Supporting Information

Cyanation of glycine derivatives

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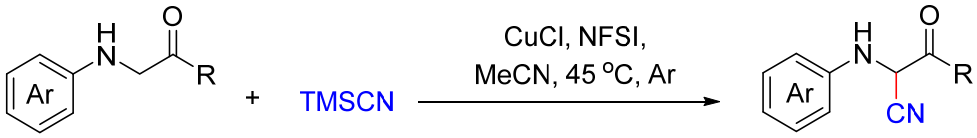

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Experimental Section

General Information

The starting materials, reagents and solvents, purchased from commercial suppliers, were used without further purification. Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. Flash chromatography was carried out using silica gel 200−300. ^{1}HNMR (400 MHz or 600 MHz) and ^{13}CNMR (151 MHz) spectra were measured with $CDCl_3$ as solvent. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. High resolution mass spectra (HR-MS) were recorded under electrospray ionization (ESI) conditions.

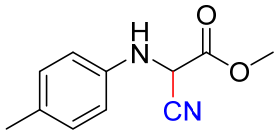
General procedure for the cyanation of glycine derivatives

To a dried reaction tube (10 mL) with a magnetic stirring bar were added glycine esters (**1,** 0.2 mmol), TNSCN (2.5 equiv), CuCl (15 mol %), and NFSI (1 equiv) successively. Air was then withdrawn and backfilled with argon for 3 times. Subsequently, degassed acetonitrile (1 mL) was added and the resulting reaction mixture was performed at 45 °C and completed within 8-12 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **2** (ethyl acetate/petroleum ether = 1:20 to 1:10).

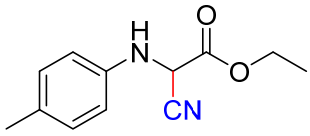
Scale-up experiment

To a dried reaction tube (50 mL) with a magnetic stirring bar were added glycine esters (**1a,** 10 mmol), TNSCN (25 mmol), CuCl (1.5 mmol), and NFSI (10 mmol) successively. Air was then withdrawn and backfilled with argon for 3 times. Subsequently, degassed acetonitrile (15 mL) was added and the resulting reaction mixture was performed at 45 °C for 12 hours. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **2a** (ethyl acetate/petroleum ether = 1:10).

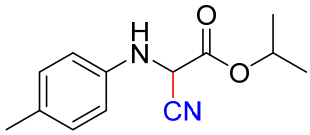
Characterization of the substrates and products



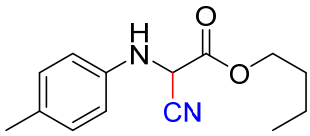
methyl 2-cyano-2-(p-tolylamino)acetate (2a) The desired pure product was obtained in 72% yield (29.4mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.1 Hz, 2H), 6.66 (d, *J* = 8.1 Hz, 2H), 4.92 (d, *J* = 6.3 Hz, 1H), 4.45 (s, 1H), 3.93 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 141.2, 130.1, 130.0, 114.9, 114.4, 54.3, 48.6, 20.5. HRMS (ESI) exact mass calcd for $C_{11}H_{13}N_2O_2$ [M+H] m/z 205.0972, found 205.0971.



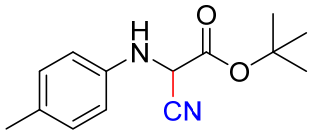
ethyl 2-cyano-2-(p-tolylamino)acetate (2b) The desired pure product was obtained in 71% yield (31.0 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.06 (d, *J* = 8.3 Hz ,2H), 6.65 (d, *J* = 8.4 Hz, 2H), 4.88 (d, *J* = 6.9 Hz, 1H), 4.46 – 4.33 (m, 2H), 2.27 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.2, 141.3, 130.1, 130.0, 115.0, 114.4, 64.0, 48.7, 20.5, 13.9. HRMS (ESI) exact mass calcd for $C_{12}H_{15}N_2O_2$ [M+H] m/z 219.1128, found 219.1126.



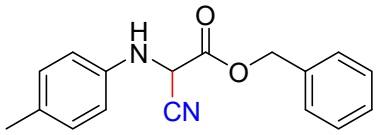
isopropyl 2-cyano-2-(p-tolylamino)acetate (2c) The desired pure product was obtained in 45% yield (20.9 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.5Hz, 2H), 6.66 (d, *J* = 8.4 Hz, 2H), 5.28 – 5.14 (m, 1H), 4.84 (d, *J* = 7.0 Hz, 1H), 4.40 (d, *J* = 7.0 Hz, 1H), 2.26 (s, 3H), 1.39 – 1.29 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.7, 141.3, 130.1, 129.9, 115.0, 114.3, 72.5, 48.9, 21.6, 21.4, 20.5. HRMS (ESI) exact mass calcd for $C_{13}H_{17}N_2O_2$ [M+H] m/z 233.1285, found 233.1284.



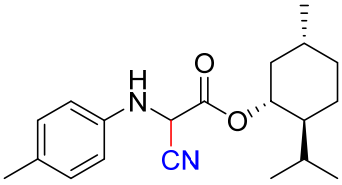
butyl 2-cyano-2-(p-tolylamino)acetate (2d) The desired pure product was obtained in 52% yield (25.6mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, J = 7.9 Hz, 2H), 6.67 (d, J = 7.6 Hz, 2H), 4.92 (d, J = 7.0 Hz, 1H), 4.42 (d, J = 7.0 Hz, 1H), 3.95 (s, 3H), 2.53 (t, J = 7.7 Hz, 2H), 1.61 – 1.49 (m, 2H), 1.41 – 1.27 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.3, 135.3, 129.5, 114.8, 114.3, 54.3, 48.6, 34.7, 33.7, 22.3, 13.9. HRMS (ESI) exact mass calcd for $C_{14}H_{19}N_2O_2$ [M+H] m/z 247.1441, found 247.1437.



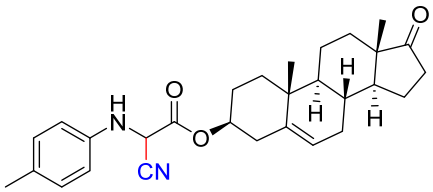
tert-butyl 2-cyano-2-(p-tolylamino)acetate (2e) The desired pure product was obtained in 35% yield (17.2 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.06 (d, *J* = 8.2 Hz, 2H), 6.63 (d, *J* = 8.4 Hz, 2H), 4.77 (s, 1H), 2.26 (s, 3H), 1.55 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.0, 141.5, 130.0, 129.7, 115.4, 114.3, 85.9, 49.3, 27.8, 20.4. HRMS (ESI) exact mass calcd for $C_{14}H_{19}N_2O_2$ [M+H] m/z 247.1441, found 247.1440.



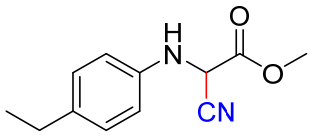
benzyl 2-cyano-2-(p-tolylamino)acetate (2f) The desired pure product was obtained in 33% yield (18.5 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (s, 5H), 7.06 (d, *J* = 8.3 Hz, 2H), 6.63 (d, *J* = 8.4 Hz, 2H), 5.33 (q, *J* = 12.1 Hz, *J* =21.8Hz, 2H), 4.92 (s, 1H), 2.26 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.2, 141.1, 133.9, 130.1, 129.1, 128.8, 128.5, 114.7, 114.4, 110.0, 69.4, 48.8, 20.5. HRMS (ESI) exact mass calcd for $C_{17}H_{17}N_2O_2$ [M+H] m/z 281.1285, found 281.1288.



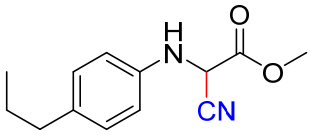
(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-cyano-2-(p-tolylamino)acetate (2g) The desired pure product was obtained in 42% yield (27.6 mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.2 Hz, 2H), 6.66 (dd, *J* = 8.2, 3.4 Hz, 2H), 4.87 (s, 1H), 4.85 (d, *J* = 2.2 Hz, 1H), 4.42 (d, *J* = 7.5 Hz, 1H), 2.27 (s, 3H), 2.09 – 1.96 (m, 1H), 1.82 – 1.65 (m, 2H), 1.61 – 1.54 (m, 1H), 1.55 – 1.44 (m, 2H), 1.19 – 1.01 (m, 2H), 0.94 – 0.88 (m, 6H), 0.76 (dd, *J* = 15.7, 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.8, 141.3, 130.1, 129.9, 114.3, 78.9, 78.7, 48.9, 48.7, 47.0, 46.7, 40.5, 40.0, 33.93, 33.89, 31.42, 31.40, 26.3, 26.0, 23.2, 23.1, 21.87, 21.85, 20.7, 20.6, 20.4, 16.1, 15.9. HRMS (ESI) exact mass calcd for $C_{20}H_{29}N_2O_2$ [M+H] m/z 329.2224, found 329.2223.



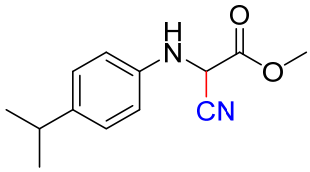
(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 2-cyano-2-(p-tolylamino)acetate (2h) The desired pure product was obtained in 31% yield (28.6 mg) as a white solid. Mp:193-194℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.81 (s, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 2H), 5.45 (d, *J* = 5.1 Hz, 1H), 4.85 – 4.77 (m, 1H), 2.61 – 2.53 (m, 1H), 2.50 – 2.42 (m, 2H), 2.33 (s, 3H), 2.15 – 2.05 (m, 3H), 1.99 – 1.92 (m, 3H), 1.88 – 1.82 (m, 2H), 1.70 – 1.65 (m, 3H), 1.57 – 1.48 (m, 2H), 1.33 – 1.24 (m, 3H), 1.22 – 1.16 (m, 1H), 1.07 (s, 3H), 0.89 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 220.9, 160.5, 153.8, 139.3, 135.2, 133.8, 129.7, 122.6, 119.7, 71.6, 51.7, 50.1, 47.5, 37.6, 36.8, 36.7, 35.8, 31.4, 31.4, 30.8, 27.3, 21.9, 20.9, 20.3, 19.4, 19.3, 13.5. HRMS (ESI) exact mass calcd for $C_{29}H_{37}N_2O_3$ [M+H] m/z 461.2799, found 461.2793.



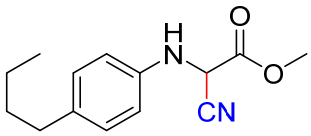
methyl 2-cyano-2-((4-ethylphenyl)amino)acetate (2i) The desired pure product was obtained in 73% yield (31.9mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 – 7.05 (m, 2H), 6.69 – 6.66 (m, 2H), 4.92 – 4.89 (m, 1H), 3.93 (s, 3H), 2.60 – 2.53 (m, 2H), 1.21 – 1.17 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.4, 136.6, 128.9, 114.8, 114.4, 54.3, 48.6, 28.0, 15.7. HRMS (ESI) exact mass calcd for $C_{12}H_{15}N_2O_2$ [M+H] m/z 219.1128, found 219.1131.



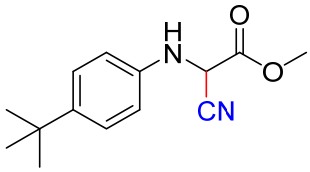
methyl 2-cyano-2-((4-propylphenyl)amino)acetate (2j) The desired pure product was obtained in 70% yield (32.5mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.5 Hz, 2H), 6.67 (d, *J*=8.5 Hz 2H), 4.91 (d, *J*=7.6 Hz 1H), 4.40 (d, *J* = 7.4 Hz, 1H), 3.94 (s, 3H), 2.53 – 2.47 (m, 2H), 1.63 – 1.53 (m, 2H), 0.95 – 0.86 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.4, 135.1, 129.5, 114.8, 114.4, 54.2, 48.7, 37.1, 24.5, 13.7. HRMS (ESI) exact mass calcd for $C_{13}H_{17}N_2O_2$ [M+H] m/z 233.1285, found 233.1288.



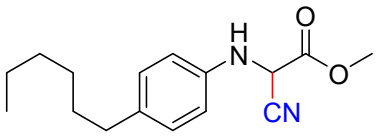
methyl 2-cyano-2-((4-isopropylphenyl)amino)acetate (2k) The desired pure product was obtained in 63% yield (29.3 mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.5 Hz, 2H), 6.69 (d, *J* = 8.6 Hz, 2H), 4.92 (d, *J* = 7.4 Hz, 1H), 4.44 (d, *J* = 7.2 Hz, 1H), 3.95 (s, 3H), 2.94 – 2.79 (m, 1H), 1.23 (s, 3H), 1.21 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.5 141.3, 127.5, 114.8, 114.4, 54.2, 48.6, 33.2, 24.0. HRMS (ESI) exact mass calcd for $C_{13}H_{17}N_2O_2$ [M+H] m/z 233.1285, found 233.1286.



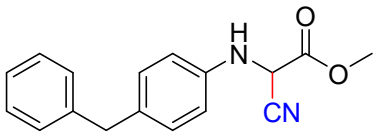
methyl 2-((4-butylphenyl)amino)-2-cyanoacetate (2l) The desired pure product was obtained in 66% yield (32.5mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.5 Hz, 2H), 6.67 (d, *J* = 8.4, 2.3 Hz, 2H), 4.92 (d, *J* = 7.2 Hz, 1H), 4.42 (d, *J* = 7.1 Hz, 1H), 3.94 (s, 3H), 2.53 (t, *J* = 7.7Hz, 2H), 1.60 – 1.47 (m, 2H), 1.40 – 1.29 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H).^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.4, 135.3, 129.4, 114.8, 114.4, 54.2, 48.7, 34.7, 33.7, 22.2, 13.8. HRMS (ESI) exact mass calcd for $C_{14}H_{19}N_2O_2$ [M+H] m/z 247.1441, found 247.1443.



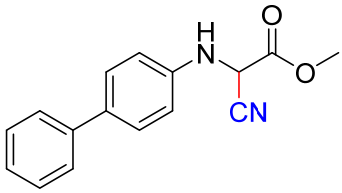
methyl 2-((4-(tert-butyl)phenyl)amino)-2-cyanoacetate (2m) The desired pure product was obtained in 63% yield (31.0 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 (d, *J* = 12.0 Hz, 2H), 6.69 (d, *J* = 12.0 Hz, 2H), 4.92 (s, 1H), 4.44 (s, 1H), 3.94 (s, 3H), 1.29 (s, 9H).^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 143.5, 141.1, 126.4, 114.9, 114.0, 54.3, 48.5, 34.1, 31.4. HRMS (ESI) exact mass calcd for $C_{14}H_{19}N_2O_2$[M+H] m/z 247.1441, found 247.1438.



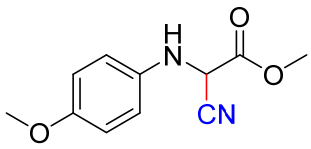
methyl 2-cyano-2-((4-hexylphenyl)amino)acetate (2n) The desired pure product was obtained in 67% yield (33.1mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.2 Hz, 2H), 6.66 (d, *J* = 8.4 Hz, 2H), 4.91 (s, 1H), 3.95 (s, 3H), 2.52 (t, *J* = 7.7 Hz, 2H), 1.56 (m, 2H), 1.29 (s, 6H), 0.92 – 0.80 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.3, 135.3, 129.5, 114.9, 114.3, 54.3, 48.6, 35.0, 31.7, 31.6, 28.9, 22.6, 14.1. HRMS (ESI) exact mass calcd for $C_{16}H_{23}N_2O_2$ [M+H] m/z 275.1754, found 275.1751.



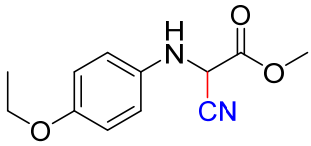
methyl 2-((4-benzylphenyl)amino)-2-cyanoacetate (2o) The desired pure product was obtained in 39% yield (21.9mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (m, 2H), 7.17 (m, 3H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 4.89 (d, *J* = 7.5 Hz, 1H), 4.41 (d, *J* = 6.7 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 141.7, 141.3, 133.4, 130.1, 128.8, 128.4, 126.0, 114.7, 114.4, 54.4, 48.4, 41.0. HRMS (ESI) exact mass calcd for $C_{17}H_{17}N_2O_2$ [M+H] m/z 281.1285, found 281.1280.



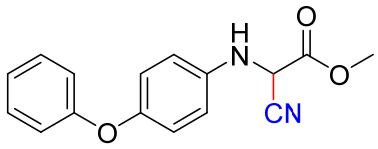
methyl 2-([1,1'-biphenyl]-4-ylamino)-2-cyanoacetate (2p) The desired pure product was obtained in 61% yield (32.5 mg) as a yellow solid. Mp:111-112 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 4H), 7.43 – 7.38 (m, 2H), 7.32 – 7.28 (m, 1H), 6.86 – 6.77 (m, 2H), 4.98 (d, *J* = 7.3 Hz, 1H), 4.61 (d, *J* = 7.3 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 142.8, 140.6, 133.6, 128.7, 128.3, 126.7, 126.6, 114.6, 114.4, 54.5, 48.1. HRMS (ESI) exact mass calcd for $C_{16}H_{17}N_2O_2$ [M+H] m/z 267.1128, found 267.1127.



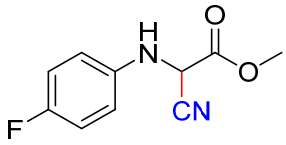
methyl 2-cyano-2-((4-methoxyphenyl)amino)acetate (2q) The desired pure product was obtained in 60% yield (26.4 mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 8.8 Hz, 2H), 6.73 (d, J = 8.8 Hz, 2H), 4.87 (s, 1H), 4.26 (s, 1H), 3.94 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.2, 130.1, 130.1, 114.8, 114.4, 54.3, 48.6, 20.5. HRMS (ESI) exact mass calcd for $C_{11}H_{13}N_2O_3$ [M+H] m/z 221.0921 found 221.0920.



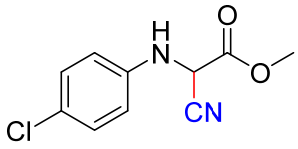
methyl 2-cyano-2-((4-ethoxyphenyl)amino)acetate (2r) The desired pure product was obtained in 56% yield (26.2 mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83 (d, *J*=8.8 Hz, 2H), 6.71 (d, *J*=8.9 Hz, 2H), 4.86 (s, 1H), 3.97 (dd, *J* = 14.0, 7.0 Hz, 2H), 3.93 (s, 3H), 1.38 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 153.9, 137.4, 116.4, 115.9, 114.8, 64.0, 54.1, 50.0, 14.8. HRMS (ESI) exact mass calcd for $C_{12}H_{15}N_2O_3$ [M+H] m/z 235.1077, found 235.1071.



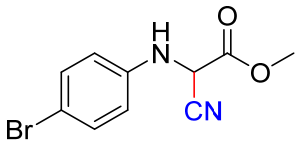
methyl 2-cyano-2-((4-phenoxyphenyl)amino)acetate (2s) The desired pure product was obtained in 42% yield (23.7 mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 2H), 7.08 – 7.01 (m, 1H), 7.00 – 6.93 (m, 4H), 6.73 (d, *J*=8.9Hz, 2H), 4.91 (d, *J* = 7.6 Hz, 1H), 4.46 (d, *J* = 7.6 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 158.2, 150.6, 139.7, 129.6, 122.6, 121.0, 117.8, 115.6, 114.7, 54.4, 48.8. HRMS (ESI) exact mass calcd for $C_{16}H_{15}N_2O_3$ [M+H] m/z 283.1077, found 283.1074.



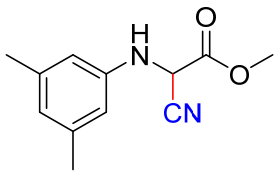
methyl 2-cyano-2-((4-fluorophenyl)amino)acetate (2t) The desired pure product was obtained in 66% yield (27.5 mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.95 – 6.87 (m, 2H), 6.65 – 6.57 (m, 2H), 4.81 (d, *J* = 7.6 Hz, 1H), 4.38 (d, *J* = 7.3 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 158.3, 156.7, 139.8, 139.8, 116.3, 116.2, 115.6, 115.6, 114.6, 54.4, 48.8. HRMS (ESI) exact mass calcd for $C_{10}H10FN_2O_2$ [M+H] m/z 209.0721, found 209.0725.



