.29. HRMS-ESI (m/z): calcd for $C_{18}H_{11}ClN_3O$ [M + H]$^+$: 320.0585, found 320.0587.



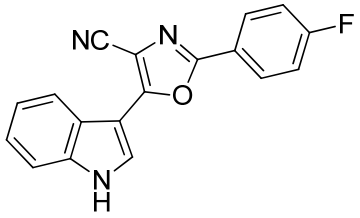
3h

2-(4-bromophenyl)-5-(1*H*-indol-3-yl)oxazole-4-carbonitrile (3h): Brown solid, 107 mg, 59% yield, mp 309.6-310.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.18 (s, 1H), 8.16 (s, 1H), 8.10 – 8.02 (m, 1H), 8.00 – 7.92 (m, 2H), 7.75 (dt, J = 8.5, 1.6 Hz, 2H), 7.54 (dd, J = 7.8, 1.8 Hz, 1H), 7.26 (td, J = 6.4, 5.3, 3.6 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.96, 157.67, 136.65, 132.78, 128.45, 128.15, 125.33, 125.02, 123.87, 123.60, 122.00, 120.42, 115.08, 113.16, 104.55, 101.41. HRMS-ESI (m/z): calcd for $C_{18}H_{11}BrN_3O$ [M + H]$^+$: 364.0080, found 364.0083.



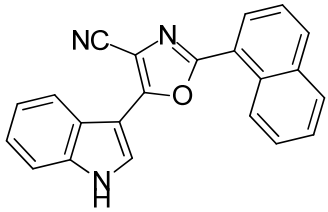
3i

2-(2-bromophenyl)-5-(1H-indol-3-yl)oxazole-4-carbonitrile (3i): Pale yellow solid, 115 mg, 63% yield, mp 203.7-205.4 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.21 (s, 1H), 8.19 (dd, J = 3.0, 1.4 Hz, 1H), 8.10 – 7.98 (m, 2H), 7.86 (dt, J = 8.0, 1.2 Hz, 1H), 7.70 – 7.42 (m, 3H), 7.34 – 7.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.72, 157.33, 136.70, 134.99, 133.13, 132.06, 128.73, 128.28, 126.74, 123.88, 123.59, 122.02, 120.72, 120.40, 115.06, 113.19, 104.45, 101.27. HRMS-ESI (m/z): calcd for $C_{18}H_{11}BrN_3O$ [M + H]$^+$: 364.0080, found 364.0081.



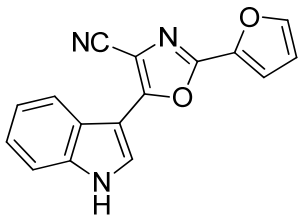
3j

2-(4-fluorophenyl)-5-(1*H*-indol-3-yl)oxazole-4-carbonitrile (3j): Pale yellow solid, 90 mg, 60% yield, mp 272.5-273.3 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.16 (d, J = 2.9 Hz, 1H), 8.14 – 8.04 (m, 3H), 7.57 – 7.52 (m, 1H), 7.41 (td, J = 8.9, 2.2 Hz, 2H), 7.26 (hept, J = 5.4 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.21 (d, J = 249.8 Hz), 157.79 (d, J = 53.7 Hz), 136.65, 129.23 (d, J = 9.0 Hz), 128.00, 123.89, 123.57, 122.57 (d, J = 3.0 Hz), 121.96, 120.42, 117.07, 116.85, 115.14, 113.14, 104.44, 101.44. HRMS-ESI (m/z): calcd for $C_{18}H_{11}FN_3O$ $[M + H]^+$: 304.0881, found 304.0882.



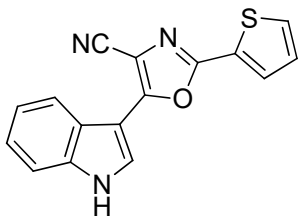
3k

5-(1*H*-indol-3-yl)-2-(naphthalen-1-yl)oxazole-4-carbonitrile (3k): Yellow solid, 112 mg, 67% yield, mp 278.9-280.8 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.22 (s, 1H), 9.21 (d, J = 8.7 Hz, 1H), 8.42 – 8.33 (m, 1H), 8.23 (d, J = 2.6 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 8.12 (dd, J = 6.9, 2.5 Hz, 1H), 8.06 (d, J = 8.2 Hz, 1H), 7.77 – 7.68 (m, 2H), 7.64 (t, J = 7.5 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.31 – 7.25 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.41, 157.00, 136.71, 133.94, 132.51, 129.48, 129.28, 128.65, 128.50, 128.19, 127.09, 125.82, 125.77, 123.98, 123.58, 122.02, 121.83, 120.36, 115.30, 113.20, 104.60, 101.46. HRMS-ESI (m/z): calcd for $C_{22}H_{14}N_3O$ $[M + H]^+$: 336.1131, found 336.1133.



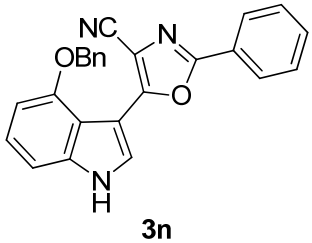
3l

2-(furan-2-yl)-5-(1*H*-indol-3-yl)oxazole-4-carbonitrile (3l): Brown solid, 82 mg, 60% yield, mp 291.3-292.5 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.21 (s, 1H), 8.18 (s, 1H), 8.13 – 7.92 (m, 2H), 7.69 – 7.49 (m, 1H), 7.43 (d, J = 3.5 Hz, 1H), 7.37 – 7.20 (m, 2H), 6.81 (dd, J = 3.6, 1.8 Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 156.92, 151.66, 146.95, 141.15, 136.69, 128.15, 123.93, 123.67, 122.04, 120.45, 115.03, 114.11, 113.23, 113.10, 104.33, 101.20. HRMS-ESI (m/z): calcd for $C_{16}H_{10}N_3O_2$ $[M + H]^+$: 276.0768, found 276.0769.



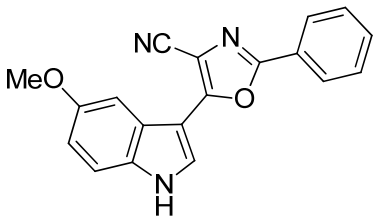
3m

5-(1*H*-indol-3-yl)-2-(thiophen-2-yl)oxazole-4-carbonitrile (3m): Pale yellow solid, 86 mg, 59% yield, mp 238.8-240.0 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.20 (s, 1H), 8.17 (s, 1H), 8.13 – 8.01 (m, 1H), 7.92 (ddd, *J* = 9.5, 4.4, 1.2 Hz, 2H), 7.63 – 7.51 (m, 1H), 7.28 (ddt, *J* = 9.2, 7.1, 3.3 Hz, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 157.03, 155.21, 136.69, 131.38, 130.00, 129.24, 128.10, 127.79, 123.93, 123.65, 122.05, 120.45, 115.02, 113.22, 104.31, 101.29. HRMS-ESI (m/z): calcd for $C_{16}H_{10}N_3OS$ $[M + H]^+$: 292.0539, found 292.0541.



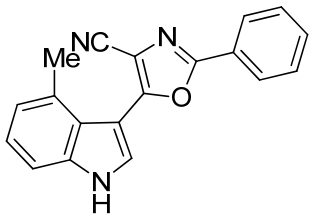
3n

5-(4-(benzyloxy)-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3n): Brown solid, 120 mg, 61% yield, mp 153.9-155.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.86 – 7.79 (m, 2H), 7.65 (d, *J* = 2.7 Hz, 1H), 7.45 – 7.36 (m, 1H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 8.2 Hz, 3H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.99 (d, *J* = 6.7 Hz, 3H), 6.72 (d, *J* = 7.8 Hz, 1H), 5.16 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.90, 156.21, 152.87, 137.94, 136.58, 130.76, 128.68, 128.25, 127.65, 126.97, 126.50, 126.11, 126.07, 124.74, 115.47, 114.51, 110.21, 105.18, 103.03, 101.23, 70.24. HRMS-ESI (m/z): calcd for $C_{25}H_{18}N_3O_2$ $[M + H]^+$: 392.1394, found 392.1396.



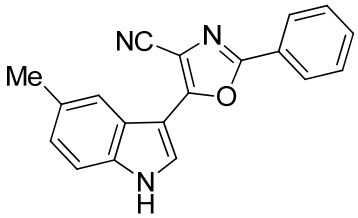
3o

5-(5-methoxy-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (**3o**). Yellow solid, 90 mg, 57% yield, mp 226.5-227.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.06 (s, 1H), 8.12 (d, *J* = 3.0 Hz, 1H), 8.08 – 8.01 (m, 2H), 7.62 – 7.56 (m, 3H), 7.52 (d, *J* = 2.4 Hz, 1H), 7.44 (d, *J* = 8.8 Hz, 1H), 6.91 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.66, 157.52, 155.40, 131.76, 131.64, 129.79, 128.32, 126.52, 125.93, 124.51, 115.34, 113.95, 113.39, 104.19, 102.11, 101.31, 55.68. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O_2$ $[M + H]^+$: 316.1081, found 316.1078.



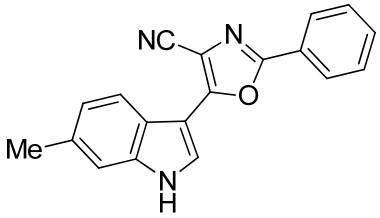
3p

5-(4-methyl-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3p): Brown solid, 102 mg, 68% yield, mp 202.1-203.4 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.31 – 11.93 (m, 1H), 8.25 – 7.96 (m, 3H), 7.58 (dd, J = 5.0, 2.0 Hz, 3H), 7.38 (d, J = 8.0 Hz, 1H), 7.20 – 7.04 (m, 1H), 7.06 – 6.84 (m, 1H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.30, 157.15, 137.26, 132.01, 129.88, 129.71, 126.69, 125.95, 124.15, 123.41, 123.01, 114.83, 110.90, 109.46, 99.98, 21.09. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1129.



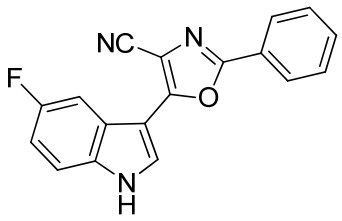
3q

5-(5-methyl-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3q): Brown solid, 104 mg, 70% yield, mp 226.7-228.4 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.06 (s, 1H), 8.14 – 7.98 (m, 3H), 7.83 (s, 1H), 7.67 – 7.51 (m, 3H), 7.43 (d, J = 8.3 Hz, 1H), 7.09 (dd, J = 8.4, 1.6 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.75, 157.66, 135.02, 131.76, 130.84, 129.79, 127.95, 126.60, 125.95, 125.16, 124.19, 119.92, 115.31, 112.83, 104.32, 101.05, 21.96. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1132.



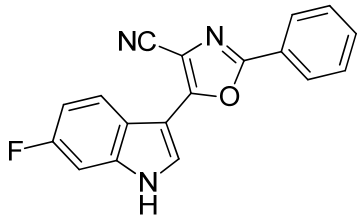
3r

5-(6-methyl-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3r): Brown solid, 104 mg, 70% yield, mp 245.5-247.2 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.03 (s, 1H), 8.25 – 8.03 (m, 3H), 7.96 (d, J = 8.2 Hz, 1H), 7.59 (dd, J = 5.2, 1.8 Hz, 3H), 7.33 (dt, J = 1.6, 0.8 Hz, 1H), 7.20 – 6.98 (m, 1H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.66, 157.57, 137.07, 132.90, 131.72, 129.74, 127.35, 126.56, 125.90, 123.68, 121.78, 120.07, 115.25, 112.79, 104.22, 101.40, 21.72. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1132.



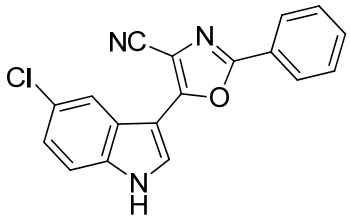
3s

5-(5-fluoro-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3s): Pale yellown solid, 101 mg, 66% yield, mp 277.4-279.1 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.29 (s, 1H), 8.25 (s, 1H), 8.09 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.76 (dd, *J* = 9.8, 2.5 Hz, 1H), 7.59 (dt, *J* = 11.1, 4.2 Hz, 4H), 7.15 (td, *J* = 9.2, 2.5 Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.09, 158.60 (d, *J* = 233.3 Hz), 157.02, 133.41, 131.91, 129.83, 129.80 (d, *J* = 5.1 Hz), 126.75, 125.86, 124.26 (d, *J* = 10.8 Hz), 115.12, 114.57 (d, *J* = 9.9 Hz), 111.98 (d, *J* = 26.0 Hz), 105.34 (d, *J* = 24.8 Hz), 104.74, 101.77 (d, *J* = 4.5 Hz). HRMS-ESI (m/z): calcd for $C_{18}H_{11}FN_3O$ $[M + H]^+$: 304.0881, found 304.0882.



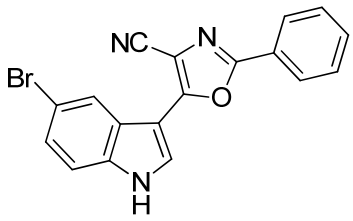
3t

5-(6-fluoro-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3t): Pale yellown solid, 108 mg, 71% yield, mp 270.4-272.0 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.21 (s, 1H), 8.19 (s, 1H), 8.15 – 7.95 (m, 3H), 7.70 – 7.52 (m, 3H), 7.36 (dd, *J* = 9.7, 2.4 Hz, 1H), 7.15 (td, *J* = 9.2, 2.4 Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ159.98 (d, *J* = 235.5 Hz), 159.10, 157.09, 136.80 (d, *J* = 13.0 Hz), 131.97, 129.85, 128.78 (d, *J* = 2.9 Hz), 126.77, 125.87, 121.80 (d, *J* = 10.0 Hz), 120.76, 115.09, 110.63 (d, *J* = 24.5 Hz), 104.93, 101.69, 99.34 (d, *J* = 26.0 Hz). HRMS-ESI (m/z): calcd for $C_{18}H_{11}FN_3O$ $[M + H]^+$: 304.0881, found 304.0882.



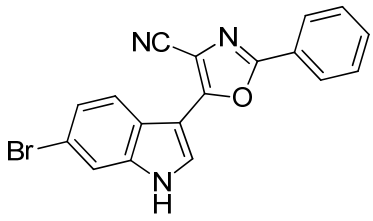
3u

5-(5-chloro-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3u): Brown solid, 110 mg, 69% yield, mp 282.4-283.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.33 (s, 1H), 8.22 (s, 1H), 8.04 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.99 (t, *J* = 1.7 Hz, 1H), 7.62 – 7.52 (m, 4H), 7.27 (dt, *J* = 8.7, 1.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.03, 156.67, 135.17, 131.85, 129.75, 129.43, 126.58, 126.45, 125.79, 124.85, 123.59, 119.44, 115.00, 114.74, 104.95, 101.26. HRMS-ESI (m/z): calcd for $C_{18}H_{11}ClN_3O$ $[M + H]^+$: 320.0585, found 320.0586.



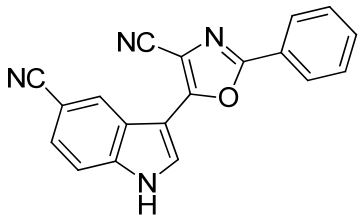
3v

5-(5-bromo-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3v): Brown solid, 127 mg, 70% yield, mp 297.6-298.2 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 – 12.30 (m, 1H), 8.23 (d, J = 2.8 Hz, 1H), 8.17 (d, J = 1.9 Hz, 1H), 8.05 (dd, J = 6.7, 2.8 Hz, 2H), 7.60 (dd, J = 5.3, 1.9 Hz, 3H), 7.53 (d, J = 8.7 Hz, 1H), 7.40 (dd, J = 8.6, 1.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.14, 156.67, 135.46, 131.91, 129.80, 129.40, 126.63, 126.18, 125.84, 125.55, 122.50, 115.20, 115.01, 114.44, 105.13, 101.15. HRMS-ESI (m/z): calcd for $C_{18}H_{11}BrN_3O$ $[M + H]^+$: 364.0080, found 364.0081.



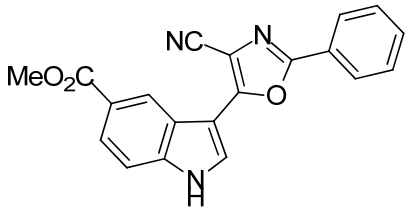
3w

5-(6-bromo-1H-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3w): Brown solid, 115 mg, 63% yield, mp 302.9-304.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.10 (dd, J = 6.7, 2.9 Hz, 2H), 8.04 (d, J = 8.6 Hz, 1H), 7.77 (d, J = 1.7 Hz, 1H), 7.67 – 7.57 (m, 3H), 7.41 (dd, J = 8.6, 1.8 Hz, 1H), 7.35 – 7.17 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.92, 161.60, 142.31, 136.71, 134.57, 133.70, 131.50, 130.58, 129.65, 127.73, 126.98, 121.02, 120.56, 119.76, 109.84, 106.50. HRMS-ESI (m/z): calcd for $C_{18}H_{11}BrN_3O$ $[M + H]^+$: 364.0080, found 364.0081.



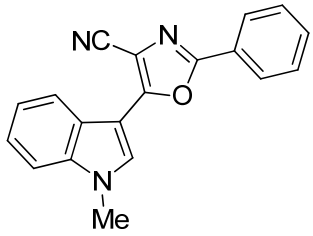
3x

5-(5-cyano-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3x): Brown solid, 85 mg, 55% yield, mp 265.4-267.0 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.40 (s, 1H), 8.31 (d, J = 1.1 Hz, 1H), 8.08 (dd, J = 6.6, 3.0 Hz, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.66 – 7.52 (m, 4H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.56, 156.05, 138.43, 132.00, 130.36, 129.76, 126.84, 126.32, 125.72, 123.59, 120.56, 114.79, 114.54, 105.86, 104.13, 102.25. HRMS-ESI (m/z): calcd for $C_{19}H_{11}N_4O$ $[M + H]^+$: 311.0927, found 311.0928.



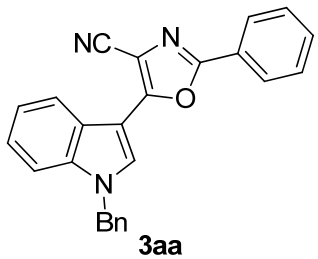
3y

Methyl 3-(4-cyano-2-phenyloxazol-5-yl)-1*H*-indole-5-carboxylate (3y): Brown solid, 102 mg, 60% yield, mp 293.9-295.7 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.72 (s, 1H), 8.25 (q, J = 2.7 Hz, 1H), 8.09 – 7.95 (m, 2H), 7.85 (d, J = 8.7 Hz, 1H), 7.61 (d, J = 5.5 Hz, 4H), 3.95 – 3.81 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.05, 158.95, 156.49, 139.07, 131.89, 129.75, 129.40, 126.42, 125.77, 124.12, 123.49, 123.12, 122.74, 114.82, 113.08, 105.17, 102.59, 52.42. HRMS-ESI (m/z): calcd for $C_{20}H_{14}N_3O_3$ $[M + H]^+$: 344.1030, found 344.1032.



3z

5-(1-methyl-1*H*-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3z): Brown solid, 77 mg, 52% yield, mp 178.8-180.6 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.14 (s, 1H), 8.07 (ddt, J = 8.1, 5.5, 1.9 Hz, 3H), 7.59 (dq, J = 5.4, 1.4 Hz, 4H), 7.33 (tt, J = 7.2, 5.6 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.78, 157.01, 137.18, 131.82, 131.40, 129.79, 126.62, 125.86, 124.25, 123.63, 122.29, 120.65, 115.10, 111.53, 104.34, 100.52, 33.67. HRMS-ESI (m/z): calcd for $C_{19}H_{14}N_3O$ $[M + H]^+$: 300.1131, found 300.1133.



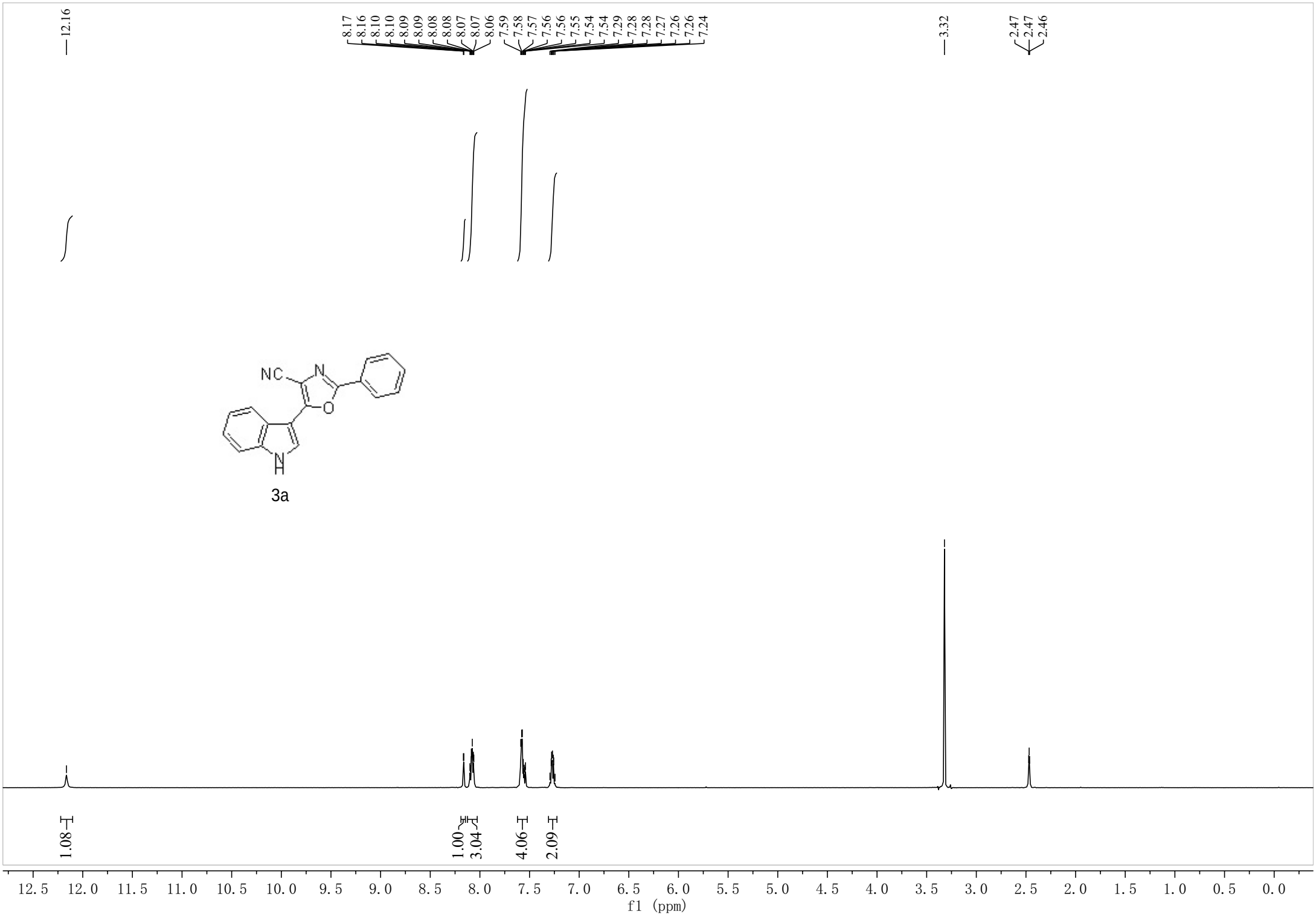
3aa

5-(1-benzyl-1H-indol-3-yl)-2-phenyloxazole-4-carbonitrile (3aa): Brown solid, 107 mg, 57% yield, mp 194.5-196.4 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.42 (s, 1H), 8.11 (ddd, J = 12.5, 6.6, 3.0 Hz, 3H), 7.62 (td, J = 6.4, 2.7 Hz, 4H), 7.30 (tt, J = 8.3, 4.6 Hz, 7H), 5.62 (s, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.06, 156.85, 137.52, 136.56, 131.91, 130.97, 129.83, 129.17, 128.18, 127.66, 126.70, 125.88, 124.62, 123.85, 122.44, 120.90, 115.06, 112.08, 104.91, 101.29, 50.11. HRMS-ESI (m/z): calcd for $C_{25}H_{18}N_3O$ $[M + H]^+$: 376.1444, found 376.1446.

4. References

(1) R. M. Abdel-Motaleb, A.-M. A.-S. Makhloof, H. M. Ibrahim and M. H. Elnagdi, *J. Heterocycl. Chem.*, 2007, **44**, 109.

