Supporting Information

Copper-catalyzed N-arylation and aerobic oxidative C-H/C-H coupling: one-pot synthesis of indoloimidazoquinoline derivatives

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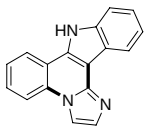
General experimental procedure

Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) and the remained DMSO in the solvent of DMSO-d_6 as the internal standards (^{1}H NMR: TMS at 0.00 ppm, DMSO at 2.50 ppm; ^{13}C NMR: DMSO at 40.0 ppm).

Synthesis of compounds 1a-e. Compounds **1a-e** were synthesized according to the known method.[1]

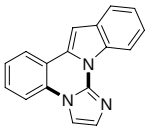
General procedure for synthesis of compounds 3a-q. A 25 mL Schlenk tube was charged with a magnetic stirrer and DMSO (1.5 mL), substituted 2-(2-bromophenyl)-1*H*-indole (**1**) (0.25 mmol), imidazole or substituted benzoimidazole (**2**) (0.5 mmol), 1,10-phenanthroline (0.01 mmol, 18 mg), Cs_2CO_3 (0.5 mmol, 163 mg), and CuBr (0.05 mmol, 7.2 mg) was added to the tube after stirring of the mixture for 10 min under nitrogen atmosphere. The N-arylation reaction was performed at 110 ^{o}C for 12 h under nitrogen atmosphere, then pivalic acid (1.75 mmol, 179 mg) was added to the resulting solution, and nitrogen atmosphere was changed into air atmosphere (*other conditions were kept*). The following aerobic oxidative intramolecular C-H/C-H coupling was carried out at 110 ^{o}C for 12 h. The resulting mixture was filtered, and the solid was washed with ethyl acetate for two times (2 × 3 mL). The combined filtrate was concentrated by the rotary evaporator, and the residue was purified by column chromatography on silica gel using petroleum ether/ ethyl acetate as eluent to provide the desired target product (**3**).



3a

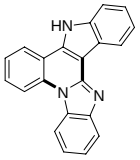
9*H*-Imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3a). Eluent: petroleum ether/ethyl acetate (2:1 to 1:2). Yield 52 mg (80%). Pale green solid, mp 209-211 ^{o}C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.50 (s, 1H), 8.54 (s, 1H), 8.49-8.47 (d, J = 7.9 Hz, 1H), 8.40-8.38 (d, J = 8.2 Hz, 1H), 8.34-8.31 (d, J = 7.5 Hz, 1H), 7.72-7.59 (m, 3H), 7.54 (s, 1H), 7.42-7.37 (t, J = 7.6 Hz, 1H), 7.31-7.26 (t, J = 7.4 Hz, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 141.4, 138.6, 133.1, 131,8, 131.3, 128.8, 125.3 124.8, 123.7,

122.6, 121.6, 121.0, 117.3, 115.5, 112.3, 112.0, 105.5. ESI-MS $[M+H]^+$ m/z 258.10.



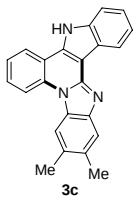
3a'

Imidazo[1,2-*a*]indolo[1,2-*c*]quinazoline (3a'). Eluent: petroleum ether/ethyl acetate (3:1). Pale yellow solid. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 8.82-8.79 (d, J = 8.3 Hz, 1H), 8.03-8.01 (d, J = 7.9 Hz, 1H), 7.77-7.75 (d, J = 7.9 Hz, 1H), 7.53-7.51 (t, J = 3.3 Hz, 2H), 7.48-7.29 (m, 5H), 7.14 (s, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 132.5, 130.8, 129.7, 128.9, 128.3, 125.7, 124.6, 123.5, 122.9, 120.5, 117.4, 114.9, 109.4, 97.5. ESI-MS $[M+H]^+$ m/z 258.10.



3b

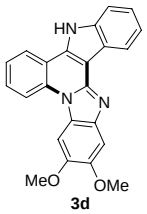
5*H*-Benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3b). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 52 mg (67%). Pale yellow solid, mp 300-302 ^{o}C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.74 (s, 1H), 8.90-8.88 (d, J = 8.3 Hz, 1H), 8.65-8.62 (d, J = 8.3 Hz, 1H), 8.56-8.54 (d, J = 7.9 Hz, 1H), 8.48-8.45 (d, J = 7.6 Hz, 1H), 7.94-7.91 (d, J = 7.9 Hz, 1H), 7.86-7.81 (t, J = 6.7 Hz, 1H), 7.71-7.65 (q, J = 6.6 Hz, 2H), 7.50-7.34 (m, 4H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.7, 145.6, 138.8, 135.8, 134.4, 131.2, 129.9, 125.1, 124.8, 124.2, 124.0, 123.5, 122.1, 121.8, 121.6, 119.4, 117.0, 115.8, 114.5, 112.5, 104.4. ESI-MS $[M+H]^+$ m/z 308.10.



3c

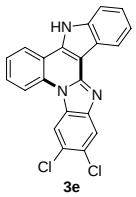
12,13-Dimethyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3c). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 71 mg (84%). Pale yellow solid, mp above 300 ^{o}C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.90 (s, 1H), 8.88-8.85 (d, J = 8.6 Hz, 1H), 8.62-8.59 (d, J = 7.6 Hz, 1H), 8.45-8.40 (t, J = 6.9 Hz, 2H), 7.84-7.79 (t, J = 8.1 Hz, 1H), 7.70-7.61 (q, J = 9.3 Hz, 3H), 7.45-7.40 (t, J = 7.5 Hz, 1H), 7.36-7.31 (t,

J = 7.0 Hz, 1H), 2.49 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.0, 144.0, 138.8, 135.6, 134.4, 132.6, 130.7, 129.7, 129.6, 124.9, 124.5, 124.1, 123.4, 121.7, 119.5, 116.9, 115.7, 114.6, 112.5, 20.7, 20.5. ESI-MS $[M+H]^+$ m/z 336.15.



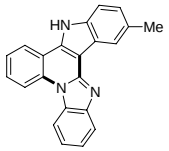
3d

12,13-Dimethoxy-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3d). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 56 mg (61%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.69 (s, 1H), 8.85-8.82 (d, *J* = 8.6 Hz, 1H), 8.56-8.53 (d, *J* = 7.9 Hz, 1H), 8.46-8.43 (d, *J* = 7.5 Hz, 1H), 8.06 (s, 1H), 7.88-7.83 (t, *J* = 7.7 Hz, 1H), 7.72-7.66 (m, 2H), 7.51 (s, 1H), 7.48-7.43 (t, *J* = 7.5 Hz, 1H), 7.39-7.34 (t, *J* = 7.4 Hz, 1H), 4.01 (s, 3H), 3.92 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 148.0, 146.1, 138, 135.1, 133.9, 132.0, 129.7, 129.1, 125.0, 124.6, 124.1, 123.8, 123.2, 121.7, 121.4, 116.8, 115.6, 112.4, 104.5, 101.8, 99.2, 57.4, 56.3. ESI-MS $[M+H]^+$ m/z 368.10.



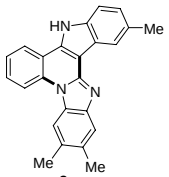
3e

12,13-Dichloro-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3e). Eluent: petroleum ether/ethyl acetate (5:1 to 1:1). Yield 84 mg (89%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.73 (s, 1H), 8.76-8.70 (t, *J* = 8.2 Hz, 2H), 8.49-8.46 (d, *J* = 7.9 Hz, 1H), 8.36-8.33 (d, *J* = 7.9 Hz, 1H), 8.03 (s, 1H), 7.80-7.74 (t, *J* = 7.7 Hz, 1H), 7.69-7.61 (q, *J* = 7.7 Hz, 2H), 7.47-7.42 (t, *J* = 7.6 Hz, 1H), 7.37-7.32 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 147.9, 144.8, 138.2, 135.8, 133.1, 129.9, 129.4, 126.0, 124.6, 123.4, 123.2, 122.7, 121.2, 121.1, 119.2, 116.7, 115.1, 115.0, 112.0, 103.2. ESI-MS $[M+H]^+$ m/z 376.00.



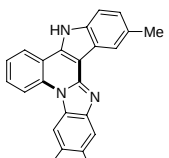
3f

2-Methyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3f). Eluent: petroleum ether/ethyl acetate (5:1 to 1:1). Yield 53 mg (66%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 13.64 (s, 1H), 8.98-8.95 (d, J = 8.6 Hz, 1H), 8.80-8.78 (d, J = 8.2 Hz, 1H), 8.71-8.69 (d, J = 7.9 Hz, 1H), 8.54 (s, 1H), 8.01-7.99 (d, J = 7.9 Hz, 1H), 7.96-7.91 (t, J = 7.7 Hz, 1H), 7.81-7.76 (t, J = 7.6 Hz, 1H), 7.71-7.59 (m, 2H), 7.52-7.49 (d, J = 8.2 Hz, 1H), 7.26-7.23 (d, J = 8.2 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 140.7, 139.1, 136.9, 133.4, 132.2, 131.9, 131.3, 128.6, 127.7, 126.9, 126.8, 125.0, 124.2, 120.9, 120.3, 117.9, 115.9, 114.9, 114.6, 112.4, 98.3, 21.6. ESI-MS $[M+H]^+$ m/z 322.15.