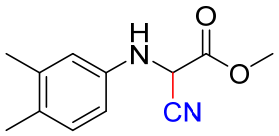
methyl 2-((4-chlorophenyl)amino)-2-cyanoacetate (2u) The desired pure product was obtained in 56% yield (25.2mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (d, J = 8.8 Hz, 2H), 6.67 (d, J = 8.8 Hz, 2H), 4.90 (d, J = 7.3 Hz, 1H), 4.57 (d, J = 6.8 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4, 142.0, 129.6, 125.6, 115.3, 114.3, 54.5, 48.1. HRMS (ESI) exact mass calcd for $C_{10}H_{10}ClN_2O_2$ [M+H] m/z 225.0425 found 225.0424.



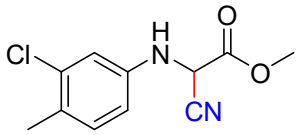
methyl 2-((4-bromophenyl)amino)-2-cyanoacetate (2v) The desired pure product was obtained in 61% yield (32.8mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J*= 8.9 Hz, 2H), 6.63 (d, *J*= 8.9 Hz, 2H), 4.90 (d, *J* = 7.1 Hz, 1H), 4.59 (d, *J* = 6.9 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.3, 142.5, 132.5, 115.7, 114.2, 112.7, 54.6, 47.9. HRMS (ESI) exact mass calcd for $C_{10}H_{10}BrN_2O_2$ [M+H] m/z 268.9920, found 268.9919.



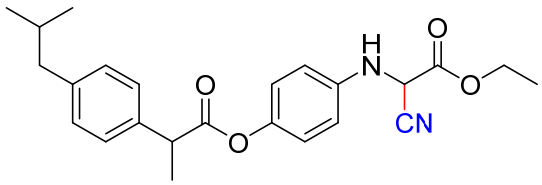
methyl 2-cyano-2-((3,5-dimethylphenyl)amino)acetate (2w) The desired pure product was obtained in 56% yield (24.4mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 – 6.92 (m, 2H), 6.57 (d, *J*= 8.0 Hz, 1H), 4.91 (d, *J* = 8.0 Hz, 1H), 4.33 (d, *J* = 4.0 Hz, 1H), 3.96 (s, 3H), 2.25 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 140.0, 131.7, 129.7, 127.5, 124.0, 114.9, 111.8, 54.4, 48.5, 20.4, 17.2. HRMS (ESI) exact mass calcd for $C_{12}H_{15}N_2O_2$ [M+H] m/z 219.1128, found 219.1133.



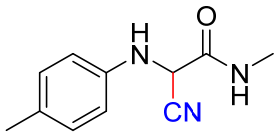
methyl 2-cyano-2-((3,4-dimethylphenyl)amino)acetate (2x) The desired pure product was obtained in 73% yield (31.9mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.03 (d, J = 8.0 Hz, 1H), 6.56 (s, 1H), 6.50 (dd, J = 8.0, 2.2 Hz, 1H), 4.92 (s, 1H), 4.35 (s, 1H), 3.95 (s, 3H), 2.23 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 141.5, 137.9, 130.6, 128.9, 116.1, 114.9, 111.6, 54.3, 48.6, 20.0, 18.8. HRMS (ESI) exact mass calcd for $C_{12}H_{15}N_2O_2$ [M+H] m/z 219.1128, found 219.1131.



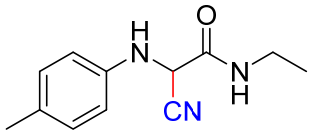
methyl 2-((3-chloro-4-methylphenyl)amino)-2-cyanoacetate (2y) The desired pure product was obtained in 34% yield (16.2mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 (d, *J* = 8.2 Hz, 1H), 6.75 (d, *J* = 1.9 Hz, 1H), 6.55 (dd, *J* = 8.2, 1.9 Hz, 1H), 4.88 (d, *J* = 7.5 Hz, 1H), 4.47 (d, *J* = 7.1 Hz, 1H), 3.95 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4, 142.5, 135.2, 131.7, 127.9, 118.1, 114.8, 114.4, 112.6, 54.5, 48.1, 19.0. HRMS (ESI) exact mass calcd for $C_{11}H_{12}ClN_2O_2$ [M+H] m/z 239.0582, found 239.0578.



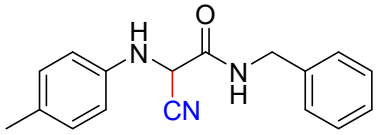
4-((1-cyano-2-ethoxy-2-oxoethyl)amino)phenyl 2-(4-isobutylphenyl)propanoate (2z) The desired pure product was obtained in 65% yield (53.1mg) as a yellow oily. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 (d, *J* = 7.7 Hz, 2H), 7.14 (d, *J* = 7.7 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 9.0 Hz, 2H), 4.85 (d, *J* = 7.2 Hz, 1H), 4.56 (d, *J* = 7.2 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.92 (q, *J* = 7.1 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.94 – 1.81 (m, 1H), 1.59 (d, *J* = 7.2 Hz, 3H), 1.37 (t, *J* = 7.1 Hz, 3H), 0.91 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.5, 164.0, 144.5, 141.3, 140.8, 137.3, 129.5, 127.2, 122.5, 114.7, 64.2, 48.5, 45.2, 45.0, 30.2, 22.4, 18.5, 13.9. HRMS (ESI) exact mass calcd for $C_{24}H_{29}N_2O_4$ [M+H] m/z 409.2122, found 409.2127.



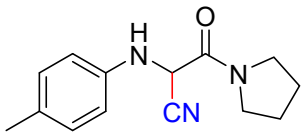
2-cyano-N-methyl-2-(p-tolylamino)acetamide (3a) The desired pure product was obtained in 58% yield (23.6mg) as a yellow oily. ^{1}H NMR (600 MHz, DMSO) δ 8.19 (d, *J* = 4.5 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 2H), 6.62 (d, *J* = 8.4 Hz, 2H), 5.43 (s, 1H), 2.63 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, CD_3OD) δ 165.8, 142.2, 129.3, 129.1, 116.1, 114.4, 50.6, 25.3, 19.1. HRMS (ESI) exact mass calcd for $C_{11}H_{14}N_3O$ [M+H] m/z 204.1131, found 204.1132.



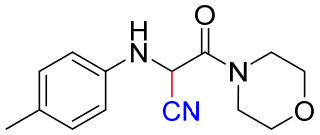
2-cyano-N-ethyl-2-(p-tolylamino)acetamide (3b) The desired pure product was obtained in 57% yield (24.8mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.0 Hz, 2H), 6.78 (s, 1H), 6.65 (d, *J* = 8.5 Hz, 2H), 4.82 (s, 1H), 4.50 (s, 1H), 3.45 – 3.32 (m, 2H), 2.28 (s, 3H), 1.18 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.0, 141.2, 130.8, 130.1, 115.9, 114.9, 51.1, 35.2, 20.5, 14.4. HRMS (ESI) exact mass calcd for $C_{12}H_{16}N_3O$ [M+H] m/z 218.1288, found 218.1290.



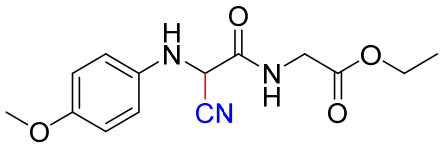
N-benzyl-2-cyano-2-(p-tolylamino)acetamide (3c) The desired pure product was obtained in 47% yield (26.3mg) as a yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 3H), 7.23 – 7.20 (m, 2H), 7.11 (s, 1H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.63 (d, *J* = 8.3 Hz, 2H), 4.85 (d, *J* = 7.7 Hz, 1H), 4.48 (d, *J* = 5.7 Hz, 2H), 2.26 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.4, 141.0, 136.9, 130.8, 130.1, 128.8, 127.9, 127.8, 115.8, 115.0, 51.2, 44.1, 20.5. HRMS (ESI) exact mass calcd for $C_{17}H_{18}N_3O$ [M+H] m/z 280.1444, found 280.1449.



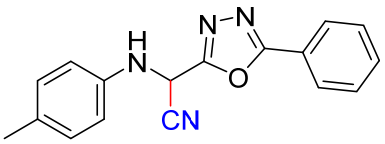
3-oxo-3-(pyrrolidin-1-yl)-2-(p-tolylamino)propanenitrile (3d) The desired pure product was obtained in 32% yield (15.6mg) as a white solid. Mp:112-113 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.0 Hz, 2H), 6.66 (d, *J* = 8.4 Hz, 2H), 4.93 (d, *J* = 7.3 Hz, 1H), 4.82 (d, *J* = 7.4 Hz, 1H), 3.80 – 3.69 (m, 1H), 3.60 (t, *J* = 7.0 Hz, 2H), 3.55 – 3.48 (m, 1H), 2.27 (s, 3H), 2.15 – 2.01 (m, 2H), 1.98 – 1.91 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.1, 141.6, 130.0, 129.2, 115.2, 114.3, 47.7, 47.2, 46.3, 26.0, 24.0, 20.5. HRMS (ESI) exact mass calcd for $C_{14}H_{18}N_3O$ [M+H] m/z 244.1444, found 244.1442.



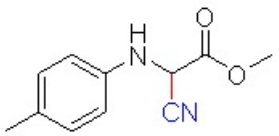
3-morpholino-3-oxo-2-(p-tolylamino)propanenitrile (3e) The desired pure product was obtained in 39% yield (20.2mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 4.96 (s, 1H), 3.90 – 3.60 (m, 8H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.9, 141.4, 130.1, 129.6, 115.1, 114.3, 66.4, 65.9, 46.5, 46.0, 43.6, 20.5. HRMS (ESI) exact mass calcd for $C_{14}H_{18}N_3O_2$ [M+H] m/z 260.1394, found 260.1395.



ethyl (2-cyano-2-(p-tolylamino)acetyl)glycinate (4a) The desired pure product was obtained in 26% yield (14.3mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 4.92 (d, *J* = 8.2 Hz, 1H), 4.55 (s, 1H), 4.23 – 4.17 (m, 2H), 4.09 (d, *J* = 5.5 Hz, 2H), 2.27 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.0, 163.9, 141.0, 130.9, 130.1, 115.4, 115.1, 61.9, 51.1, 41.7, 20.5, 14.1. HRMS (ESI) exact mass calcd for $C_{14}H_{18}N_3O_3$ [M+H] m/z 276.1343, found 276.1346.



2-(5-phenyl-1,3,4-oxadiazol-2-yl)-2-(p-tolylamino)acetonitrile (5a) The desired pure product was obtained in 77% yield (44.7mg) as a yellow oily. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.2 Hz, 2H), 7.61 – 7.48 (m, 3H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.79 (d, *J* = 8.1 Hz, 2H), 5.79 (d, *J* = 8.8 Hz, 1H), 4.48 (d, *J* = 8.4 Hz, 1H), 2.29 (s, 3H). ^{13}C 166.4, 159.3, 140.6, 132.6, 131.2, 130.2, 129.2, 127.2, 122.8, 115.3, 114.1, 43.3, 20.5. HRMS (ESI) exact mass calcd for $C_{17}H_{15}N_4O$ [M+H] m/z 291.1240, found 291.1241.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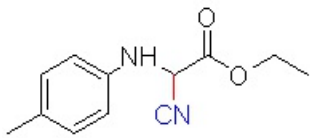
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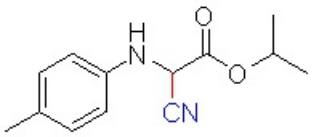
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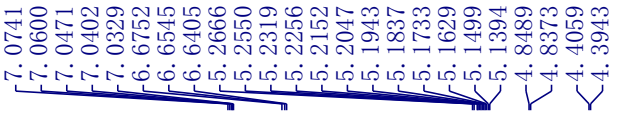
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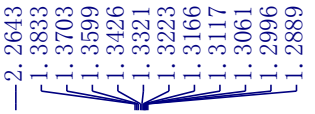
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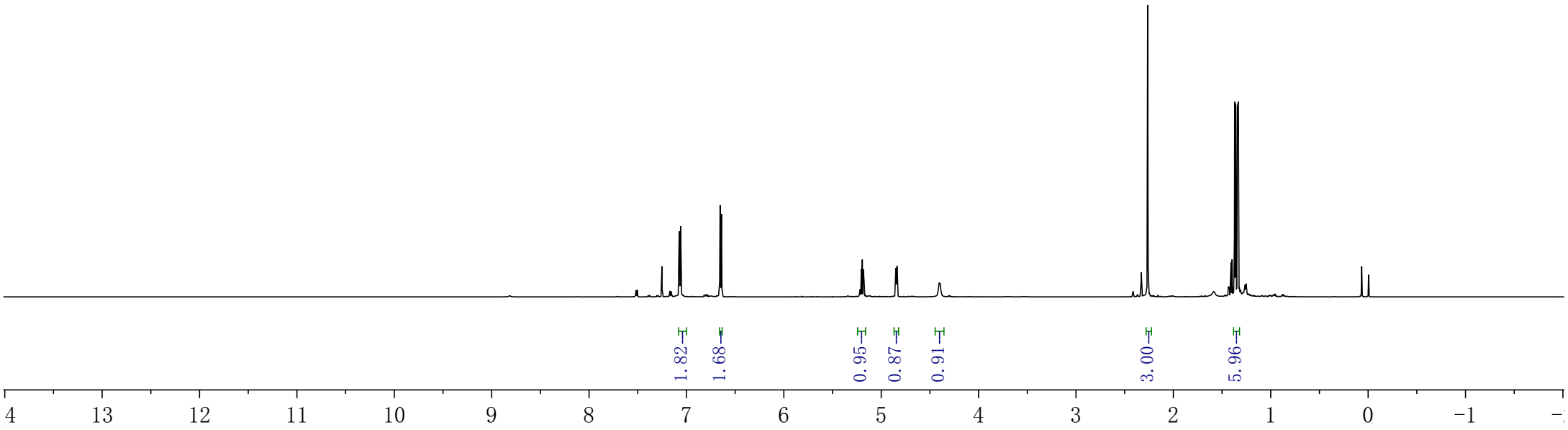
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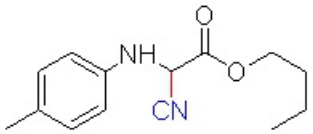
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2d

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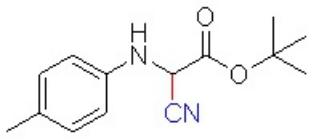
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2e

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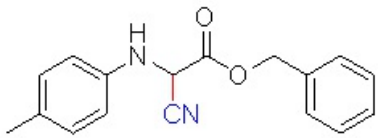

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3.07

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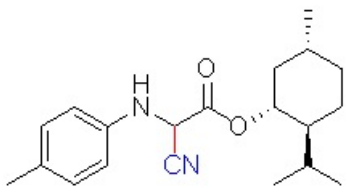
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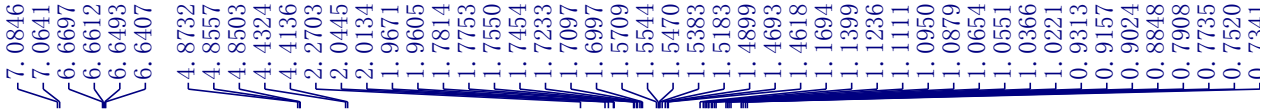
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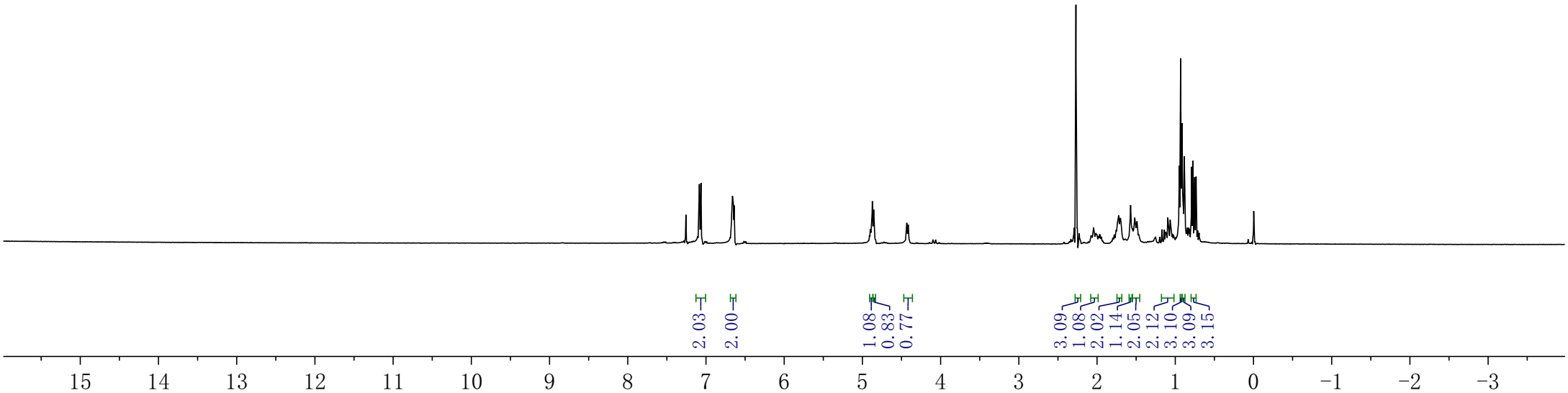
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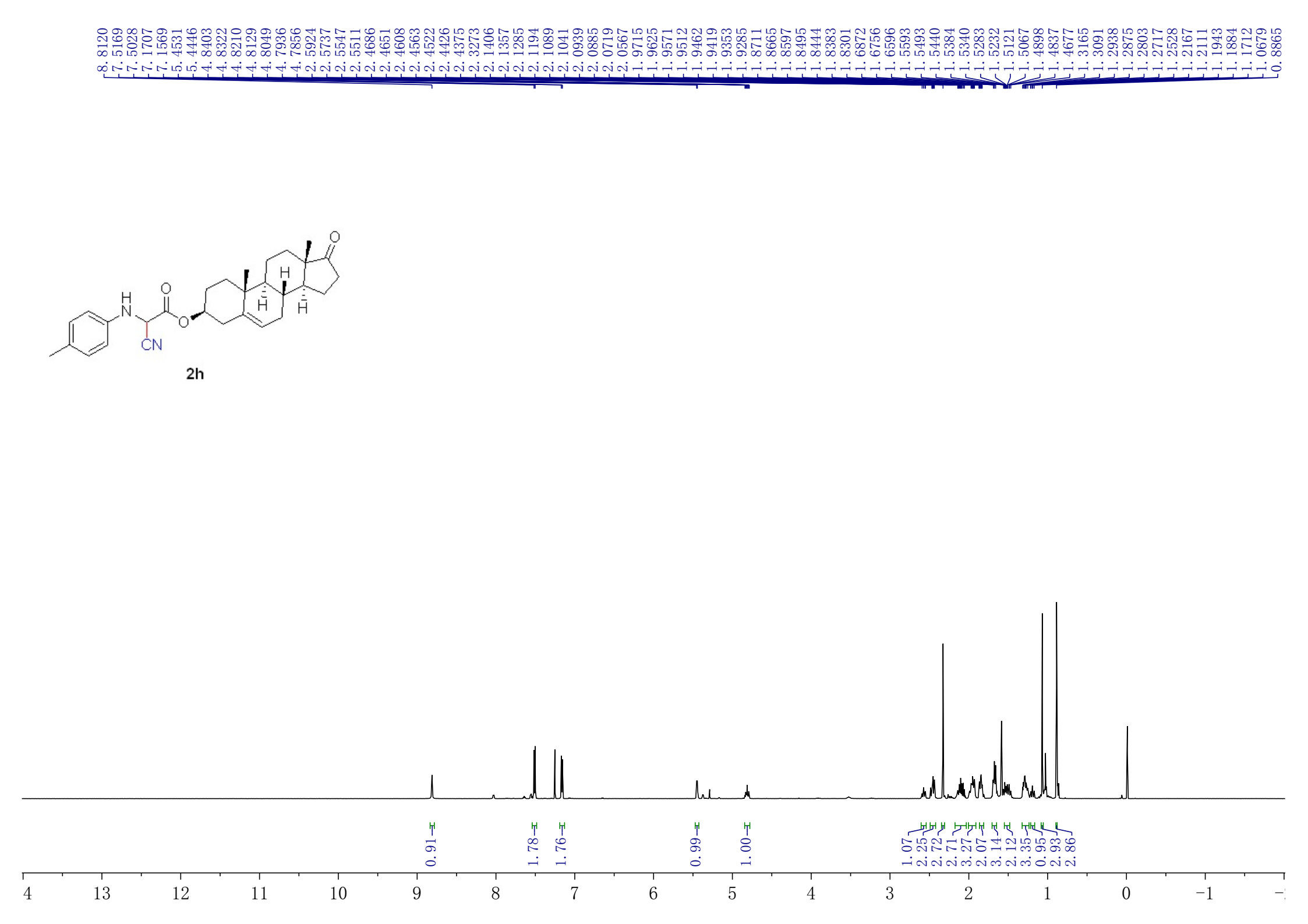
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H
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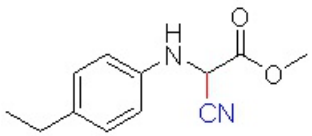
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2i