5. ^{1}H and ^{13}C NMR spectral of products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7.28
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7.27
7.26
7.26
7.24
3.32
2.47
2.47
2.46
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N
O
N
H
3a
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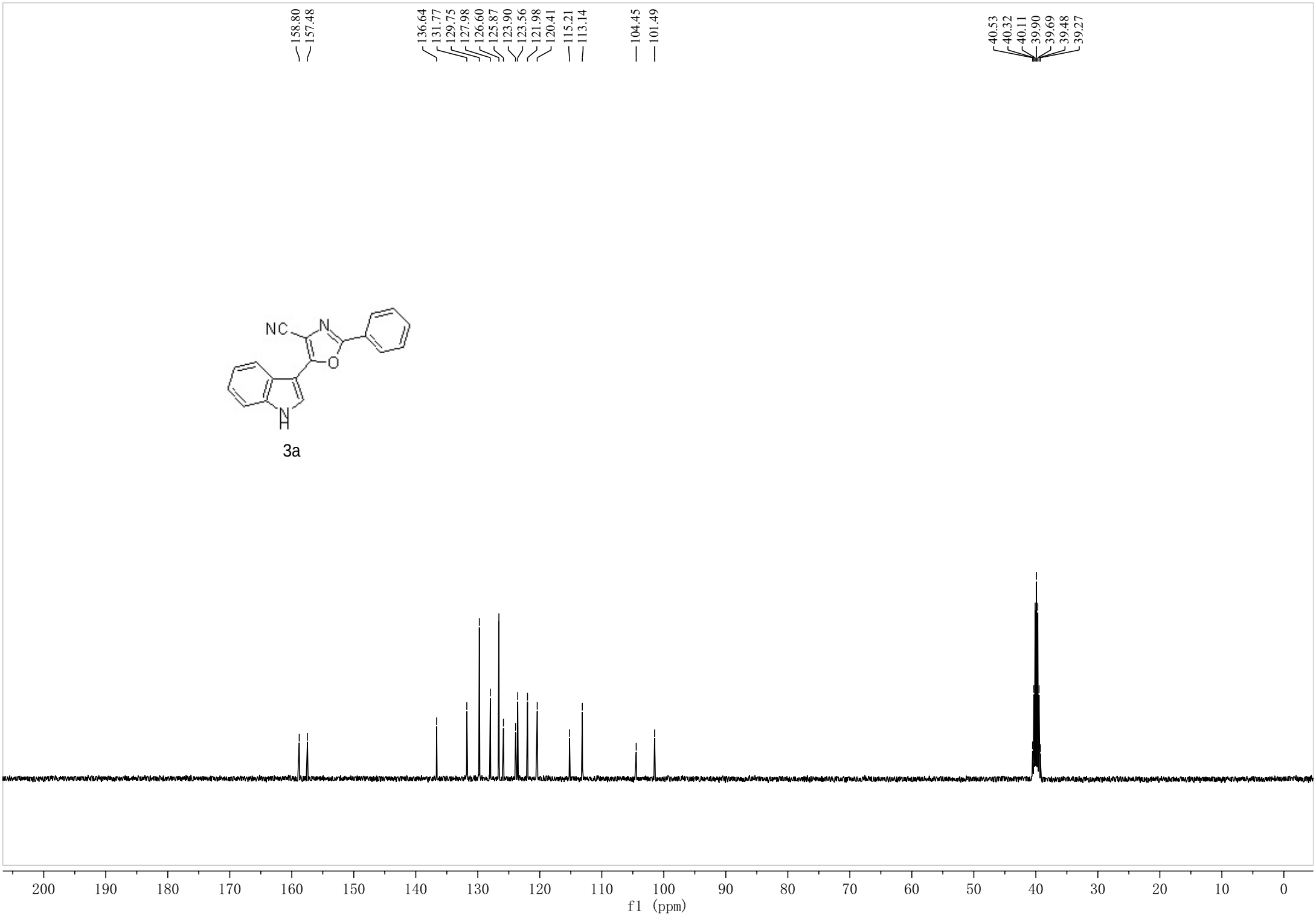
1.00
3.04
4.06
2.09
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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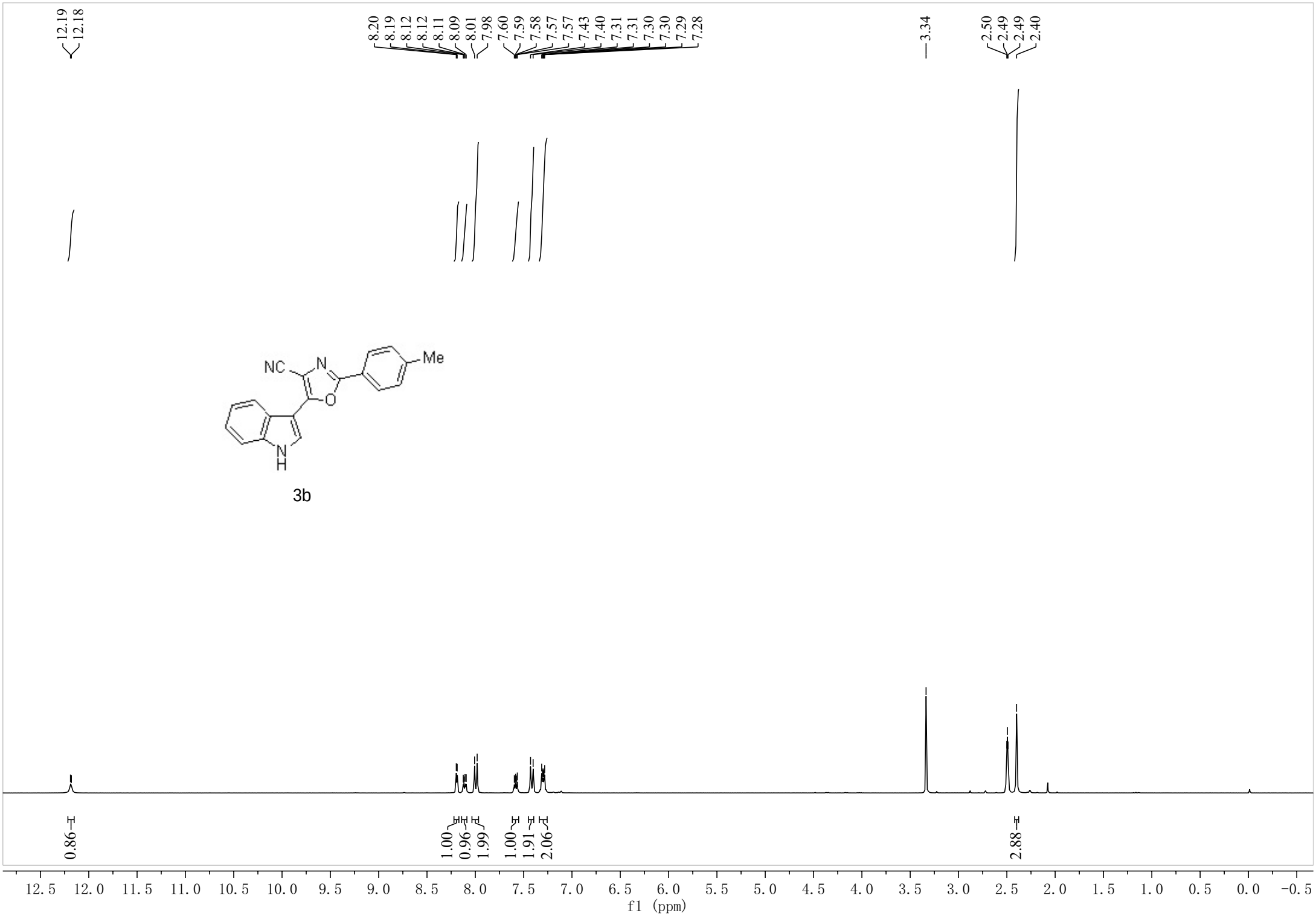
f1 (ppm)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1.99
1.00
1.91
2.06
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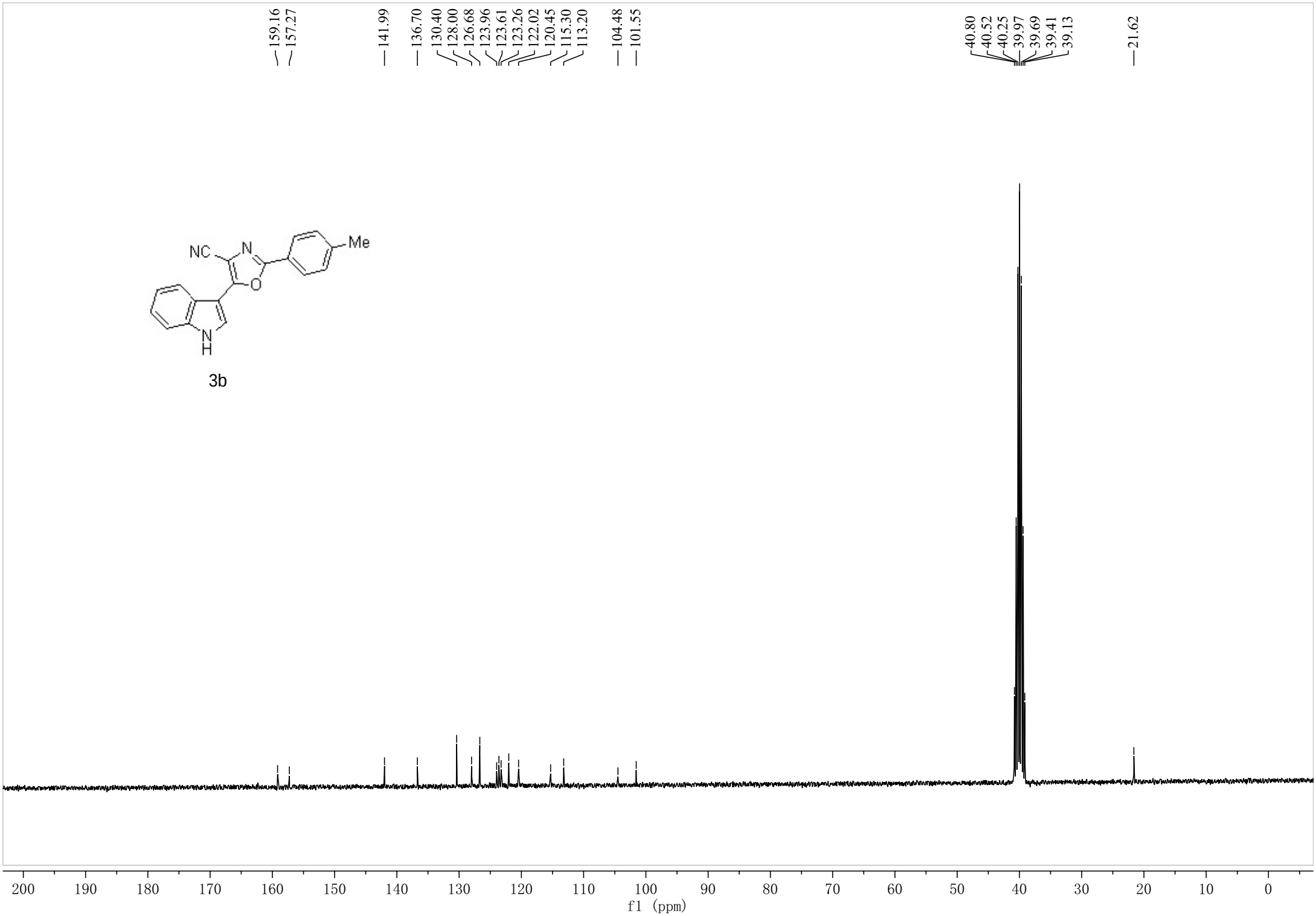
f1 (ppm)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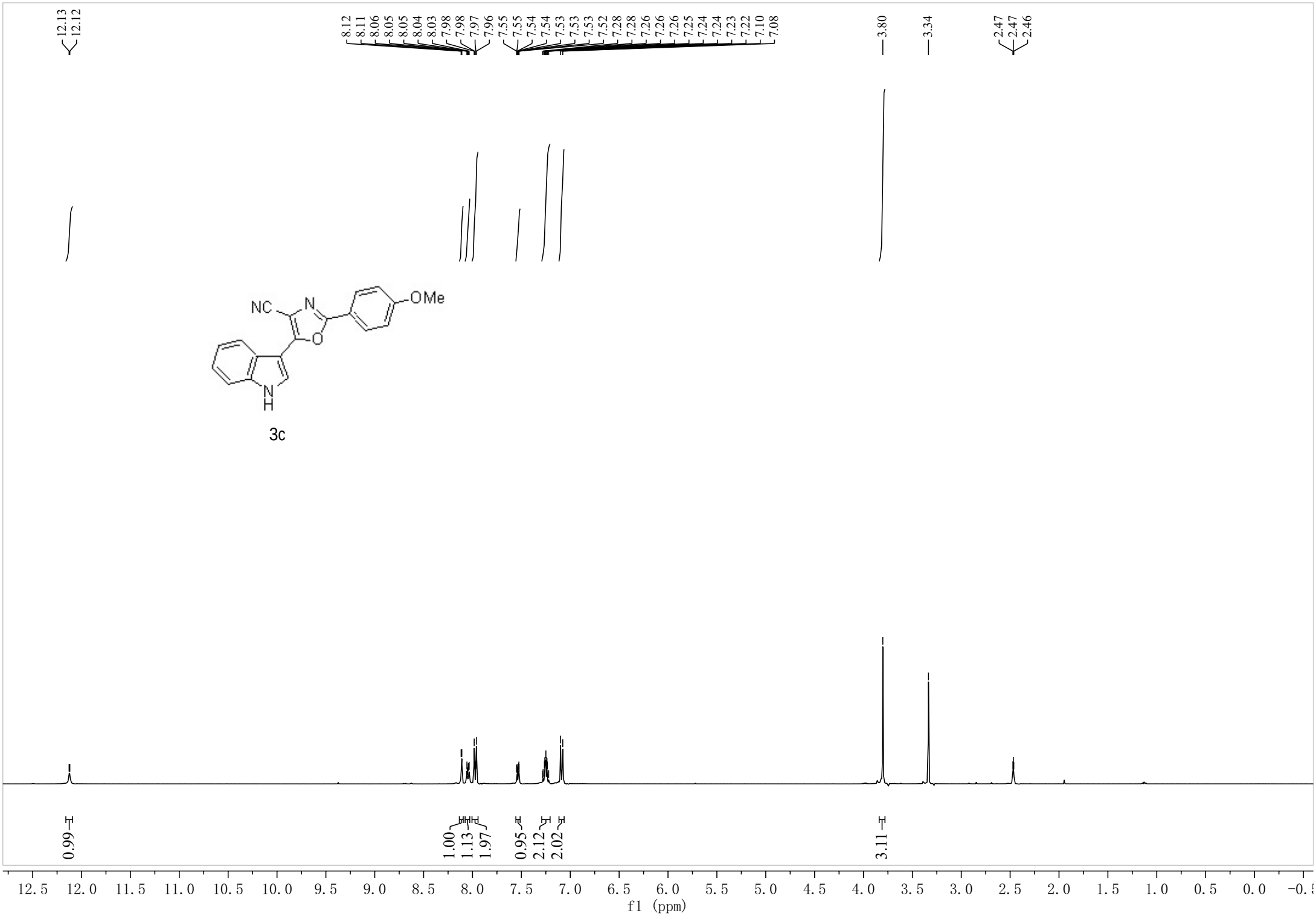
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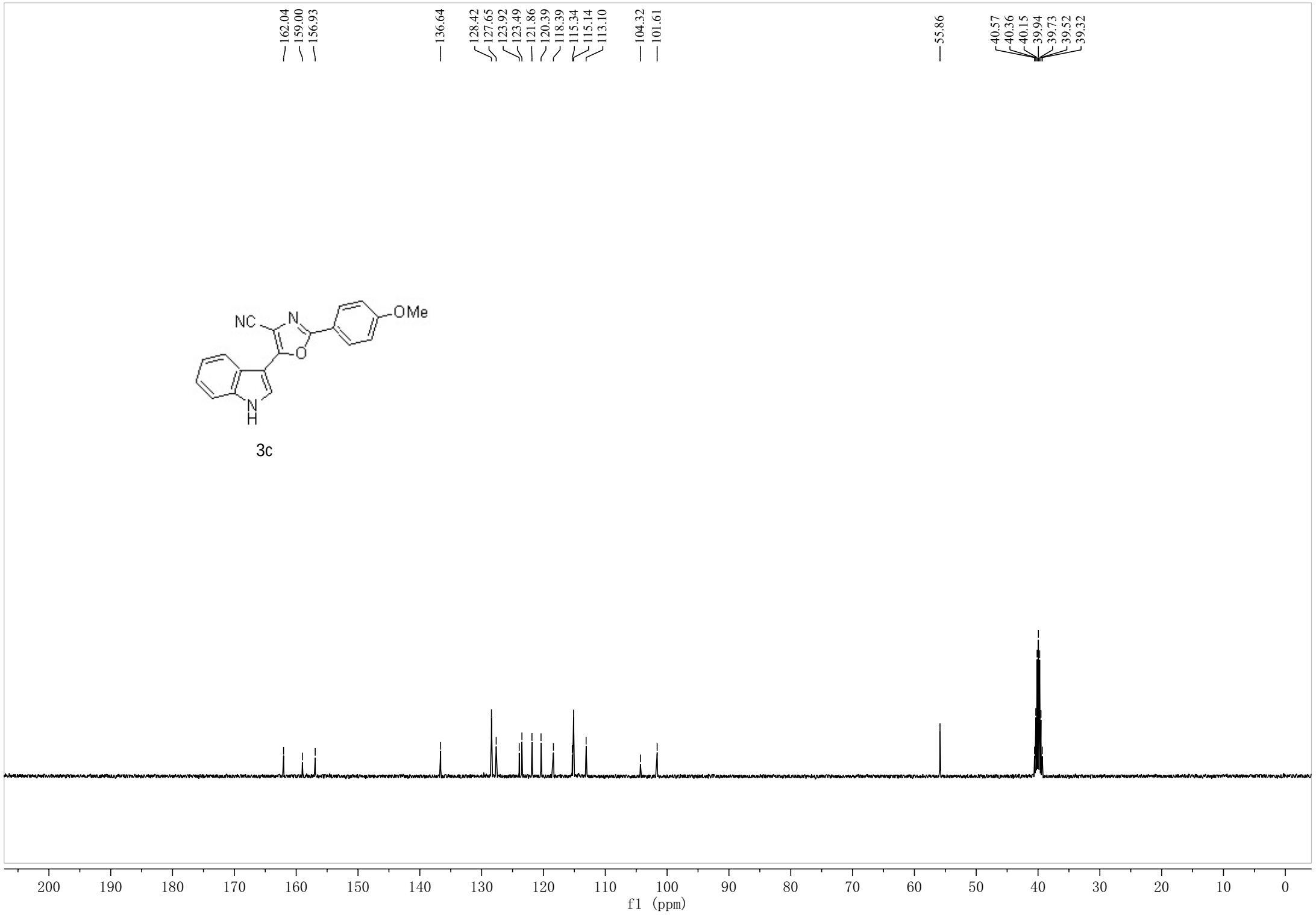
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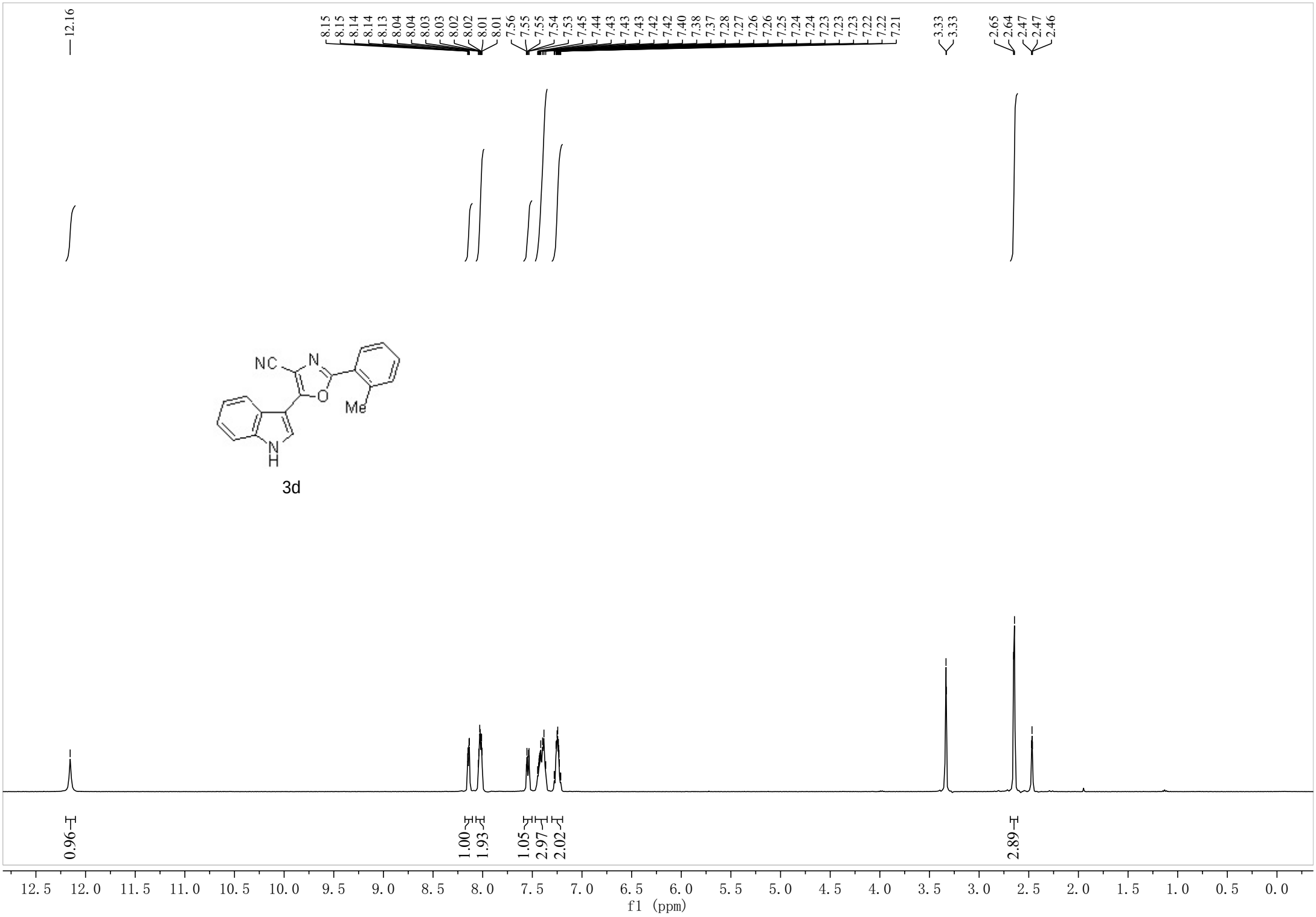
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N
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1.05
2.97
2.02
2.89
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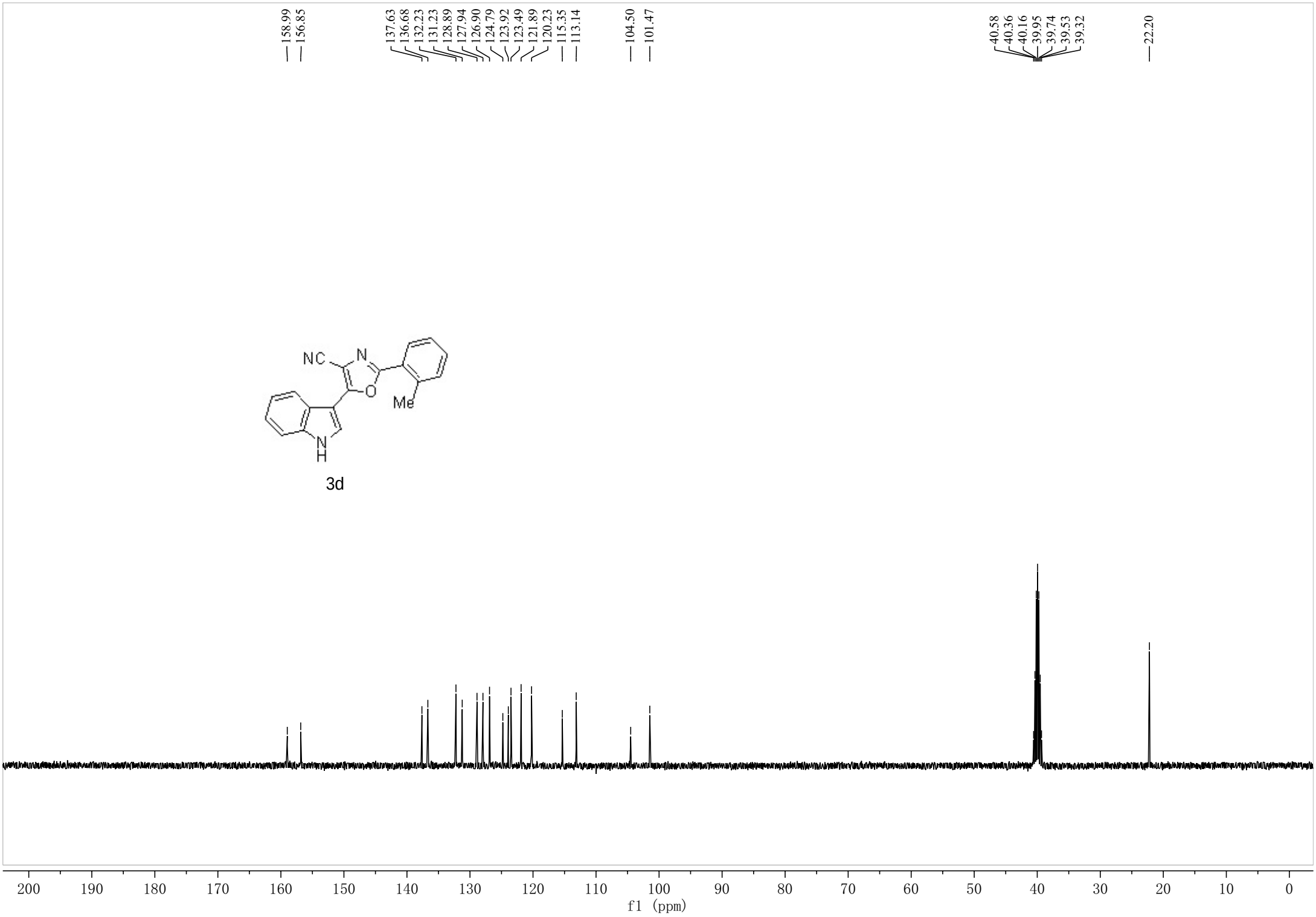
f1 (ppm)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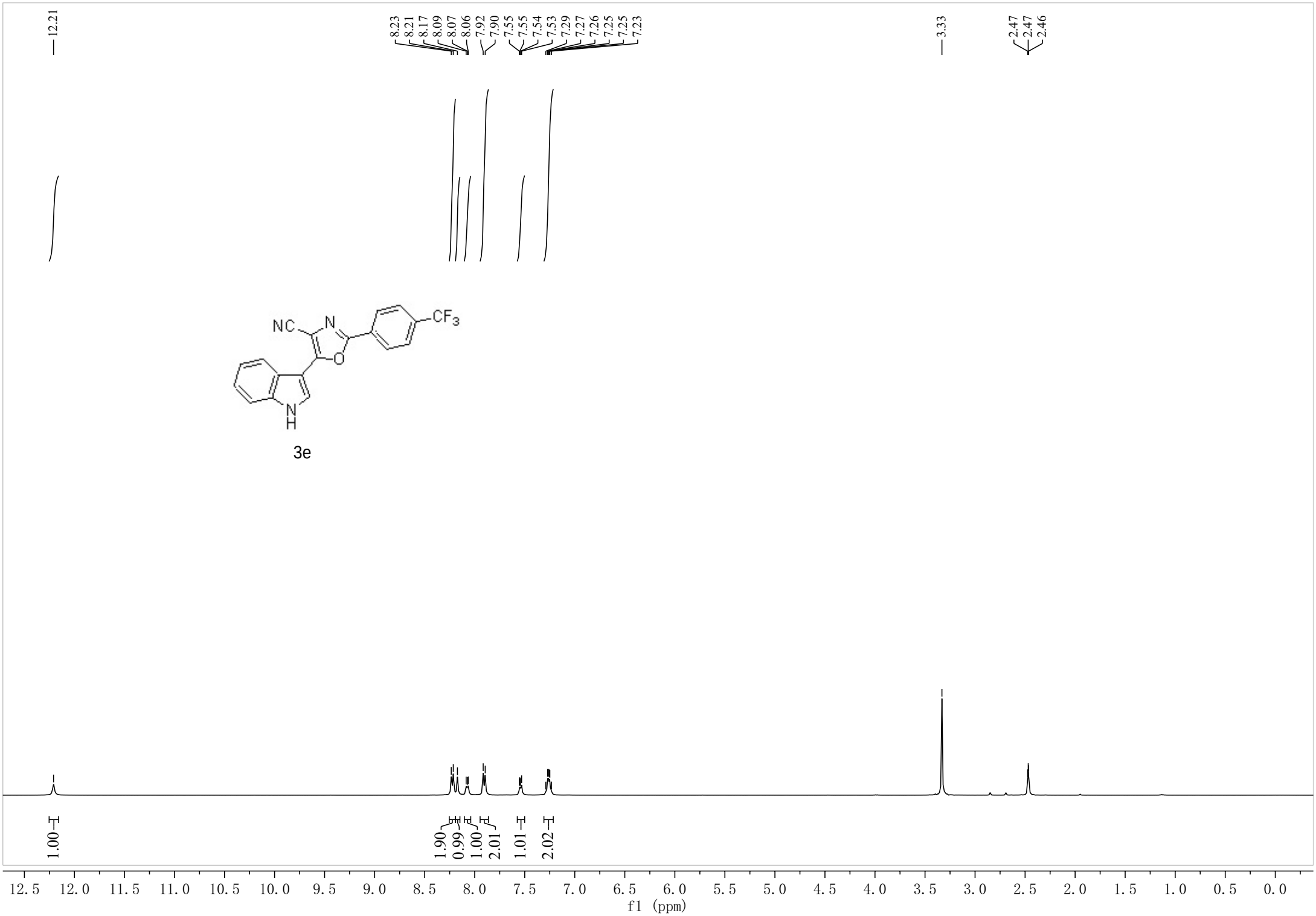
f1 (ppm)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H
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6.0
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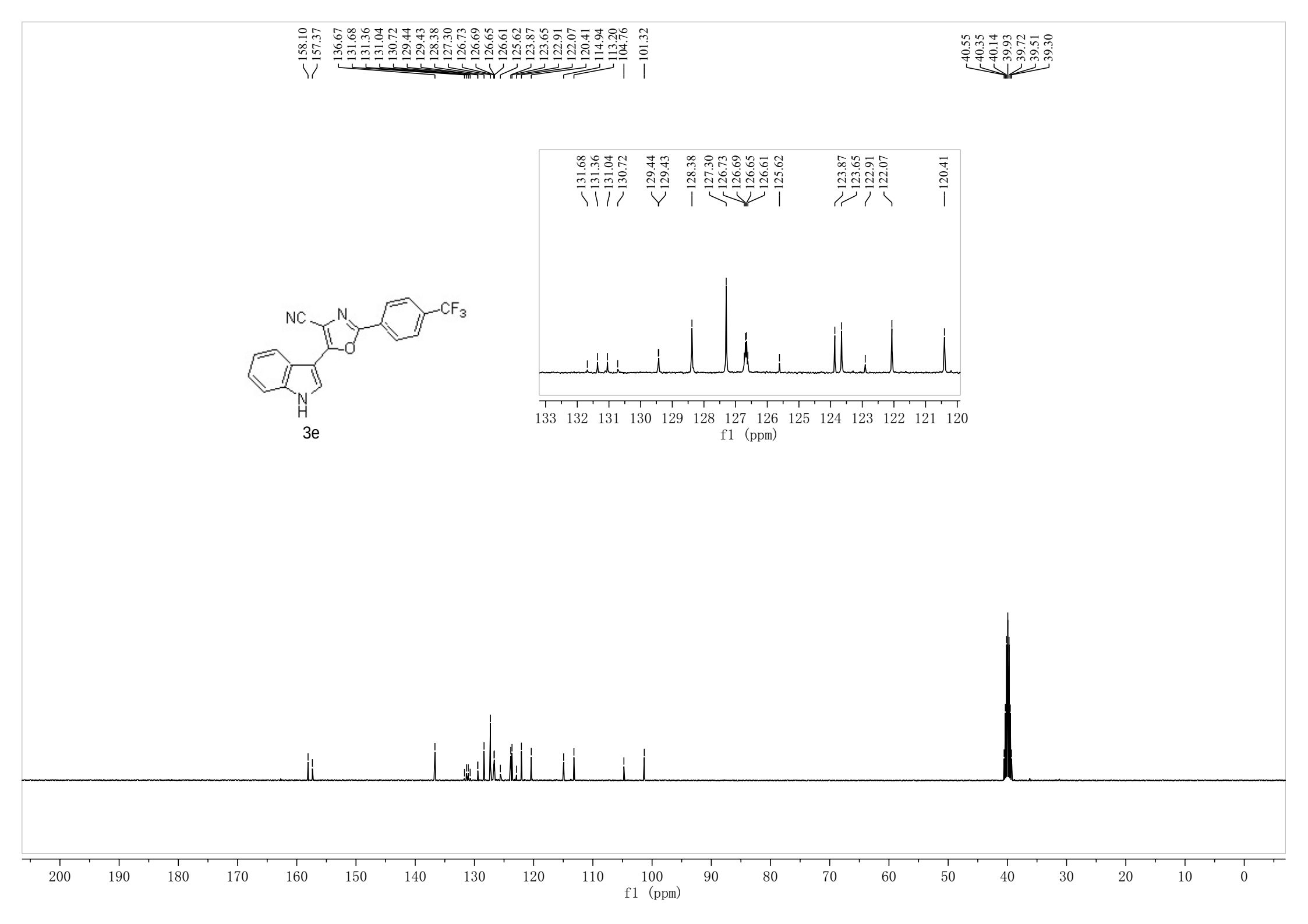
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123.65
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122.07
120.41
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113.20
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101.32
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O
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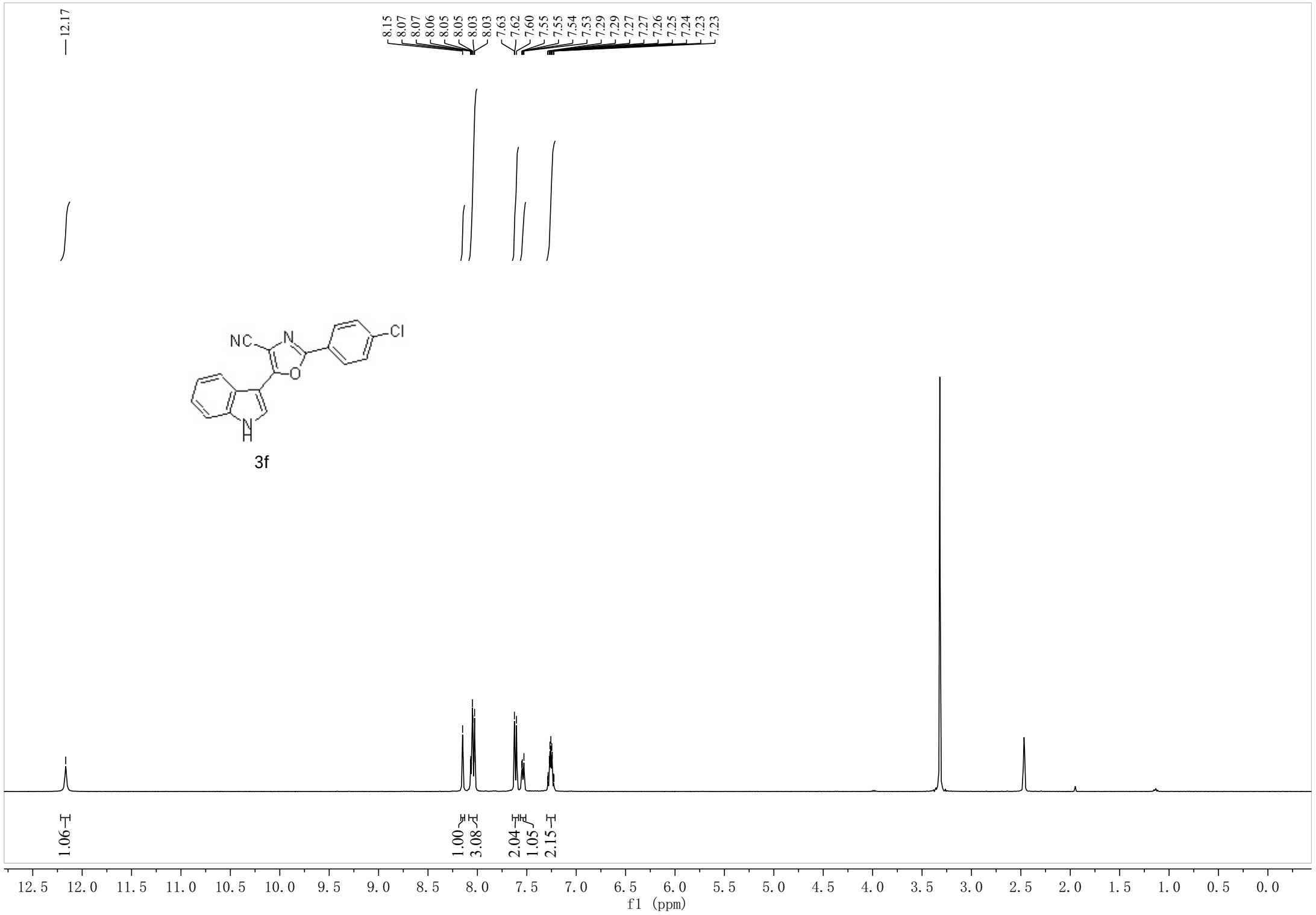
H
CF3
3e
f1 (ppm)
f1 (ppm)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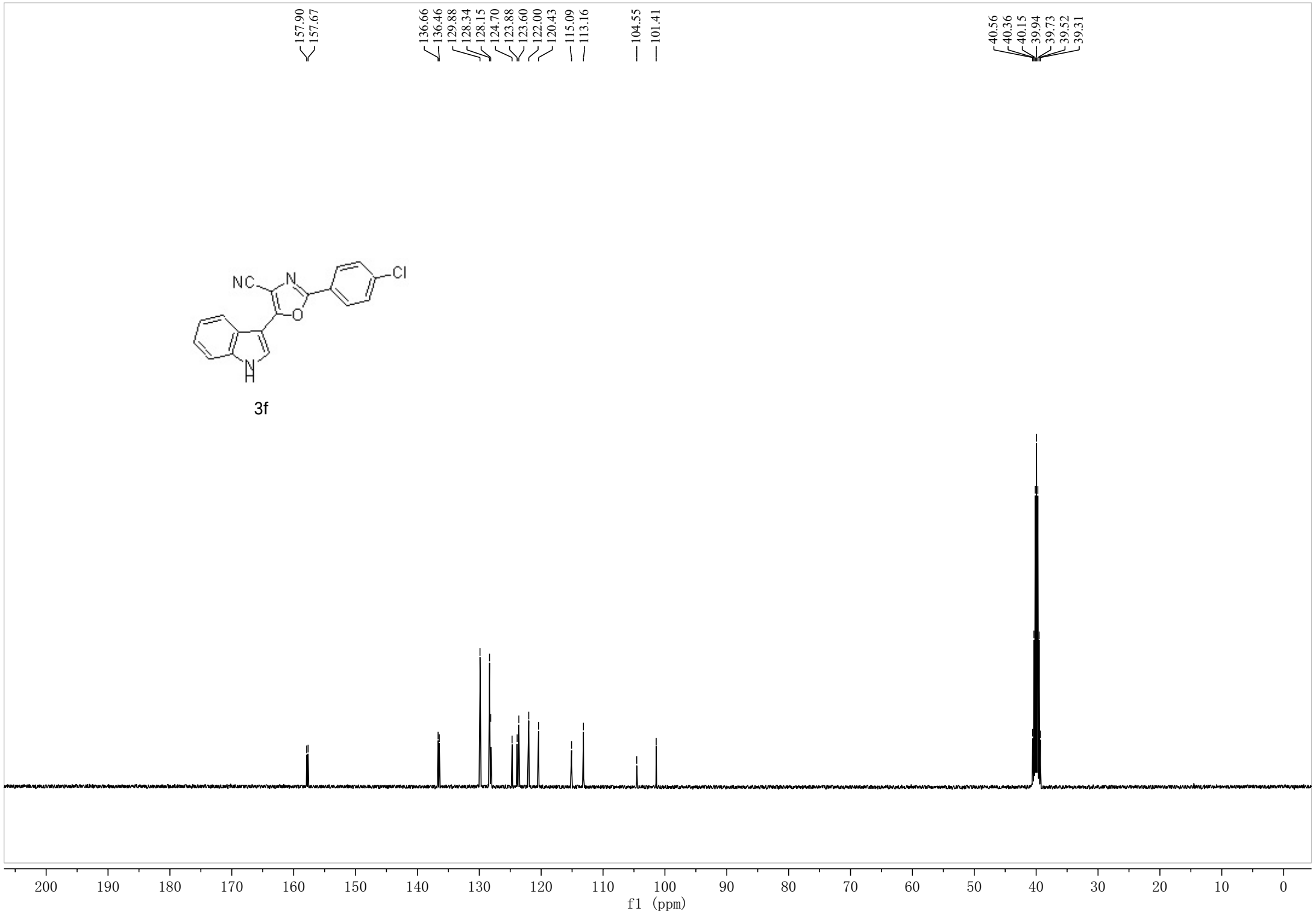
7.55
7.54
7.53
7.29
7.29
7.27
7.27
7.26
7.25
7.24
7.23
7.23
NC
N
O
N
H
Cl
3f
1.06
1.00
3.08
2.04
1.05
2.15
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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104.55
101.41
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39.52
39.31
NC
N
O
Cl
N
H
3f
200
190
180
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110
100
90
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50
40
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10
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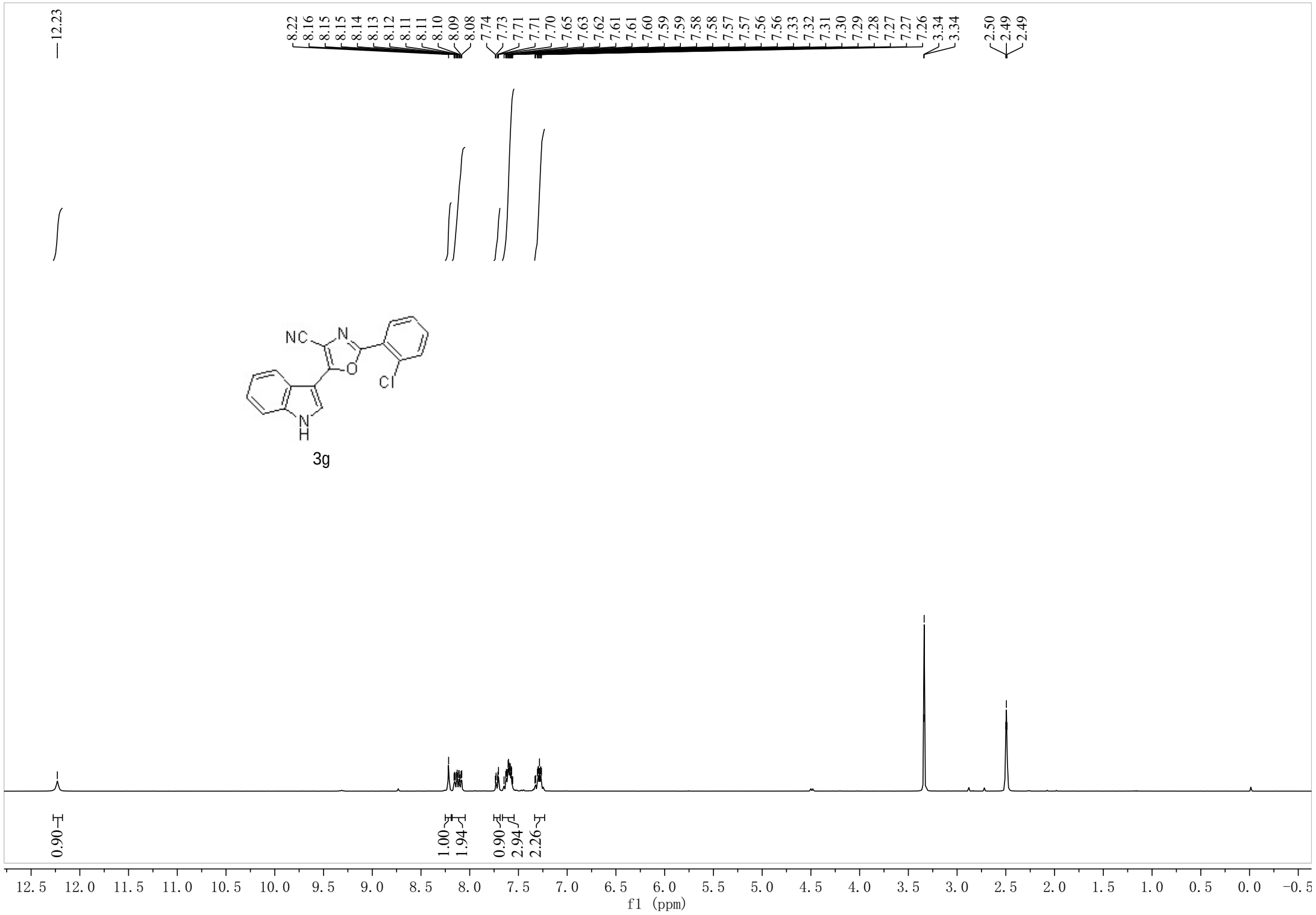
f1 (ppm)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8.10
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7.73
7.71
7.71
7.70
7.65
7.63
7.62
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.57
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7.56
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7.27
7.27
7.26
3.34
3.34