3g

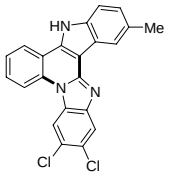
2,12,13-Trimethyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3g). Eluent: petroleum ether/ethyl acetate (5:1 to 1:1). Yield 71 mg (81%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.60 (s, 1H), 8.84-8.82 (d, J = 8.6 Hz, 1H), 8.51-8.48 (d, J = 7.9 Hz, 1H), 8.37 (s, 1H), 8.22 (s, 1H), 7.82-7.78 (t, J = 7.7 Hz, 1H), 7.66-7.59 (q, J = 7.2 Hz, 2H), 7.57-7.54 (d, J = 8.3 Hz, 1H), 7.26-7.23 (d, J = 8.2 Hz, 1H) 2.52 (s, 3H), 2.47 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.1, 144.2, 137.1, 135.5, 134.4, 132.5, 130.7, 130.3, 129.6, 126.5, 124.5, 123.8, 123.7, 121,5, 119.6, 116.9, 115.8, 114.6, 112.1, 104.2, 21.8, 20.7, 20.5. ESI-MS $[M+H]^+$ m/z 350.15.



3h

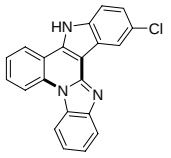
12,13-Dimethoxy-2-methyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3h). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 33 mg (34%). Pale

yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.47 (s, 1H), 8.80-8.78 (d, J = 8.6 Hz, 1H), 8.50-8.47 (d, J = 7.9 Hz, 1H), 8.21 (s, 1H), 8.03 (s, 1H), 7.83-7.77 (t, J = 7.9 Hz, 1H), 7.65-7.60 (t, J = 7.4 Hz, 1H), 7.56-7.51 (t, J = 7.9 Hz, 2H), 7.25-7.22 (d, J = 8.3 Hz, 1H), 3.99 (s, 3H), 3.89 (s, 3H), 2.48 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 147.9, 146.0, 145.7, 139.9, 137.1, 134.9, 134.0, 130.2, 129.5, 126.5, 124.5, 124.3, 123.8, 123.6, 121.4, 116.8, 115.8, 112.1, 104.4, 102.2, 99.3, 57.5, 56.3, 21.8. ESI-MS $[M+H]^+$ m/z 382.15.



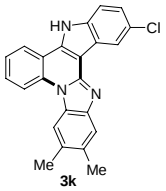
3i

12,13-Dichloro-2-methyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3i). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 83 mg (85%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.61 (s, 1H), 8.78-8.72 (t, J = 8.9 Hz, 2H), 8.46-8.43 (d, J = 6.9 Hz, 1H), 8.11 (s, 1H), 8.04 (s, 1H), 7.79-7,74 (t, J = 7.4 Hz, 1H), 7.66-7.61 (t, J = 7.5 Hz, 1H), 7.55-7.52 (d, J = 8.3 Hz, 1H), 7.25-7.22 (d, J = 7.6 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 148.6, 145.5, 137.1, 136.4, 133.6, 130.7, 130.5, 130.0, 126,8, 126.6, 125.3, 123.9, 123.7, 123.5, 121.3, 119.7, 117.3, 115.8, 115.6, 112.2, 103.5, 21.8. ESI-MS $[M+H]^+$ m/z 390.05.



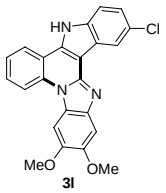
3j

2-Chloro-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3j). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 75 mg (87%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.89 (s, 1H), 8.86-8.83 (d, J = 8.6 Hz, 1H), 8.62-8.59 (d, J = 7.9 Hz, 1H), 8.51-8.48 (d, J = 7.9 Hz, 1H), 8.36 (s, 1H), 7.94-7.91 (d, J = 7.6 Hz, 1H), 7.87-7.82 (t, J = 7.7 Hz, 1H), 7.70-7.63 (m, 2H), 7.52-7.41 (m, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.0, 145.2, 137.3, 137.1, 134.6, 131.1, 130.3, 126.0, 125.0, 124.4, 124.2, 122.3, 120.6, 119.4, 117.1, 115.5, 114.6, 114.1, 103.7. ESI-MS $[M+H]^+$ m/z 342.05.



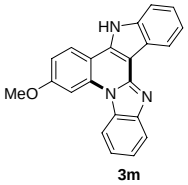
3k

2-Chloro-12,13-dimethyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3k). Eluent: petroleum ether/ethyl acetate (3:1/1:1). Yield 82 mg (88%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.71 (s, 1H), 8.68-8.65 (d, J = 8.3 Hz, 1H), 8.38-8.36 (d, J = 7.9 Hz, 1H), 8,23-8.18 (d, J = 12.4 Hz, 2H), 7.74-7.69 (t, J = 7.7 Hz, 1H), 7.60-7.51 (m, 3H), 7.35-7.33 (d, J = 8.6 Hz, 1H), 2.38 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 145.3, 143.7, 137.2, 136.6, 134.5, 132.6, 130.8, 130.0, 129.4, 125.8, 124.8, 124.5, 124.4, 124.0, 120.6, 119.5, 116.9, 115.3, 114.5, 114.0, 103.9, 20.7, 20.5. ESI-MS $[M+H]^+$ m/z 370.10.



3l

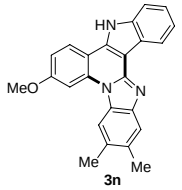
2-Chloro-12,13-dimethoxy-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3l). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 63 mg (62%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.82 (s, 1H), 8.85-8.82 (d, J = 8.6 Hz, 1H), 8.53-8.50 (d, J = 6.5 Hz, 1H), 8.37-8.36 (d, J = 2.1 Hz, 1H), 8.05 (s, 1H), 7.89-7.84 (t, J = 7.7 Hz, 1H), 7.73-7.65 (q, J = 7.2 Hz, 2H), 7.55 (s, 1H), 7.47-7.43 (q, J = 3.7 Hz, 1H), 4.02 (s, 3H), 3.92 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 148.0, 146.2, 145.1, 139.7, 137.2, 136.1, 134.3, 130.1, 125.8, 124.9, 124.7, 124.3, 124.2, 124.0, 120.6, 116.9, 115.4, 114.1, 104.2, 102.2, 99.2, 57.4, 56.3. ESI-MS $[M+H]^+$ m/z 402.05.



3m

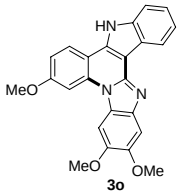
8-Methoxy-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3m). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 67 mg (79%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 13.27 (s, 1H), 8.60-8.57 (d, J = 7.9 Hz,

1H), 8.39-8.32 (q, *J* = 7.2 Hz, 2H), 7.84-7.81 (d, *J* = 8.6 Hz, 2H), 7.55-7.36 (m, 4H), 7.30-7.25 (t, *J* = 7.4 Hz, 1H), 7.15-7.12 (d, *J* = 8.9 Hz, 1H), 3.93 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 142.0, 139.2, 138.8, 134.1, 128.9, 126.2, 126.1, 125.7, 124.3, 122.1, 121.6, 121.5, 115.4, 114.4, 112.7, 108.6, 101.1, 98.3, 56.5. ESI-MS $[M+H]^+$ m/z 338.15.



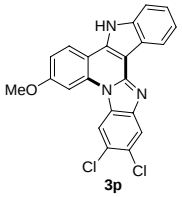
3n

8-Methoxy-12,13-dimethyl-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3n). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 74 mg (81%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.42 (s, 1H), 8.37-8.34 (t, *J* = 4.5 Hz, 2H), 7.97-7.92 (d, *J* = 13.4 Hz, 2H), 7.63-7.61 (d, *J* = 7.9 Hz, 1H), 7.56 (s, 1H), 7.40-7.28 (m, 2H), 7.20-7.17 (d, *J* = 8.6 Hz, 1H), 3.94 (s, 3H), 2.36 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.4, 144.3, 138.5, 132.5, 130.4, 129.4, 129.2, 125.3, 124.4, 123.6, 121.5, 121.3, 119.5, 114.3, 112.2, 111.5, 109.3, 102.8, 101.5, 56.2, 20.9, 20.5. ESI-MS $[M+H]^+$ m/z 366.15.



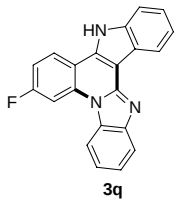
3o

8,12,13-Trimethoxy-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3o). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 66 mg (66%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.45 (s, 1H), 8.42-8.39 (d, *J* = 8.9 Hz, 1H), 8.36-8,33 (d, *J* = 7.5 Hz, 1H), 8.02 (s, 1H), 7.86 (s, 1H), 7.64-7.61 (d, *J* = 7.9 Hz, 1H), 7.46 (s, 1H), 7.38-7.25 (m, 3H), 4.03 (s, 1H), 3.96 (s, 1H), 3.89 (s, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 147.8, 146.0, 145.6, 139.8, 138.5, 135,4, 125.3, 124.4, 124.0, 121.3, 121.2, 112.2, 112.1, 109.2, 103.0, 102.1, 100.8, 98.8, 56.9, 56.3, 56.1. ESI-MS $[M+H]^+$ m/z 398.15.



3p

12,13-Dichloro-8-methoxy-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3p). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 92 mg (90%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.46-12.35 (d, J = 33.0 Hz, 1H), 8.30-8.08 (m, 3H), 7.80-7.77 (d, J = 9.6 Hz, 1H), 7.60-7.54 (t, J = 8.8 Hz, 1H), 7.44-7.22 (m, 3H), 7.14-7.01 (m, 1H), 3.93-3.83 (ss, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 148.6, 147.9, 146.3, 145.3, 138.6, 136.9, 135.2, 134.8, 130.1, 129.6, 128.6, 126.6, 125.5, 125.4, 124.7, 123.3, 121.5, 121.4, 119.4, 118.1, 115.4, 115.2, 112.6, 112.3, 109.1, 102.0, 101.5, 101.2, 79.9, 79.5, 79.0, 56.3, 56.2. ESI-MS $[M+H]^+$m/z 406.05.