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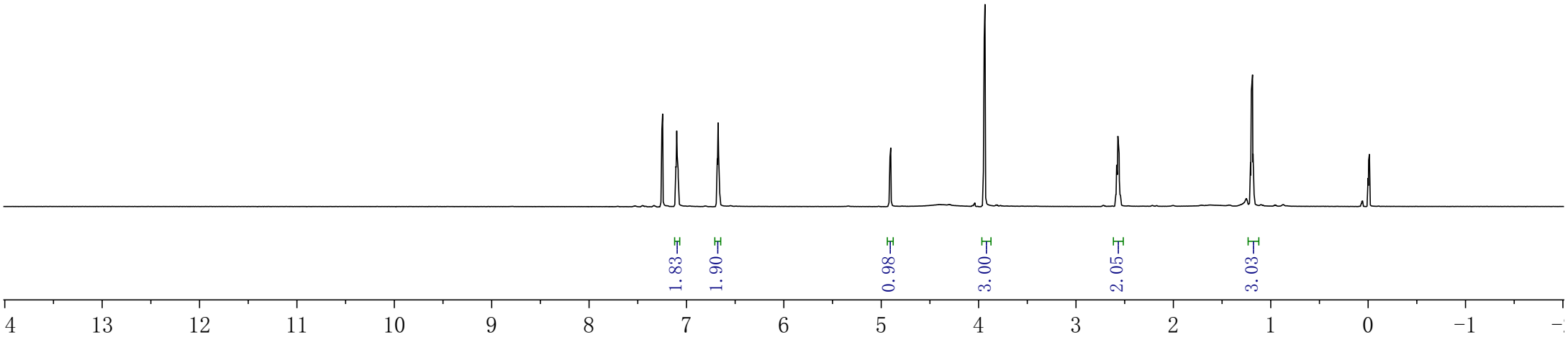
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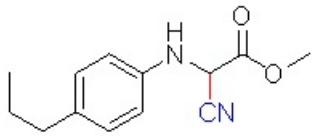
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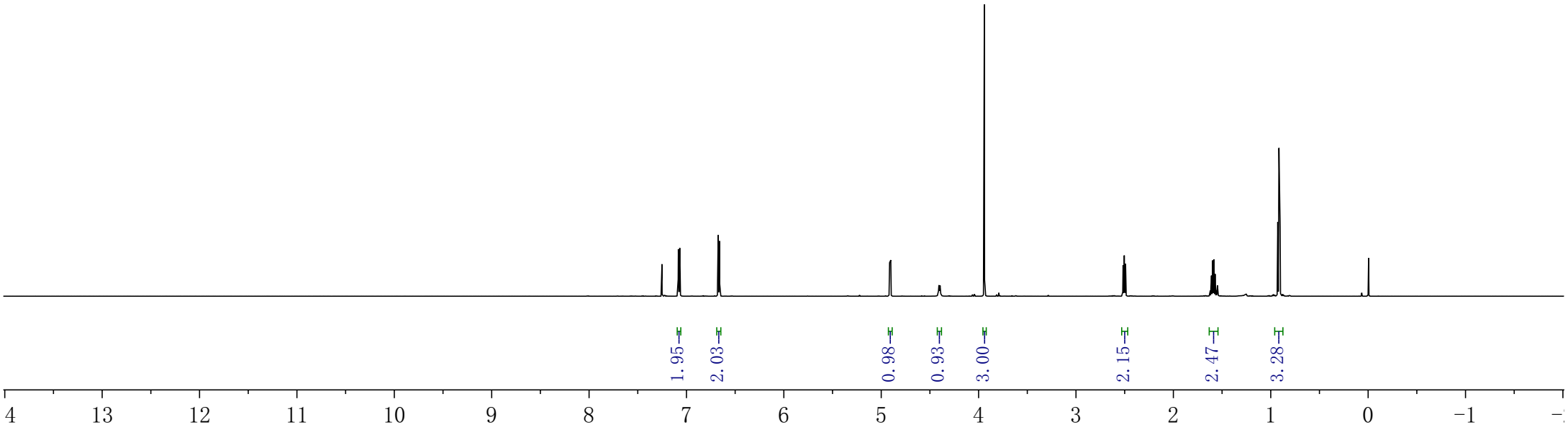
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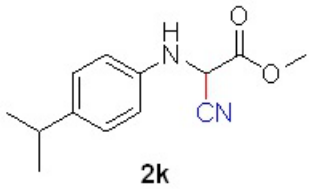

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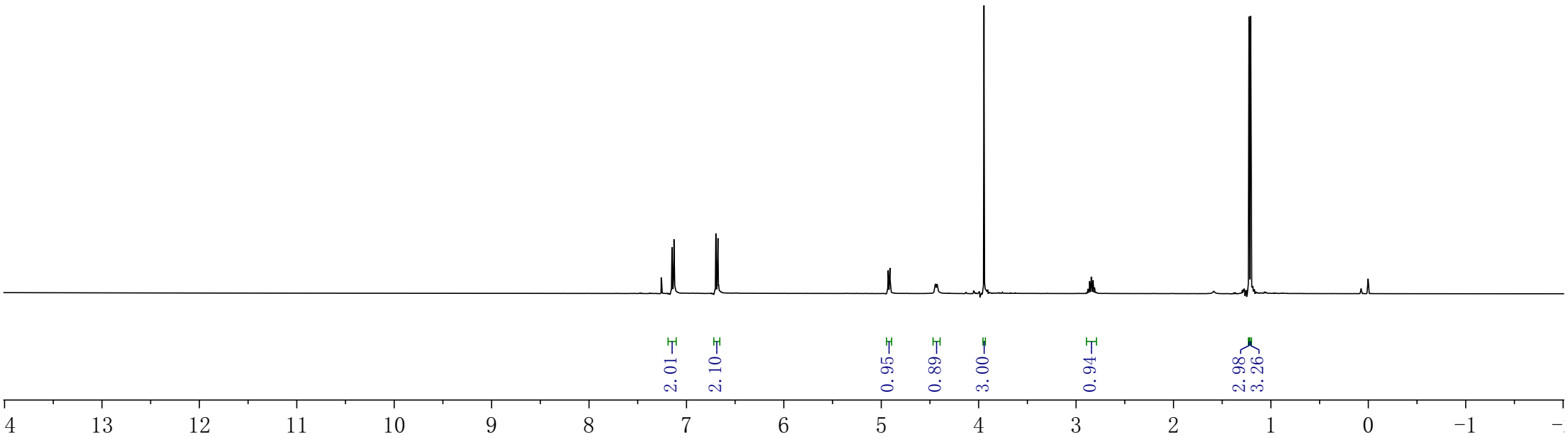

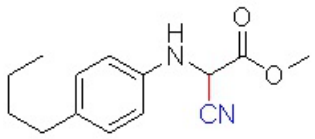
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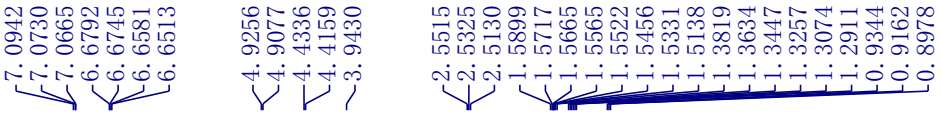
2l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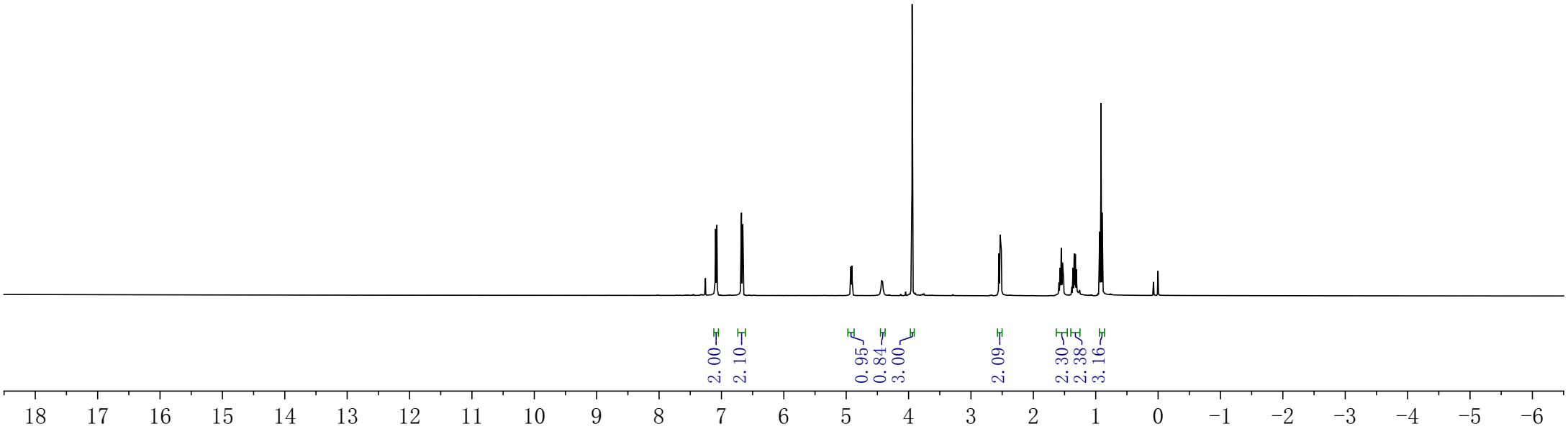
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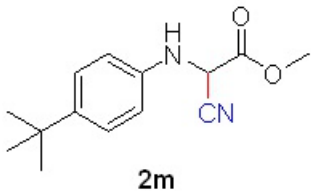
−6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2m

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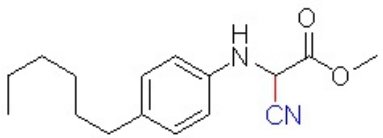

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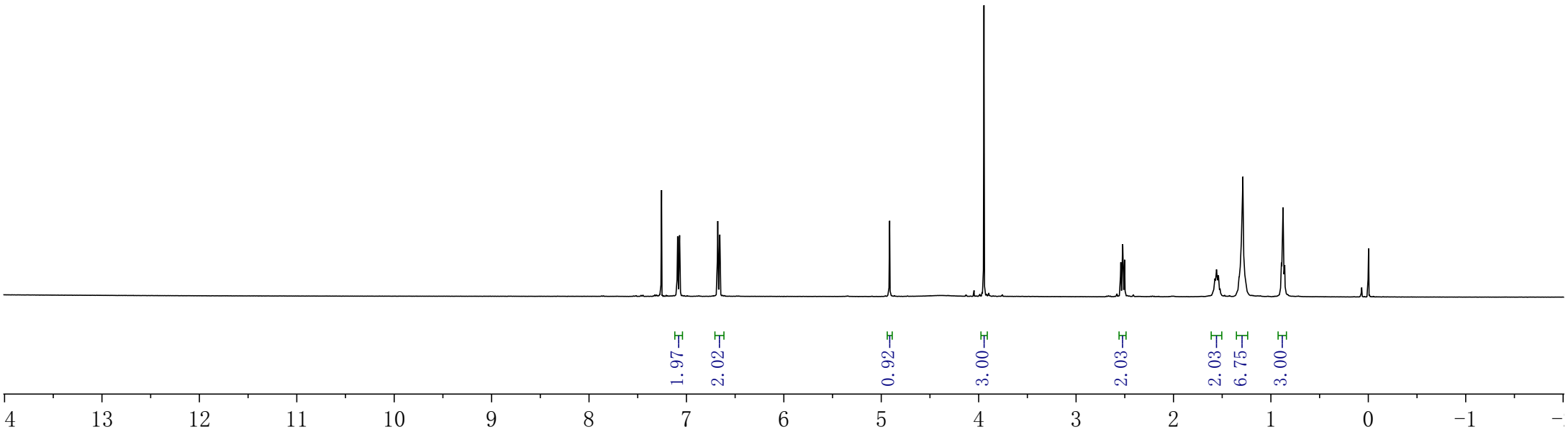

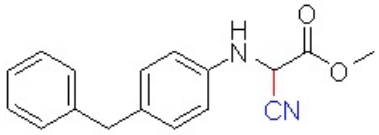

2o

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4.4155
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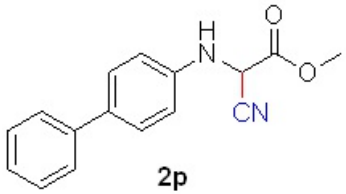
H
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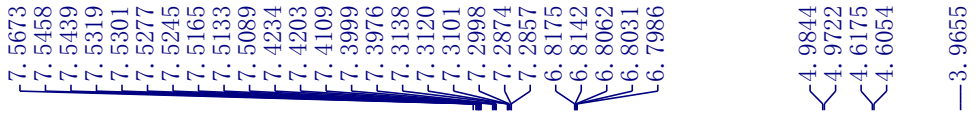
2p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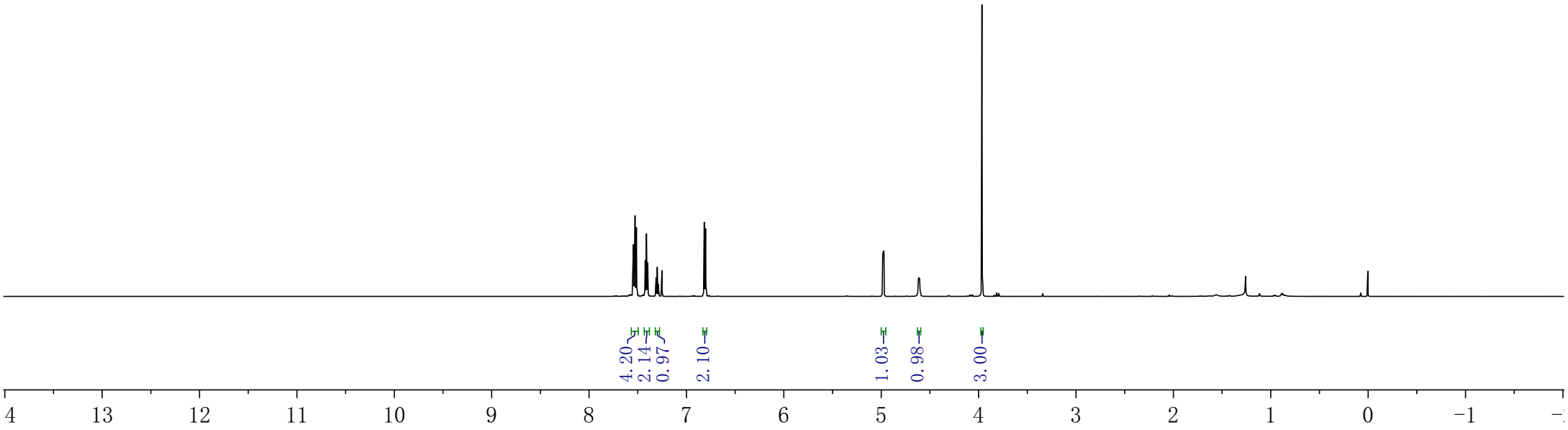
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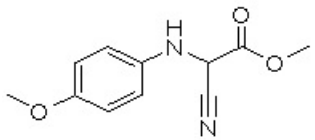

2q

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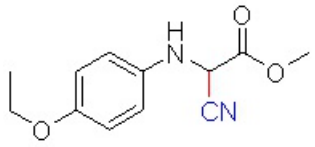
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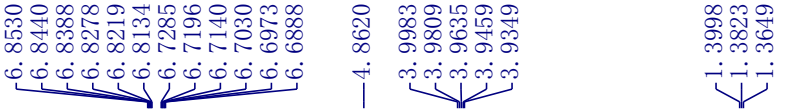
CN
O

2r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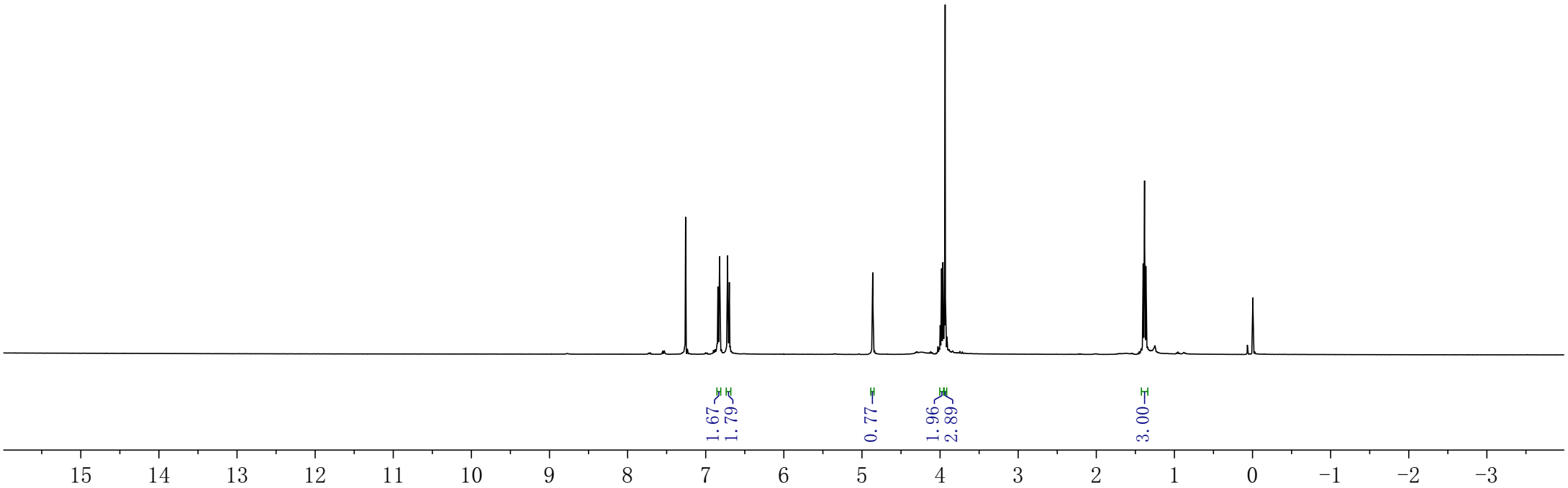
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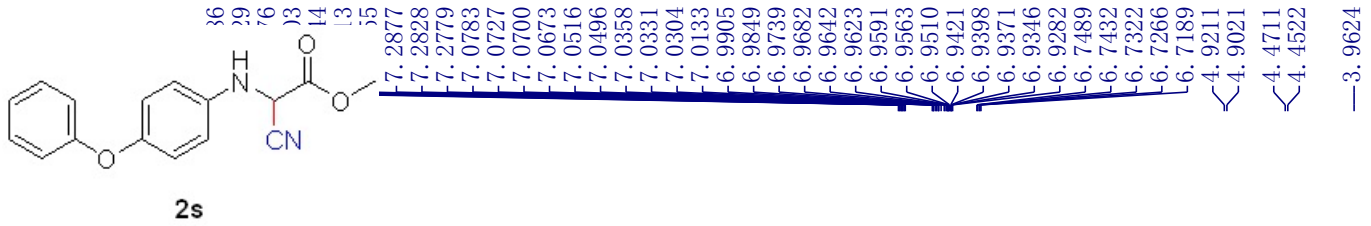
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CN
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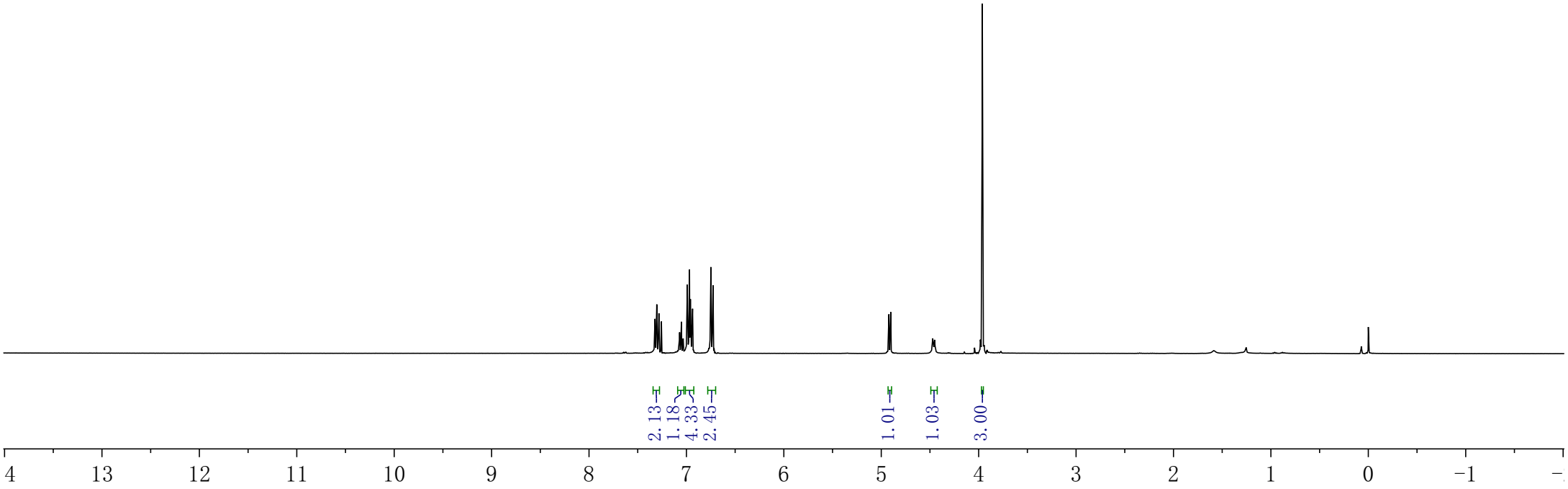
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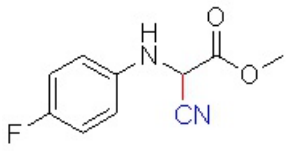
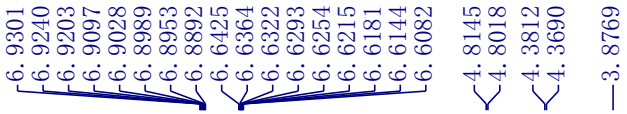