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2.49
NC
N
O
Cl
N
H
3g
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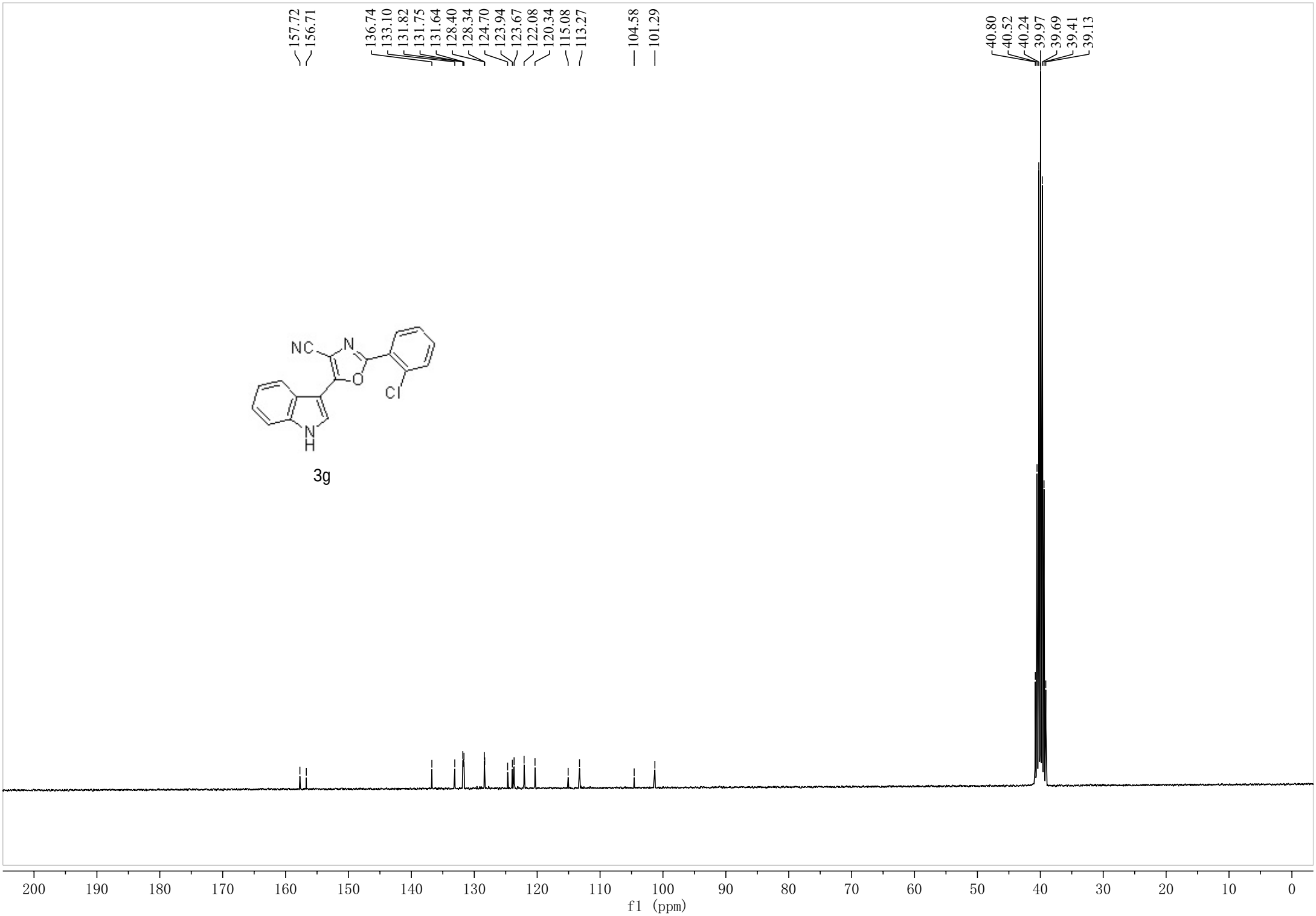
1.94
0.90
2.94
2.26
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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104.58
101.29
40.80
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40.24
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39.41
39.13
NC
N
O
Cl
N
H
3g
200
190
180
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90
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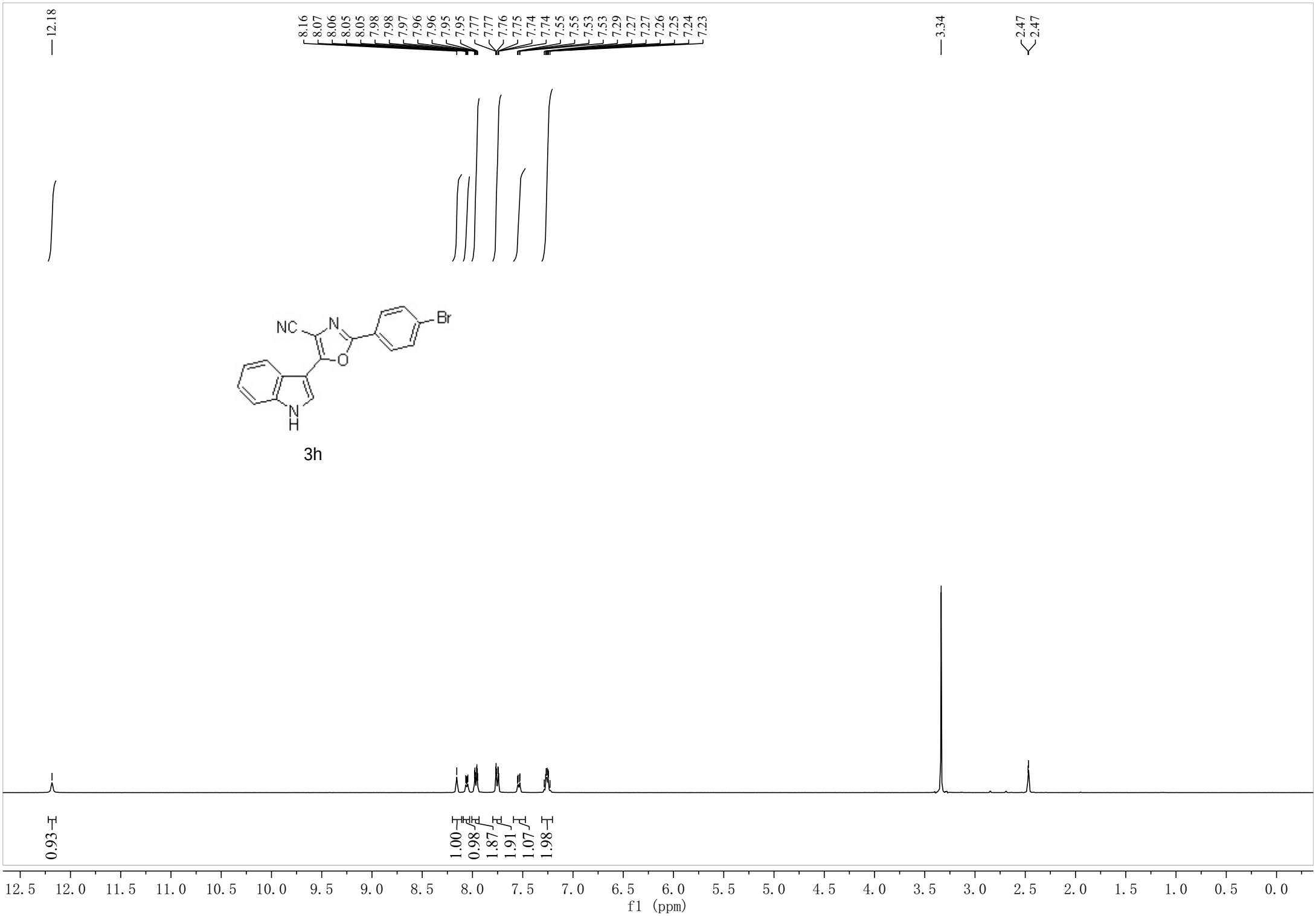
f1 (ppm)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7.76
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7.55
7.55
7.53
7.53
7.29
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7.27
7.26
7.25
7.24
7.23
3.34
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2.47
NC
N
O
Br
N
H
3h
0.93
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0.98
1.87
1.91
1.07
1.98
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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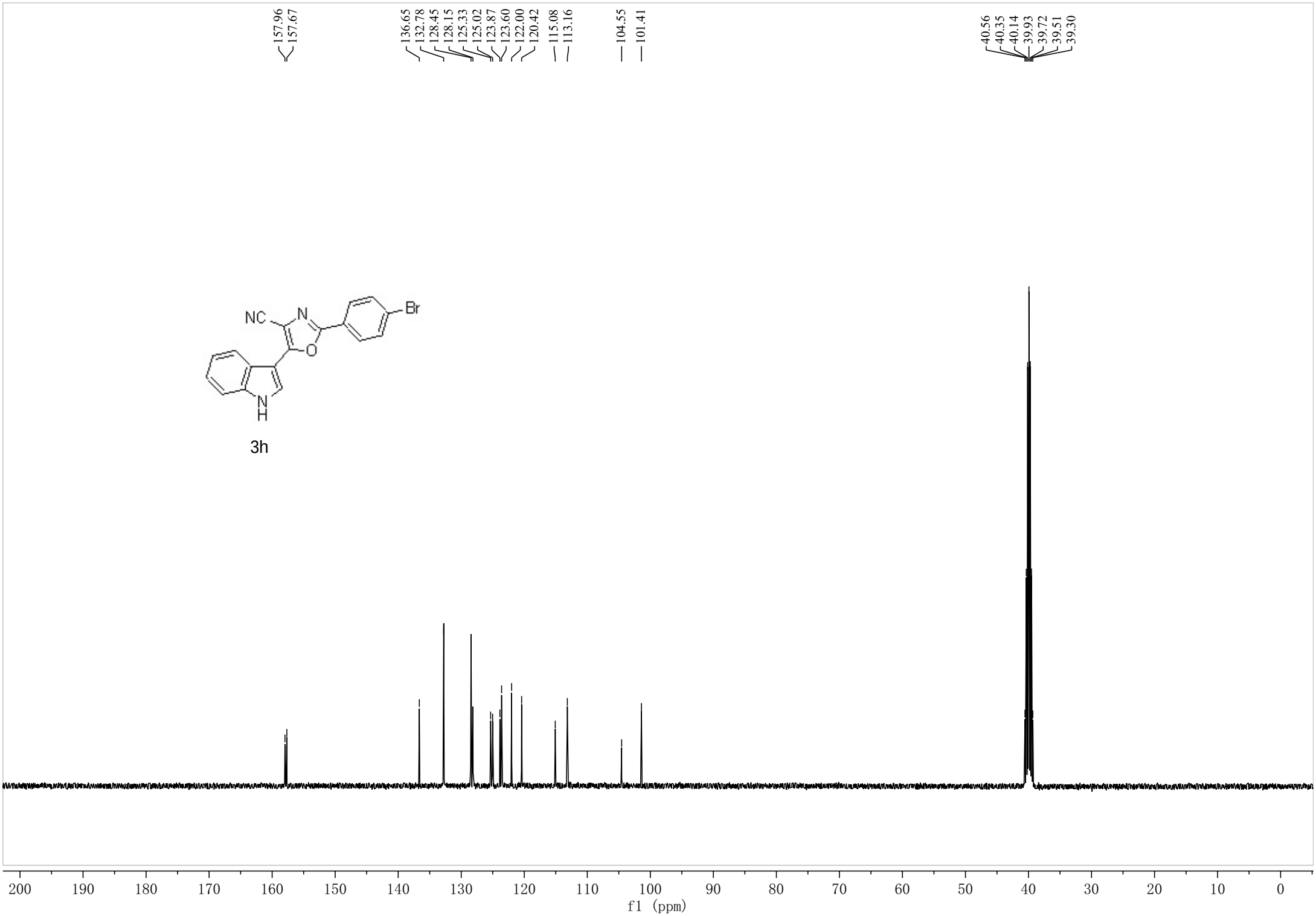
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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113.16
104.55
101.41
40.56
40.35
40.14
39.93
39.72
39.51
39.30
NC
N
O
Br
N
H
3h
200
190
180
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130
120
110
100
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30
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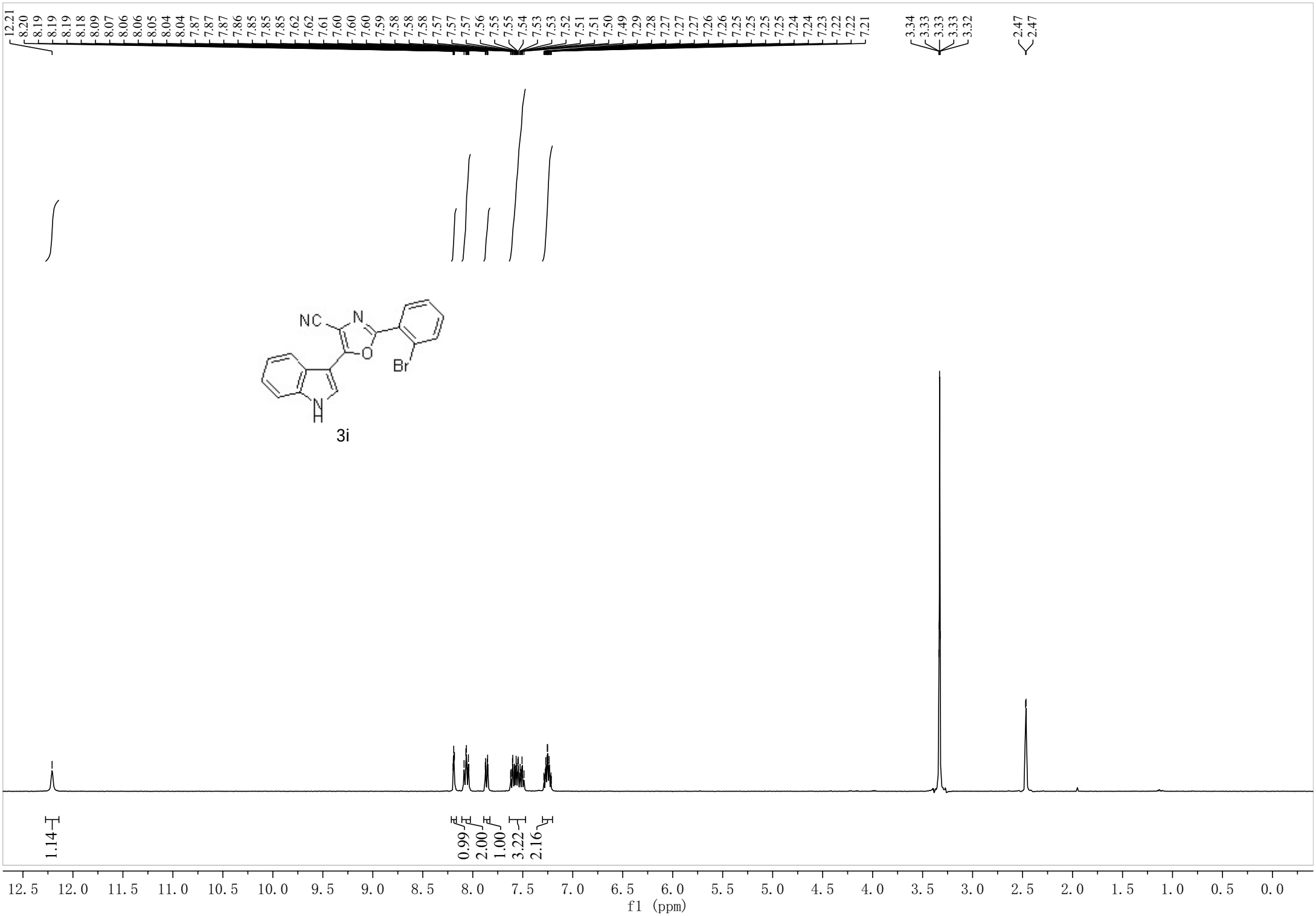
f1 (ppm)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7.28
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7.23
7.22
7.22
7.21
3.34
3.33
3.33
3.33
3.32
2.47
2.47
NC
N
O
Br
N
H
3i
1.14
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2.00
1.00
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11.0
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10.0
9.5
9.0
8.5
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6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
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1.0
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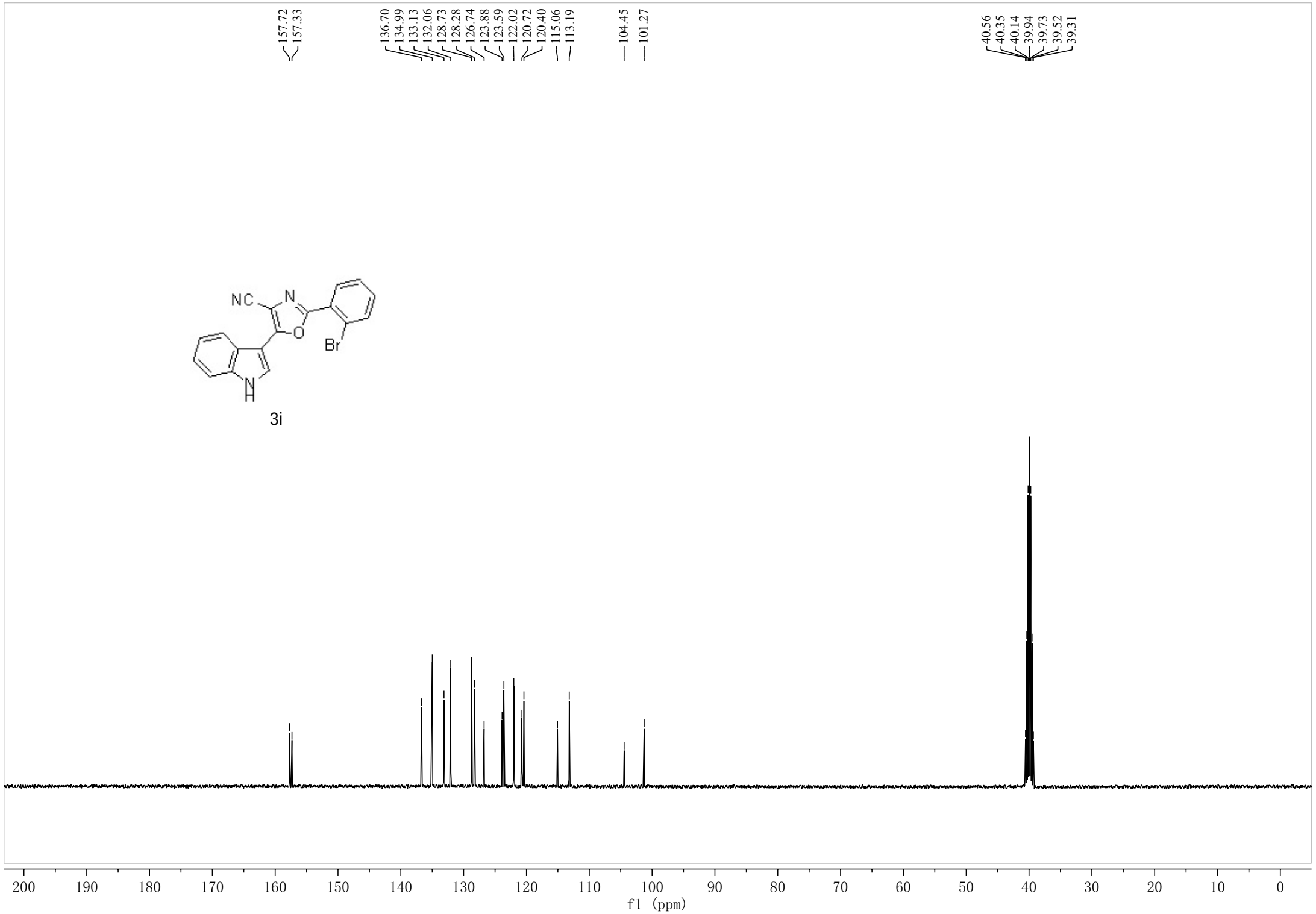
0.0
f1 (ppm)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120.40
115.06
113.19
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101.27
40.56
40.35
40.14
39.94
39.73
39.52
39.31
NC
N
O
Br
N
H
3i
200
190
180
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50
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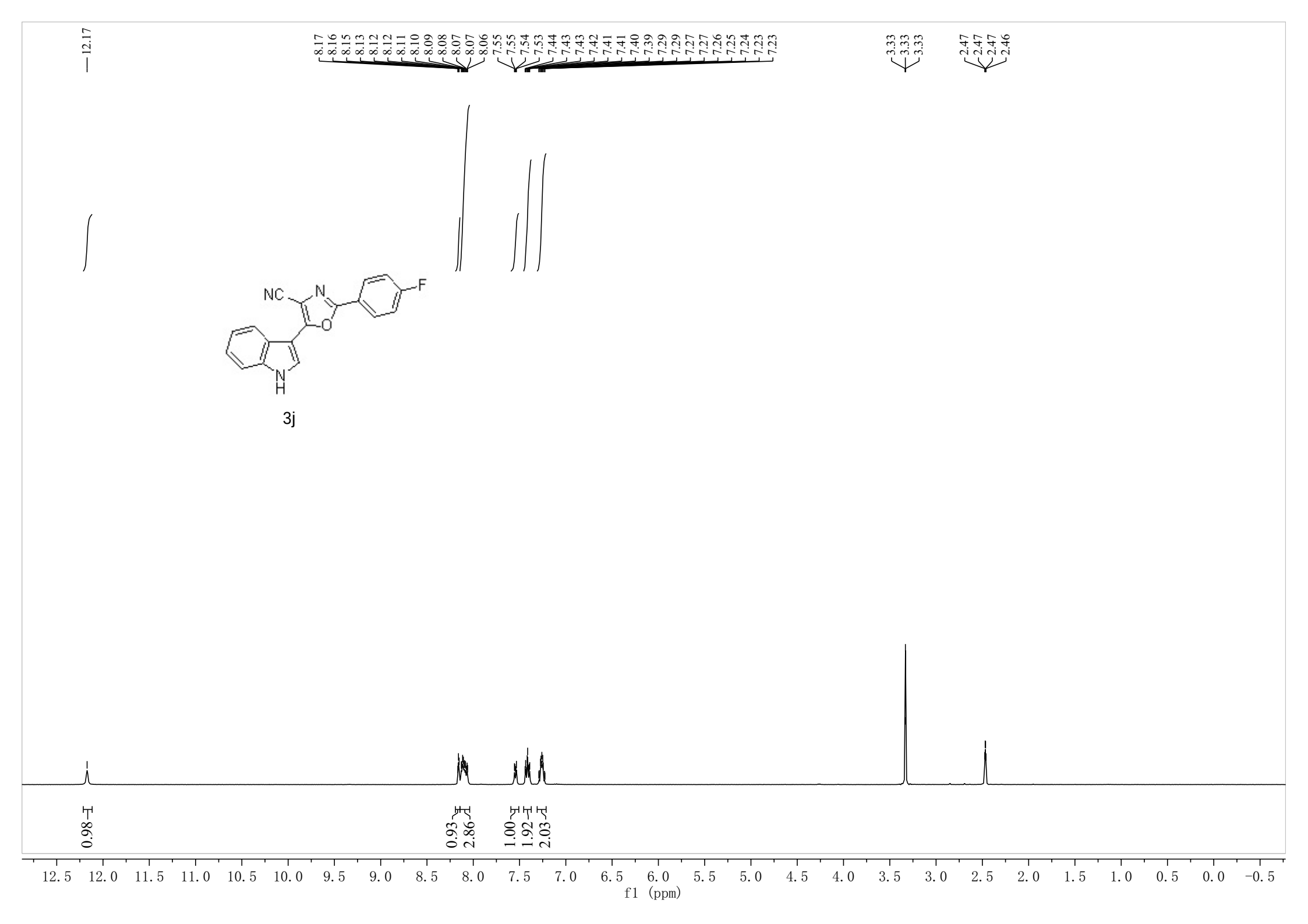
f1 (ppm)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8.06
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7.55
7.54
7.53
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7.43
7.43
7.42
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7.40
7.39
7.29
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7.24
7.23
7.23
3.33
3.33
3.33
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2.47
2.47
2.46
NC
N
O
F
N
H
3j