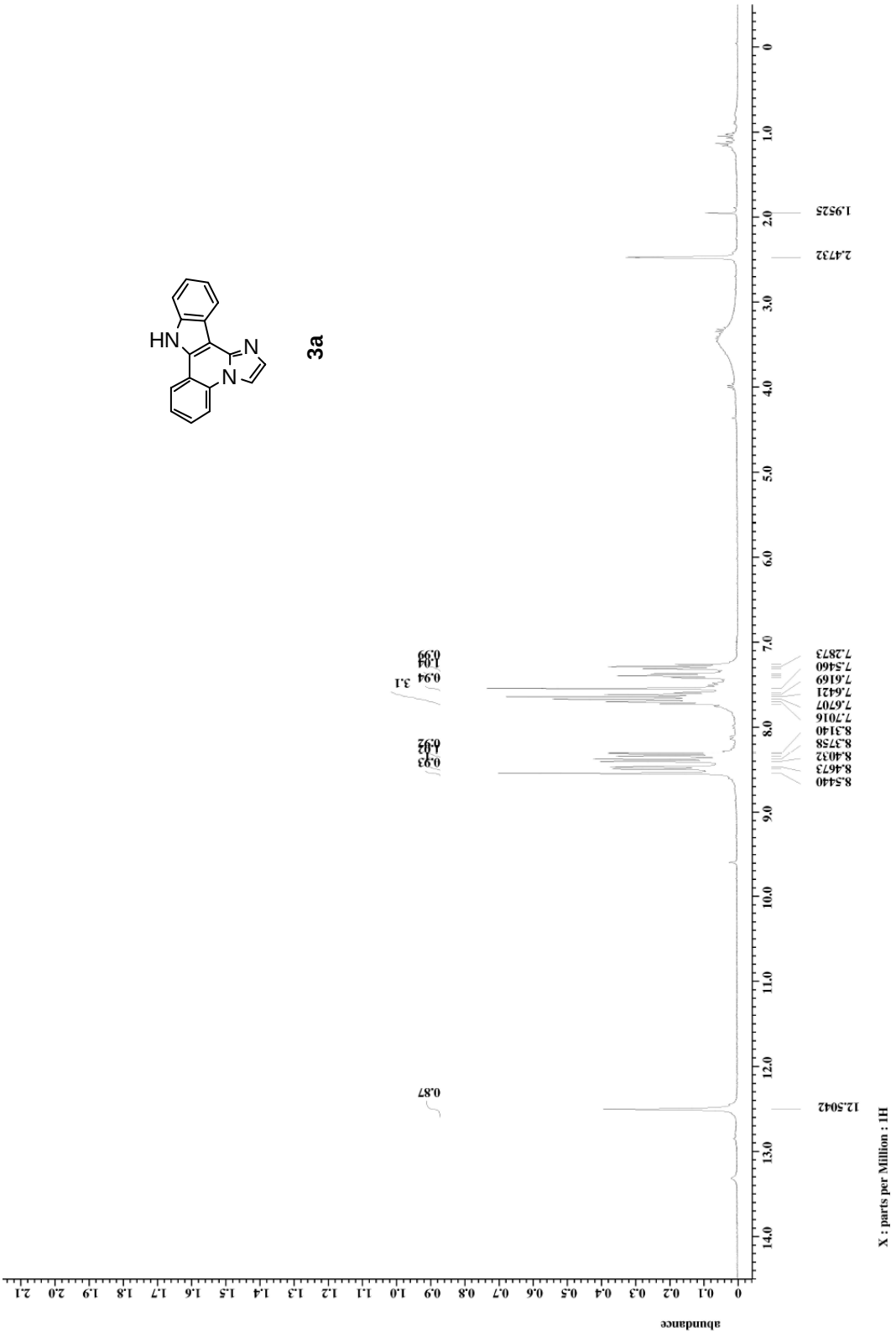


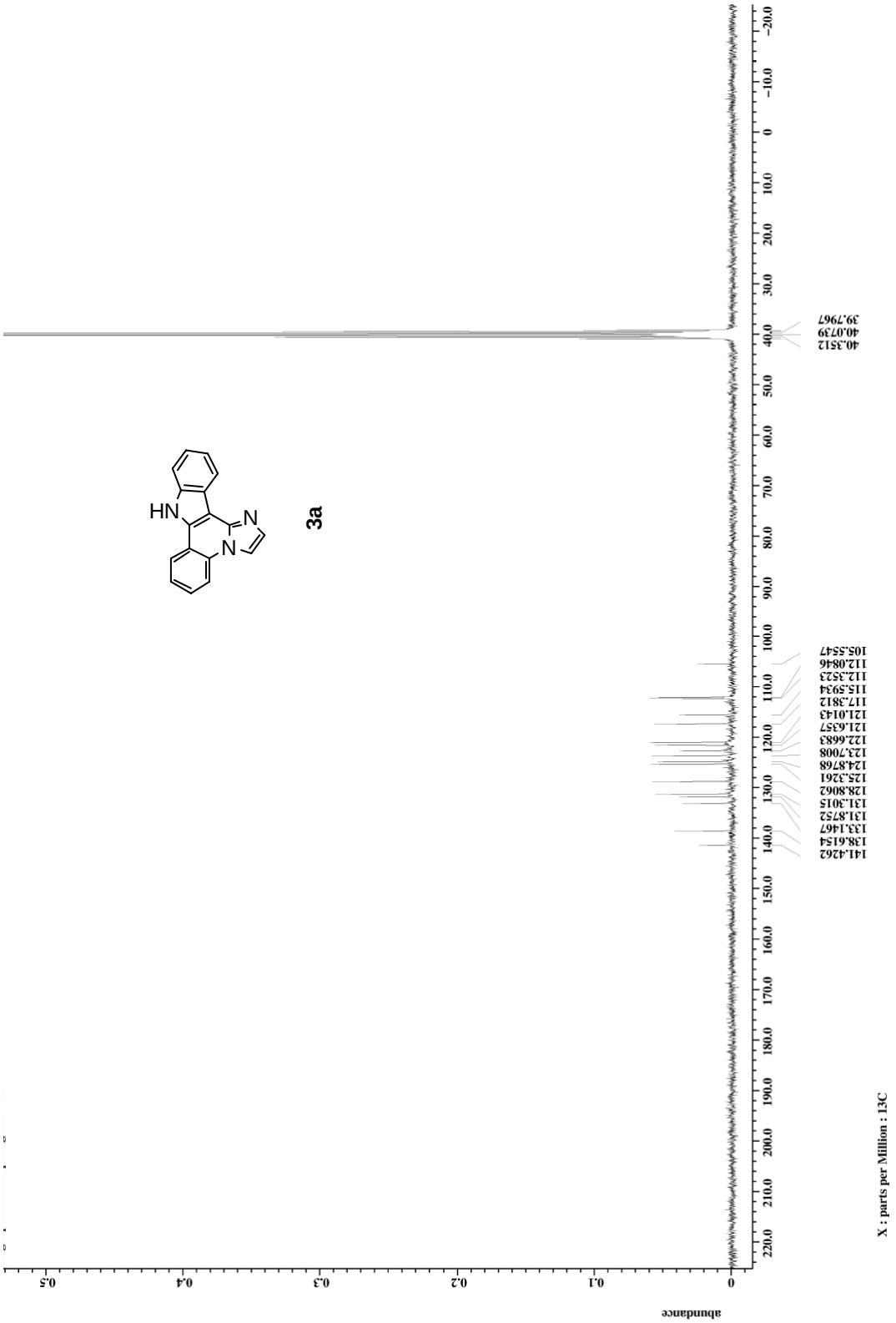
3q

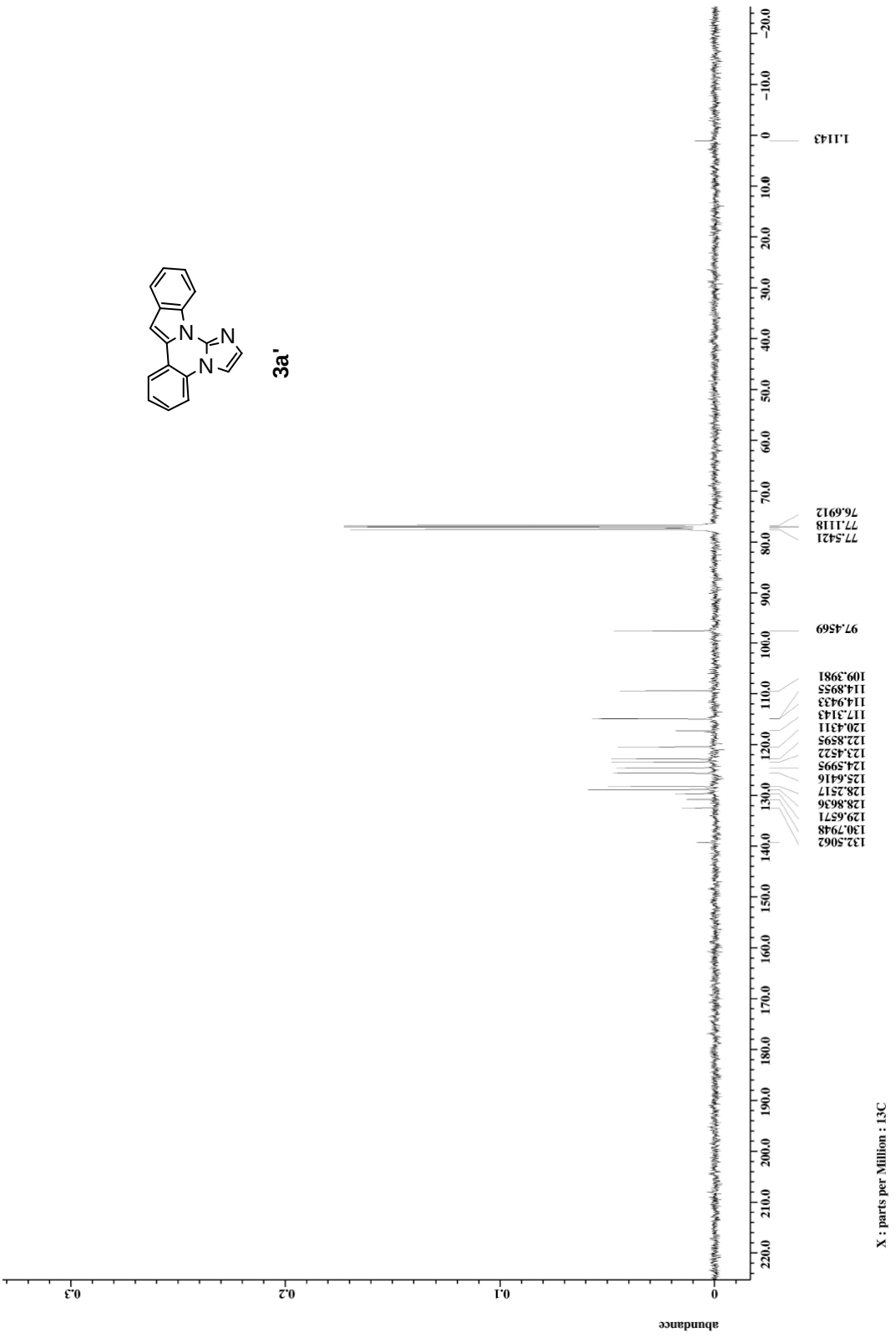
8-Fluoro-5*H*-benzo[4,5]imidazo[1,2-*a*]indolo[3,2-*c*]quinoline (3q). Eluent: petroleum ether/ethyl acetate (3:1 to 1:1). Yield 37 mg (45%). Pale yellow solid, mp 300-302 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.68 (s, 1H), 8.61-8.53 (q, J = 7.4 Hz, 3H), 8.43-8.41 (d, J = 7.5 Hz, 1H), 7.91-7.89 (d, J = 7.9 Hz, 1H), 7.68-7.65 (d, J = 8.2 