O
N
H
O
CN
F

2t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6.9240
6.9203
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6.9028
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6.8892
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6.6322
6.6293
6.6254
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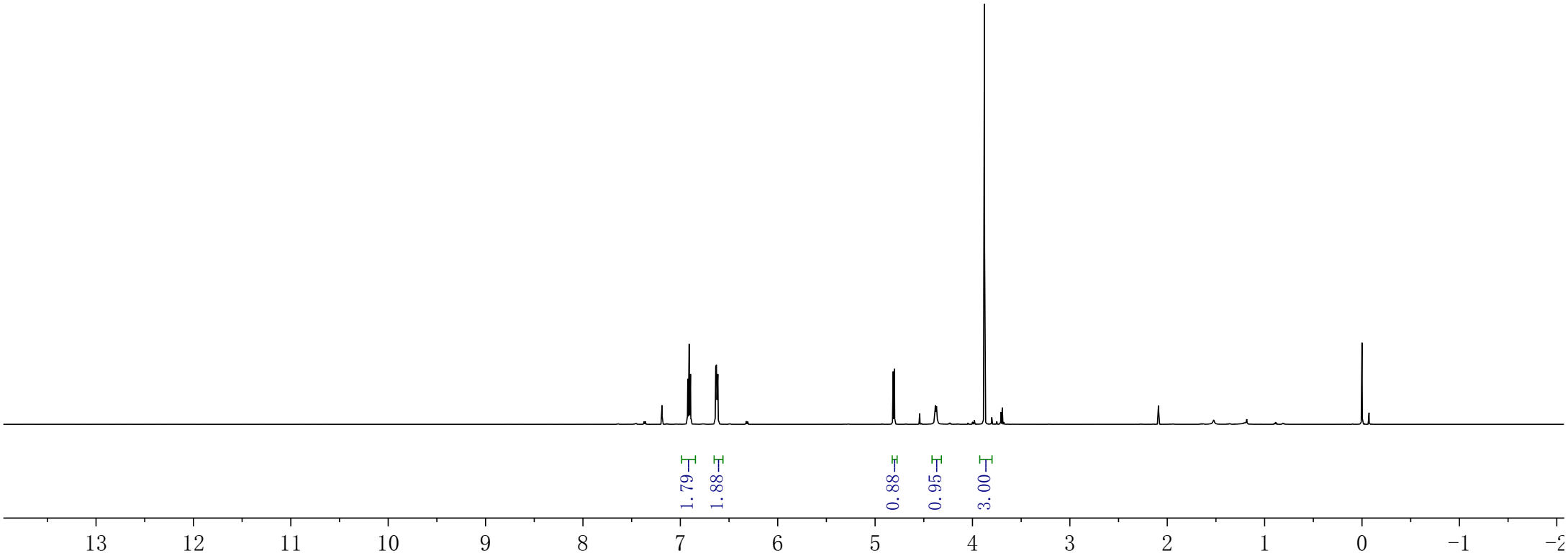
6.6181
6.6144
6.6082
4.8145
4.8018
4.3812
4.3690
3.8769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1.88
0.88
0.95
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11
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9
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5
4
3
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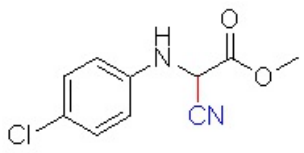
0
−1
−2


H
N
O
O
CN
Cl

2u

7.2458
7.2239
6.6810
6.6591
4.9070
4.8888
4.5756
4.5588
3.9658
2.06
2.03
0.86
0.88
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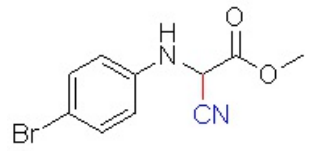
0
-1

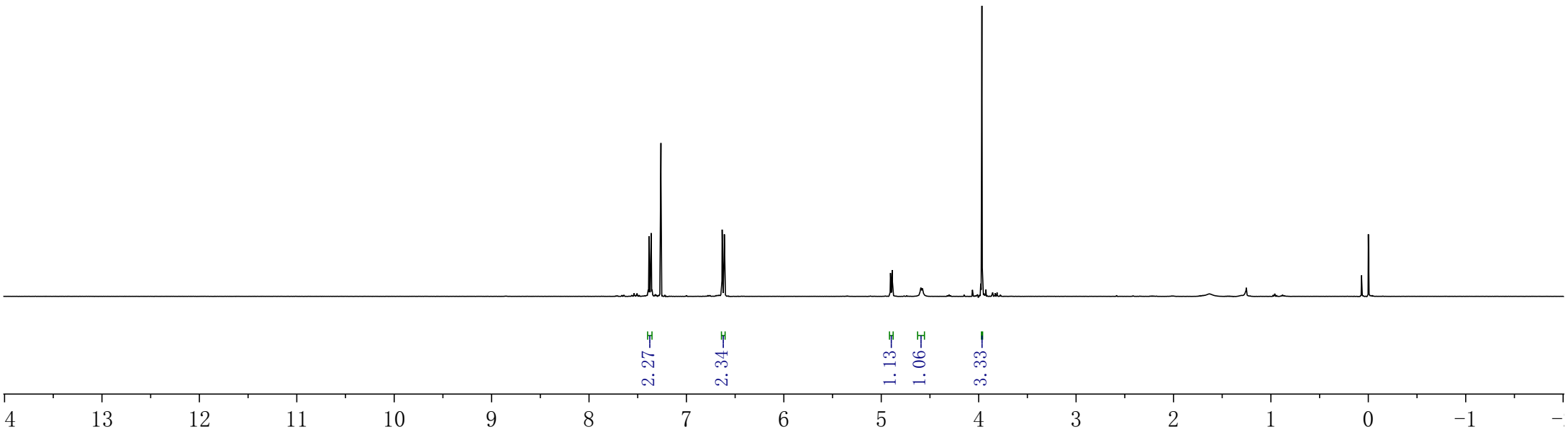


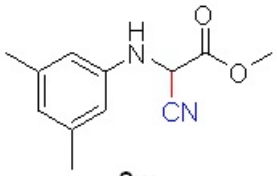
2v

7.3915
7.3836
7.3782
7.3667
7.3613
7.3535
6.6412
6.6333
6.6279
6.6165
6.6111

4.9050
4.8873
4.5943
4.5772

3.9665




H
N
O
O
CN

2w

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6.9609
6.6014
6.5804
6.5604
6.5404
4.9265
4.9081
4.8881
4.3341
4.3164
3.9790
3.9575
3.9377
2.2531
2.2087
2.23
1.11
0.93
1.00
3.26
3.10
3.05
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3


H
N
O
O
CN

2x

7.0396
7.0197
6.5595
6.5131
6.5077
6.4932
6.4877
4.9182
4.3523
3.9491
2.2302
2.1851
0.86
0.89
0.84
0.81
0.73
2.78
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10
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8
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6
5
4
3
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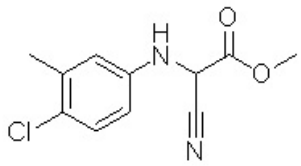
1
0
−1


Cl
N
H
O
O
N

2y

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6.7545
6.7491
6.5631
6.5576
6.5427
6.5372
4.9025
4.8845
4.5034
4.4862
3.9608
2.2792
0.95
0.90
0.95
0.89
0.85
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4
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12
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6
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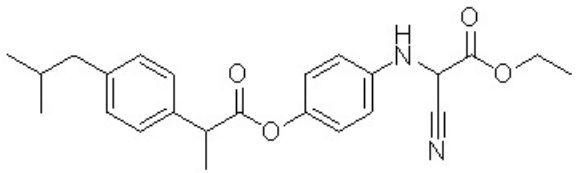
0
−1



2z

7.3010
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7.1528
7.1334
6.9172
6.8949
6.6860
6.6634

4.8620
4.8441
4.5688
4.5509
4.4135
4.3957
4.3779
4.3601
3.9425
3.9248
3.9069
3.8893
2.4795
2.4614
1.8988
1.8818
1.8651
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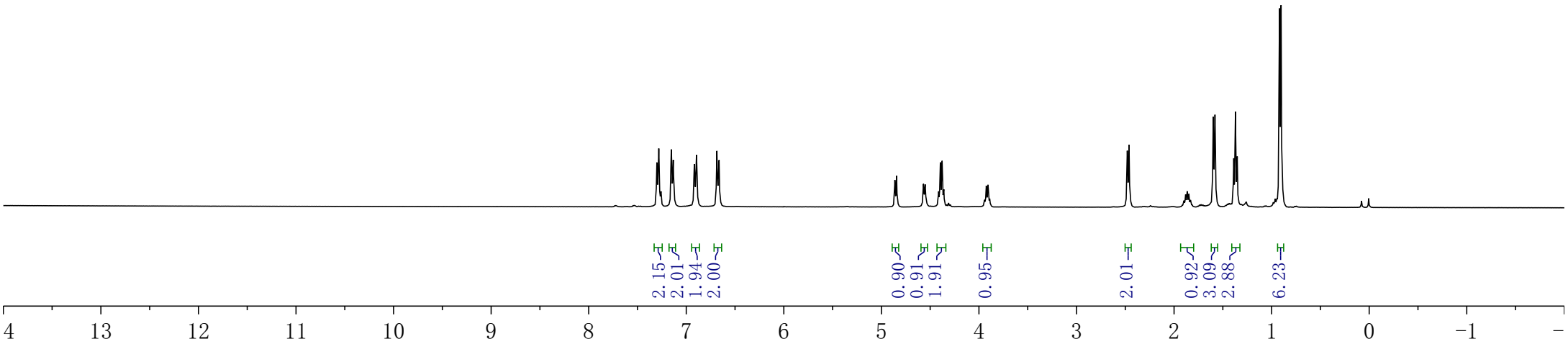
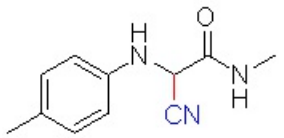
1.8313
1.5986
1.5806
1.3886
1.3709
1.3530
0.9198
0.9030



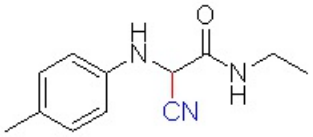


3a

8.1966
8.1891
6.9864
6.9729
6.6280
6.6140
5.4333
2.6324
2.6246
2.1638

1.09
1.95
2.14
1.04
3.00
3.00

4 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1

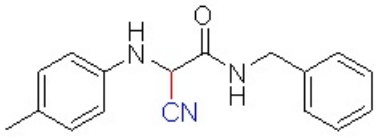


3b

7.0925
7.0724
6.7751
6.6618
6.6407
4.8183
4.5041
3.4145
3.3978
3.3803
3.3632
3.3460
2.2969
2.2787
2.2577
1.2029
1.1842
1.1660
1.1477

1.82
0.79
2.04
0.91
0.65
1.95
3.06
3.00

4 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1



3c

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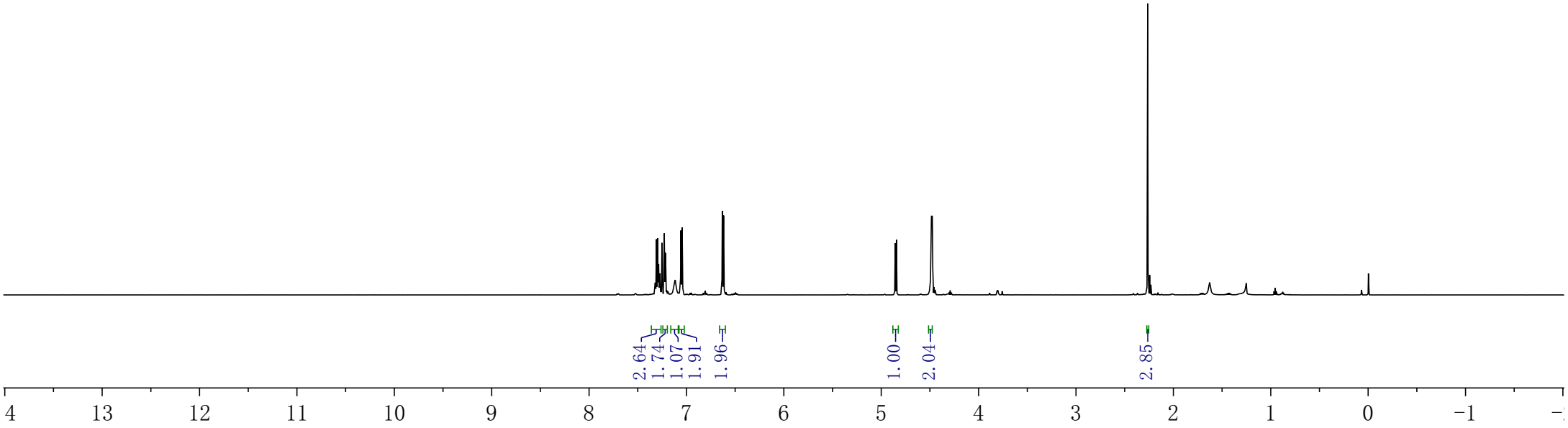
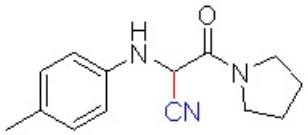
7.2962
7.2863
7.2791
7.2747
7.2692
7.2276
7.2161
7.2044
7.1148
7.0573
7.0437
6.6321
6.6182

4.8563
4.8434
4.4844
4.4757
4.4749

2.2640




H
N
O
N
CN

3d

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7.0605
6.6769
6.6607
6.6558
4.9409
4.9226
4.8264
4.8080
3.7819
3.7645
3.7578
3.7469
3.7402
3.7225
3.6130
3.5954
3.5781
3.5561
3.5389
3.5316
3.5232
3.5170
3.5138
3.4987
2.2677
2.1251
2.1083
2.0924
2.0756
2.0696
2.0519
2.0344
2.0213
2.0178
2.0054
2.0049
1.9747
1.9672
1.9586
1.9502
1.9410
1.96
2.00
0.91
1.01
0.97
2.10
1.12
3.13
2.04
2.30
4
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9
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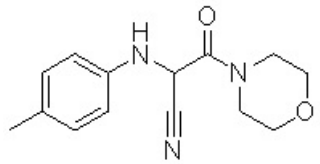
H
N
O
N
O
N

3e

7.0853
7.0650
6.6758
6.6552
4.9562
4.9381
4.9139
3.8085
3.7533
3.6967
3.6504
2.2723
1.90
1.89
1.30
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10
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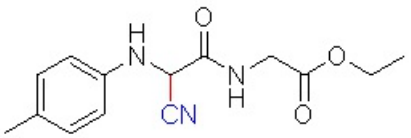
0
-1



4a

7.3055
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6.6818
6.6608
4.9344
4.9140
4.5512
4.2362
4.2183
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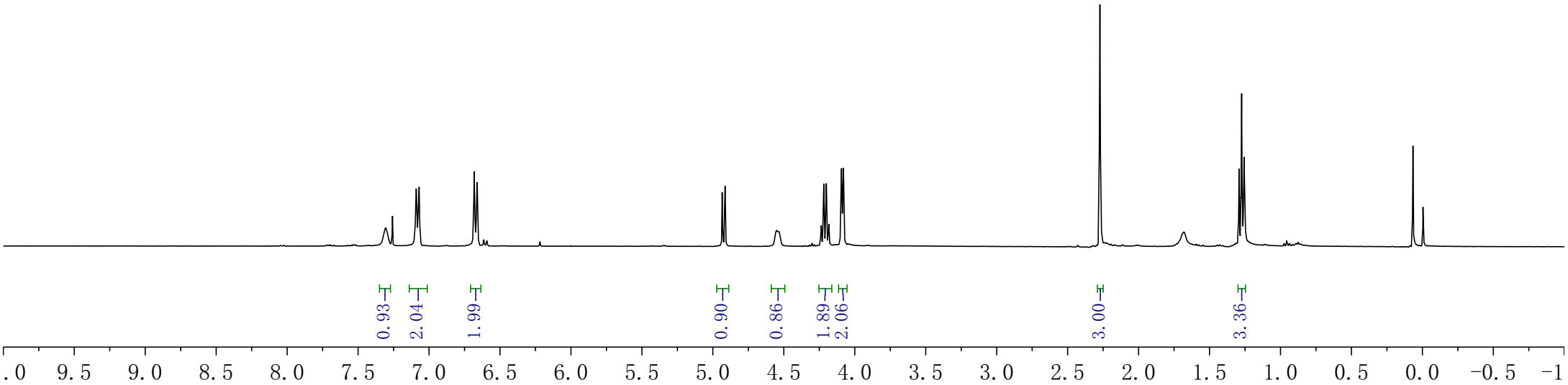
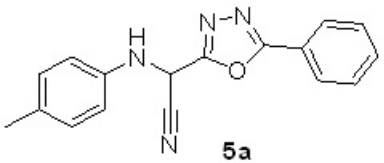
4.1827
4.0937
4.0800
2.2725
1.2918
1.2790
1.2739
1.2560



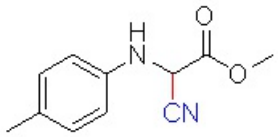


5a

8.0775
8.0595
7.5889
7.5708
7.5480
7.5292
7.5114
7.1223
7.1024
6.8019
6.7816
5.7993
5.7772
4.4948
4.4739
2.2875