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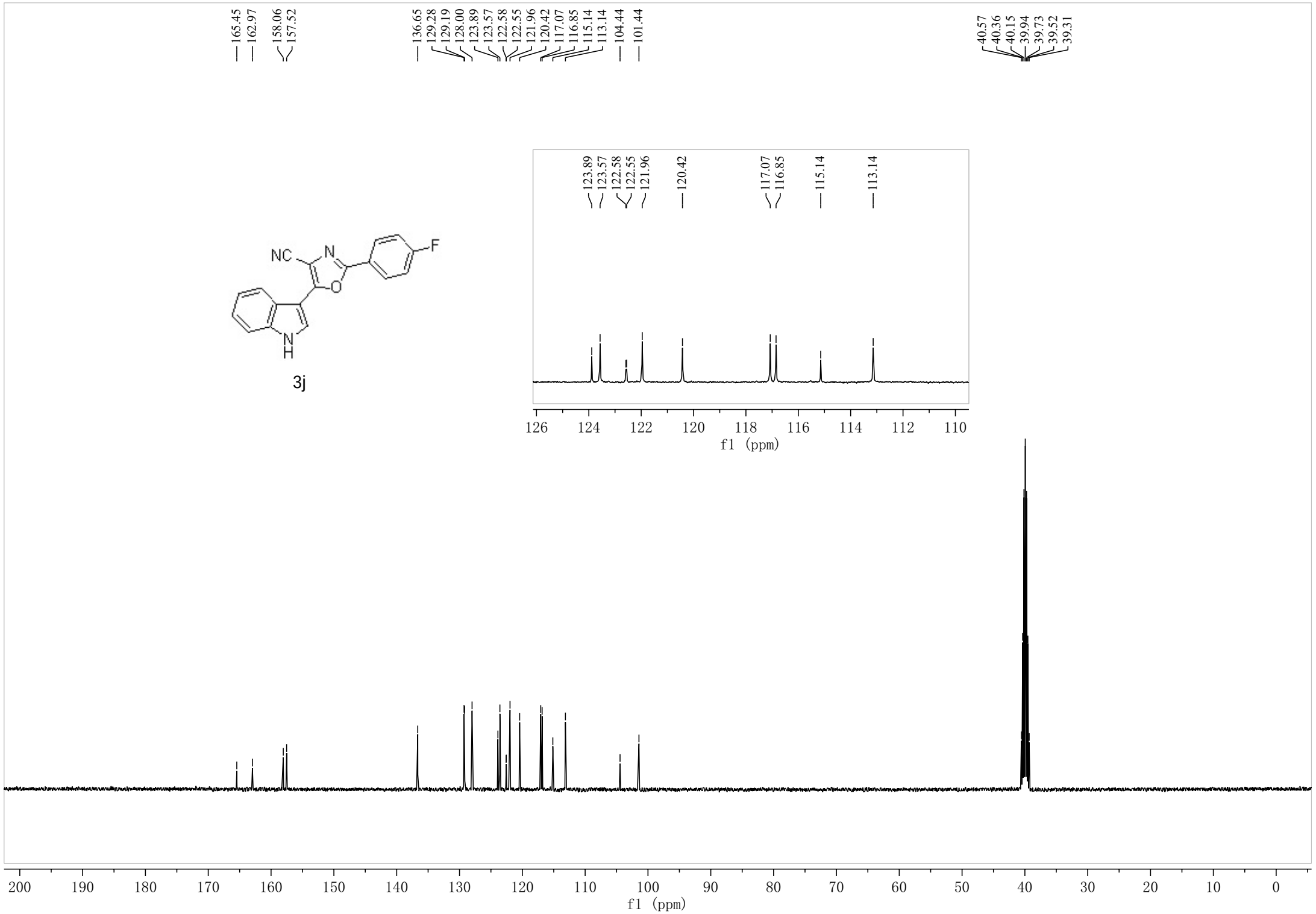
0.93
2.86
1.00
1.92
2.03
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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117.07
116.85
115.14
113.14
104.44
101.44
40.57
40.36
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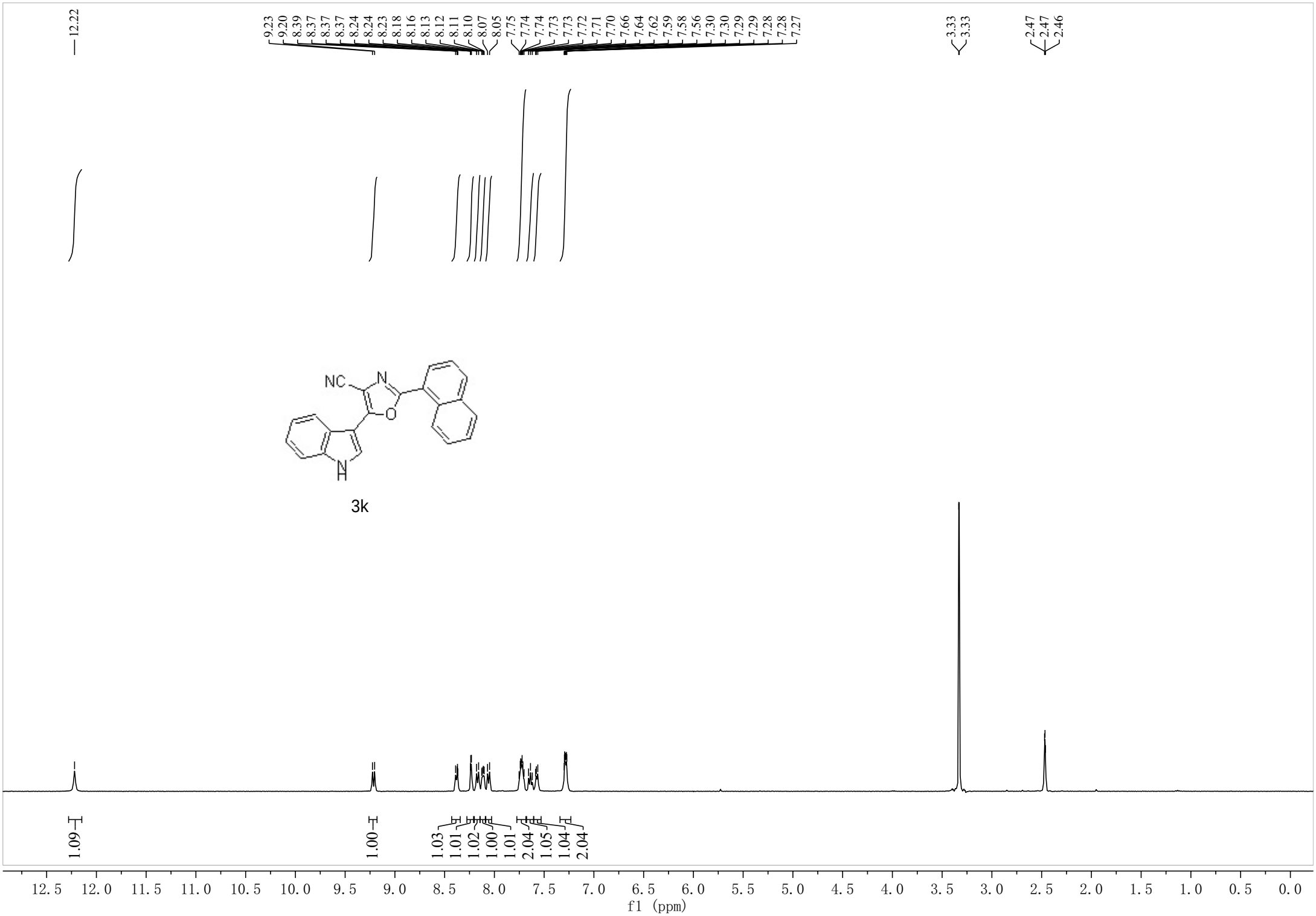
F
O
N
H
3j
f1 (ppm)
f1 (ppm)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8.12
8.11
8.10
8.07
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7.74
7.73
7.73
7.72
7.71
7.70
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7.30
7.29
7.29
7.28
7.28
7.27
3.33
3.33
2.47
2.47
2.46
NC
N
O
N
H
3k
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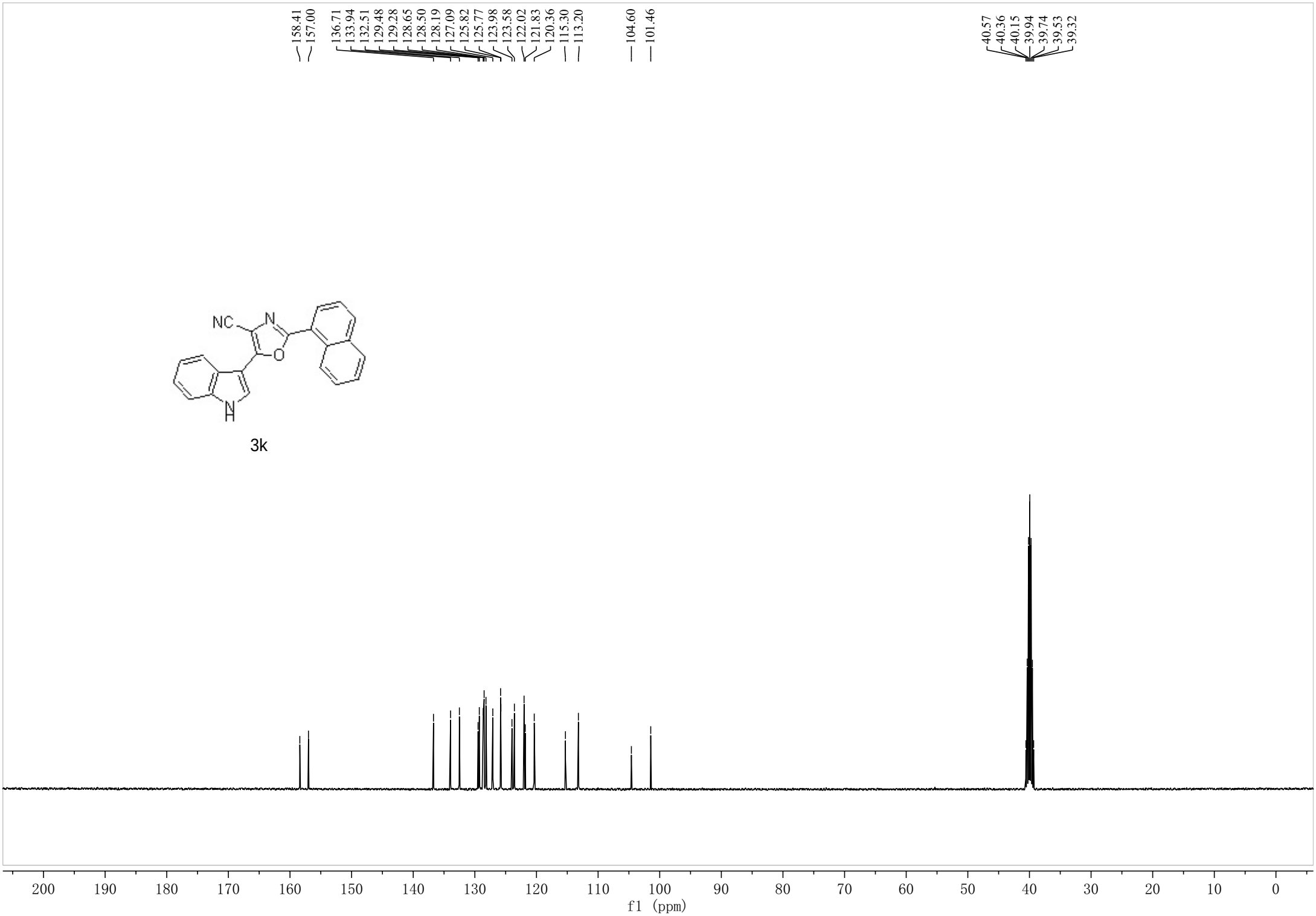
1.00
1.03
1.01
1.02
1.00
1.01
2.04
1.05
1.04
2.04
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.58
122.02
121.83
120.36
115.30
113.20
104.60
101.46
40.57
40.36
40.15
39.94
39.74
39.53
39.32
NC
N
O
N
H
3k
200
190
180
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120
110
100
90
80
70
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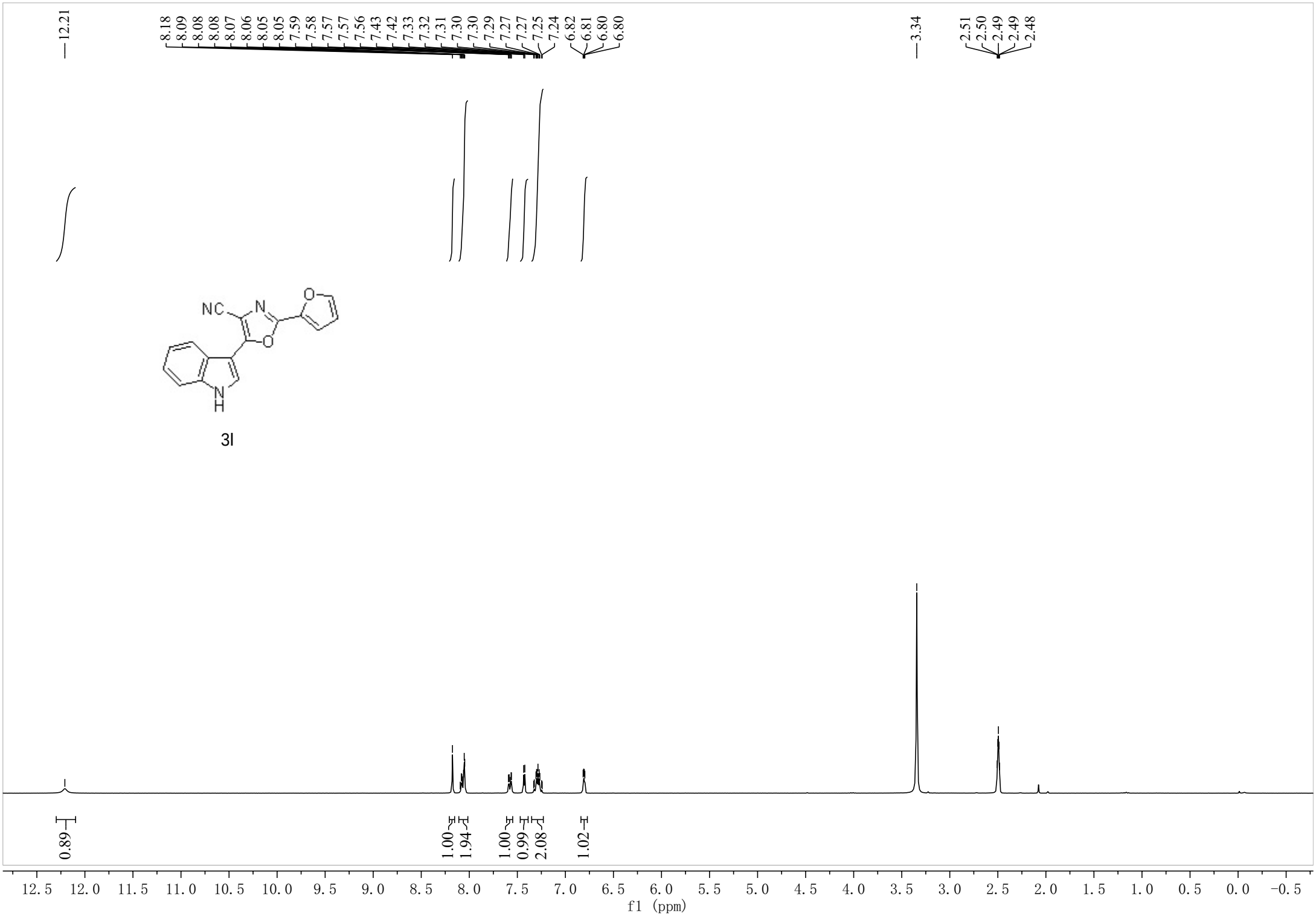
50
40
30
20
10
0
f1 (ppm)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7.56
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7.42
7.33
7.32
7.31
7.30
7.30
7.29
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7.27
7.25
7.24
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6.81
6.80
6.80
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2.50
2.49
2.49
2.48
NC
N
O
O
N
H
3l
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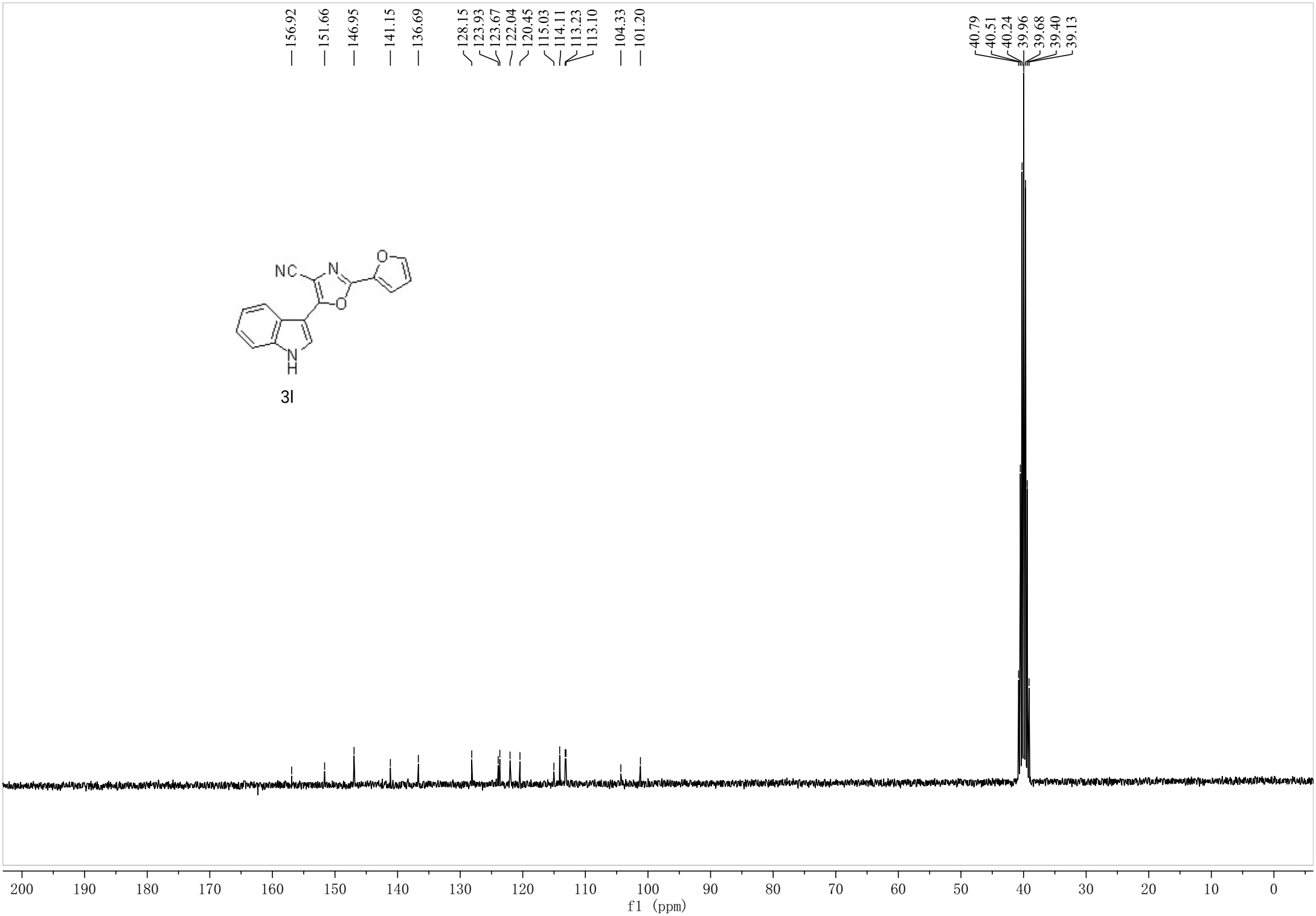
1.00
1.94
1.00
0.99
2.08
1.02
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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113.10
104.33
101.20
40.79
40.51
40.24
39.96
39.68
39.40
39.13
NC
N
O
O
N
H
3l
200
190
180
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160
150
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130
120
110
100
90
80
70
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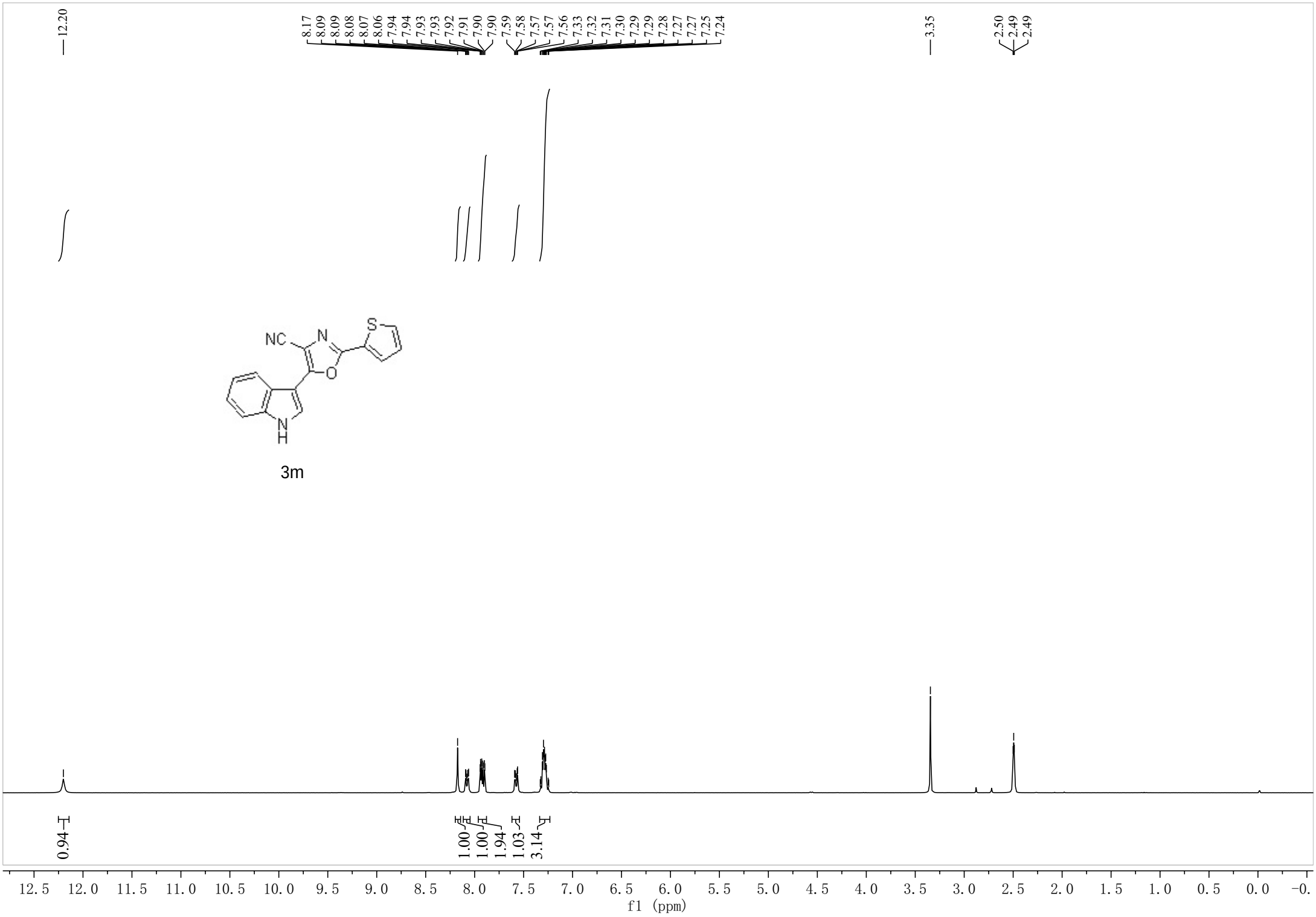
50
40
30
20
10
0
f1 (ppm)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7.93
7.93
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7.90
7.90
7.59
7.58
7.57
7.57
7.56
7.33
7.32
7.31
7.30
7.29
7.29
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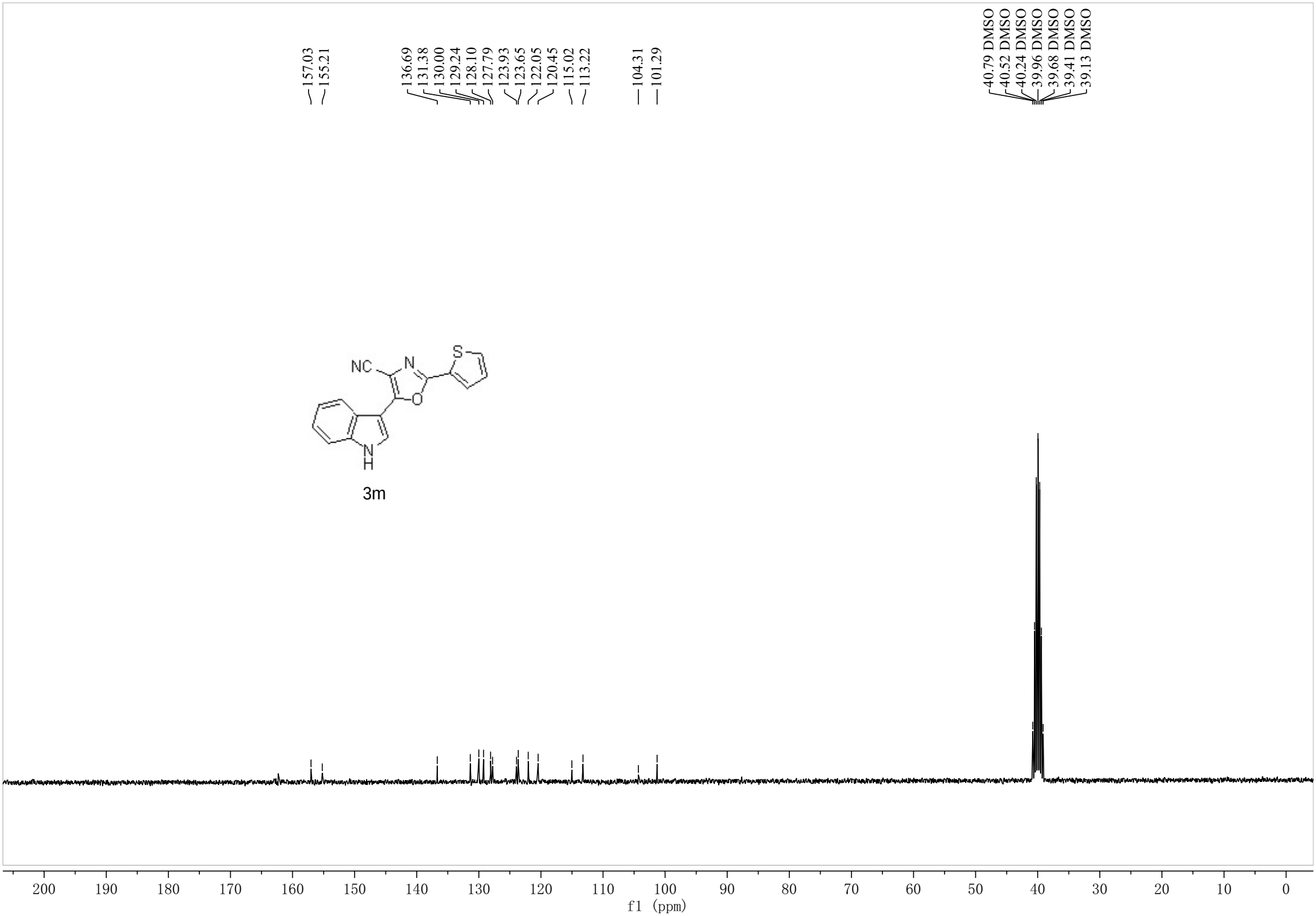
7.27
7.27
7.25
7.24
3.35
2.50
2.49
2.49
NC
N
S
O
N
H
3m
0.94
1.00
1.00
1.94
1.03
3.14
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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122.05
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115.02
113.22
104.31
101.29
40.79 DMSO
40.52 DMSO
40.24 DMSO
39.96 DMSO
39.68 DMSO
39.41 DMSO
39.13 DMSO
NC
N
S
O
N
H
3m
200
190
180
170
160
150
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120
110
100
90
80
70
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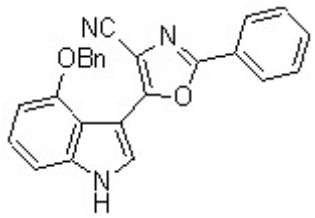
50
40
30
20
10
0
f1 (ppm)