Hz, 1H), 7.56-7.53 (t, J = 8.6 Hz, 1H), 7.50-7.32 (m, 4H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 146.8, 145.7, 138.7, 135.5, 135.3, 135.2, 132.0, 131.0, 129.2, 126.2, 126.0, 125.1,124.5, 123.4, 122.3, 121.7, 121.6, 119.4, 114.5, 112.9, 112.7, 112.5, 104.3, 103.9, 103.8. ESI-MS $[M+H]^+$m/z 326.10.

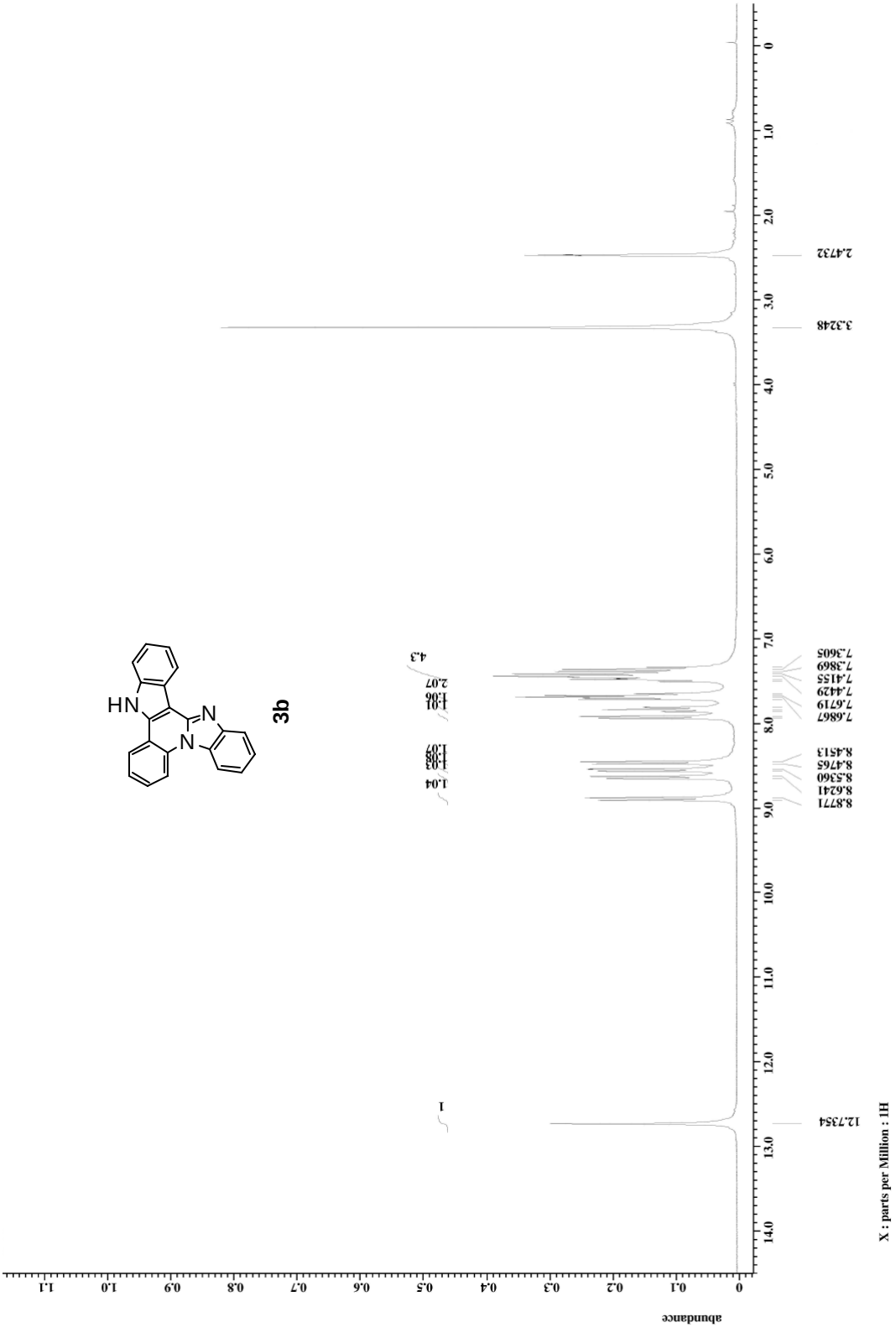
Reference

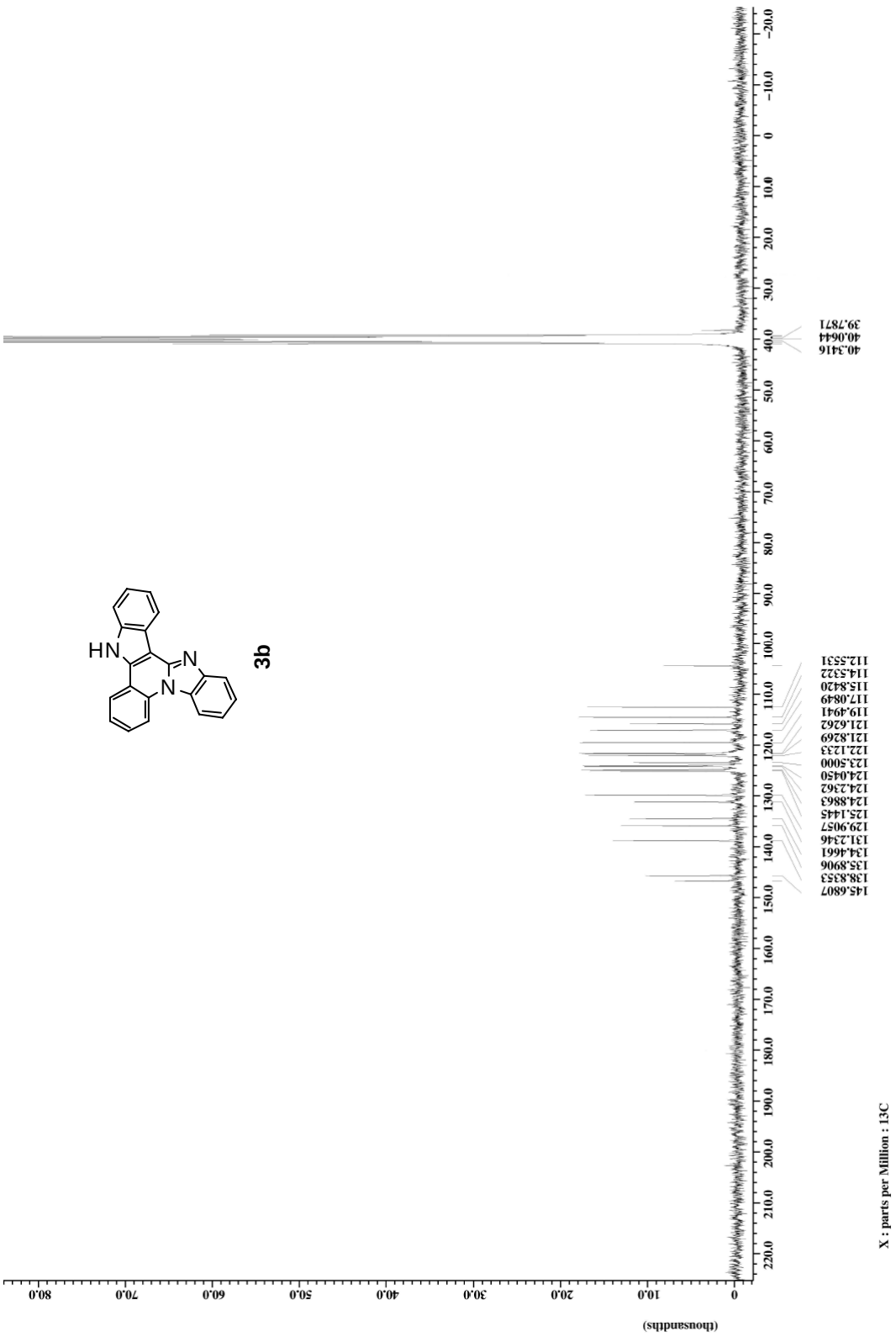
1 Y. Liu, W. W. McWhorter. Jr., *J. Am. Chem. Soc.*, 2003, **125**, 4240.