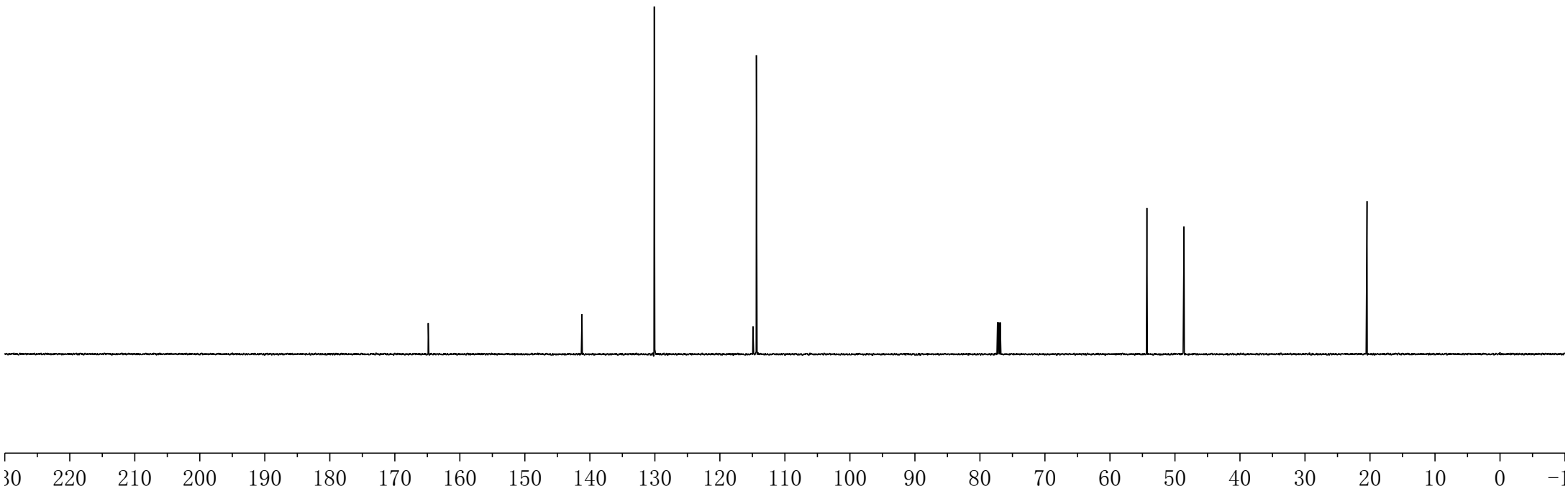
1.80
2.88
1.88
1.96
0.93
0.90
3.00

4 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −



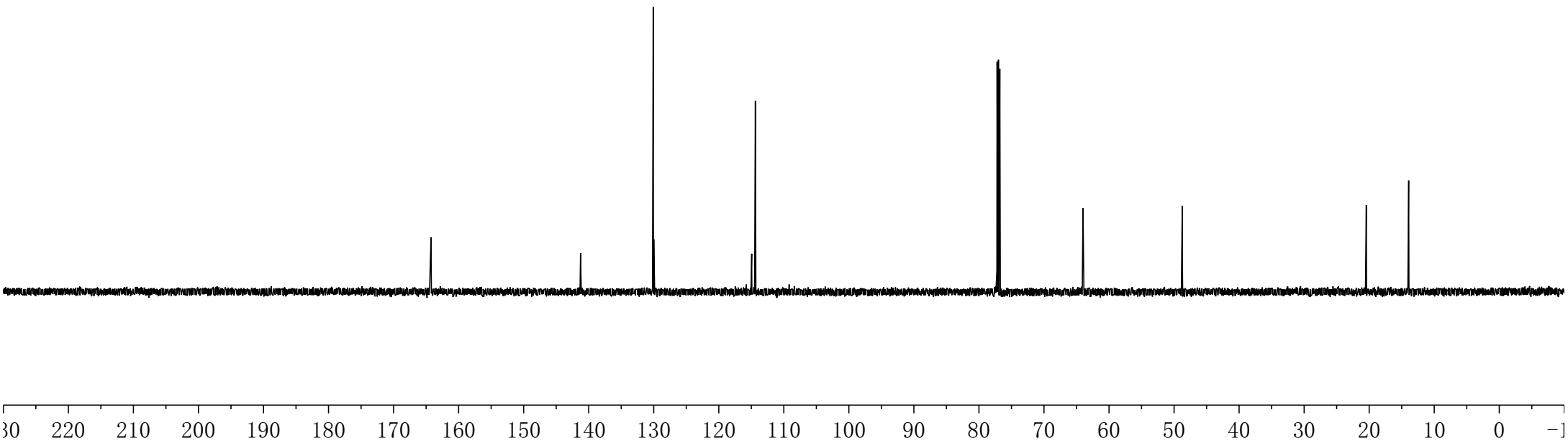
2a

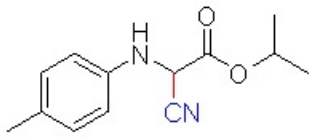
164.86
141.22
130.10
130.02
114.91
114.39
54.32
48.60
20.46



2b

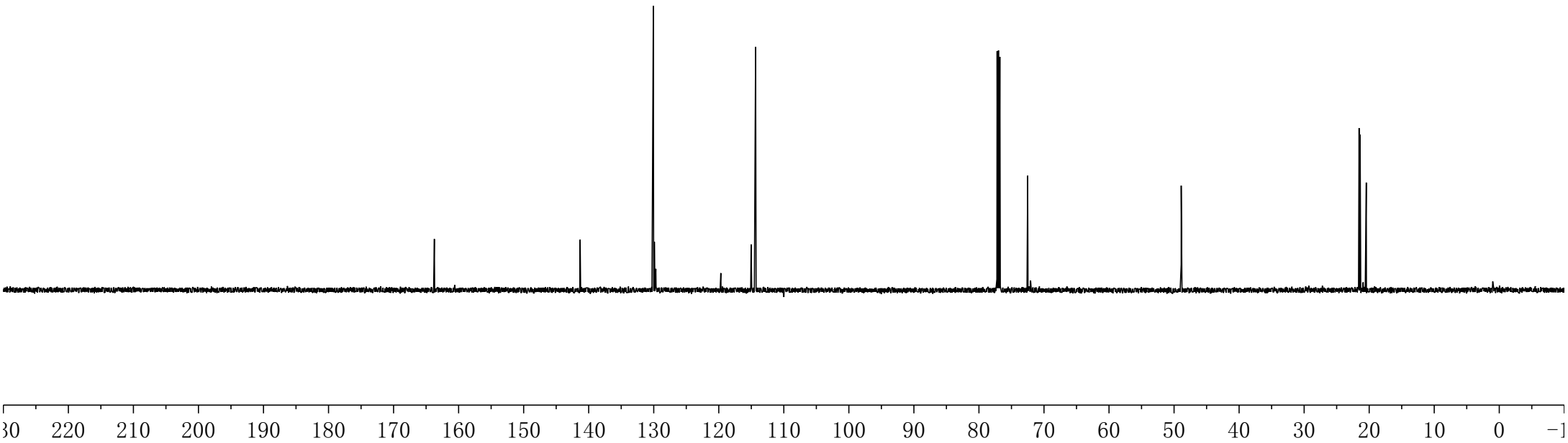
164.24
141.26
130.08
129.99
114.94
114.38
64.00
48.74
20.45
13.93

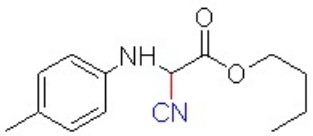




2c

163.73
141.31
130.06
129.90
115.03
114.34
72.51
48.90
21.55
21.39
20.45





2d

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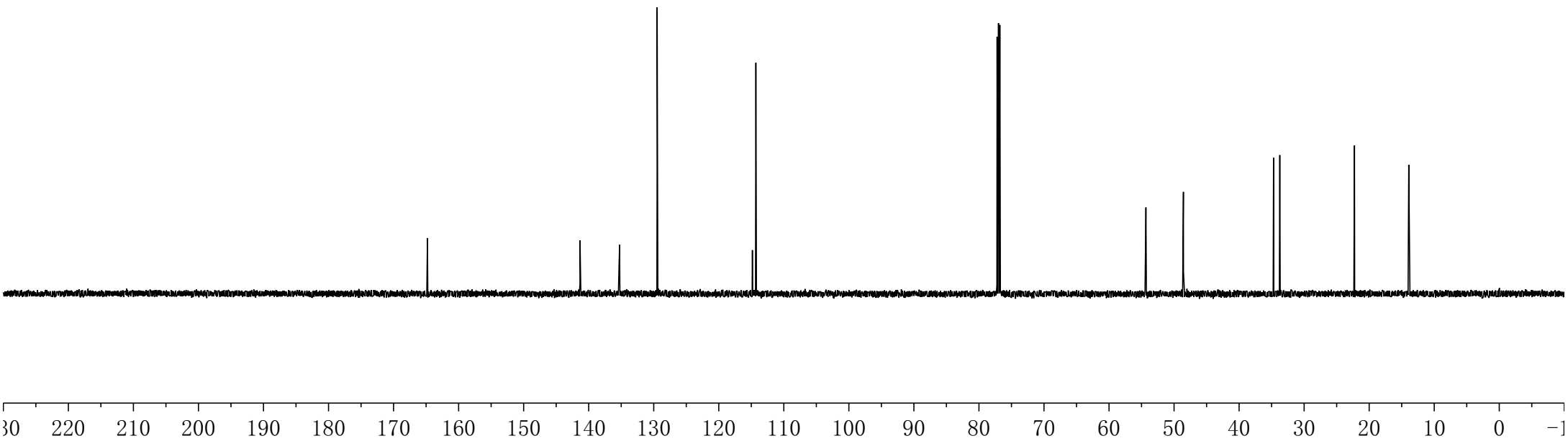
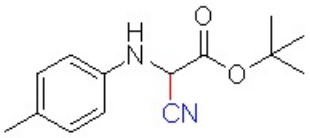
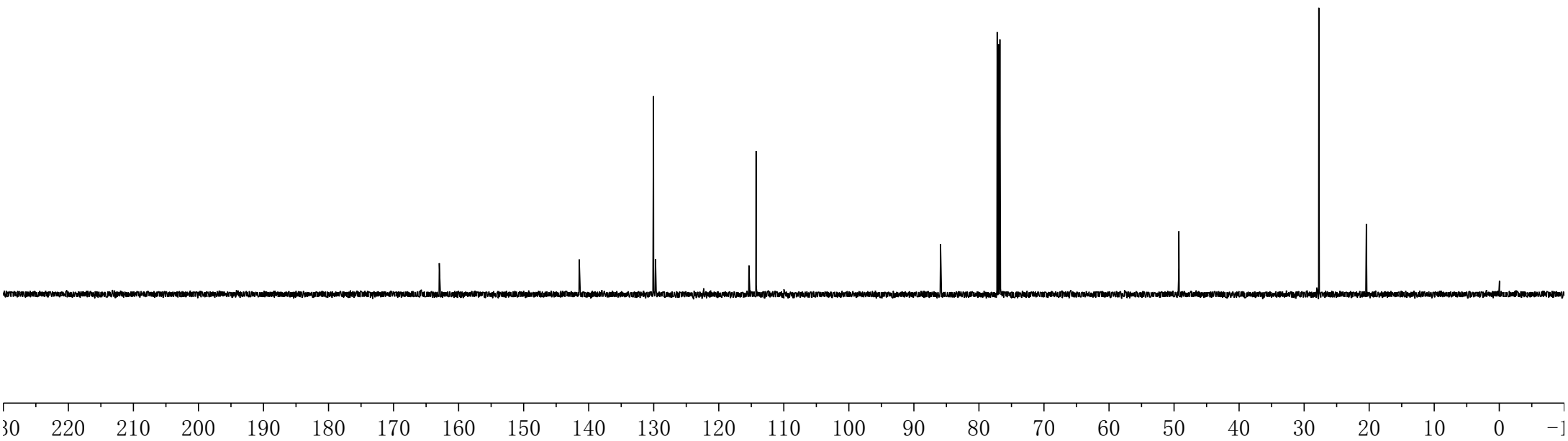
141.33
135.26
129.48
114.83
114.30
54.32
48.56
34.70
33.74
22.26
13.92

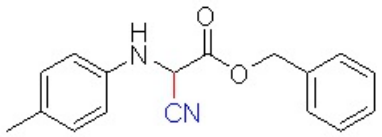




2e

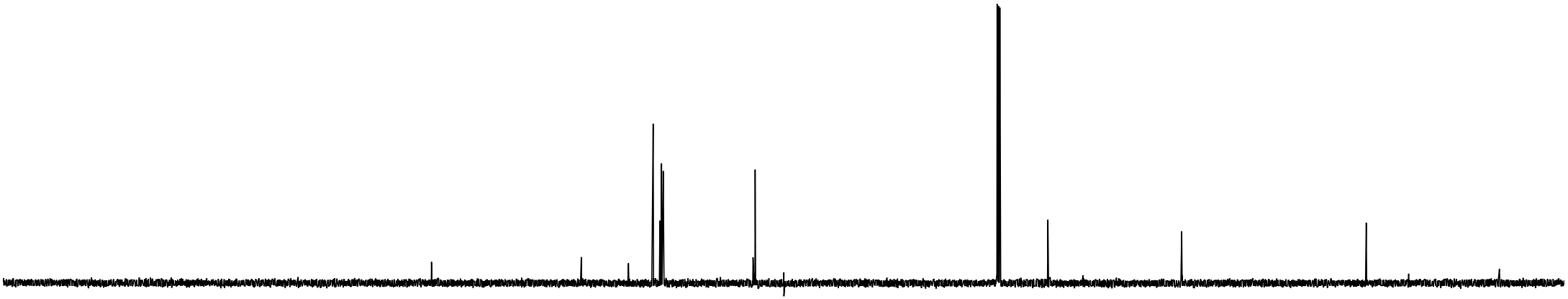
162.97
141.45
130.04
129.72
115.37
114.27
85.90
49.26
27.75
20.44

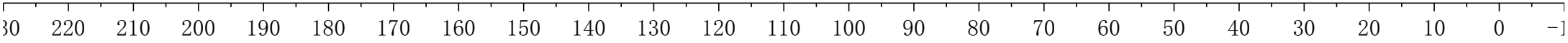


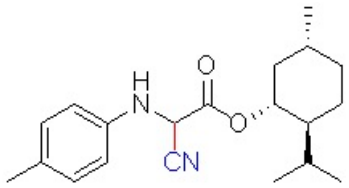


2f

164.17
141.14
133.89
130.09
129.05
128.80
128.54
114.73
114.41
109.99
69.39
48.83
20.45

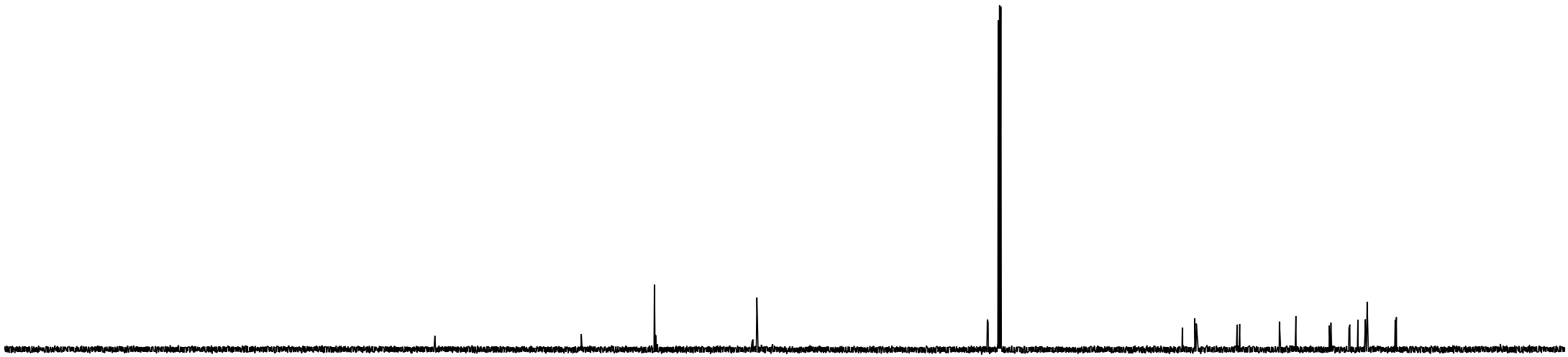


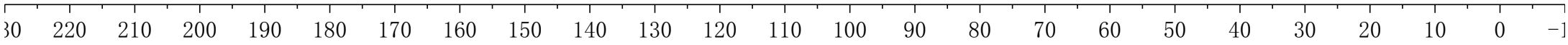


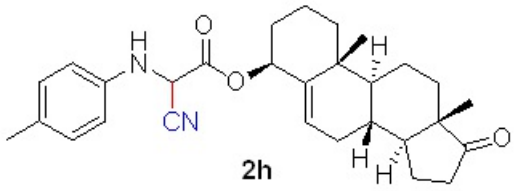


2g

163.82
141.32
130.06
129.87
114.31
78.85
78.74
48.87
48.74
46.95
46.70
40.45
40.04
33.93
33.89
31.42
31.40
26.26
26.00
23.24
23.10
21.87
21.85
20.71
20.64
20.44
16.13
15.94







2h

220.8960
160.5270
153.8408
139.2925
135.2232
133.8397
129.6942
122.5521
119.6893
71.5885
51.6899
50.1124
47.4984
37.5943
36.8037
36.7245
35.7998
31.4263
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30.7769
27.2959
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20.9411
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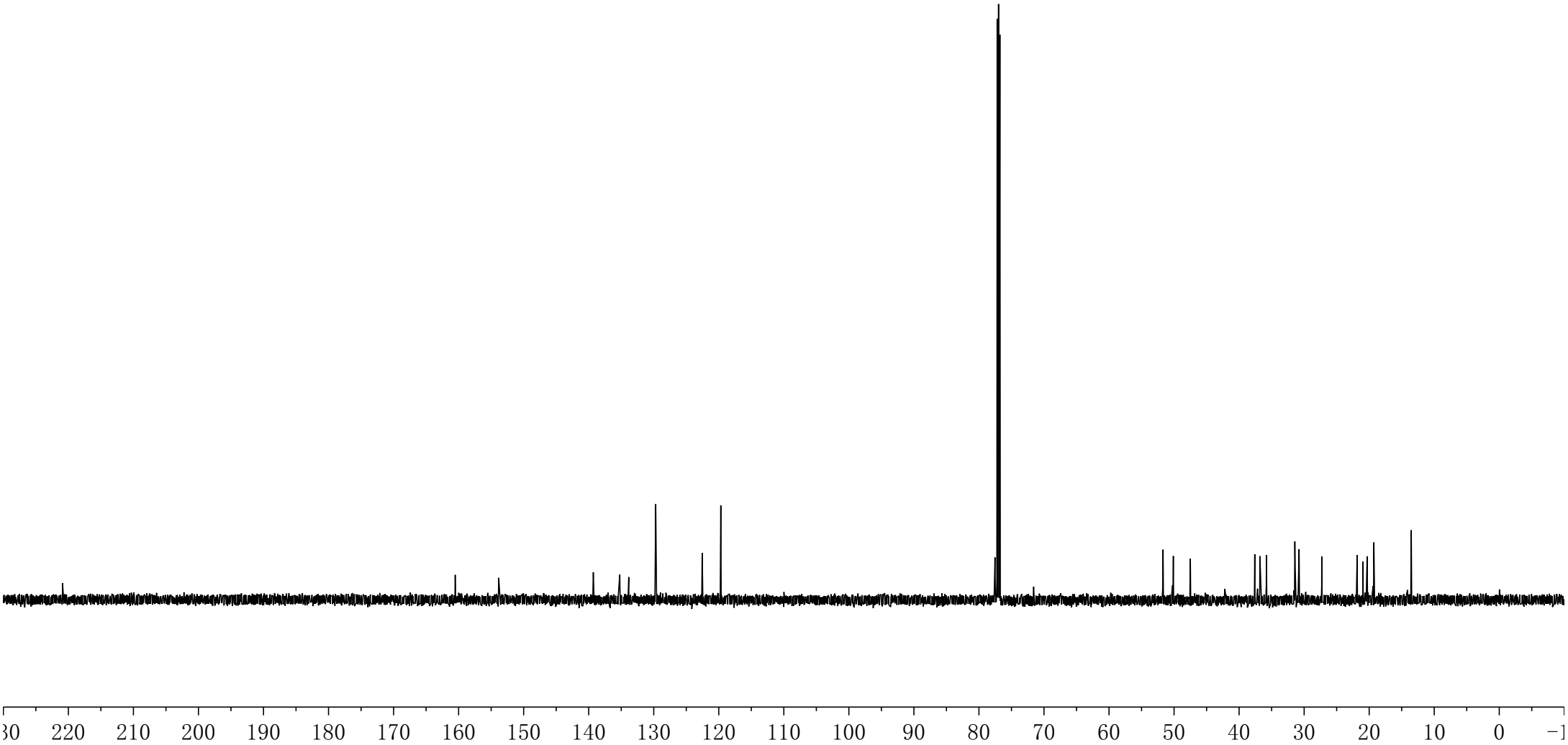
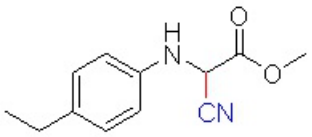
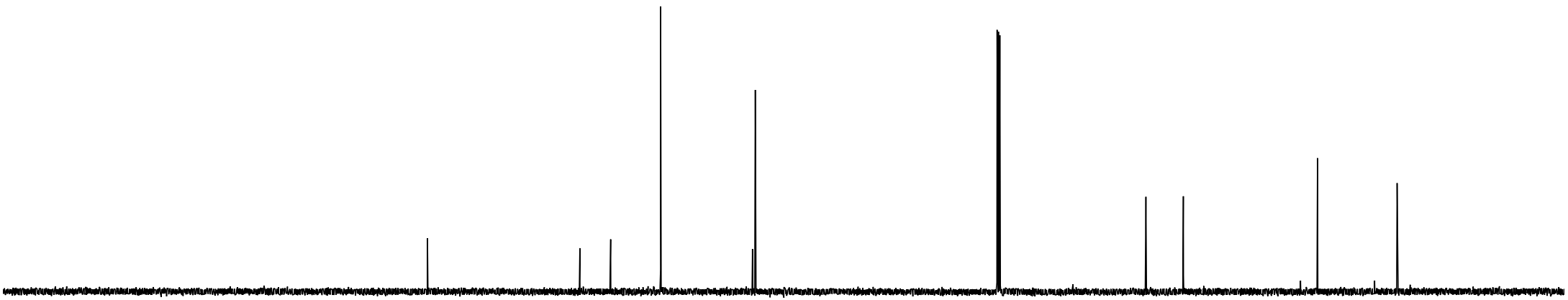
19.2783
13.5307