NC
N
OBn
O
N
H

3n

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7.65
7.40
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7.38
7.34
7.32
7.30
7.24
7.22
7.21
7.20
7.11
7.09
7.02
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1.85
0.96
1.06
2.08
3.09
0.99
2.85
1.00
1.97
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11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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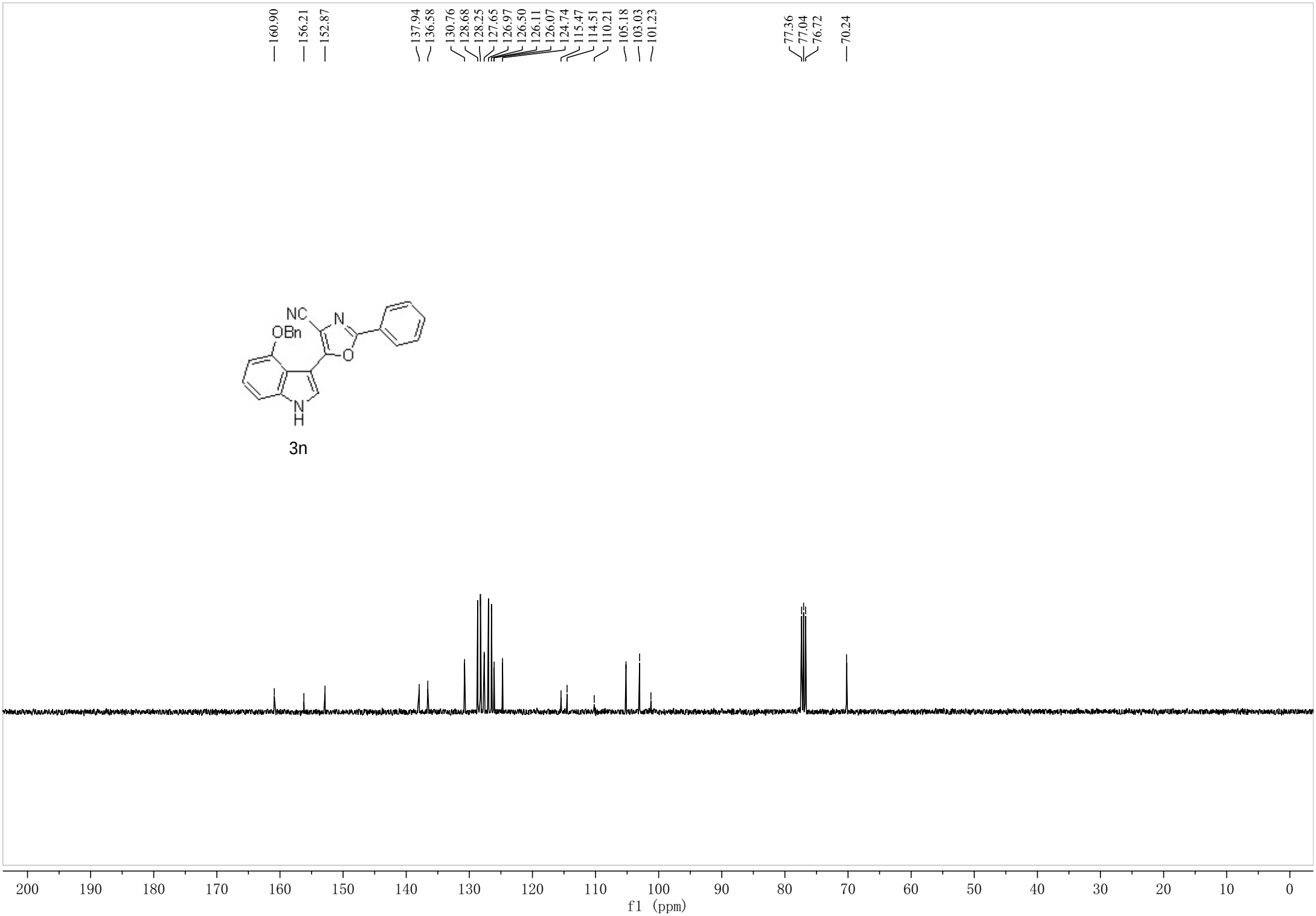
f1 (ppm)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124.74
115.47
114.51
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103.03
101.23
77.36
77.04
76.72
70.24
NC
OBn
N
O
N
H
3n
200
190
180
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110
100
90
80
70
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50
40
30
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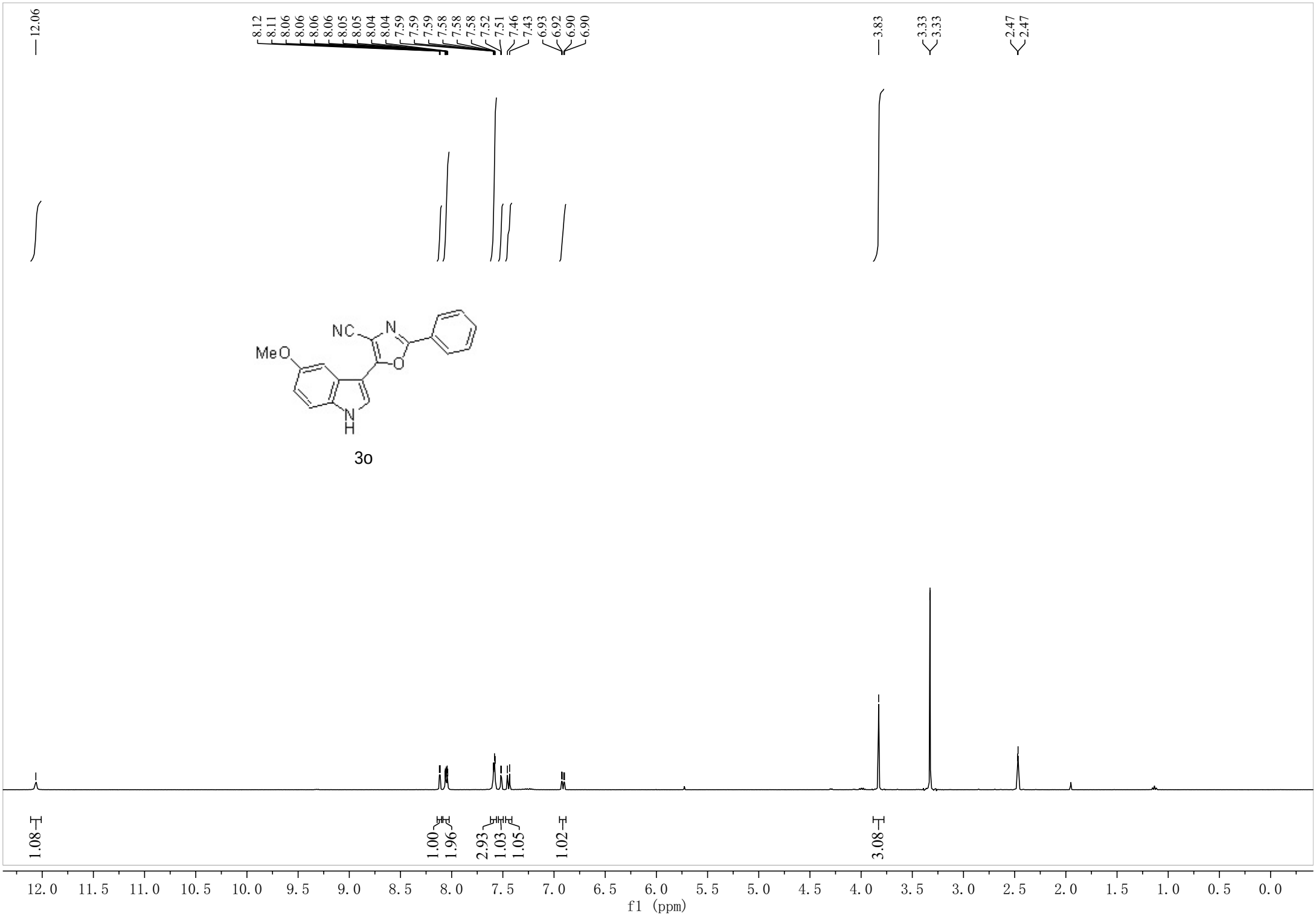
10
0
f1 (ppm)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7.52
7.51
7.46
7.43
6.93
6.92
6.90
6.90
3.83
3.33
3.33
2.47
2.47
NC
N
MeO
O
N
H
3o
1.08
1.00
1.96
2.93
1.03
1.05
1.02
3.08
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
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1.0
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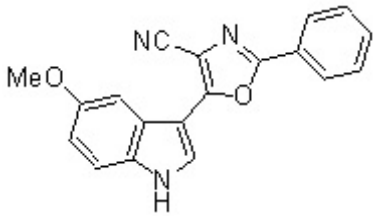
f1 (ppm)

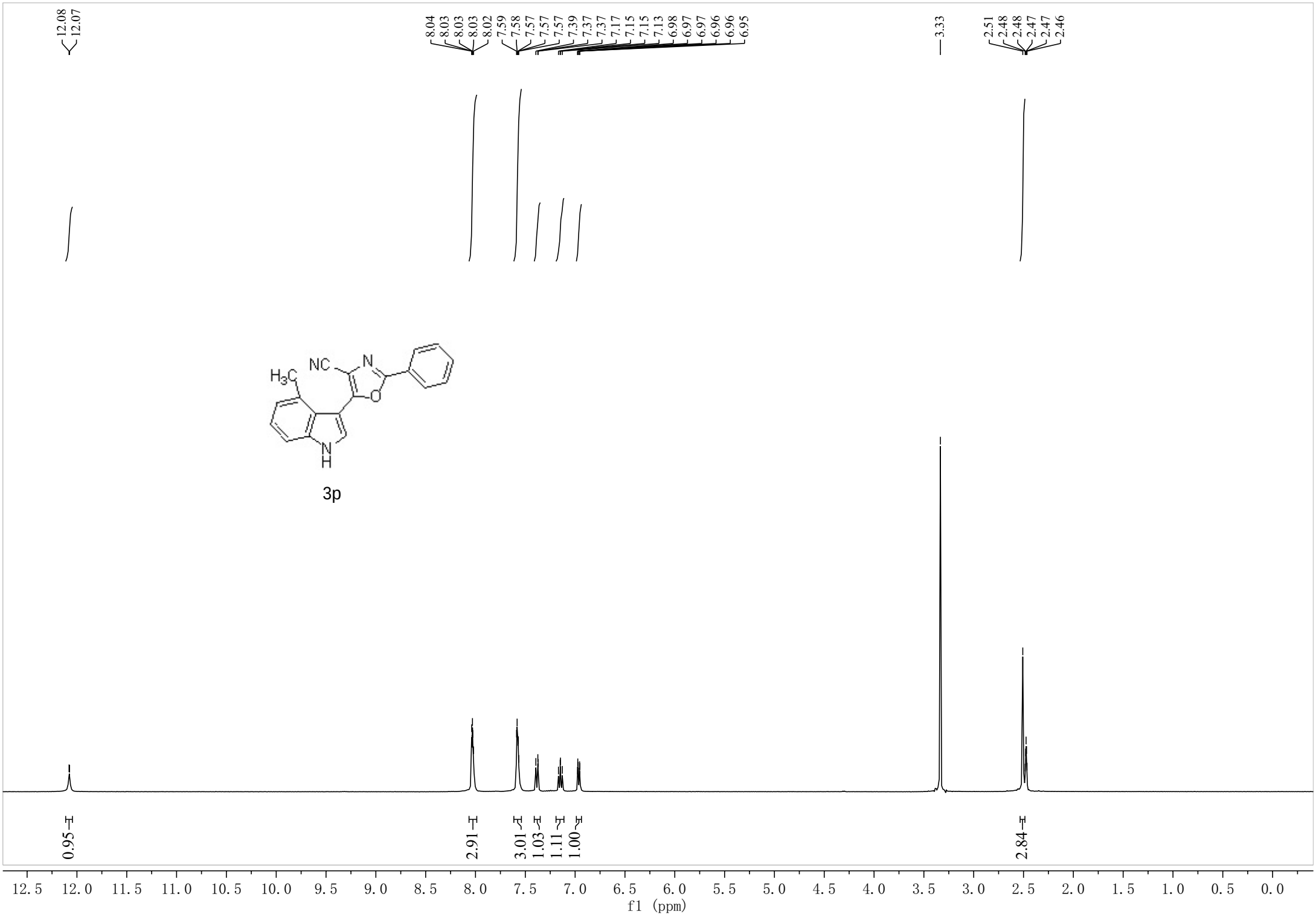


3o

158.66
157.52
155.40
131.76
131.64
129.79
128.32
126.52
125.93
124.51
115.34
113.95
113.39
104.19
102.11
101.31
55.68
40.57
40.36
40.15
39.94
39.73
39.53
39.32