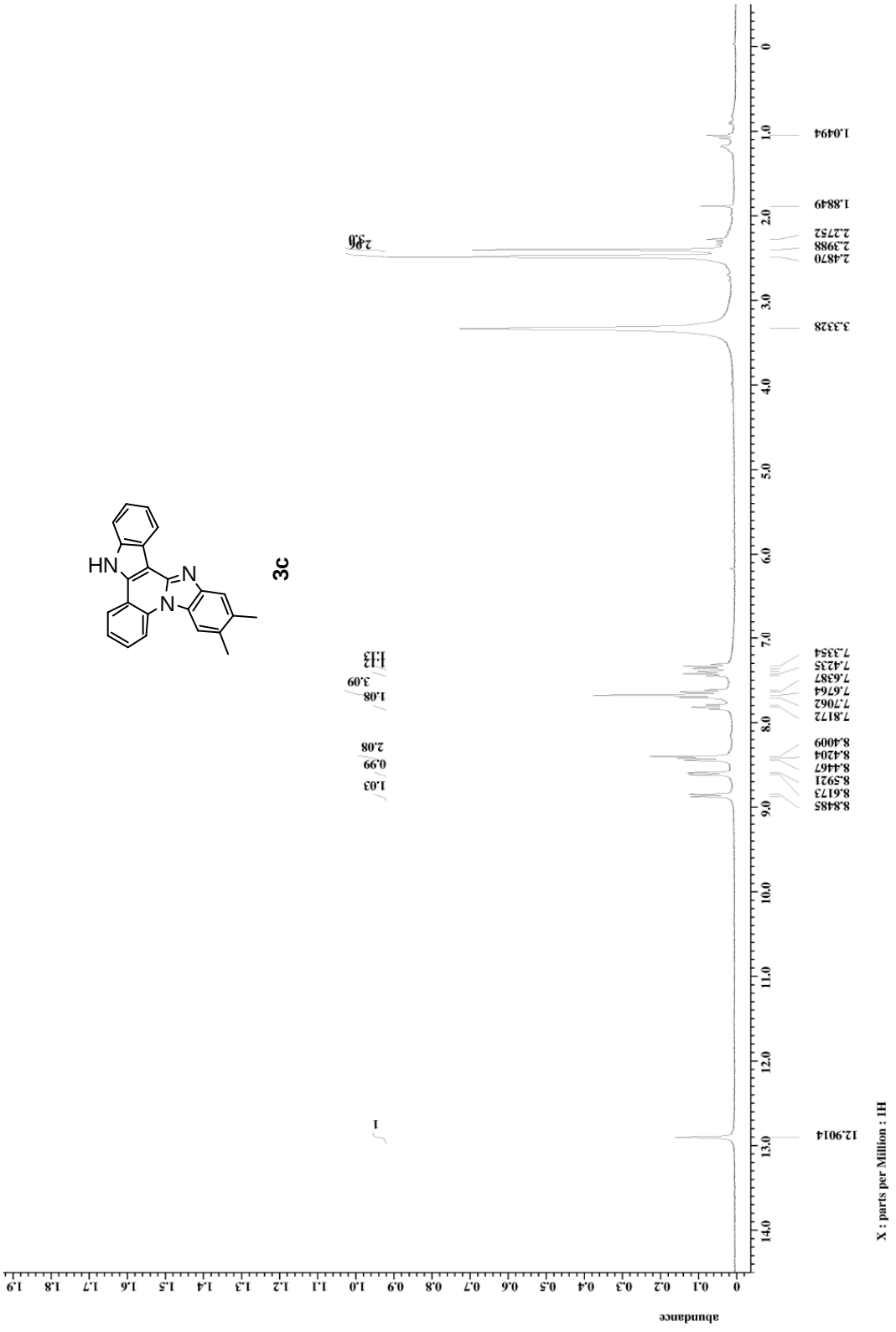


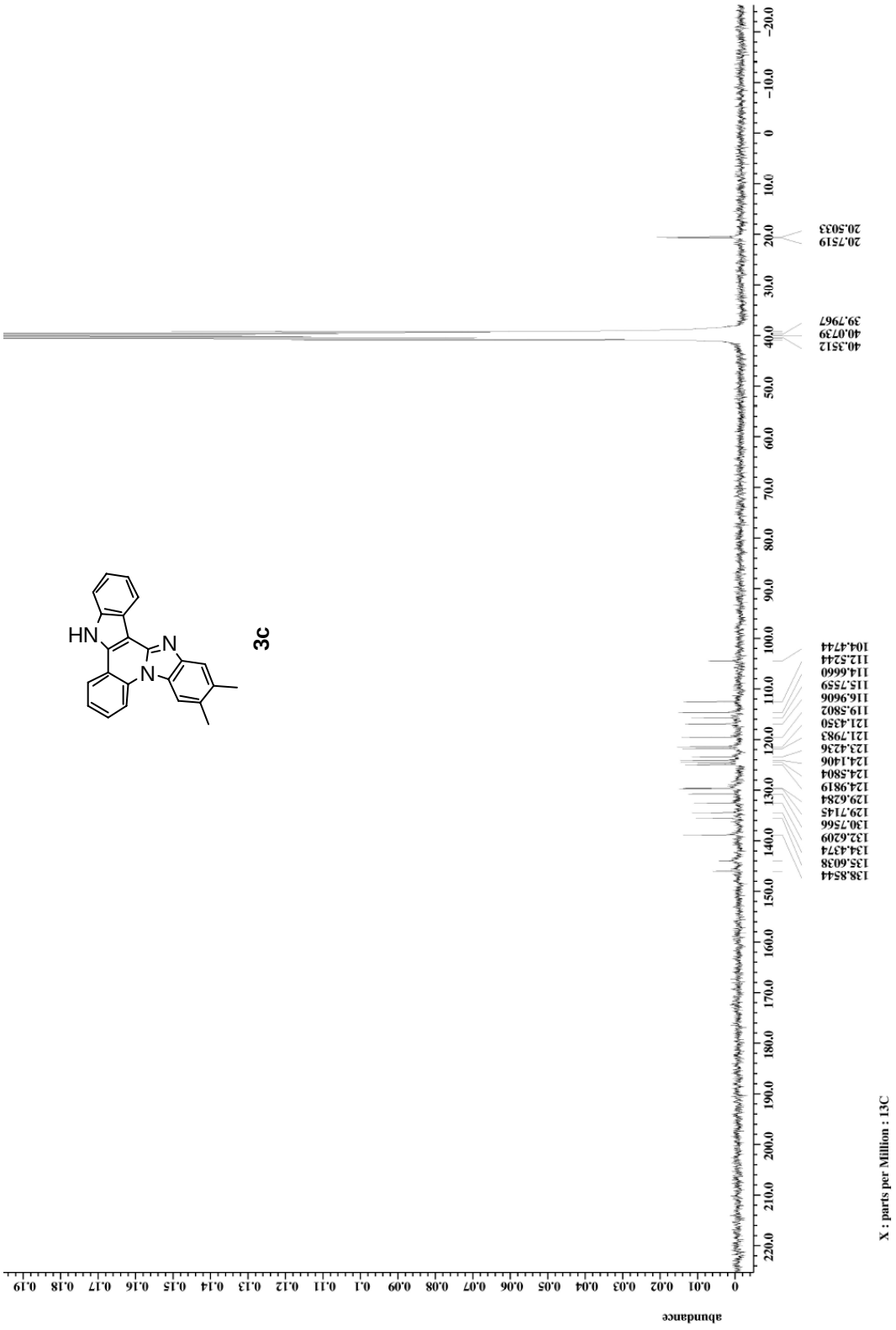


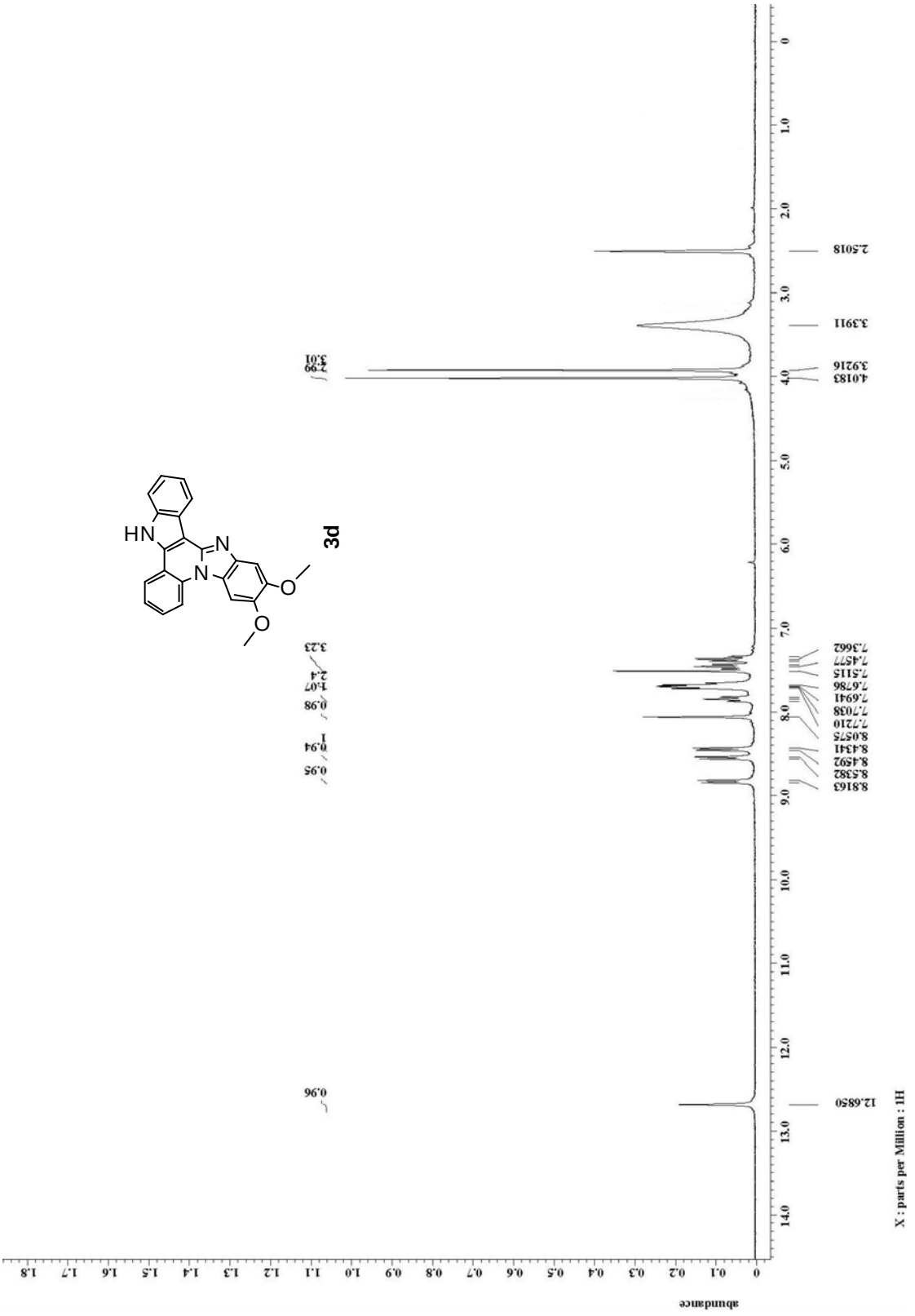


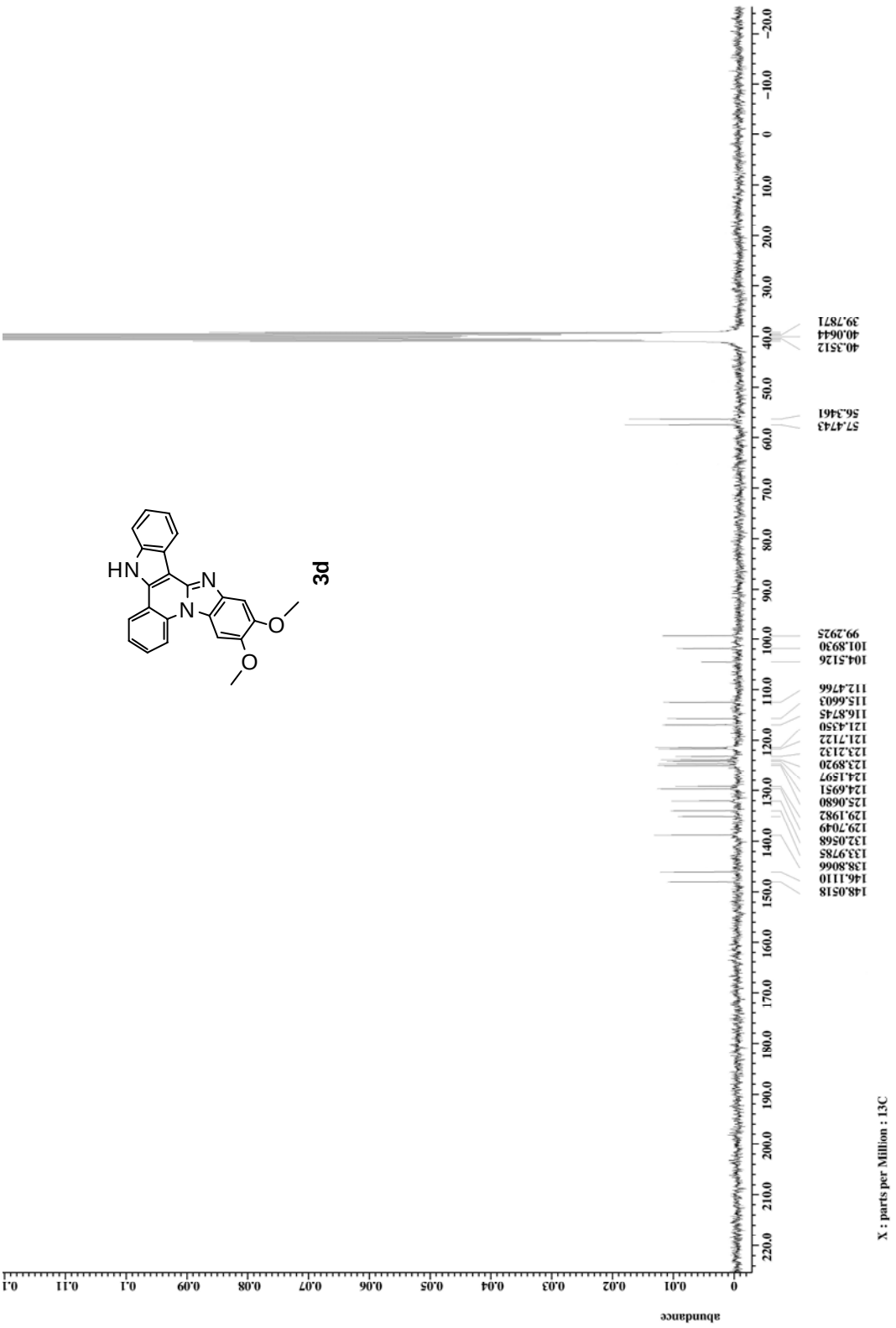