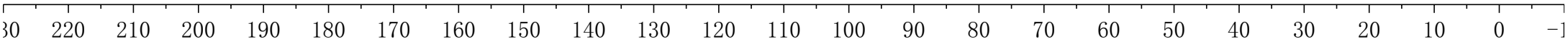


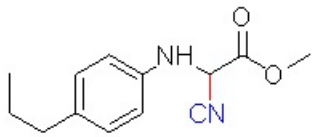


2i

164.79
141.36
136.62
128.94
114.82
114.39
54.33
48.57
27.95
15.71







2j

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135.09
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114.78
114.37
54.21
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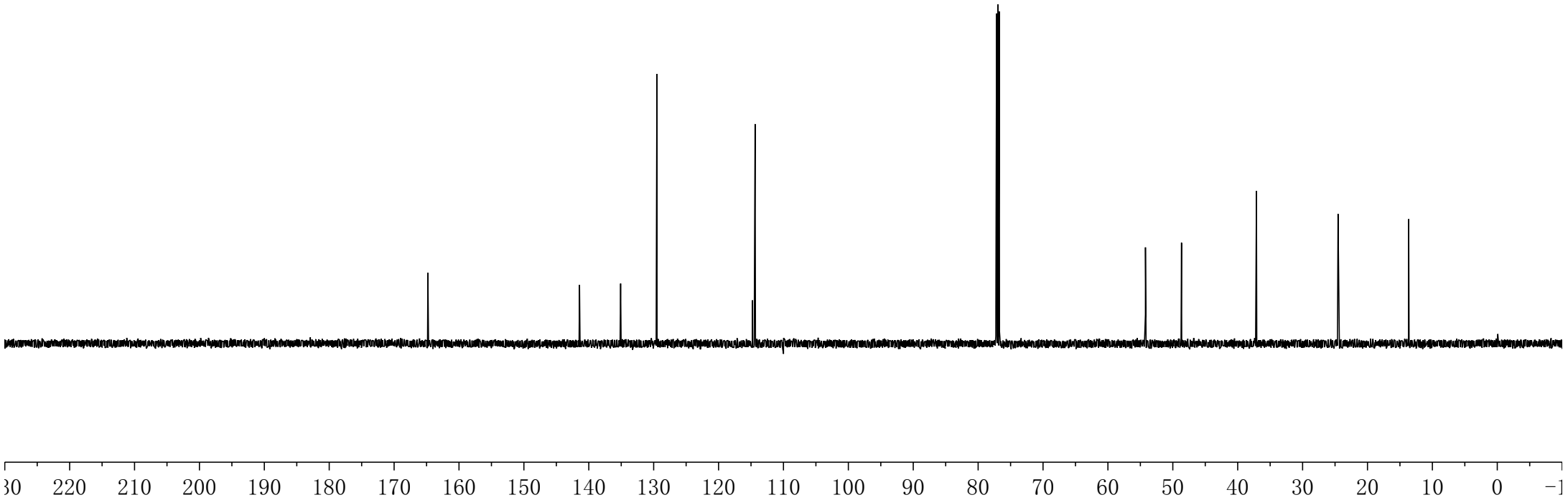
24.54
13.65



2k

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114.39
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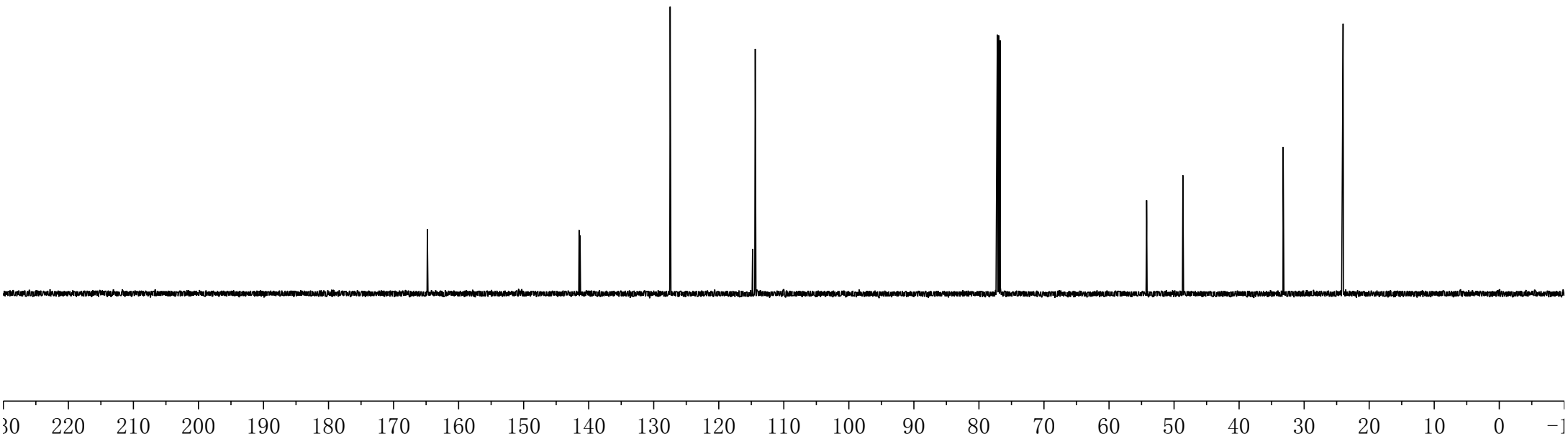
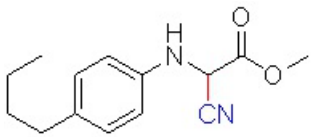
33.22
24.01





2l

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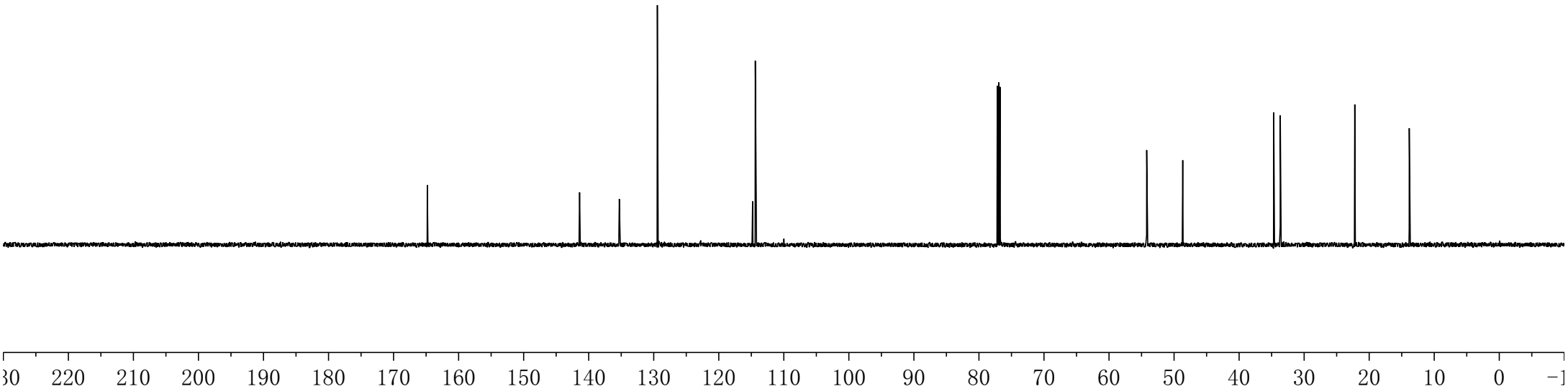
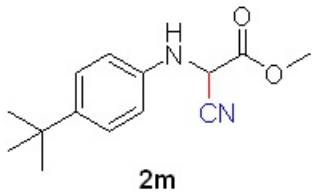
22.22
13.84





2m

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113.95
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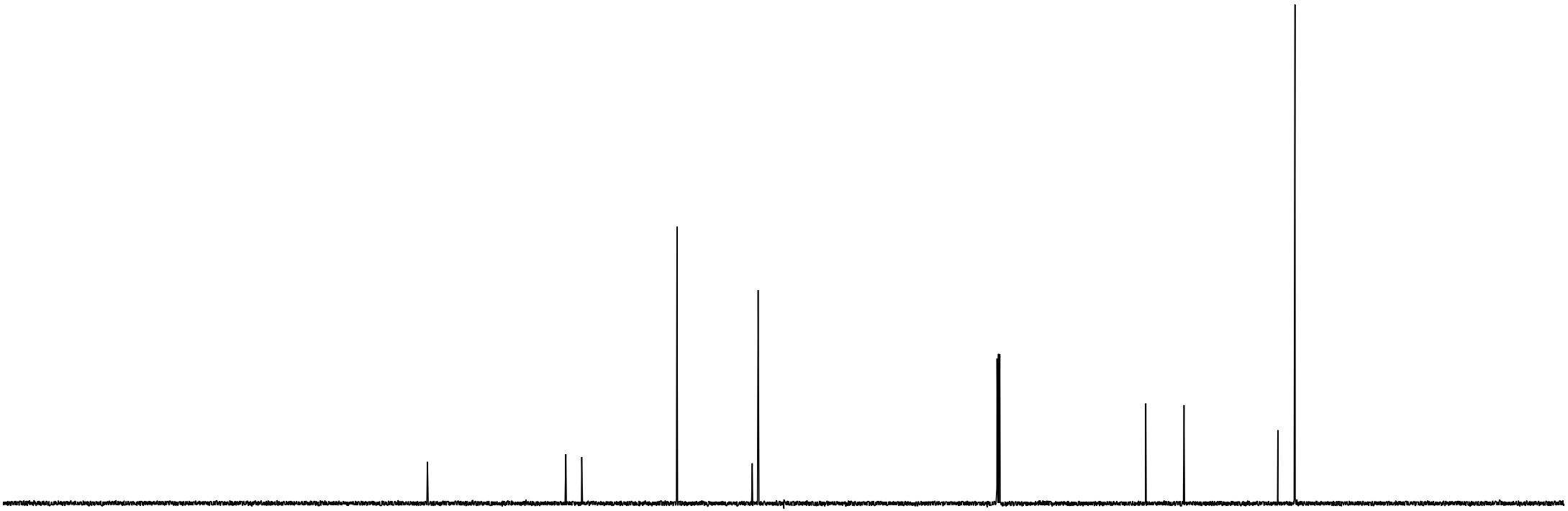
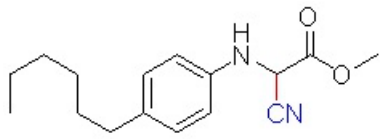
34.05
31.41





2n

164.80
141.33
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114.85
114.29
54.33
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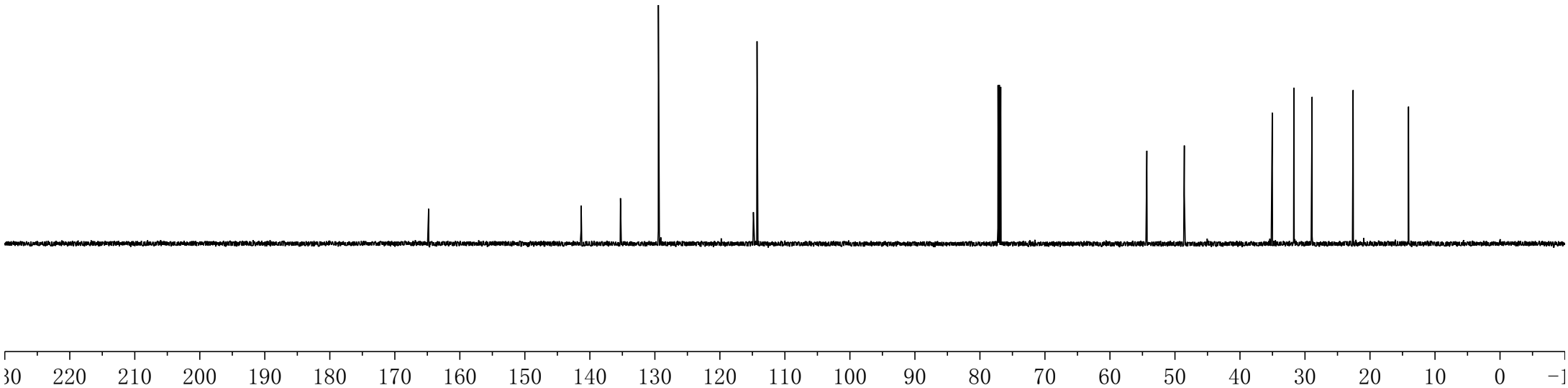
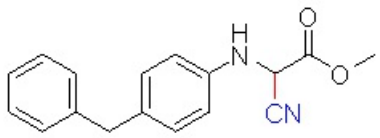
22.59
14.07





2o

164.71

141.73
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133.41
130.07
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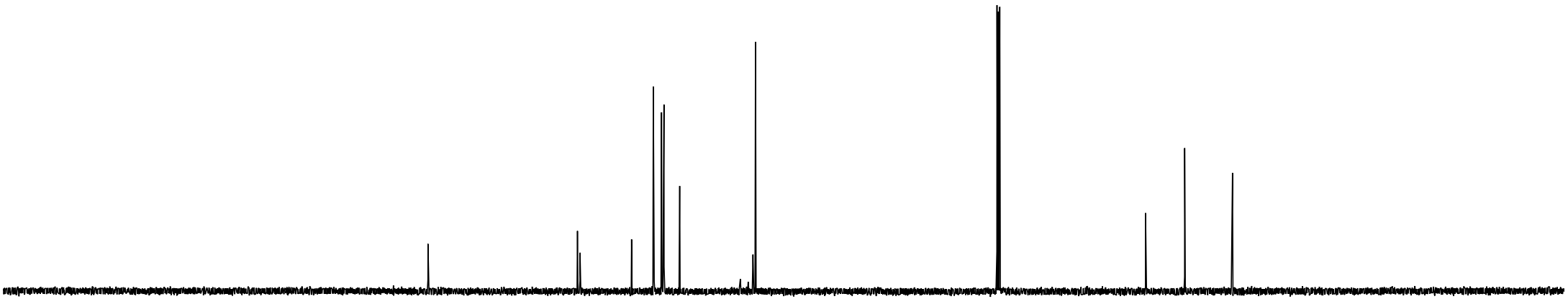
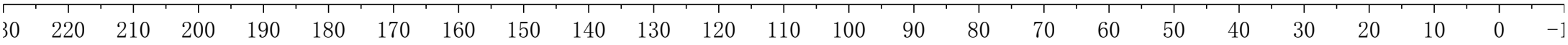
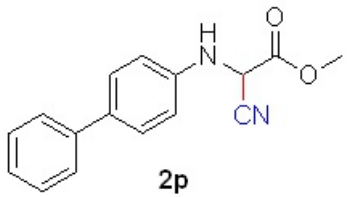
128.43
126.01
114.74
114.35

54.38
48.37
41.01







2p

164.61
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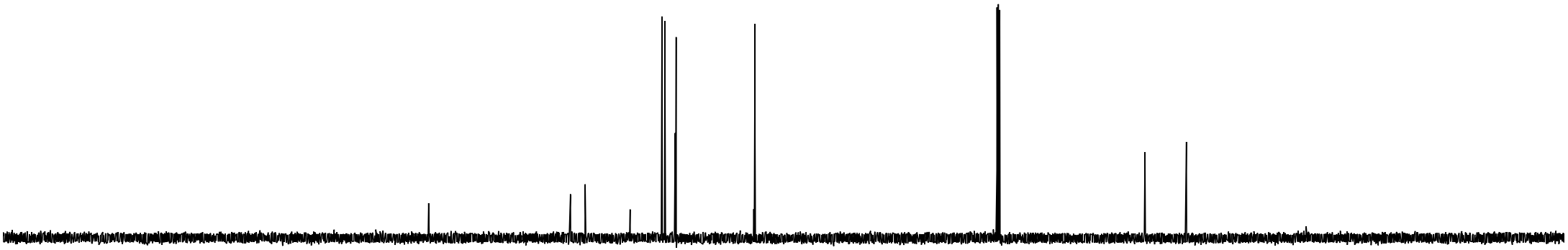
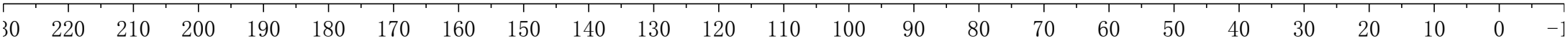
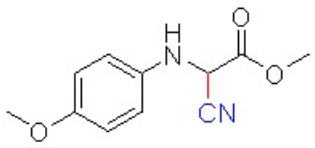
128.74
128.30
126.71
126.55
114.62
114.43
54.48
48.11







2q

164.81
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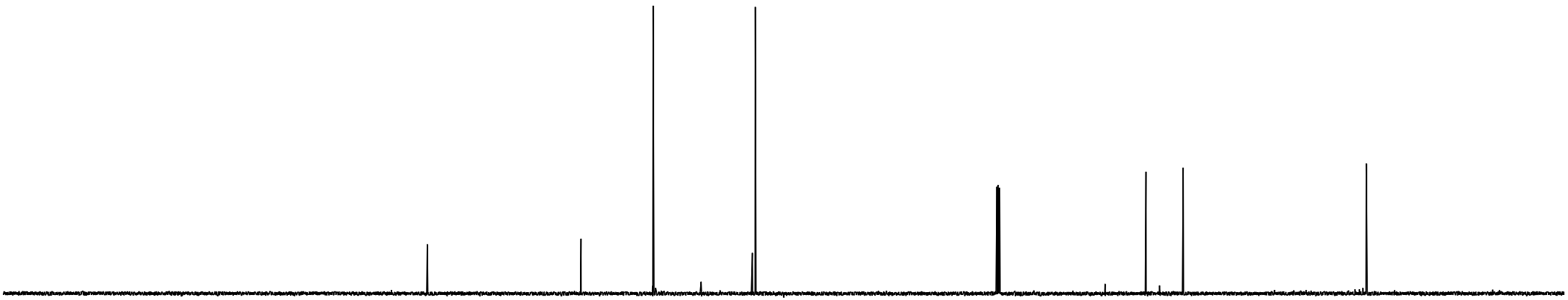
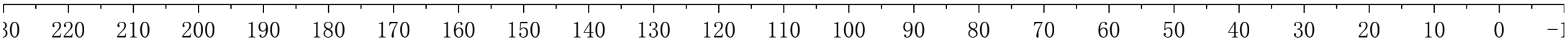
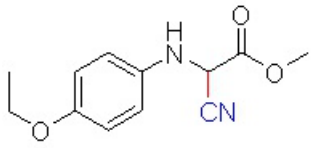
130.06
114.83
114.39
54.32
48.59
20.45







2r

164.87
153.85
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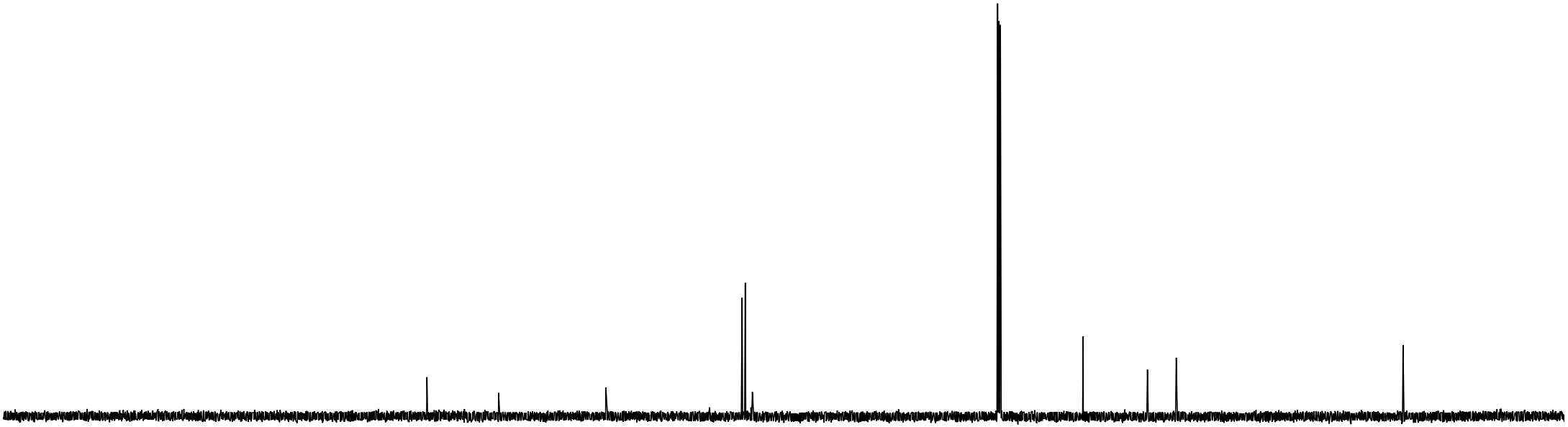
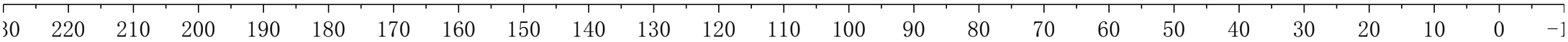
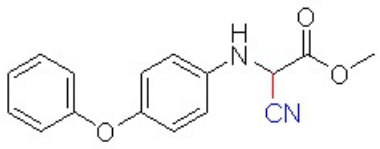
116.42
115.93
114.83
63.98
54.09
49.66
14.79