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)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12.07
8.04
8.03
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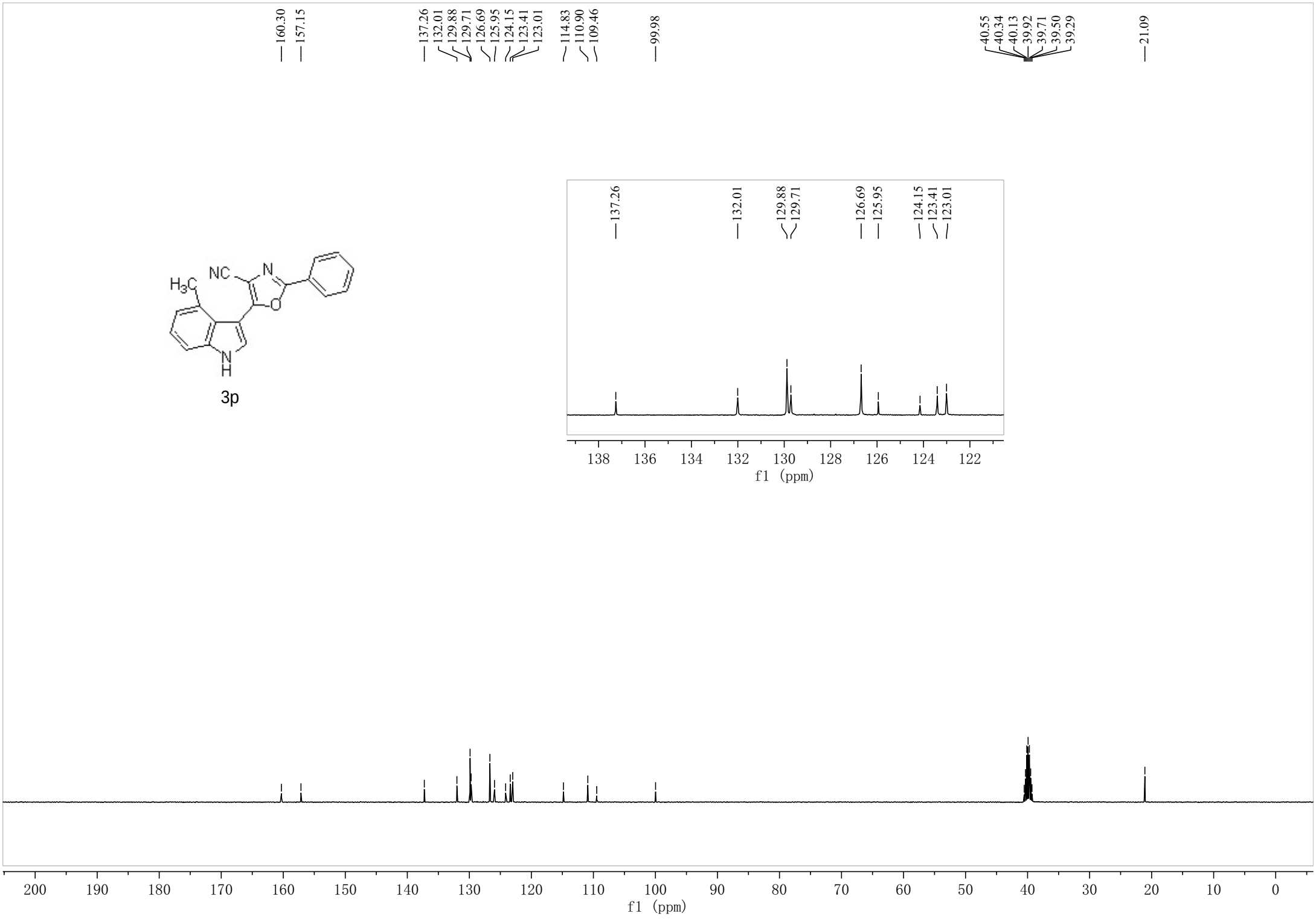
8.03
8.02
7.59
7.58
7.57
7.57
7.57
7.39
7.37
7.37
7.17
7.15
7.15
7.13
6.98
6.97
6.97
6.96
6.96
6.95
3.33
2.51
2.48
2.48
2.47
2.47
2.46
NC
N
H3C
O
N
H
3p
0.95
2.91
3.01
1.03
1.11
1.00
2.84
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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157.15
137.26
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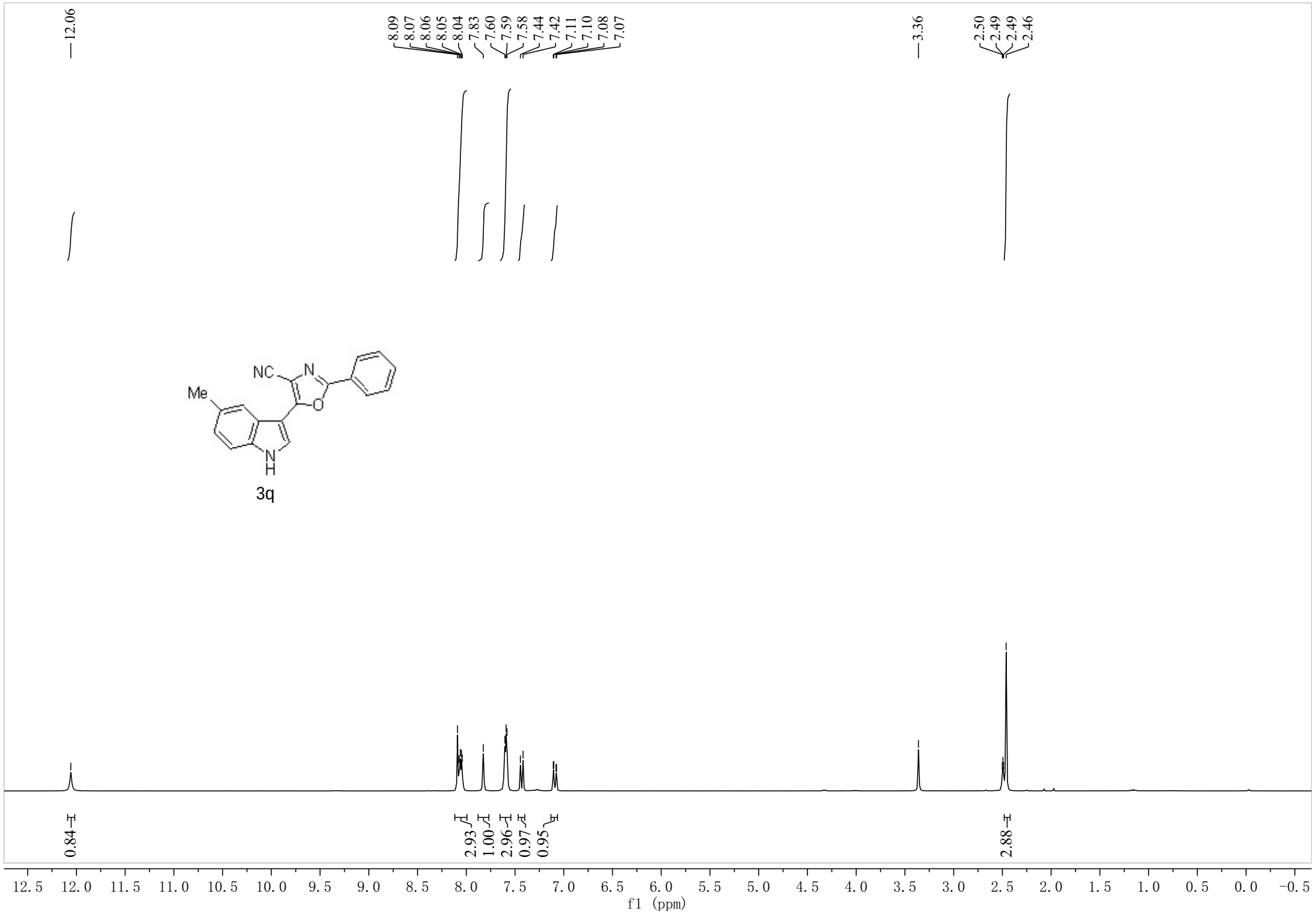
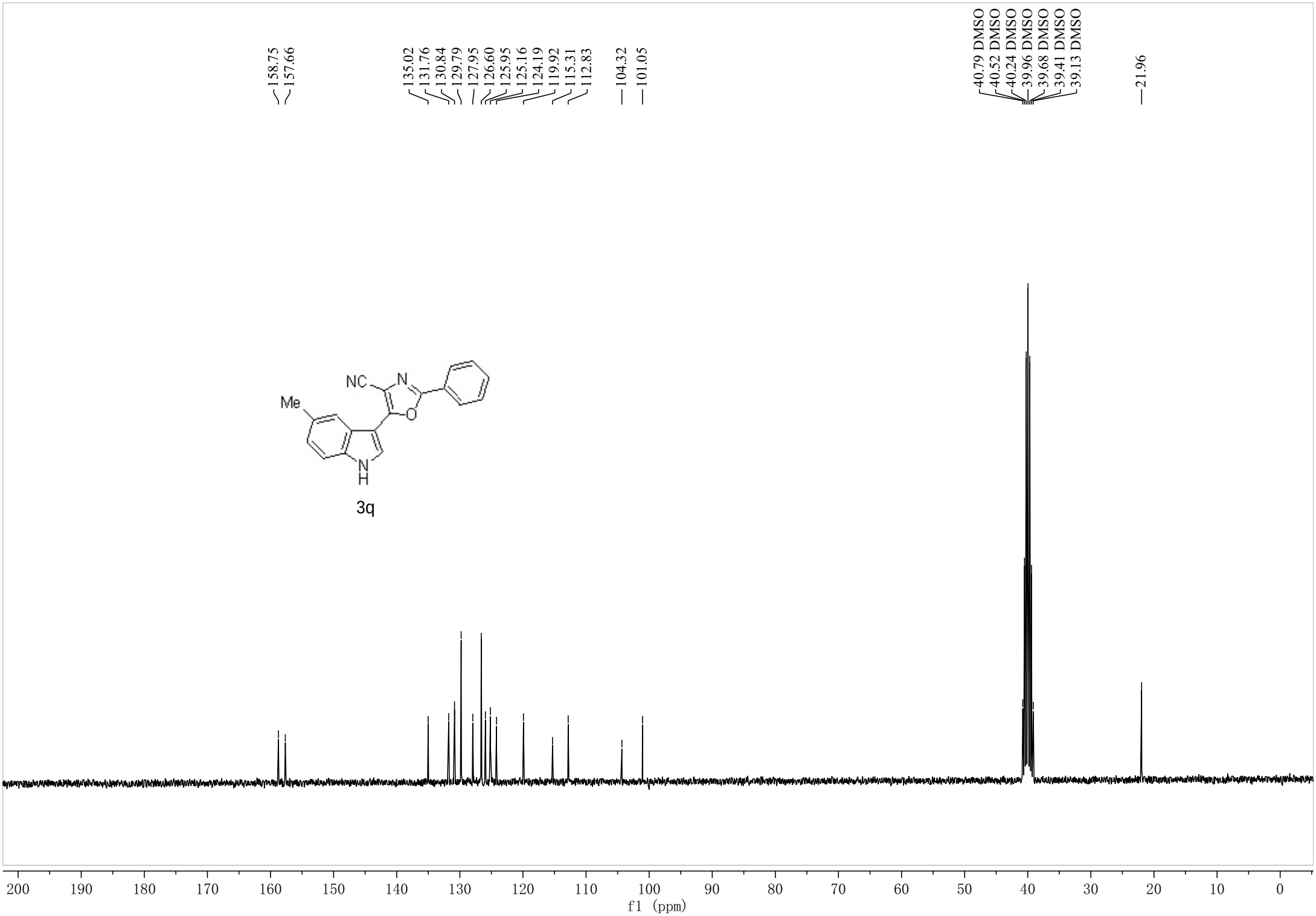
129.88
129.71
126.69
125.95
124.15
123.41
123.01
114.83
110.90
109.46
99.98
40.55
40.34
40.13
39.92
39.71
39.50
39.29
21.09
NC
N
H3C
O
N
H
3p
137.26
132.01
129.88
129.71
126.69
125.95
124.15
123.41
123.01
138
136
134
132
130
128
126
124
122
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.06
8.09
8.07
8.06
8.05
8.04
7.83
7.60
7.59
7.58
7.44
7.42
7.11
7.10
7.08
7.07
3.36
2.50
2.49
2.49
2.46
NC
N
O
Me
N
H
3q
0.84
2.93
1.00
2.96
0.97
0.95
2.88
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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157.66
135.02
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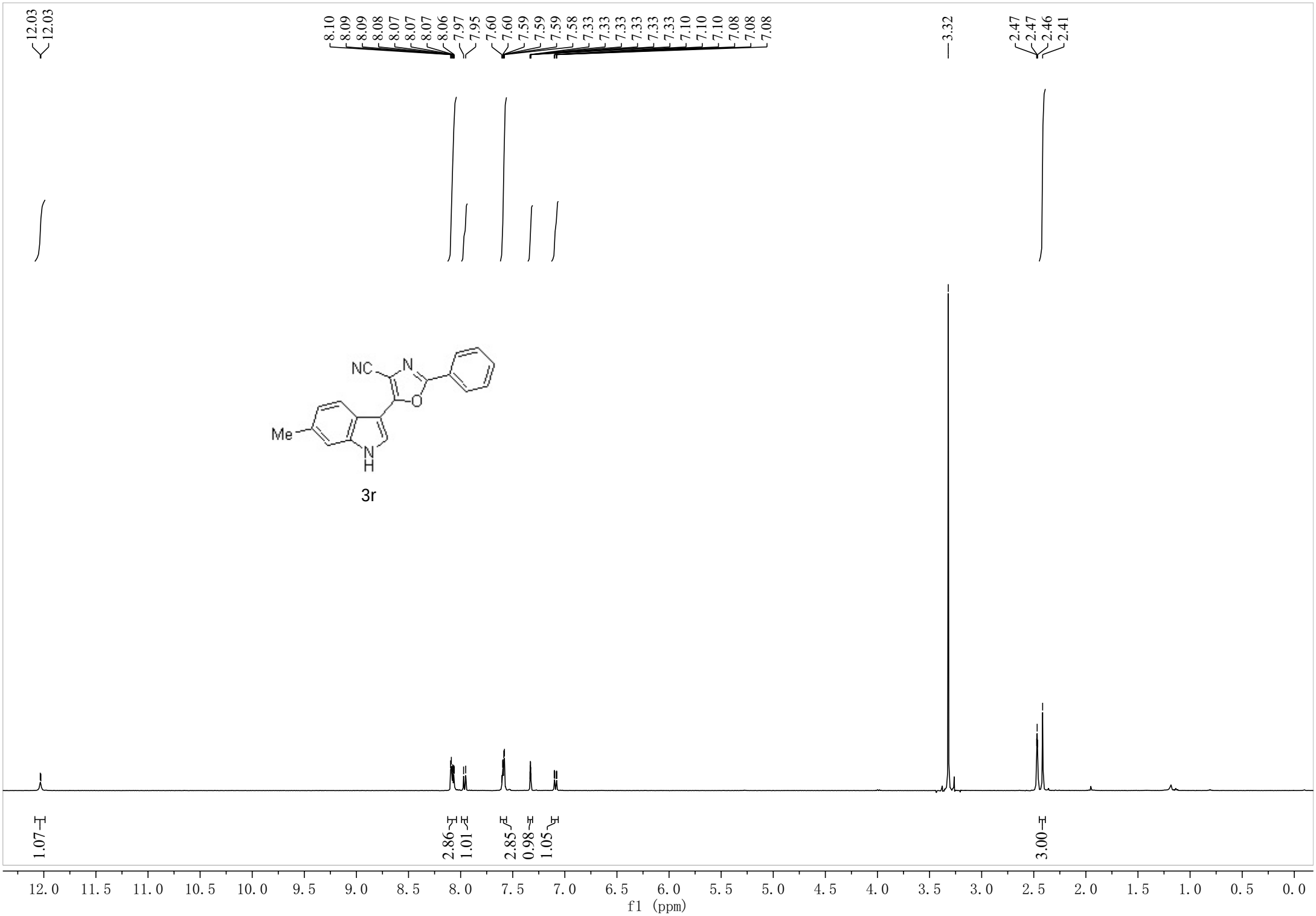
129.79
127.95
126.60
125.95
125.16
124.19
119.92
115.31
112.83
104.32
101.05
40.79 DMSO
40.52 DMSO
40.24 DMSO
39.96 DMSO
39.68 DMSO
39.41 DMSO
39.13 DMSO
21.96
NC
N
Me
O
N
H
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.03
12.03
8.10
8.09
8.09
8.08
8.07
8.07
8.07
8.06
7.97
7.95
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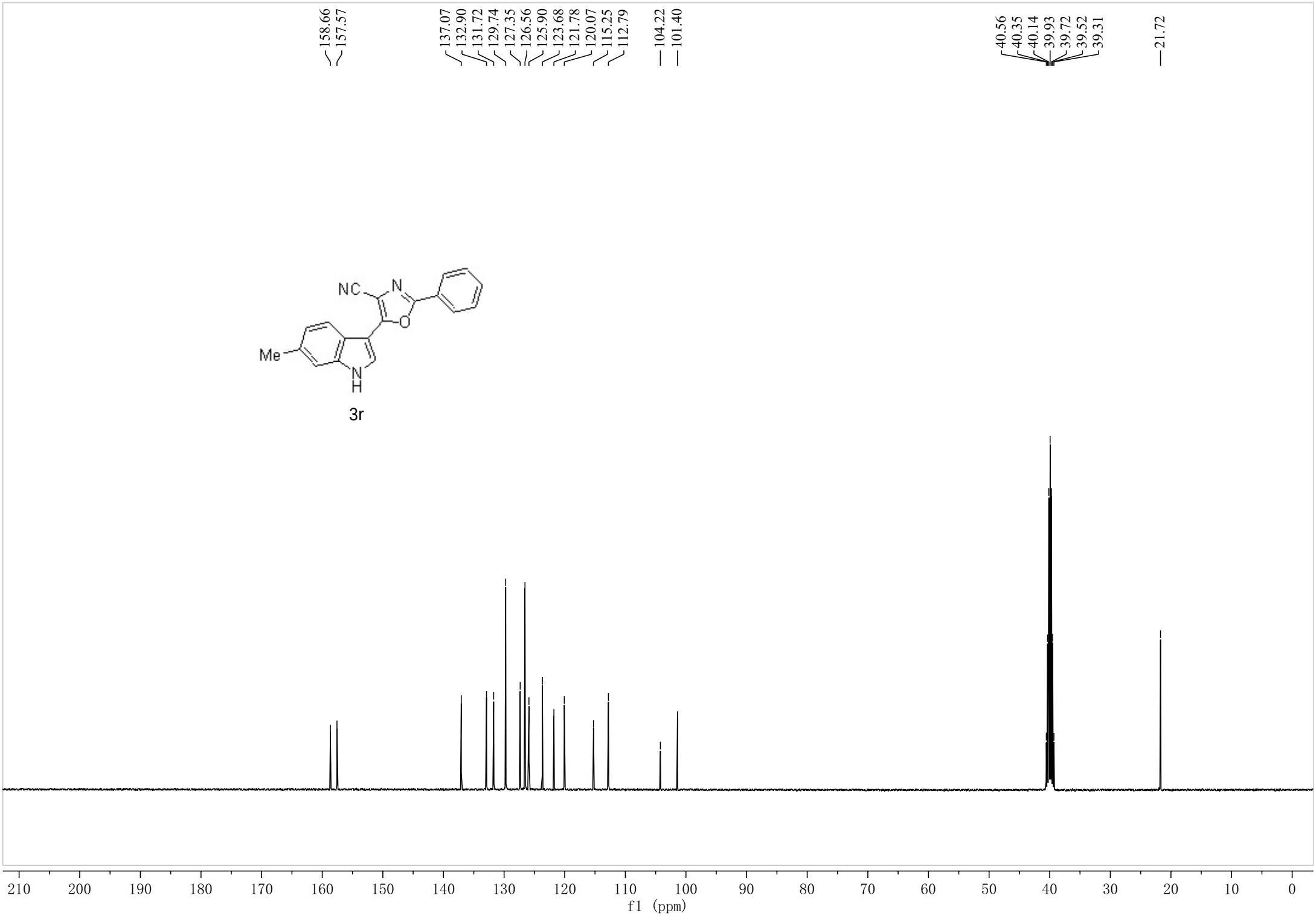
7.60
7.59
7.59
7.59
7.58
7.33
7.33
7.33
7.33
7.33
7.10
7.10
7.08
7.08
7.08
3.32
2.47
2.47
2.46
2.41
NC
N
O
Me
N
H
3r
1.07
2.86
1.01
2.85
0.98
1.05
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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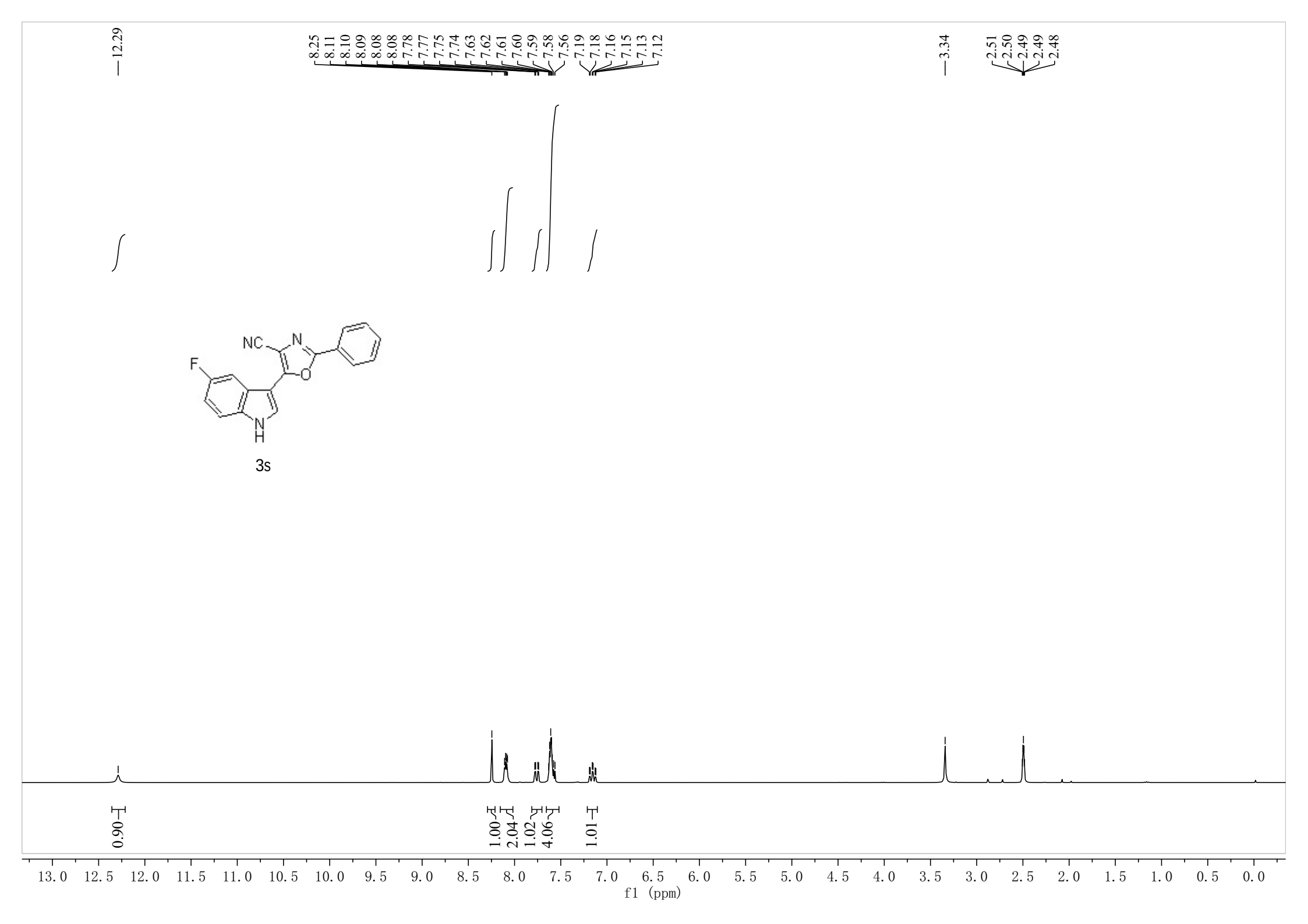
157.57
137.07
132.90
131.72
129.74
127.35
126.56
125.90
123.68
121.78
120.07
115.25
112.79
104.22
101.40
40.56
40.35
40.14
39.93
39.72
39.52
39.31
21.72
NC
N
O
Me
N
H
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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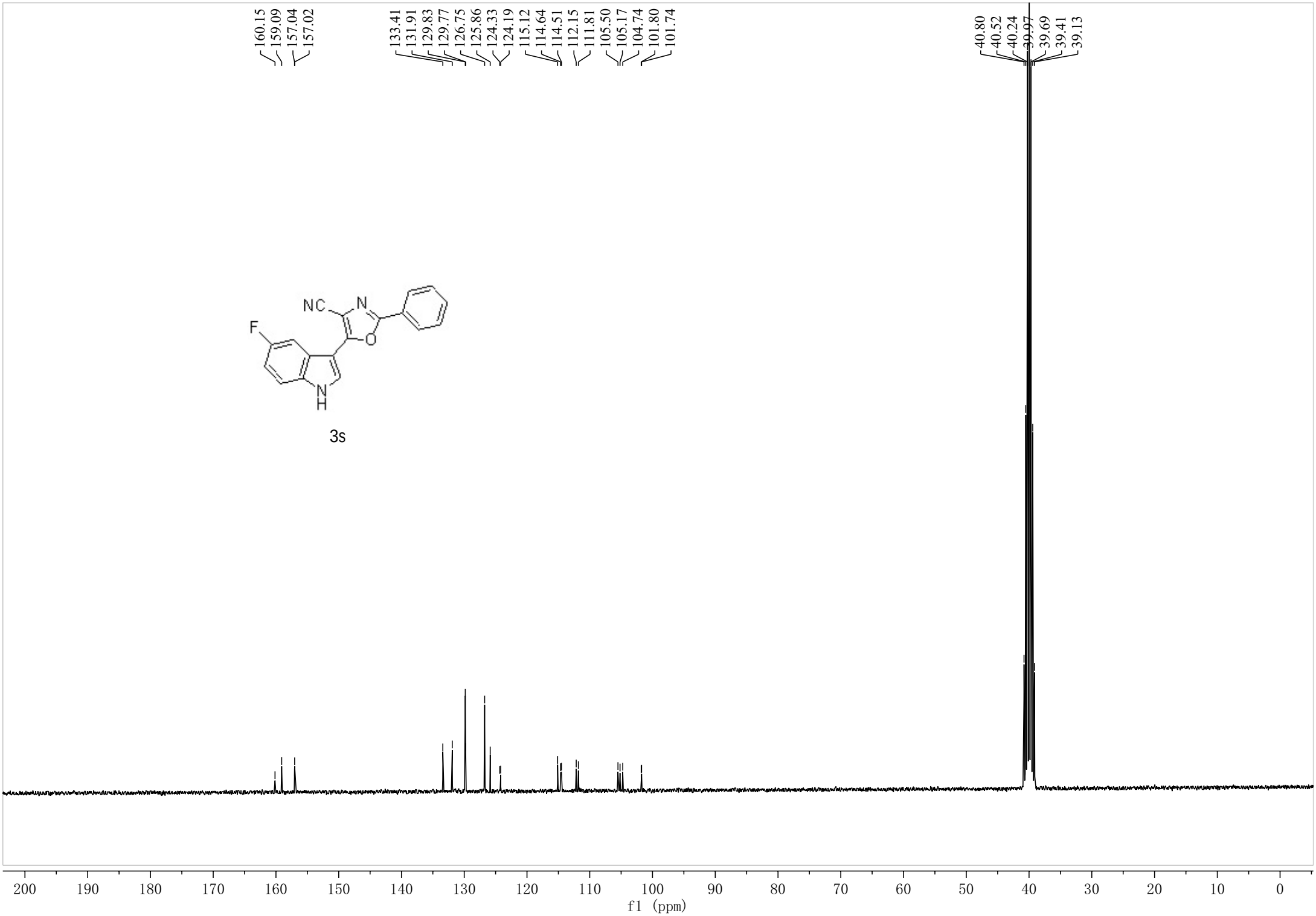
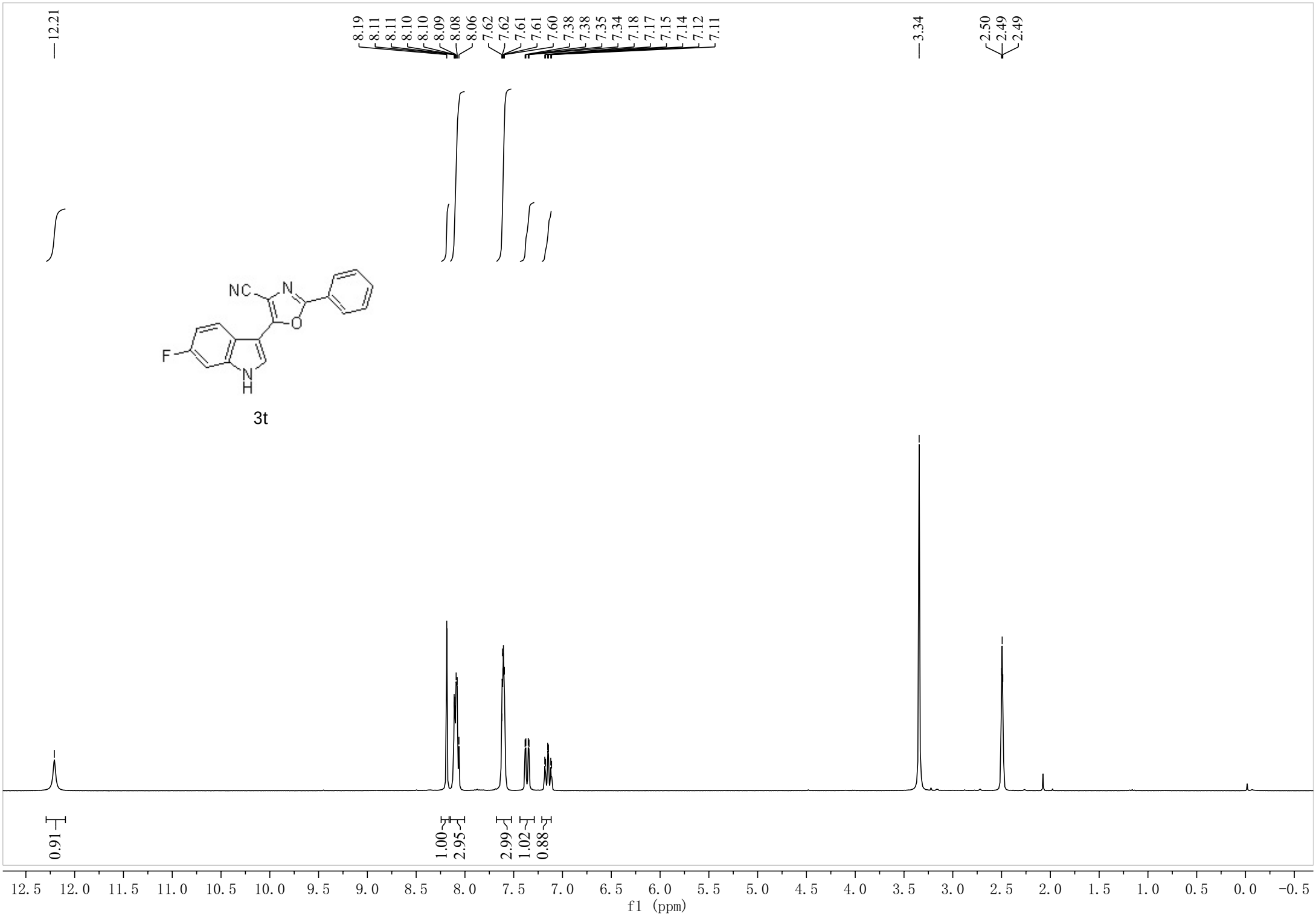
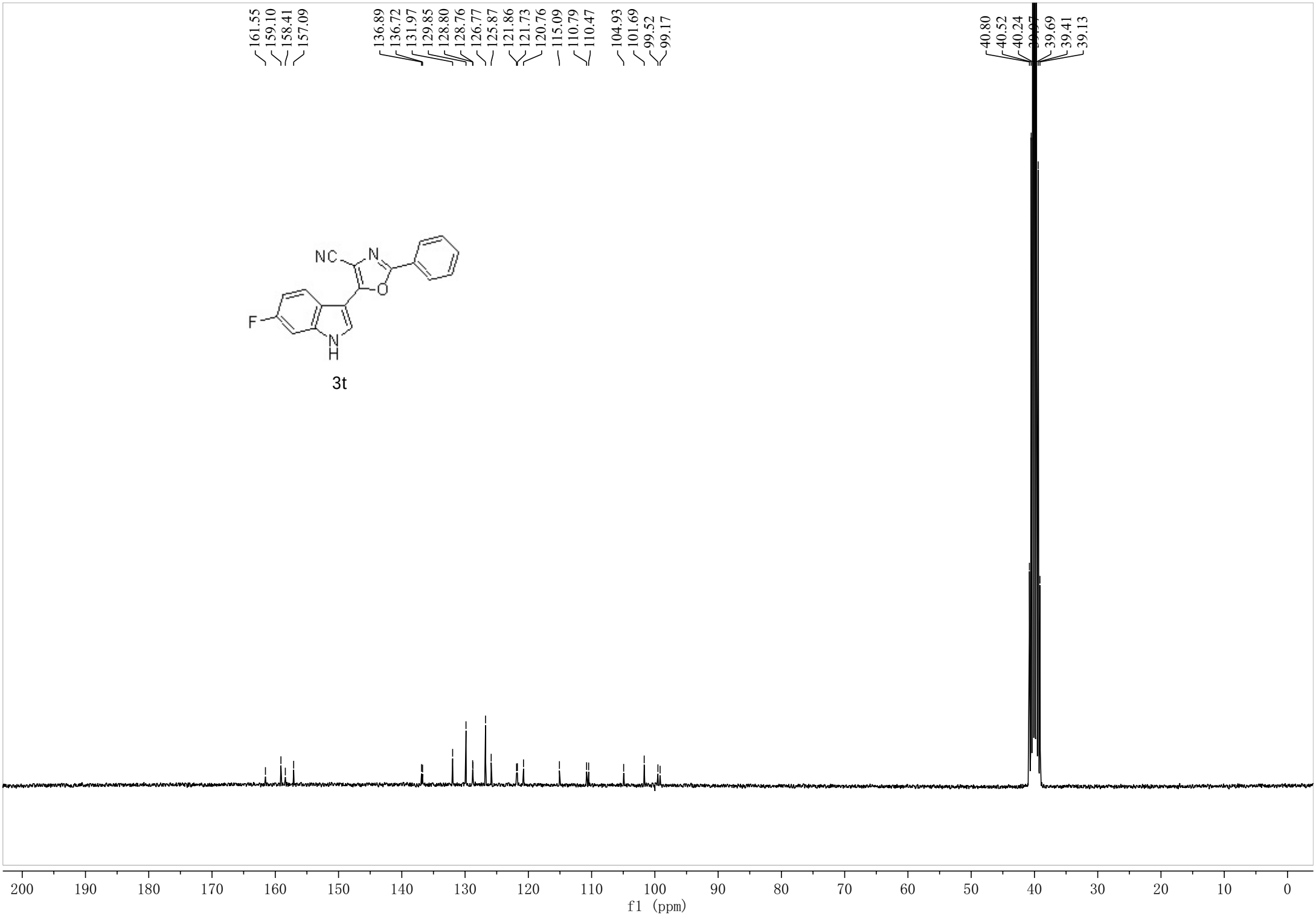
8.25
8.11
8.10
8.09
8.08
8.08
7.78
7.77
7.75
7.74
7.63
7.62
7.61
7.60
7.59
7.58
7.56
7.19
7.18
7.16
7.15
7.13
7.12
3.34
2.51
2.50
2.49
2.49
2.48
NC
N
O
F
N
H
3s
0.90
1.00
2.04
1.02
4.06
1.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.15
159.09
157.04
157.02
133.41
131.91
129.83
129.77
126.75
125.86
124.33
124.19
115.12
114.64
114.51
112.15
111.81
105.50
105.17
104.74
101.80
101.74
40.80
40.52
40.24
39.97
39.69
39.41
39.13
NC
N
F
O
N
H
3s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.21
8.19
8.11
8.11
8.10
8.10
8.09
8.08
8.06
7.62
7.62
7.61
7.61
7.60
7.38
7.38
7.35
7.34
7.18
7.17
7.15
7.14
7.12
7.11
3.34
2.50
2.49
2.49
NC
N
O
F
N
H
3t
0.91
1.00
2.95
2.99
1.02
0.88
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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159.10
158.41
157.09
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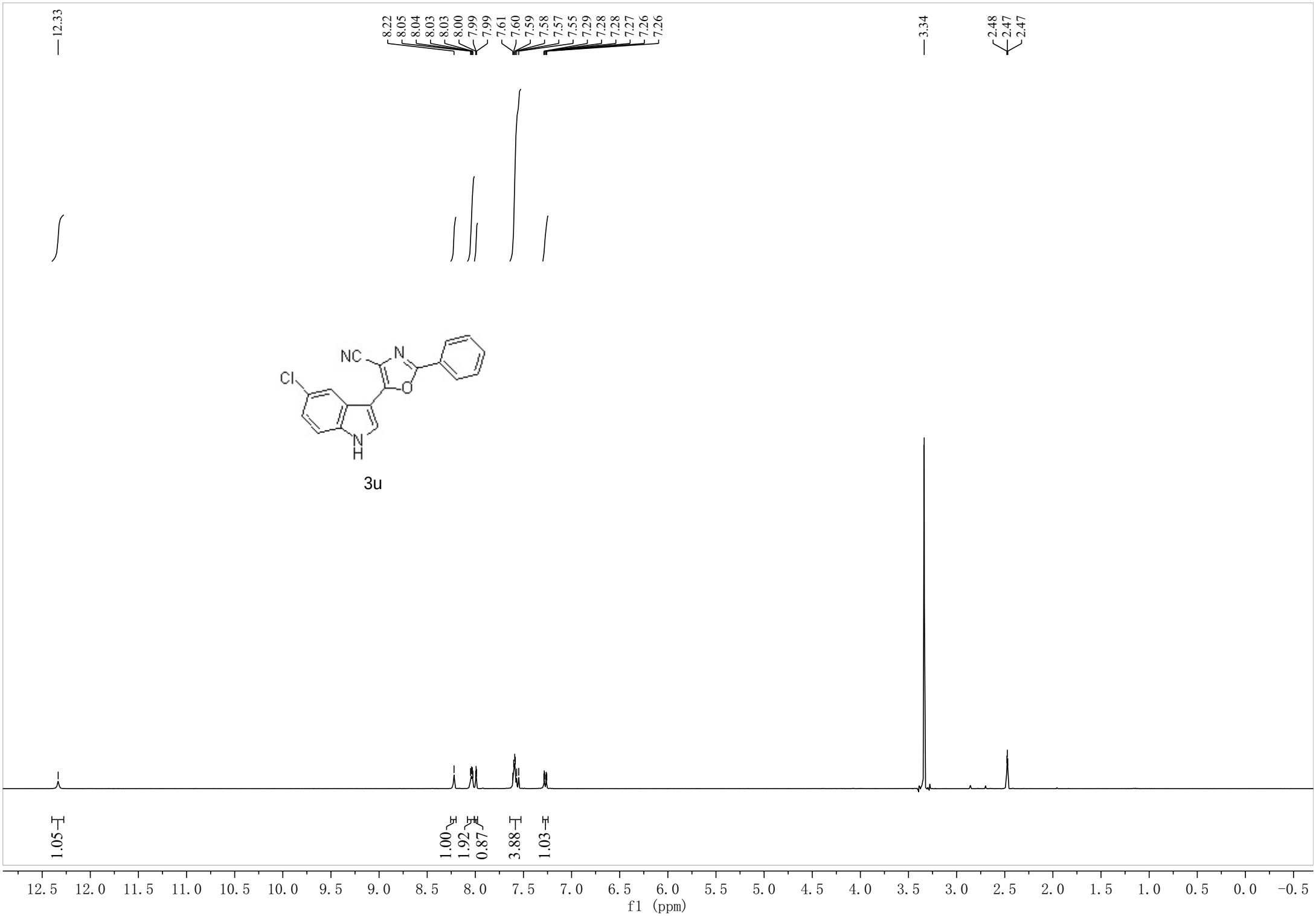
136.72
131.97
129.85
128.80
128.76
126.77
125.87
121.86
121.73
120.76
115.09
110.79
110.47
104.93
101.69
99.52
99.17
40.80
40.52
40.24
39.69
39.41
39.13
NC
N
O
F
N
H
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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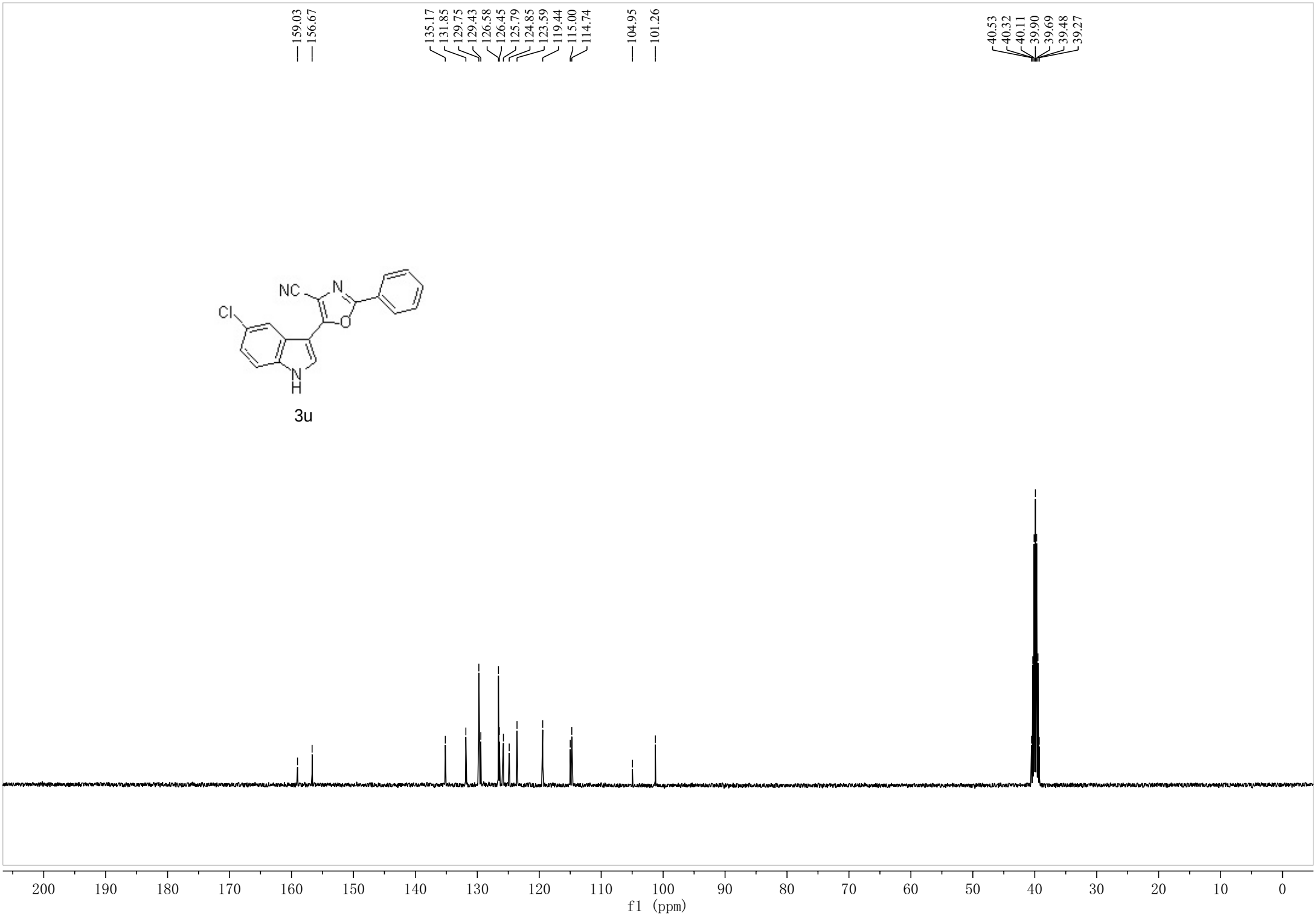
8.22
8.05
8.04
8.03
8.03
8.00
7.99
7.99
7.61
7.60
7.59
7.58
7.57
7.55
7.29
7.28
7.28
7.27
7.26
7.26
3.34
2.48
2.47
2.47
NC
N
Cl
O
N
H
3u
1.05
1.00
1.92
0.87
3.88
1.03
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