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abundance
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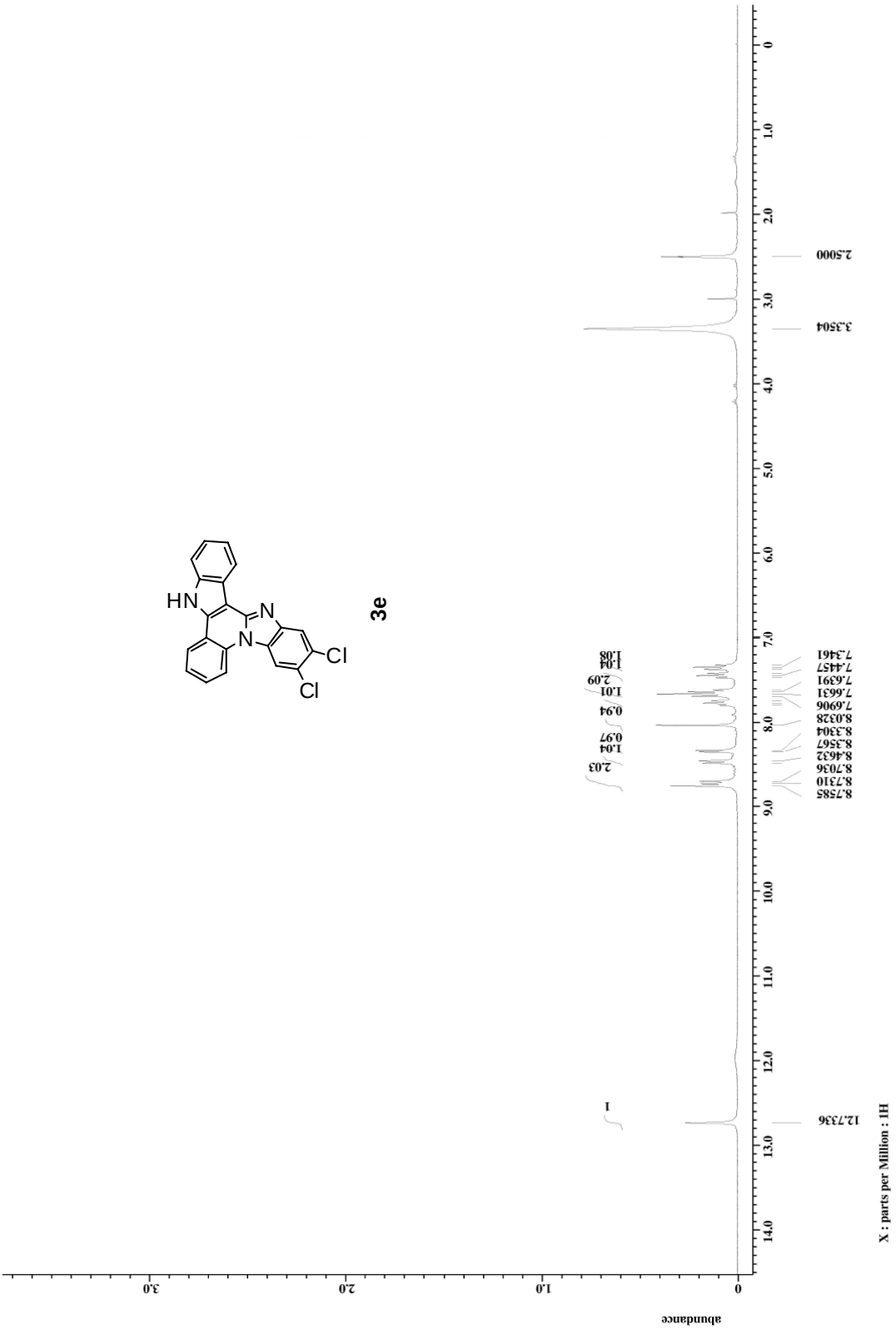