2s

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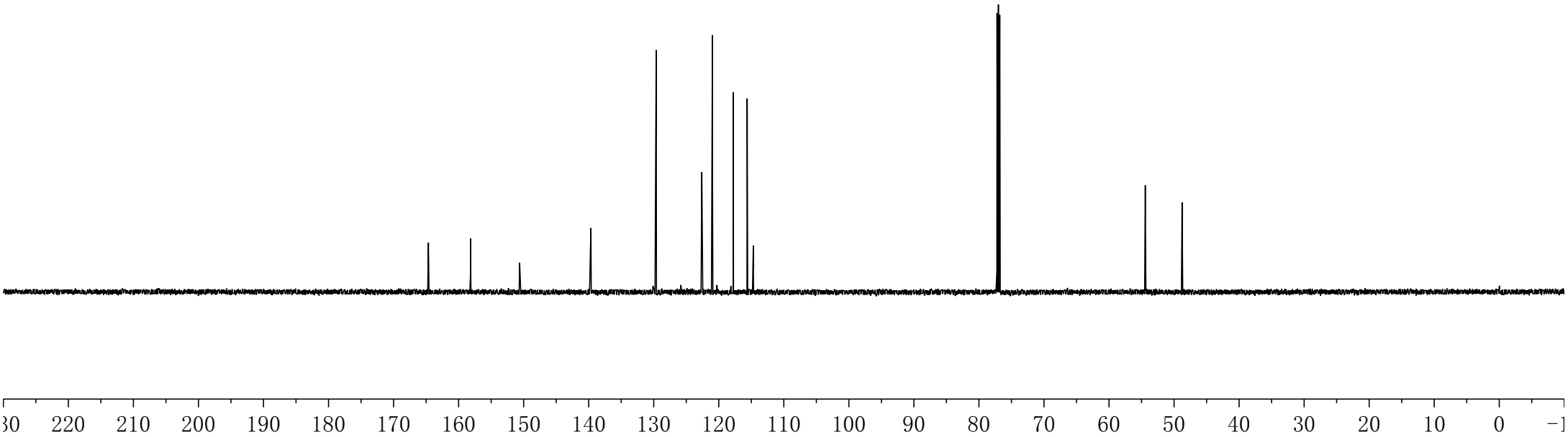
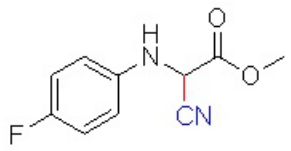
122.61
120.98
117.77
115.64
114.69
54.43
48.77





2t

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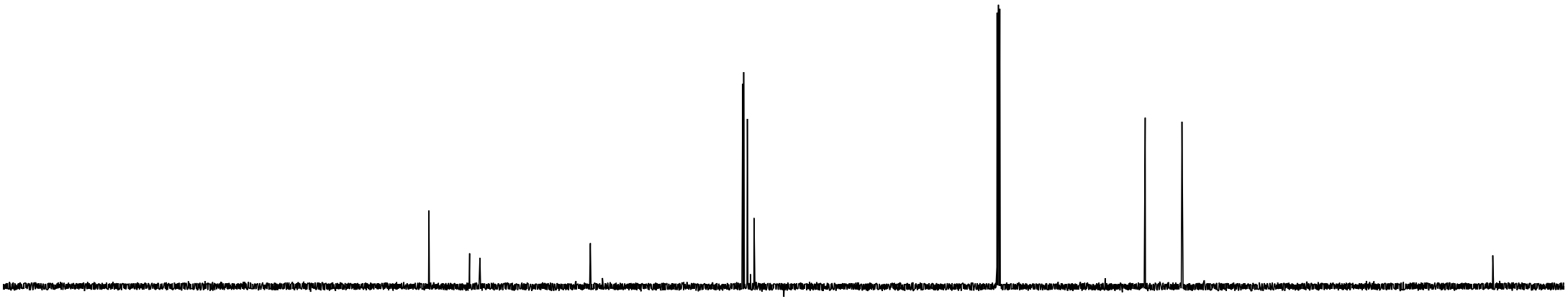
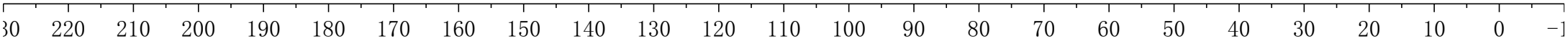
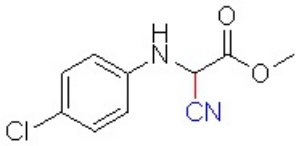
116.32
116.17
115.61
115.56
114.58
54.44
48.79







2u

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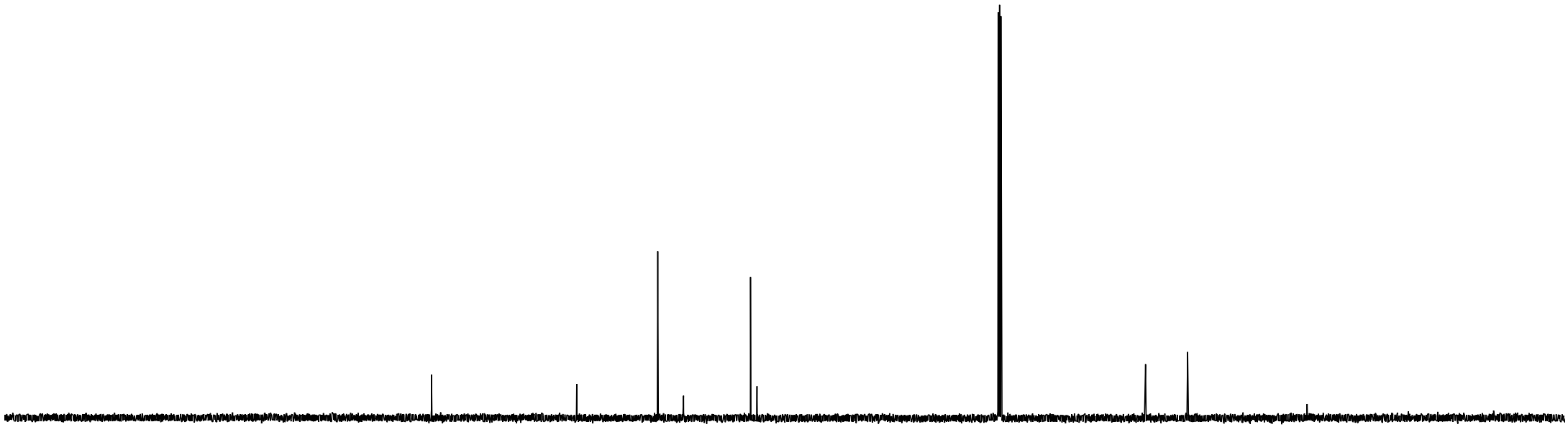
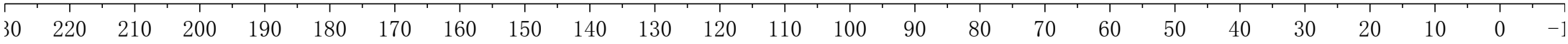
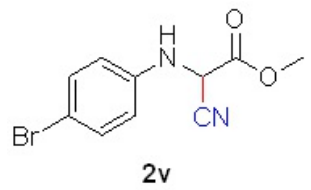
114.29
54.52
48.05







2v

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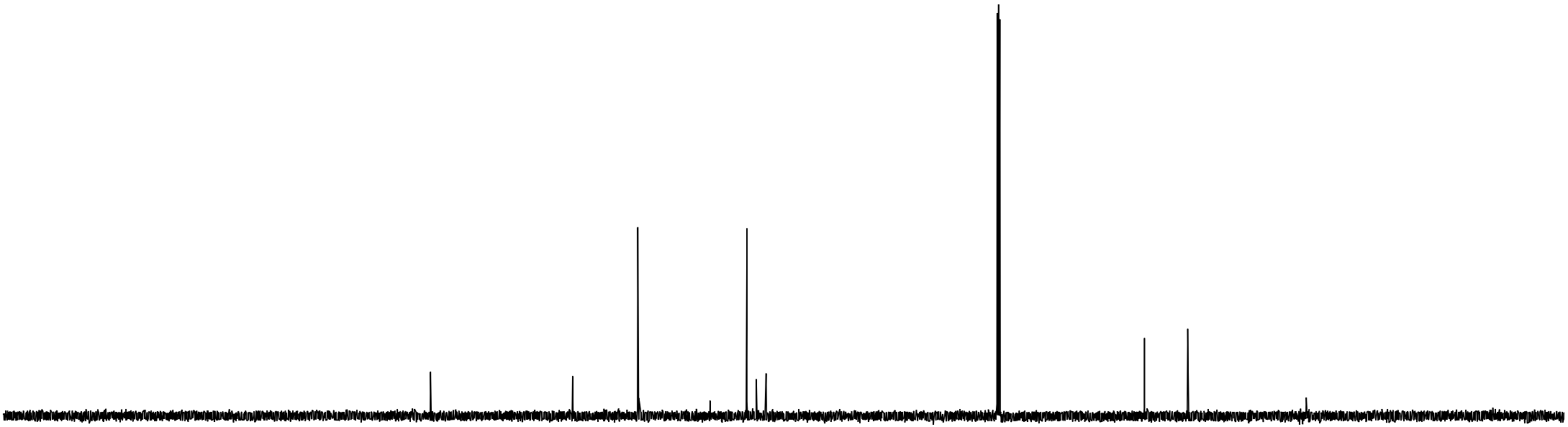
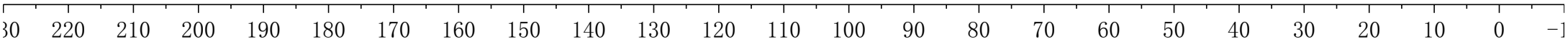
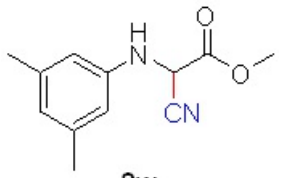
132.45
115.67
114.23
112.72
54.55
47.90







2w

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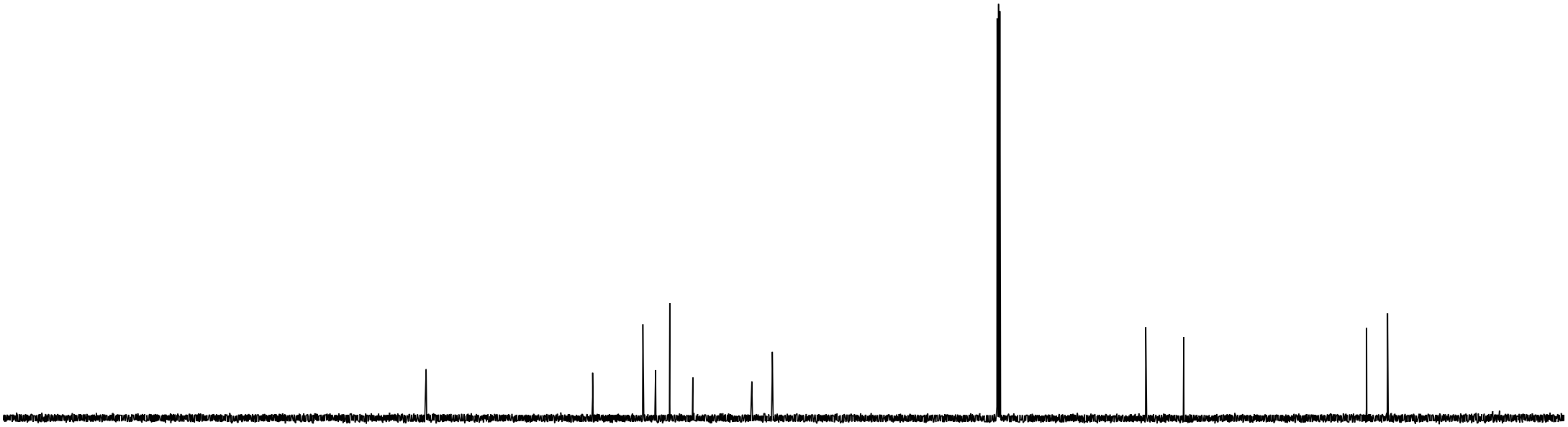
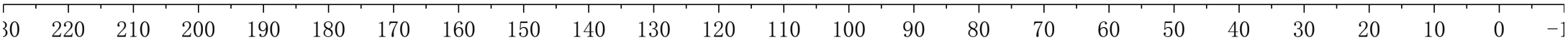
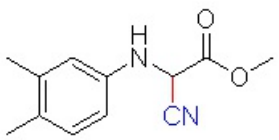
127.53
123.99
114.92
111.77
54.35
48.51
20.39
17.17







2x

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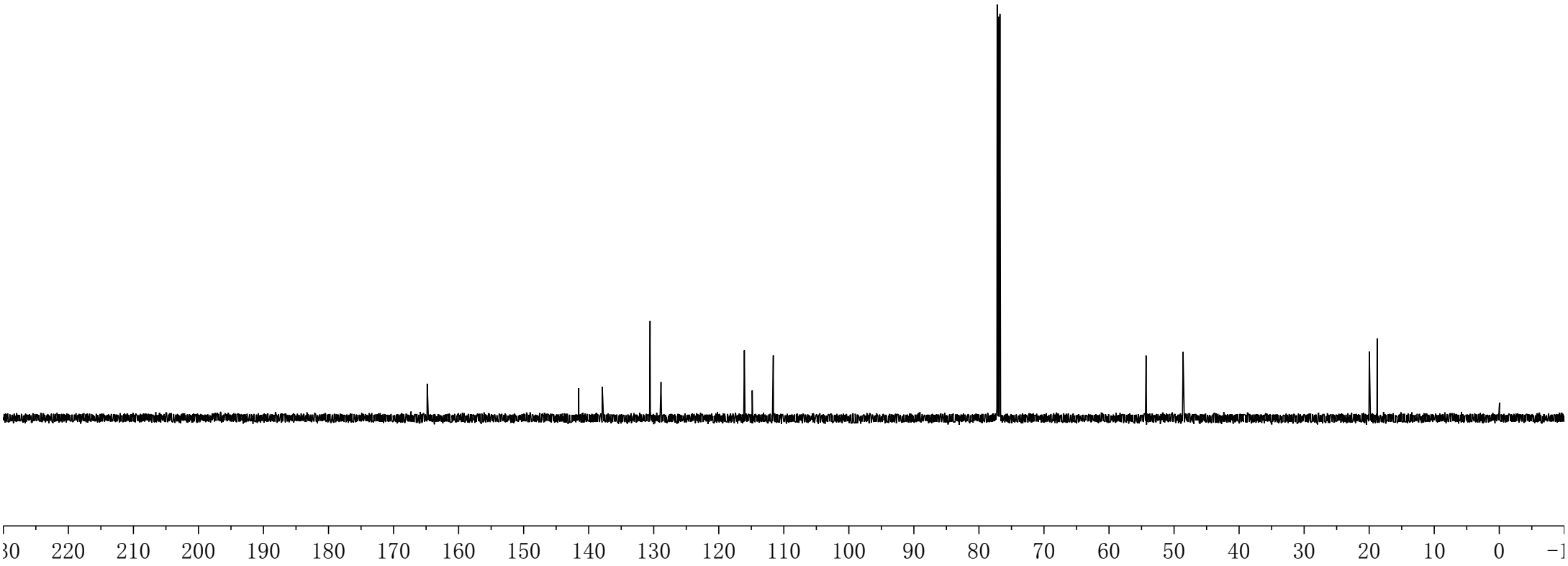
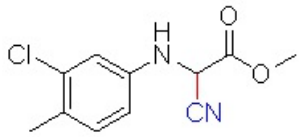
130.56
128.89
116.07
114.86
111.62
54.30
48.61
19.98
18.78





2y

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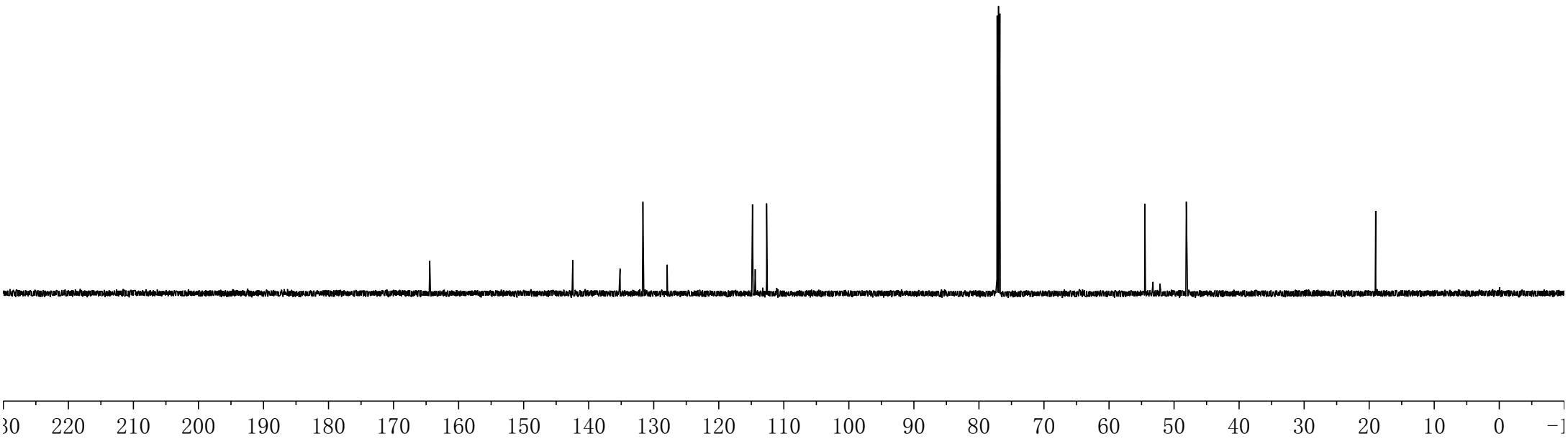
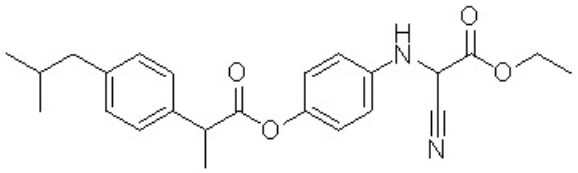
135.18
131.67
127.93
114.82
114.40
112.64
54.49
48.12
19.00





2z

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164.00
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141.33
140.76
137.26
129.46
127.17
122.45
114.67
77.22
77.01
76.80
64.15
48.54
45.18
45.03
30.16
22.38
19.17
18.51
13.91
220
210
200
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150
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70
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30
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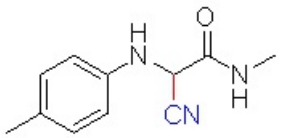
10
0