159.03
156.67
135.17
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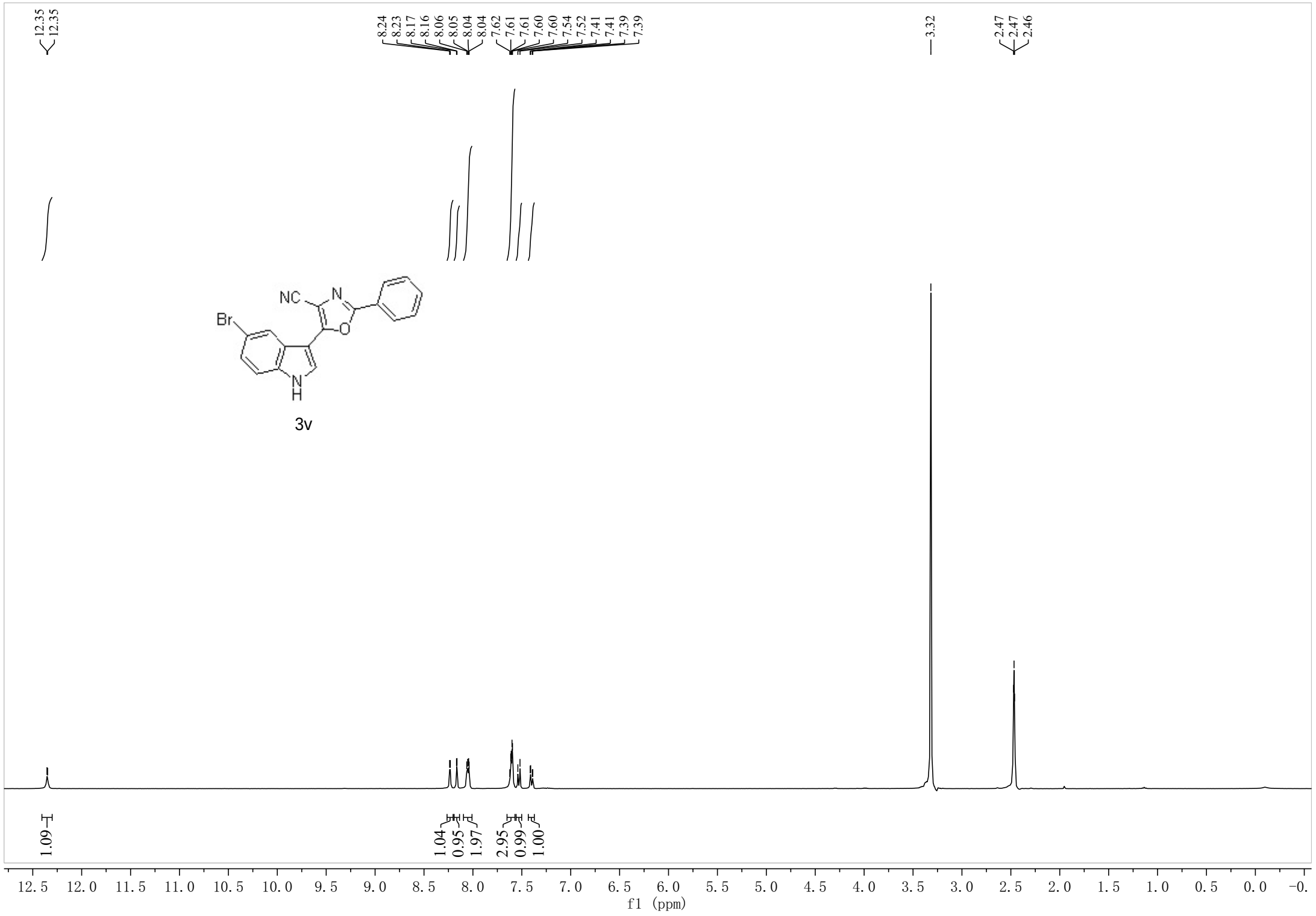
129.75
129.43
126.58
126.45
125.79
124.85
123.59
119.44
115.00
114.74
104.95
101.26
40.53
40.32
40.11
39.90
39.69
39.48
39.27
NC
N
Cl
O
N
H
3u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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12.35
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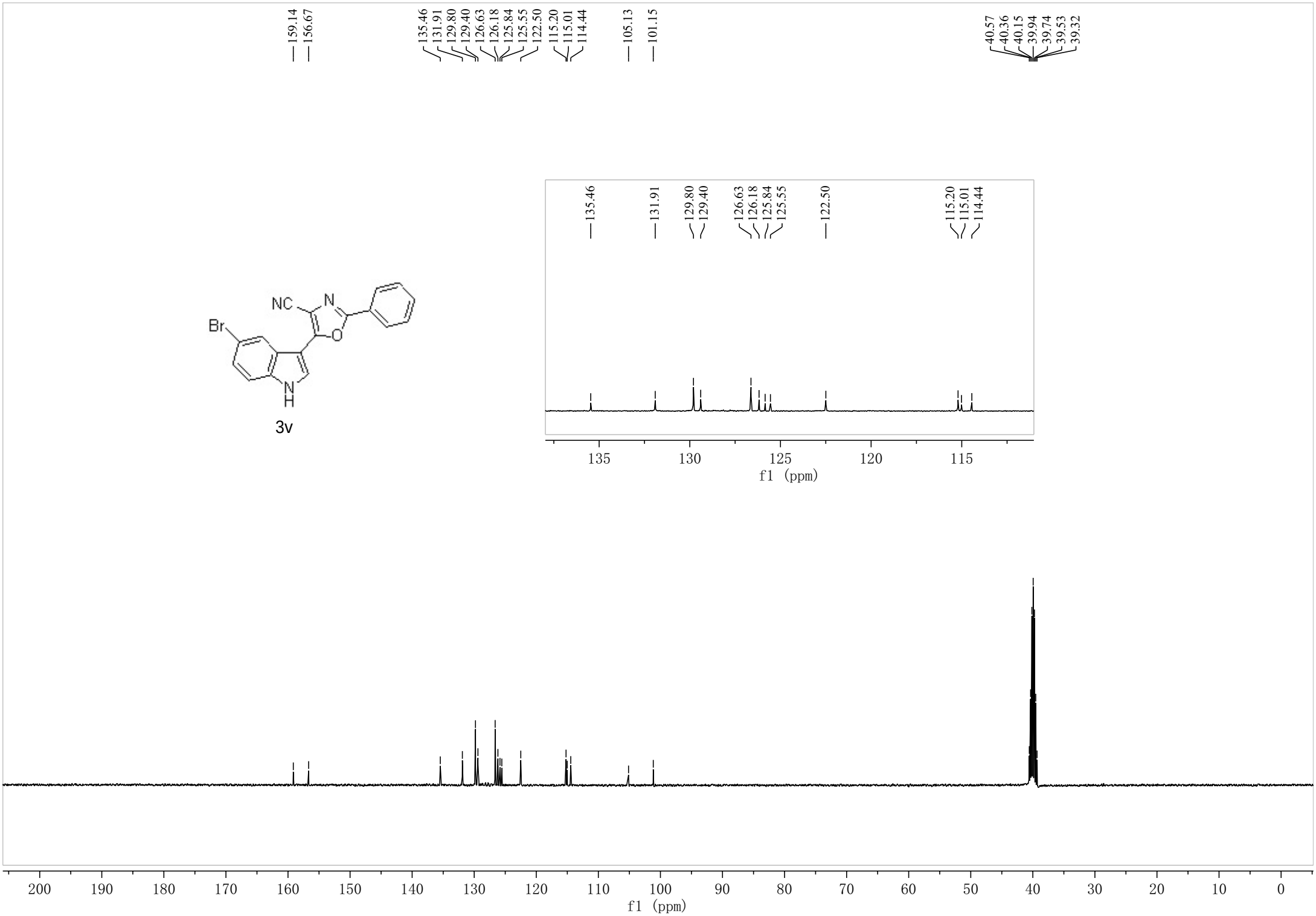
8.16
8.06
8.05
8.04
8.04
7.62
7.61
7.61
7.60
7.60
7.54
7.52
7.41
7.41
7.39
7.39
3.32
2.47
2.47
2.46
NC
N
Br
O
N
H
3v
1.09
1.04
0.95
1.97
2.95
0.99
1.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


159.14
156.67
135.46
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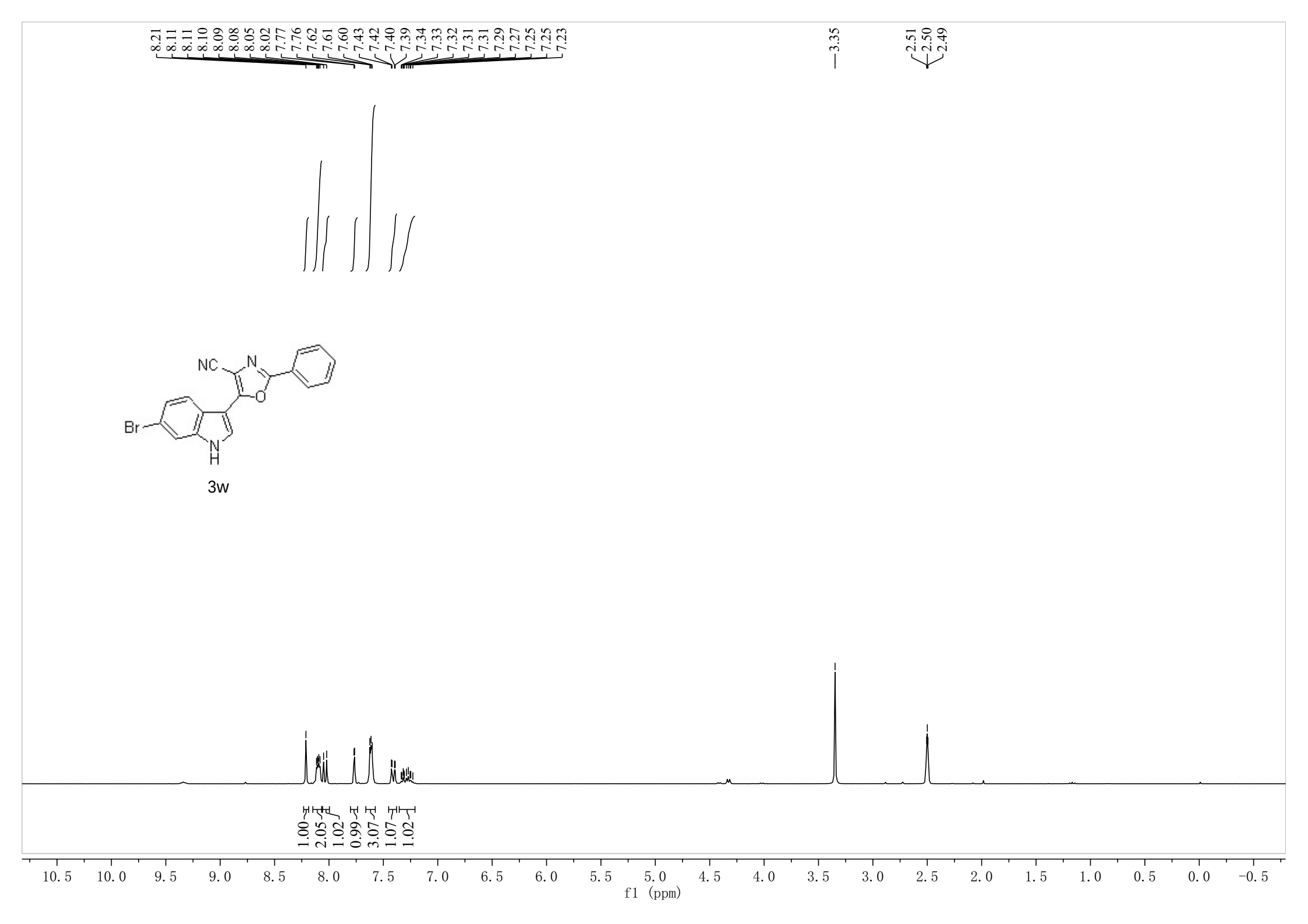
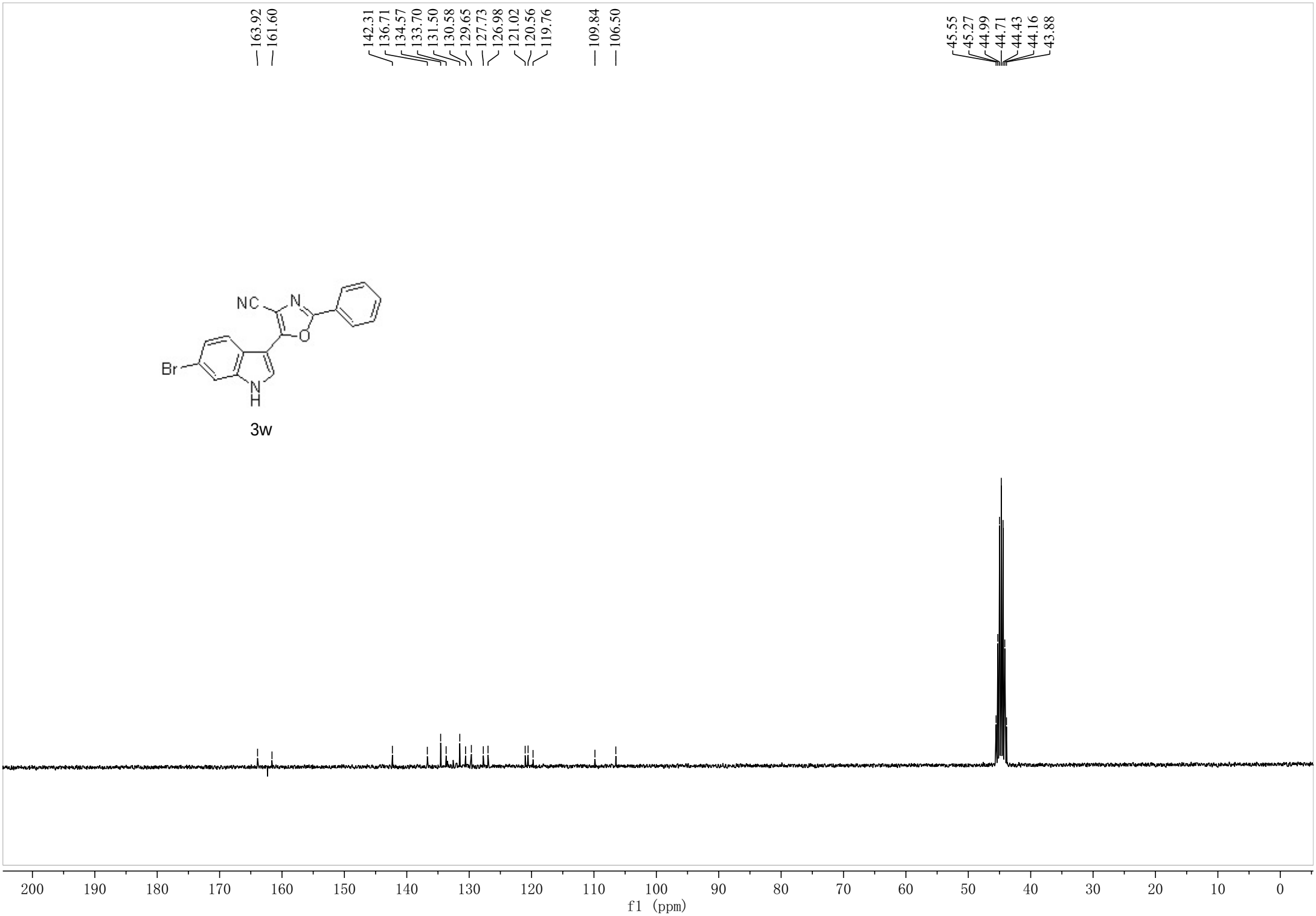
129.80
129.40
126.63
126.18
125.84
125.55
122.50
115.20
115.01
114.44
105.13
101.15
40.57
40.36
40.15
39.94
39.74
39.53
39.32
NC
N
O
Br
N
H
3v
f1 (ppm)
f1 (ppm)


8.21
8.11
8.11
8.10
8.09
8.08
8.05
8.02
7.77
7.76
7.62
7.61
7.60
7.43
7.42
7.40
7.39
7.34
7.33
7.32
7.31
7.31
7.29
7.27
7.25
7.25
7.23
3.35
2.51
2.50
2.49
NC
N
O
Br
N
H
3w
1.00
2.05
1.02
0.99
3.07
1.07
1.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.92
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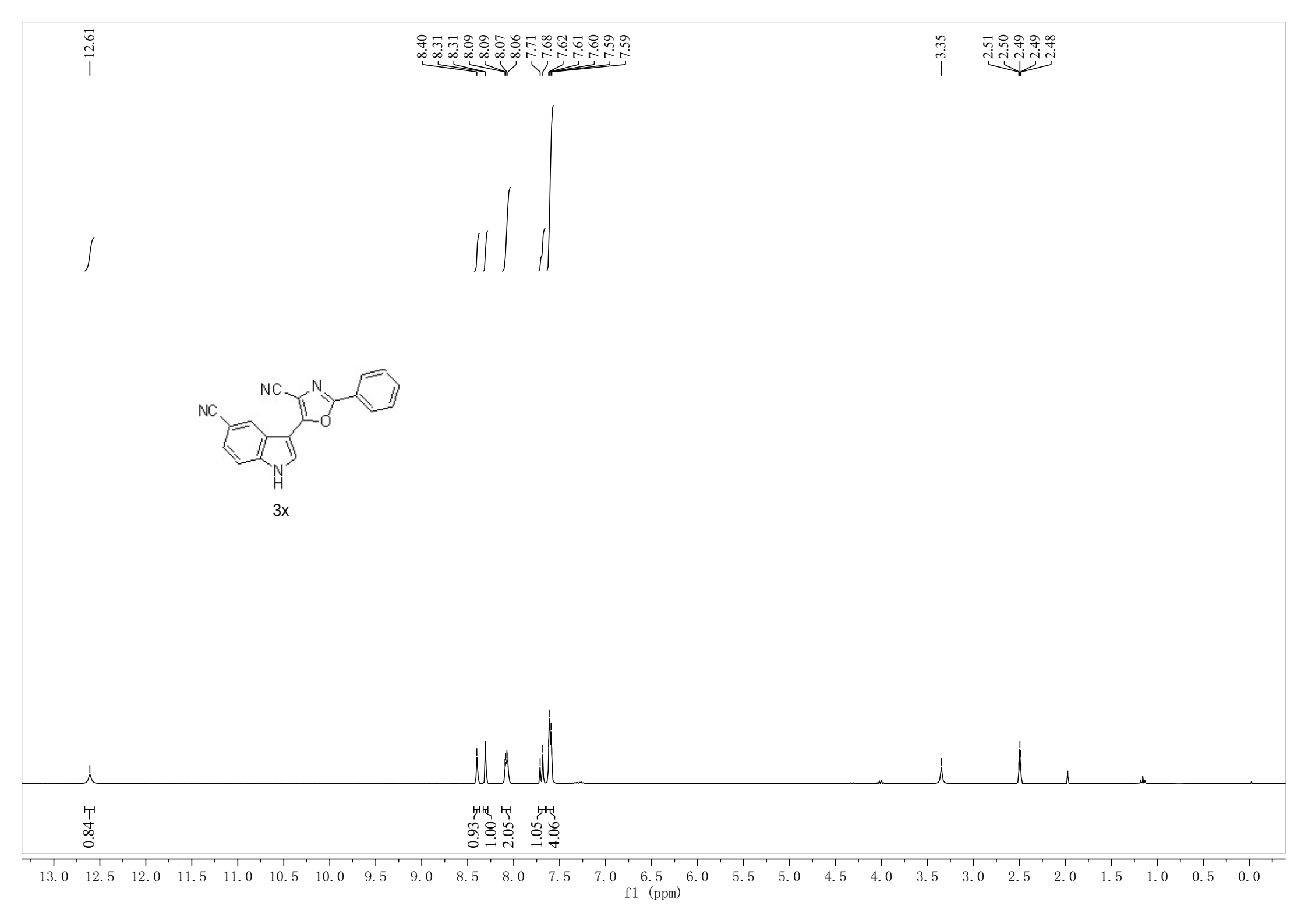
134.57
133.70
131.50
130.58
129.65
127.73
126.98
121.02
120.56
119.76
109.84
106.50
45.55
45.27
44.99
44.71
44.43
44.16
43.88
NC
N
O
Br
N
H
3w
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.61
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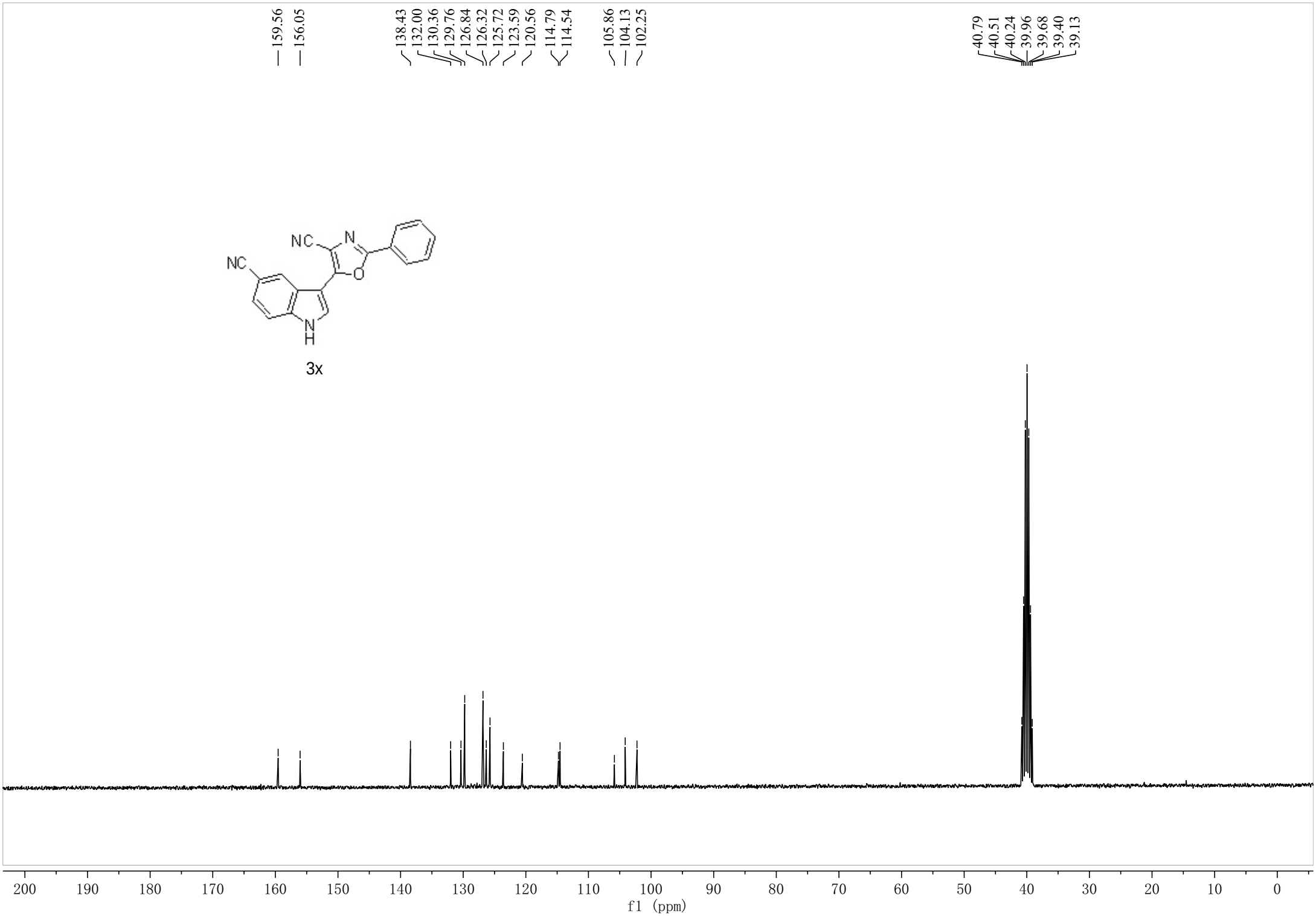
8.31
8.09
8.09
8.07
8.06
7.71
7.68
7.62
7.61
7.60
7.59
7.59
3.35
2.51
2.50
2.49
2.49
2.48
NC
N
NC
O
N
H
0.84
0.93
1.00
2.05
1.05
4.06
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3x