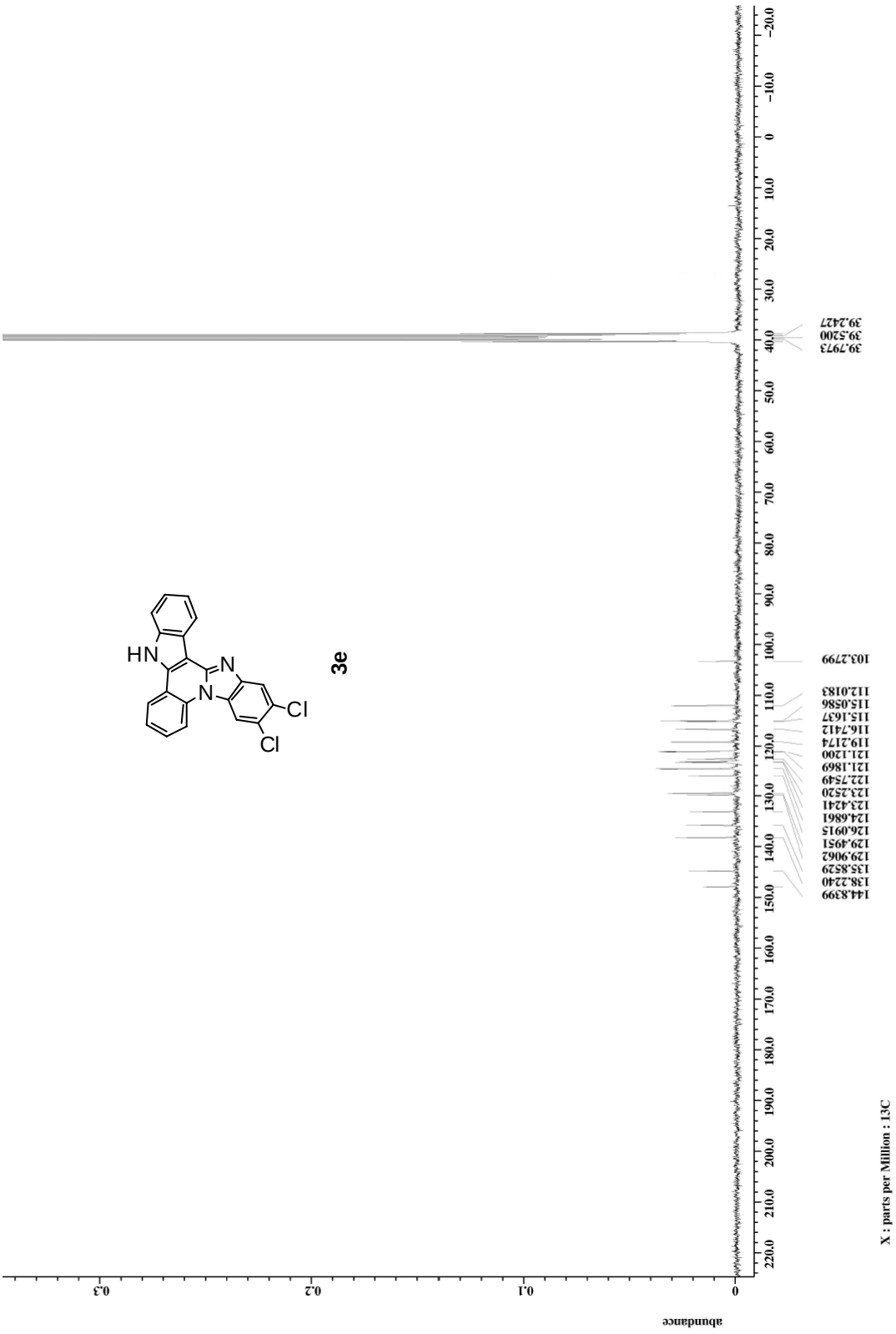
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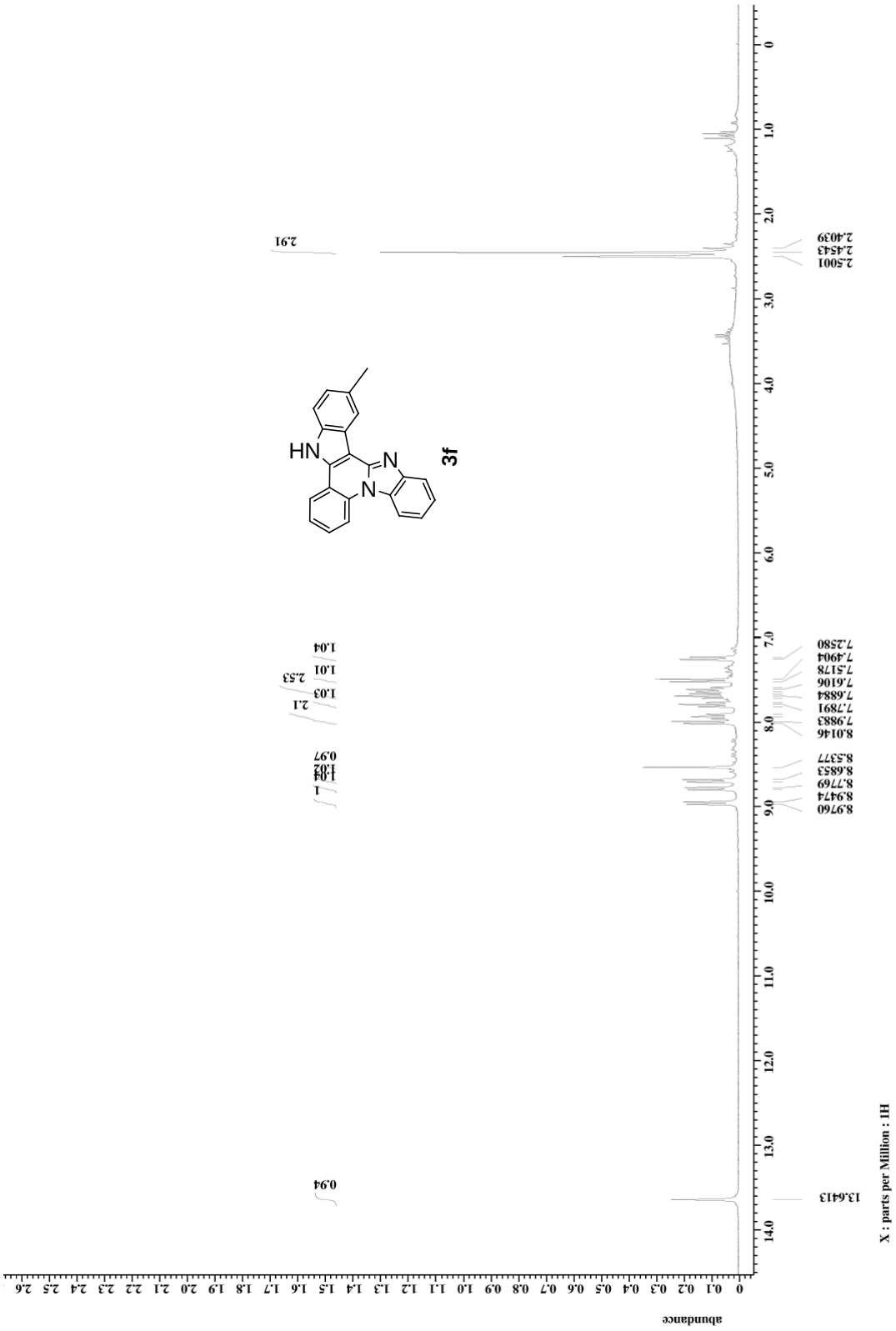