3a

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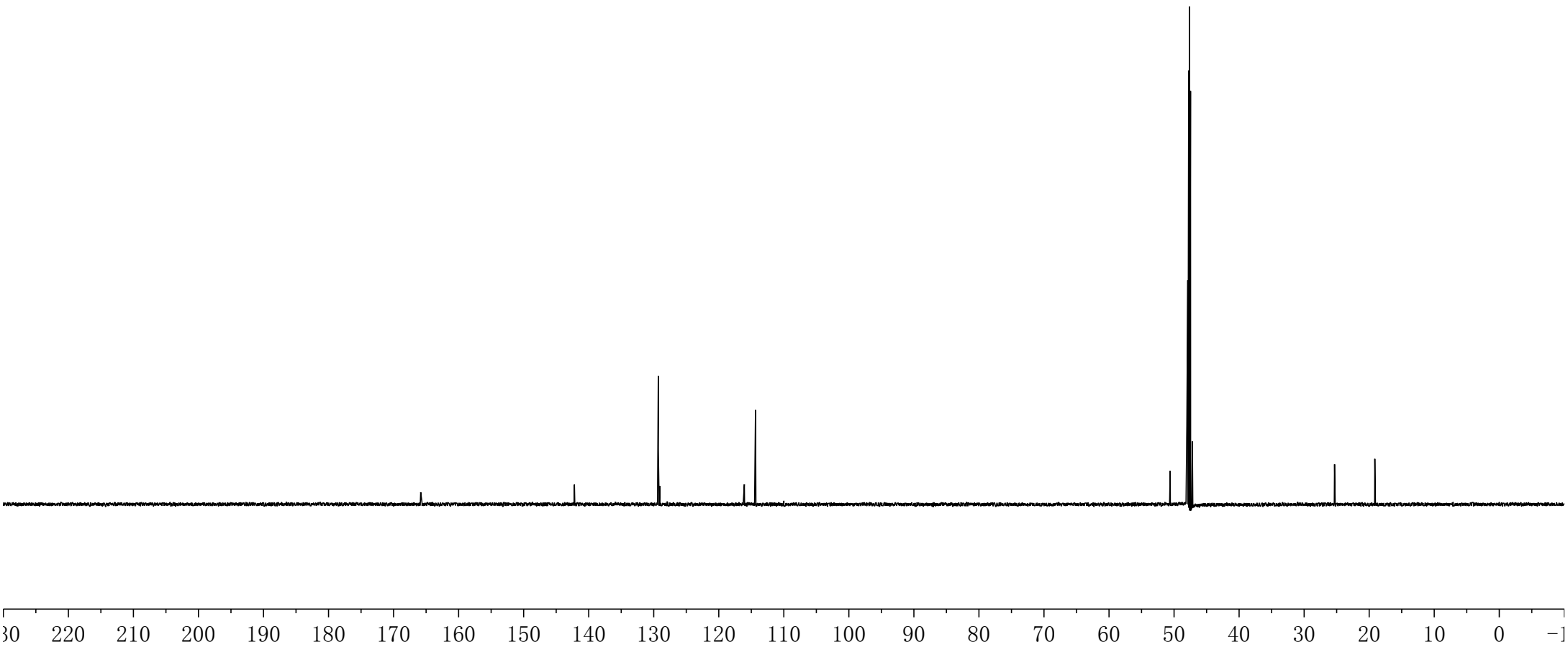
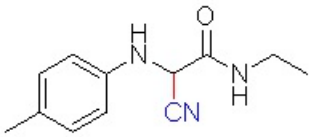
129.30
129.08
116.07
114.35
50.59
25.32
19.13




H
N
O
N
H
CN

3b

162.97
141.19
130.77
130.11
115.89
114.94
51.14
35.19
20.47
14.44
30
220
210
200
190
180
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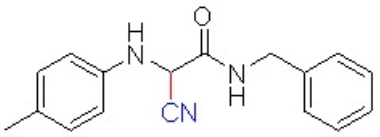

3c

163.35
141.03
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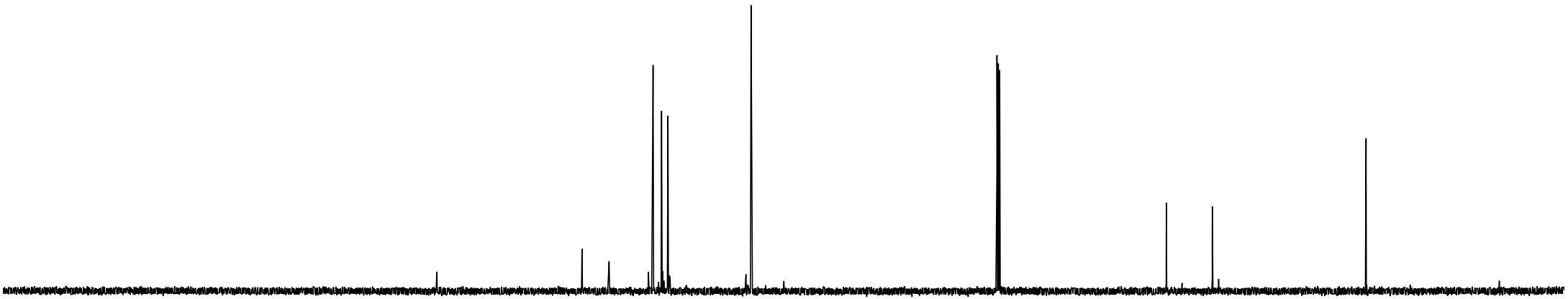
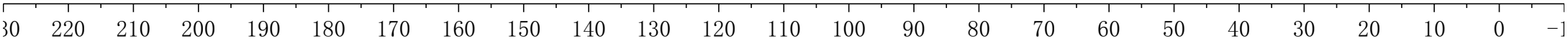
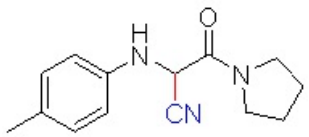
128.80
127.86
127.81
115.82
115.03
51.18
44.12
20.48







3d

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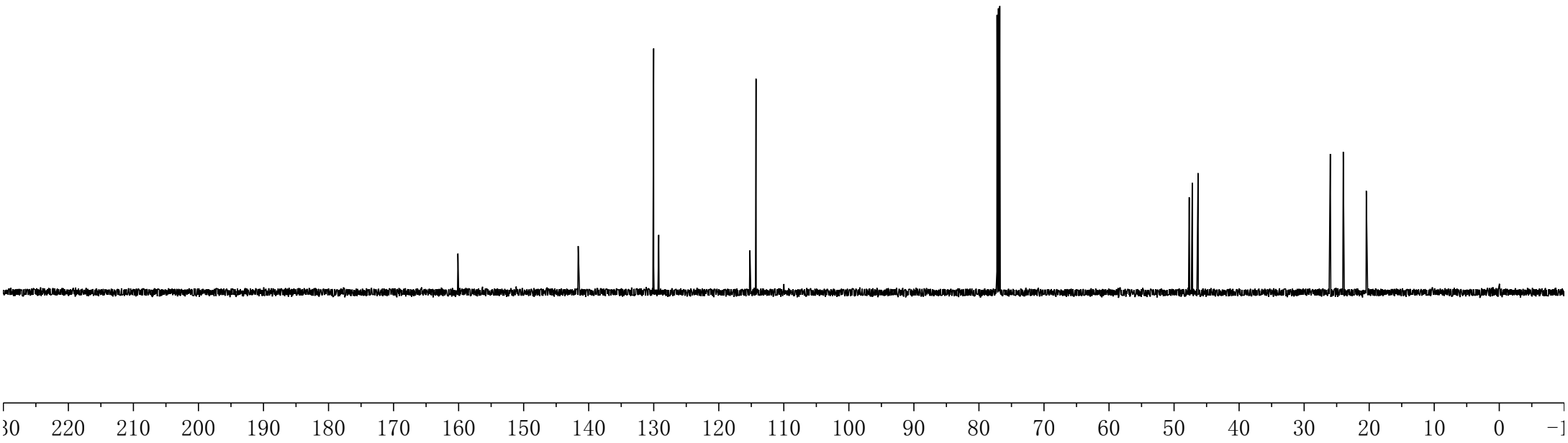
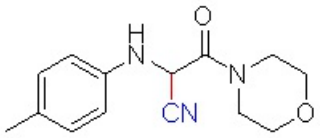
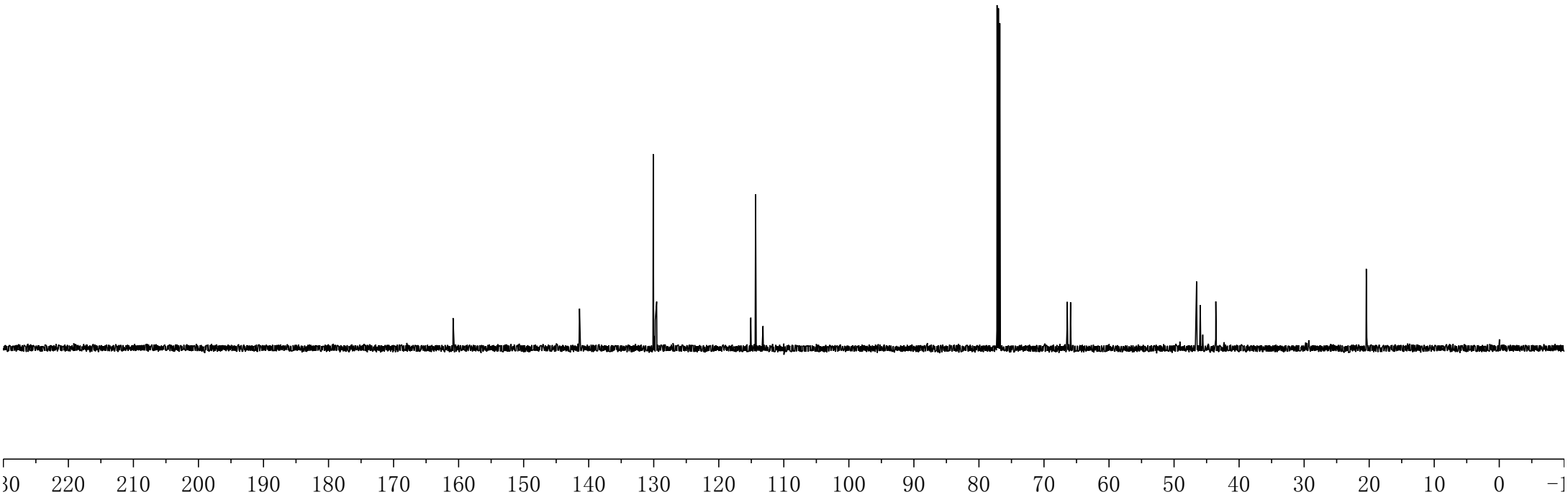
129.23
115.22
114.27
47.67
47.20
46.31
25.98
23.99
20.45

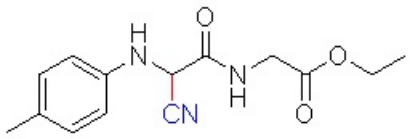




3e

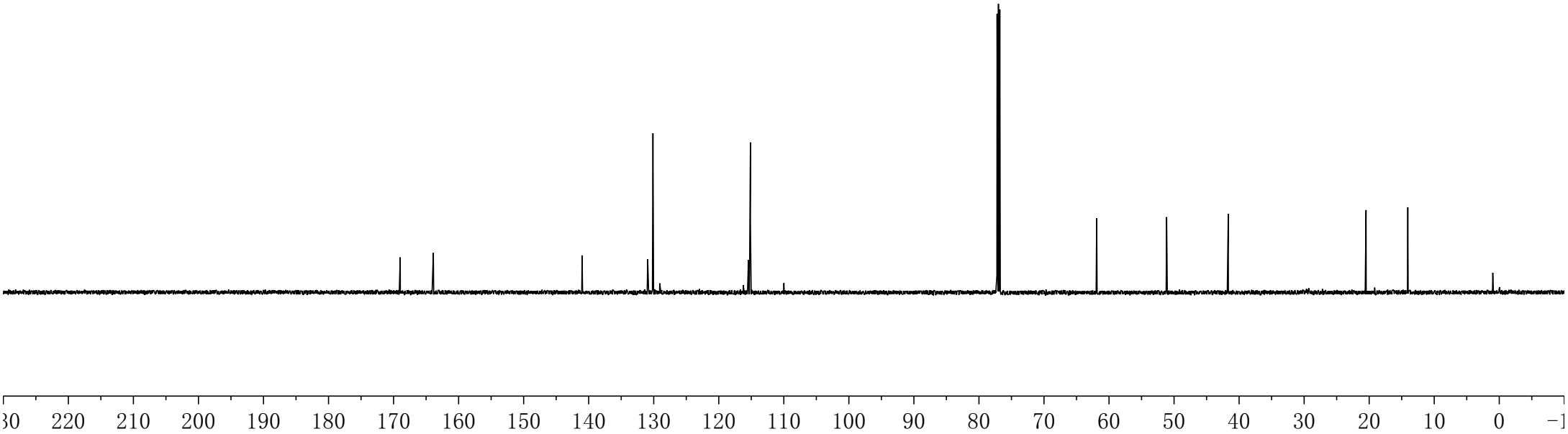
160.85
141.41
130.08
129.55
115.08
114.34
66.43
65.91
46.54
45.97
43.58
20.45

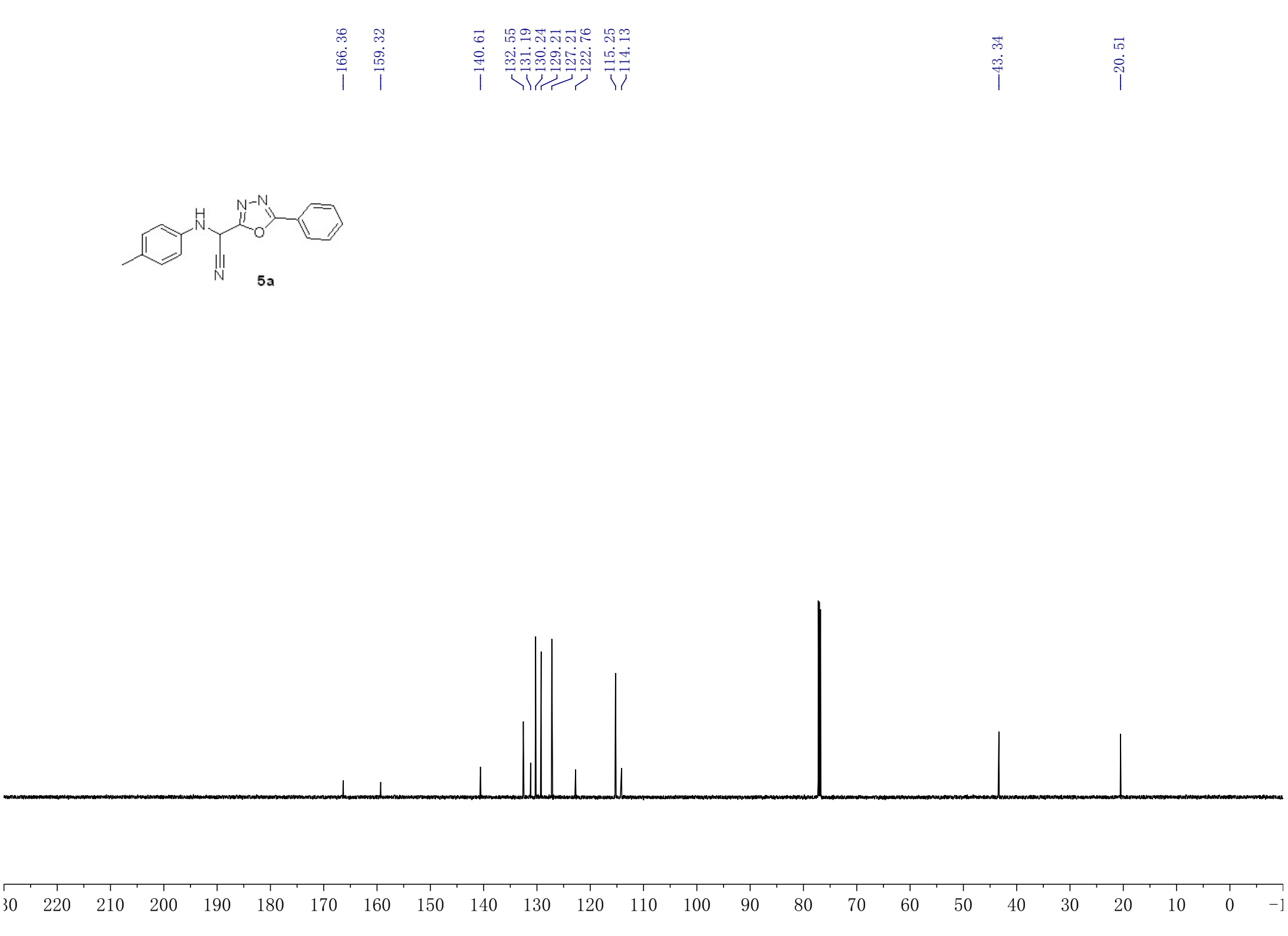


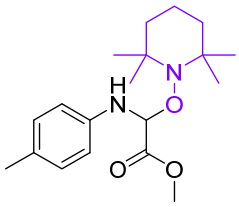


4a

168.98
163.88
141.01
130.93
130.12
115.44
115.13
61.90
51.14
41.67
20.48
14.06

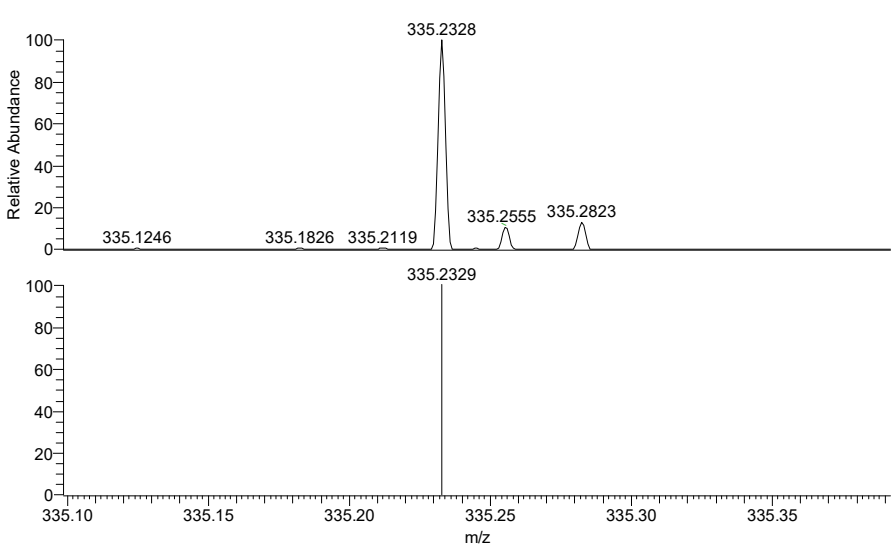


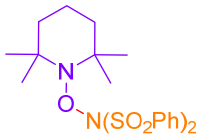

166.36
159.32
140.61
132.55
131.19
130.24
129.21
127.21
122.76
115.25
114.13
43.34
20.51
5a
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



C:\Users\...\filerecv\hcd-liangjia-2

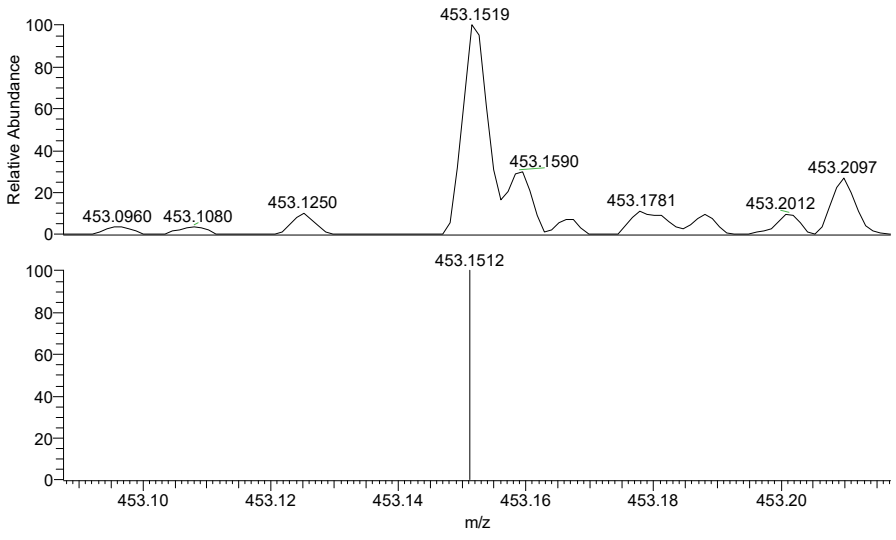
2020-6-5 17:24:11
Error = 0.3 ppm





hcd-liangjia-1_20200605170732

2020-6-5 17:07:32
Error = 1.5 ppm



$HN(SO_2Ph)_2$

C:\Users\...\filerecv\hcd-liangjia-3

2020-6-5 17:30:24
Error = 3.4 ppm