159.56
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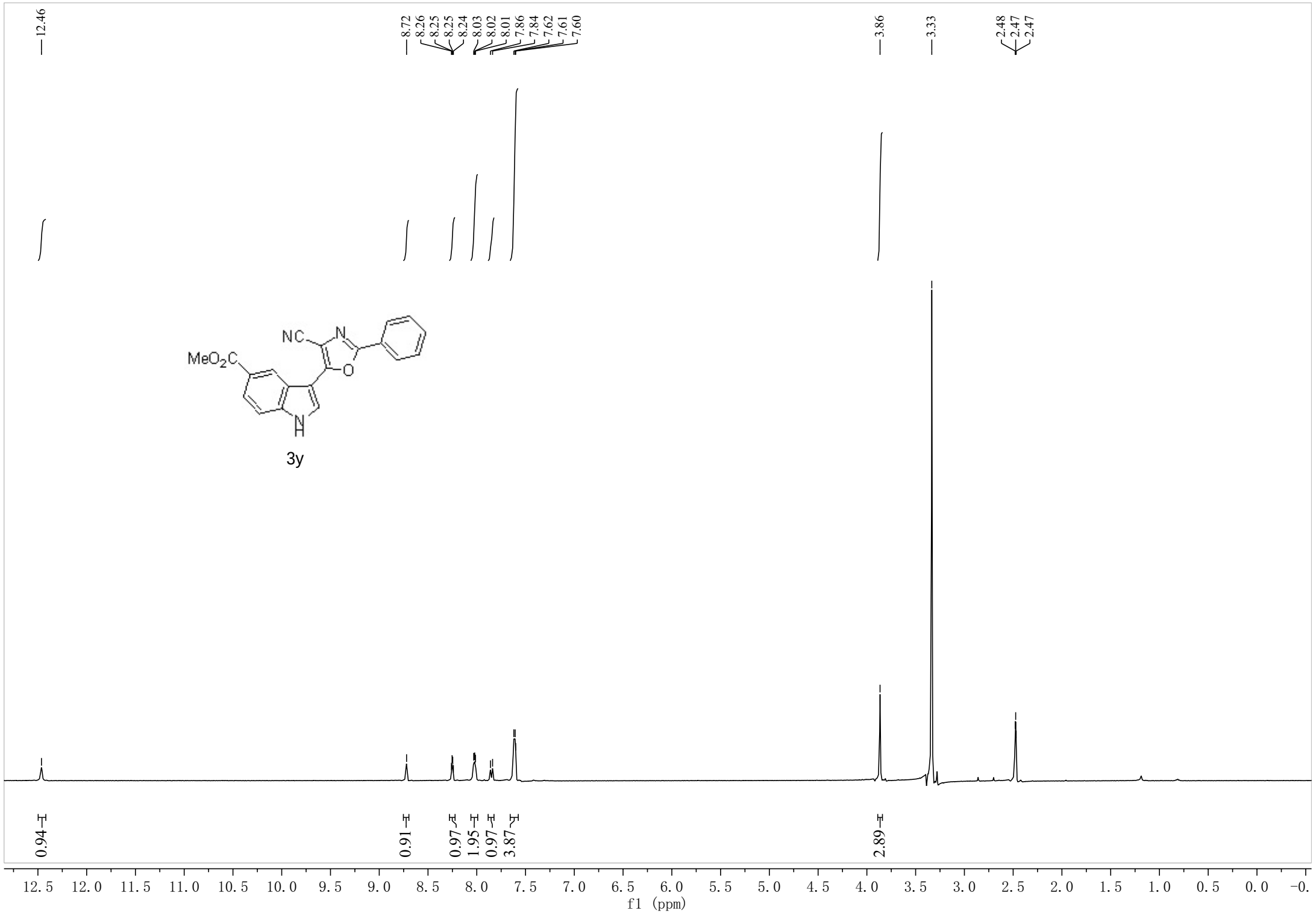
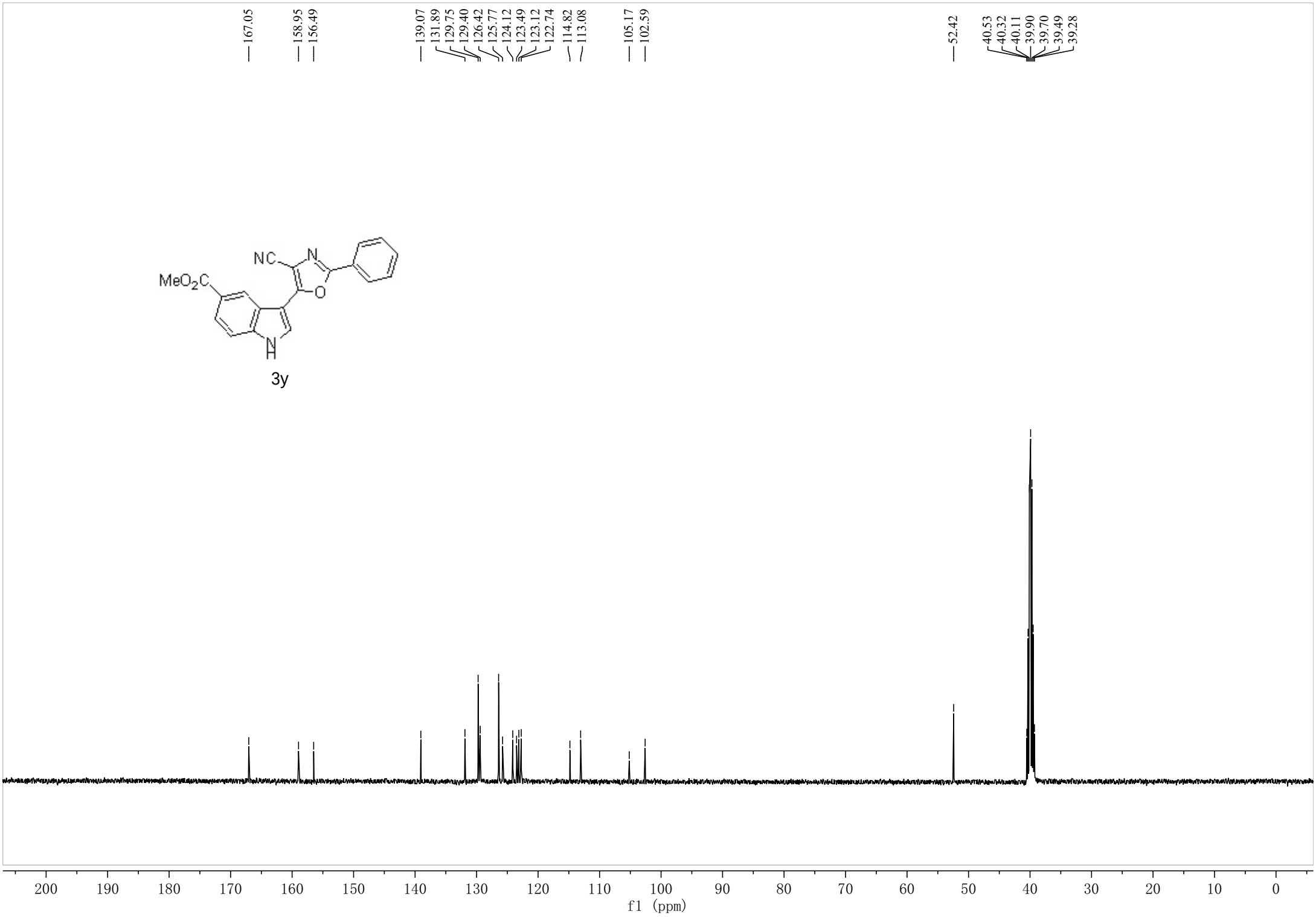
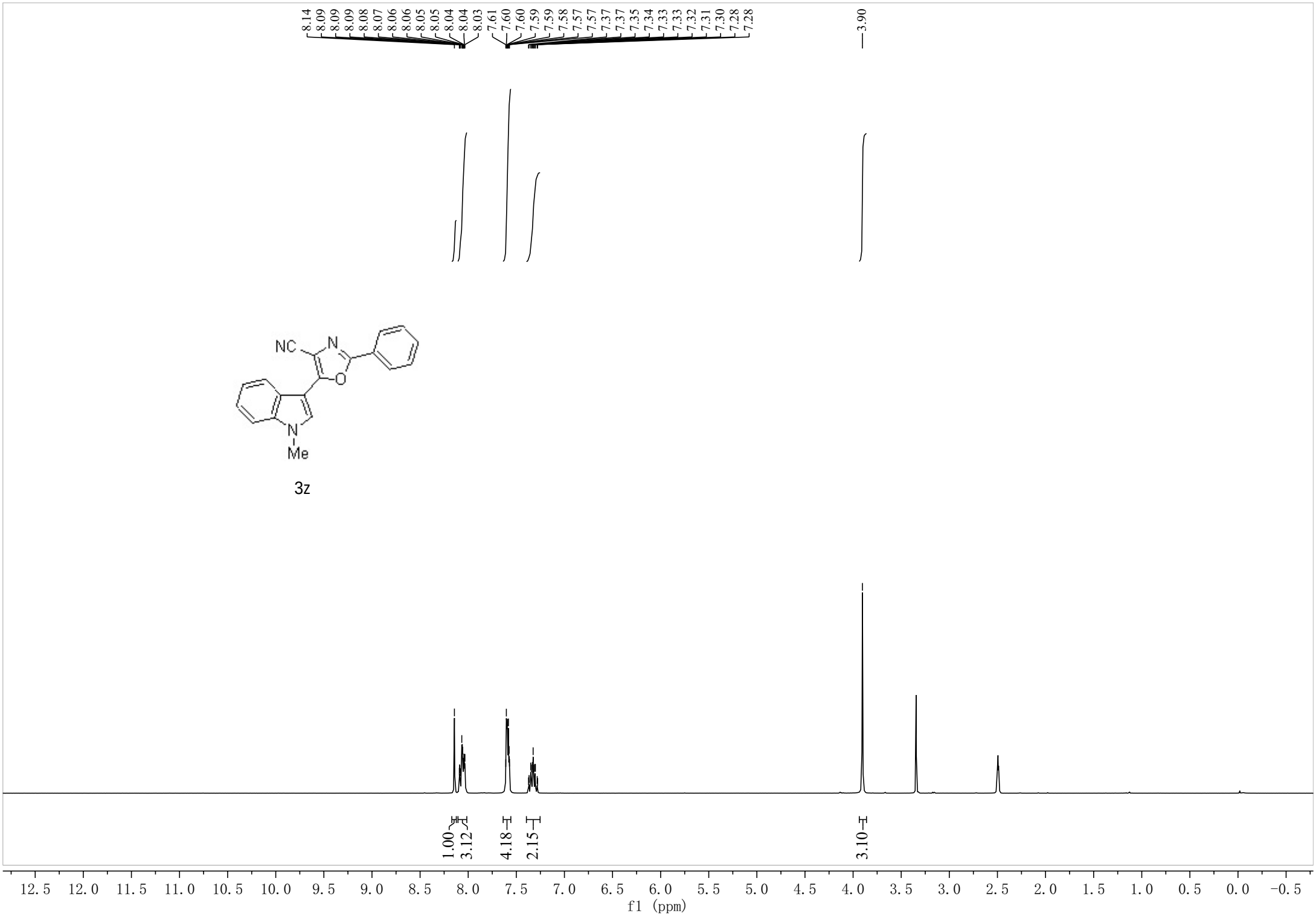
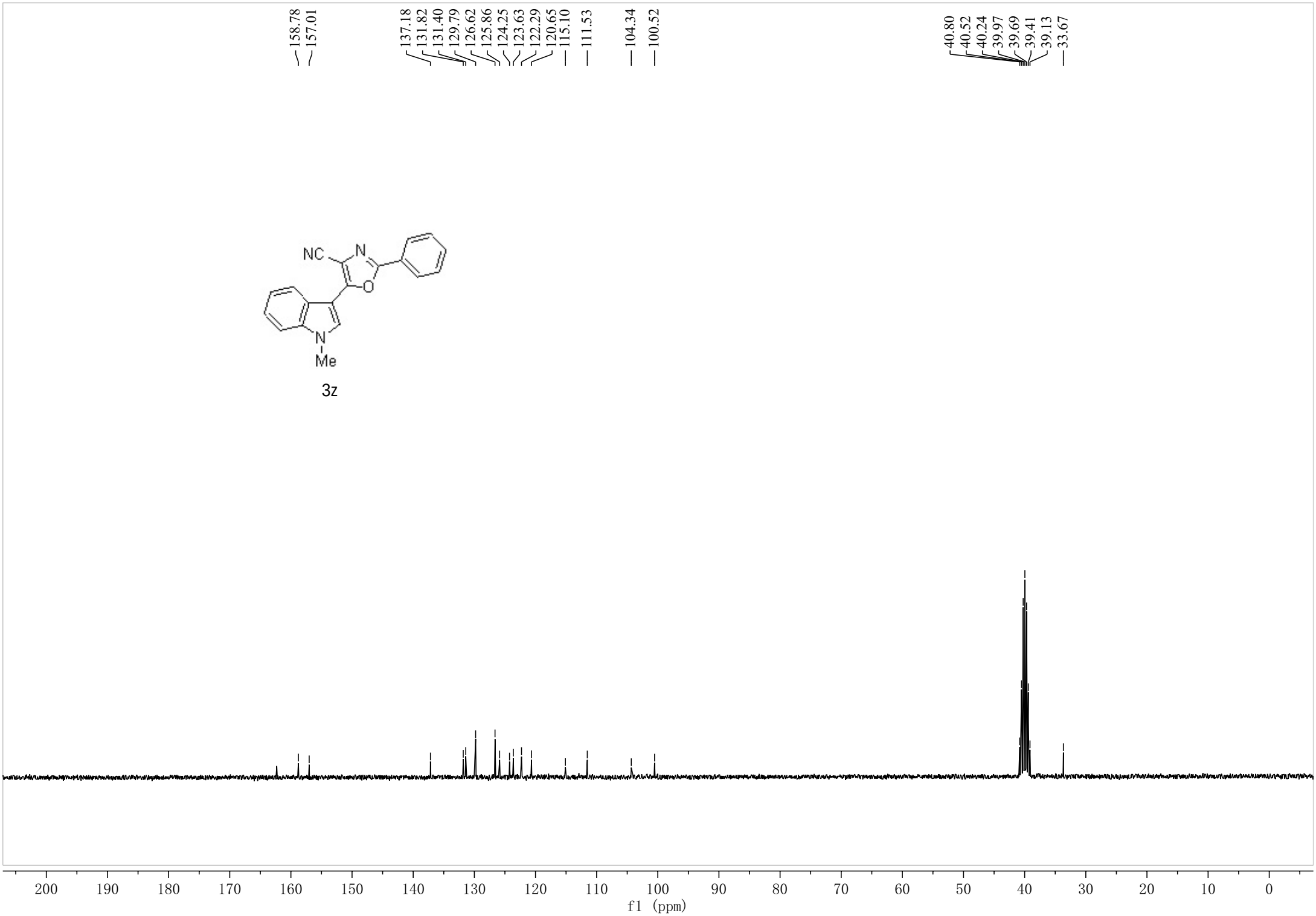
132.00
130.36
129.76
126.84
126.32
125.72
123.59
120.56
114.79
114.54
105.86
104.13
102.25
40.79
40.51
40.24
39.96
39.68
39.40
39.13
NC
N
NC
O
N
H
3x
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.46
8.72
8.26
8.25
8.25
8.24
8.03
8.02
8.01
7.86
7.84
7.62
7.61
7.60
3.86
3.33
2.48
2.47
2.47
NC
N
MeO2C
O
H
0.94
0.91
0.97
1.95
0.97
3.87
2.89
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

3y


167.05
158.95
156.49
139.07
131.89
129.75
129.40
126.42
125.77
124.12
123.49
123.12
122.74
114.82
113.08
105.17
102.59
52.42
40.53
40.32
40.11
39.90
39.70
39.49
39.28
NC
N
MeO2C
O
N
H
3y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.14
8.09
8.09
8.09
8.08
8.07
8.06
8.06
8.05
8.05
8.04
8.04
8.03
7.61
7.60
7.60
7.59
7.59
7.58
7.57
7.57
7.37
7.37
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.28
7.28
3.90
NC
N
O
N
Me
3z
1.00
3.12
4.18
2.15
3.10
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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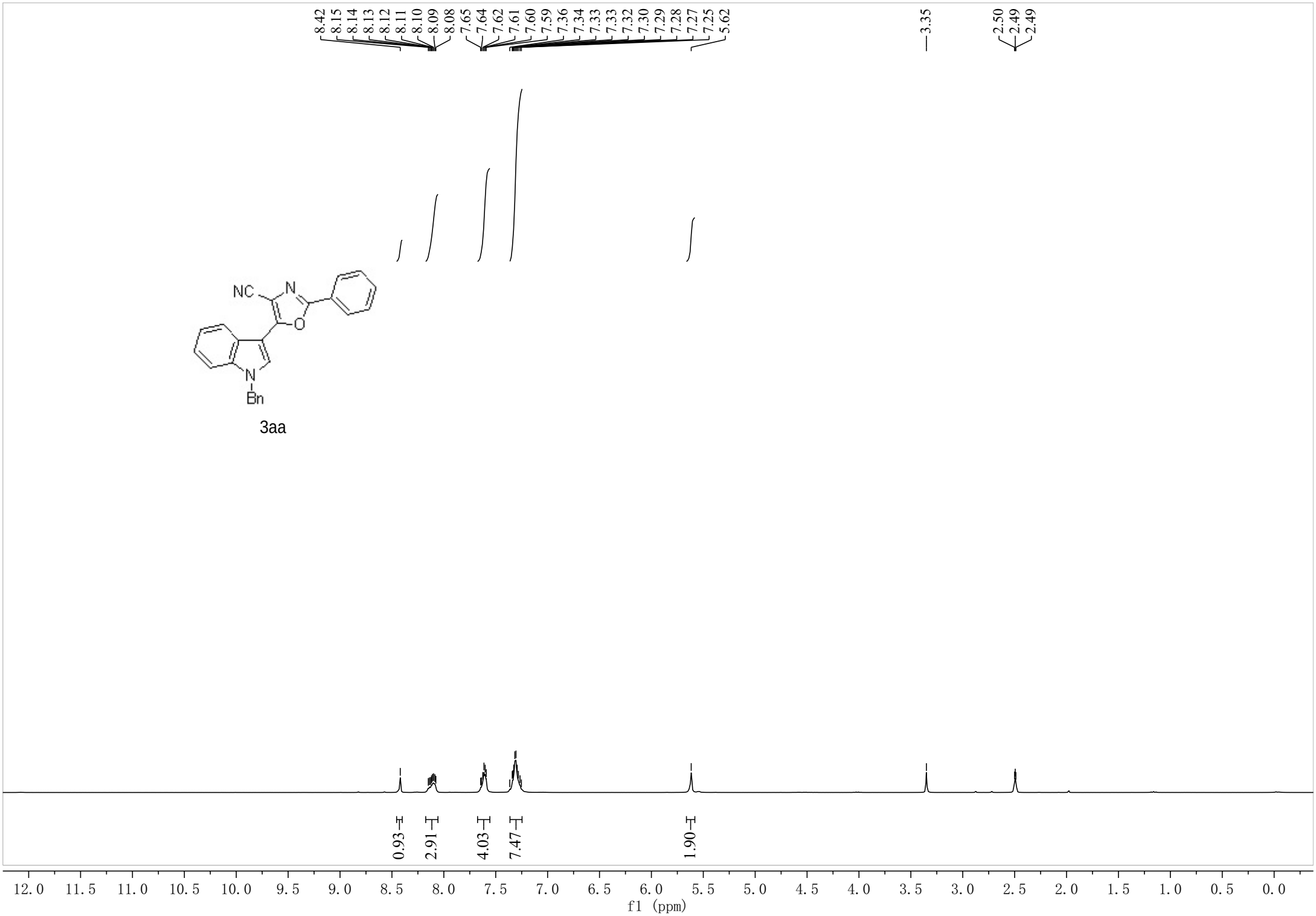
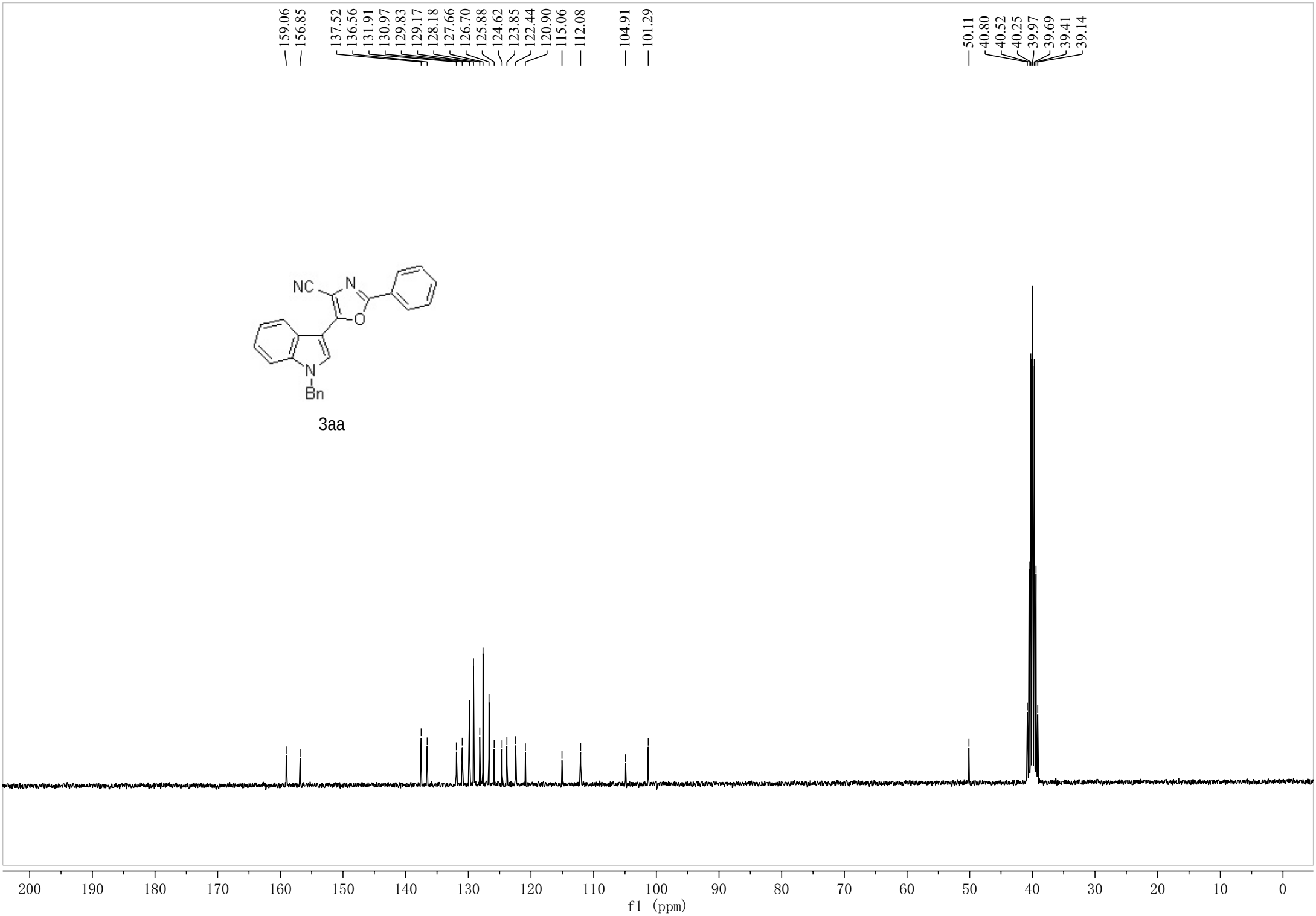
157.01
137.18
131.82
131.40
129.79
126.62
125.86
124.25
123.63
122.29
120.65
115.10
111.53
104.34
100.52
40.80
40.52
40.24
39.97
39.69
39.41
39.13
33.67
NC
N
O
N
Me
3z
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.42
8.15
8.14
8.13
8.12
8.11
8.10
8.09
8.08
7.65
7.64
7.62
7.61
7.60
7.59
7.36
7.34
7.33
7.33
7.32
7.30
7.29
7.28
7.27
7.25
5.62
3.35
2.50
2.49
2.49
NC
N
O
N
Bn
0.93
2.91
4.03
7.47
1.90
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3aa


159.06
156.85
137.52
136.56
131.91
130.97
129.83
129.17
128.18
127.66
126.70
125.88
124.62
123.85
122.44
120.90
115.06
112.08
104.91
101.29
50.11
40.80
40.52
40.25
39.97
39.69
39.41
39.14
NC
N
O
N
Bn
3aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)