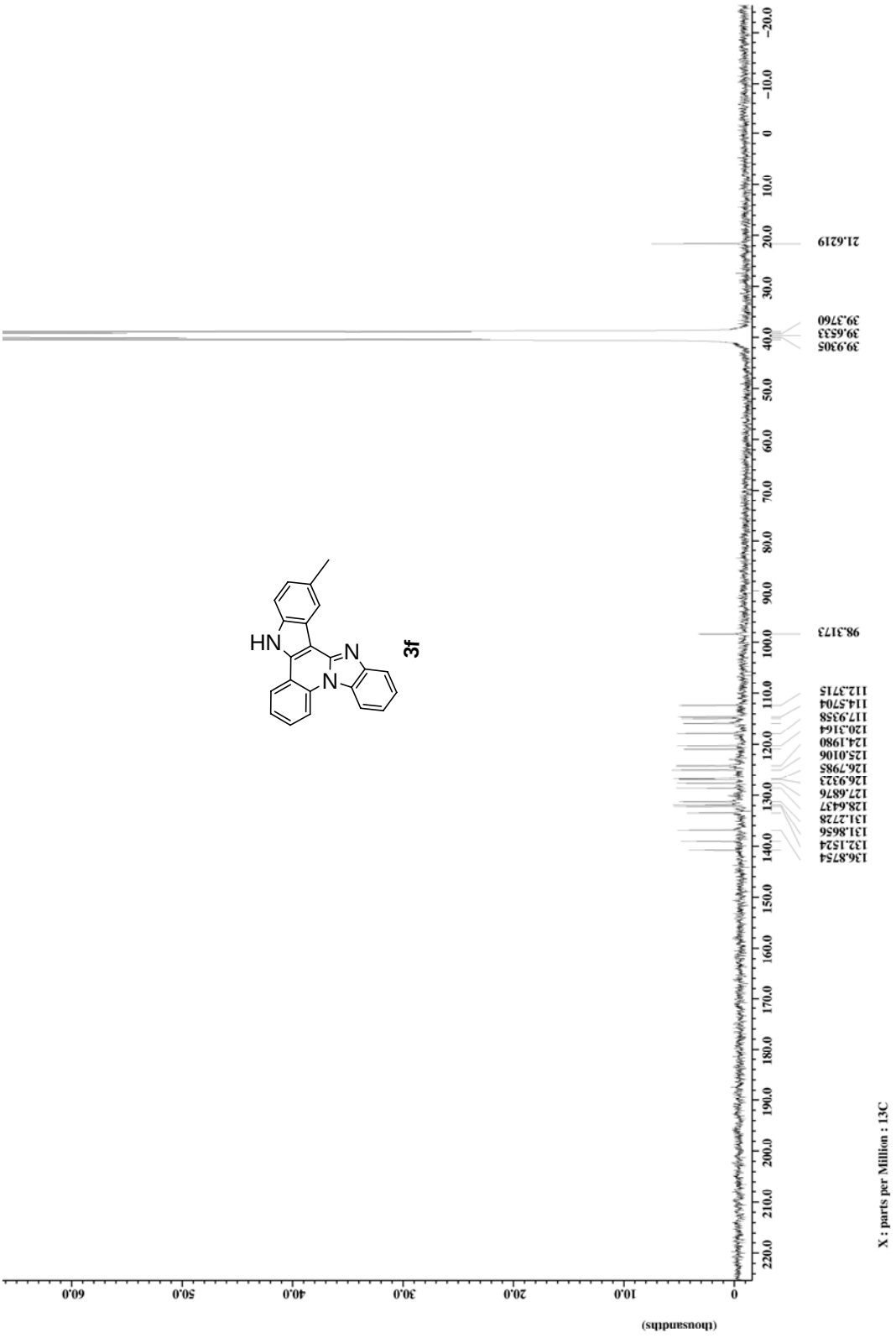
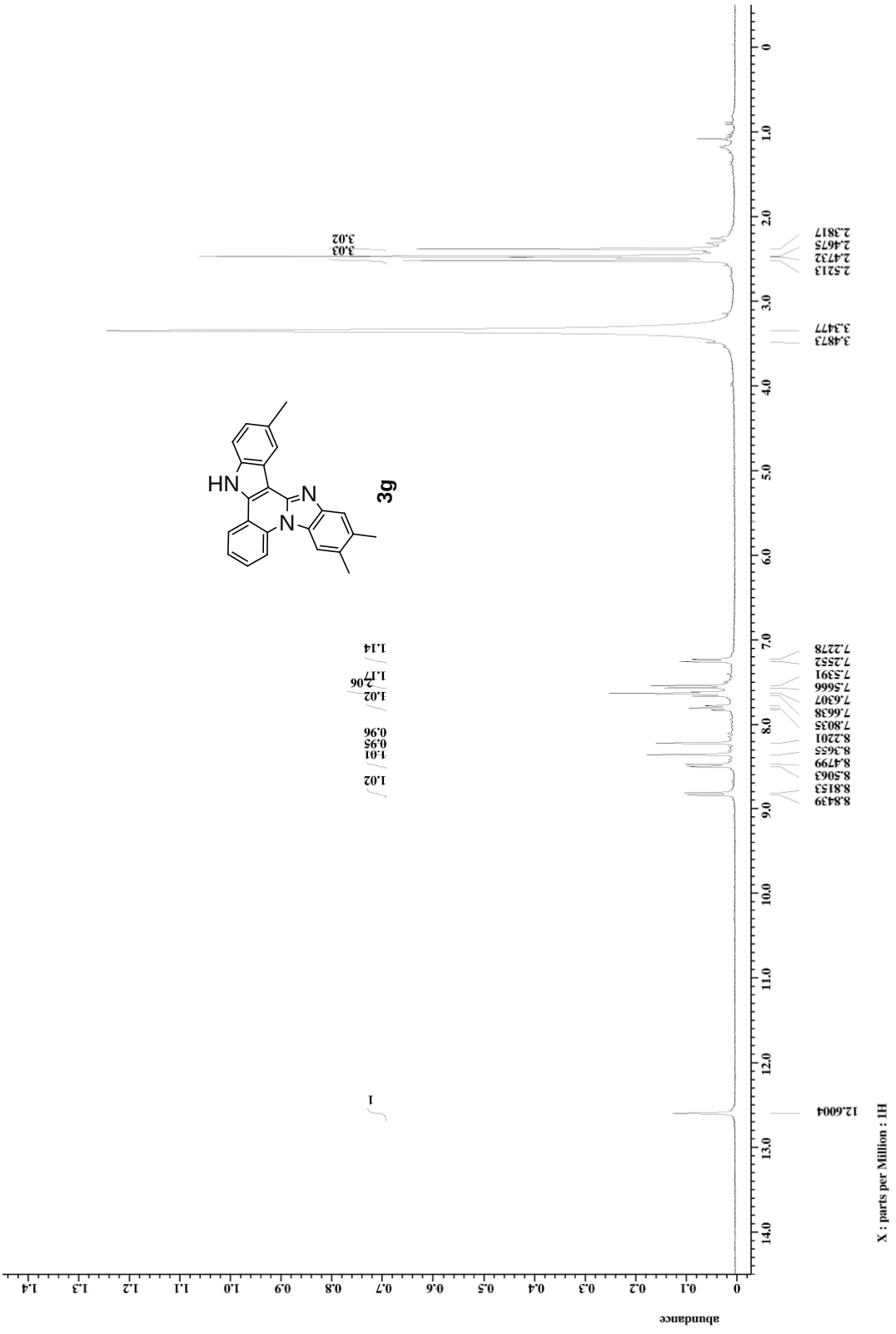
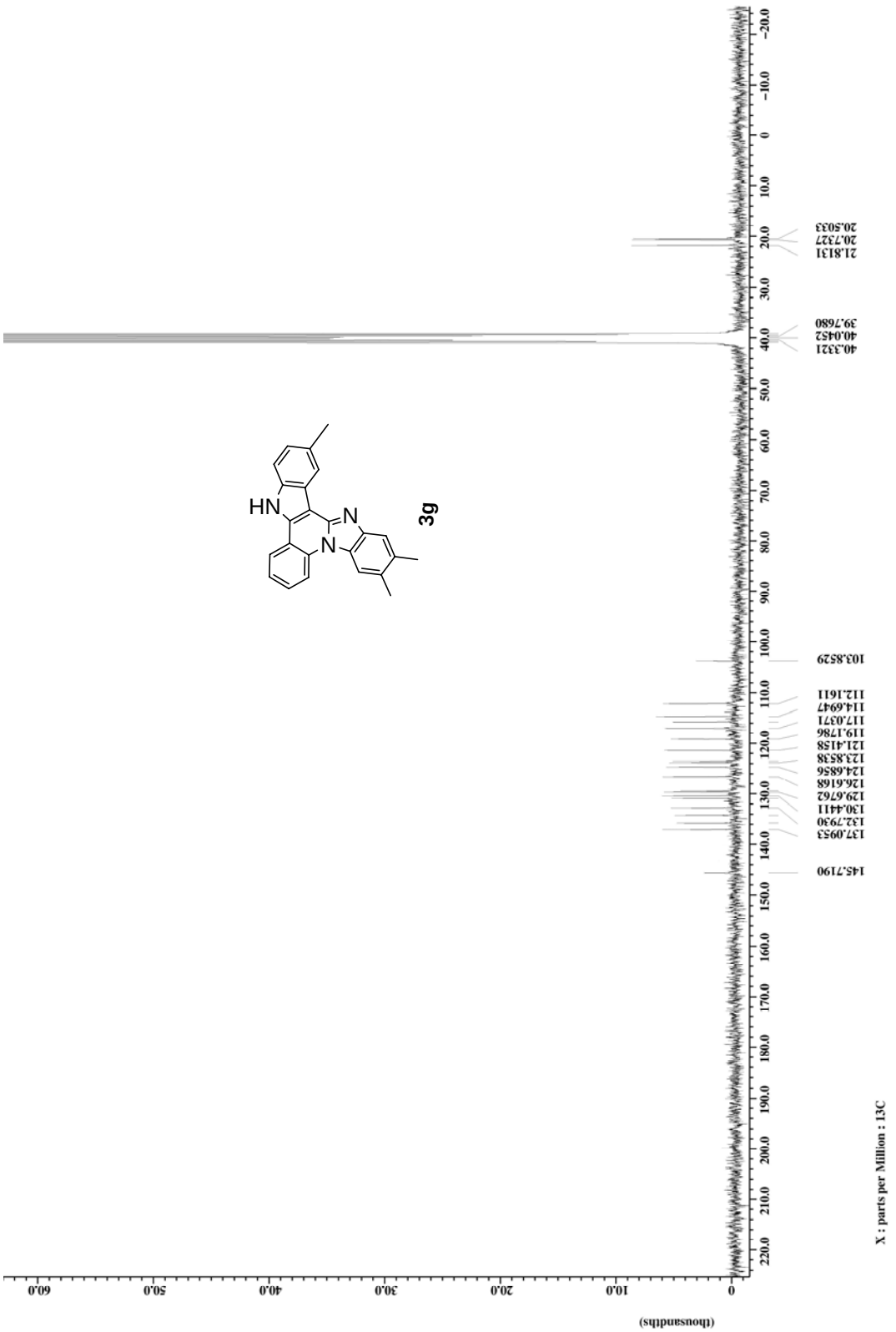
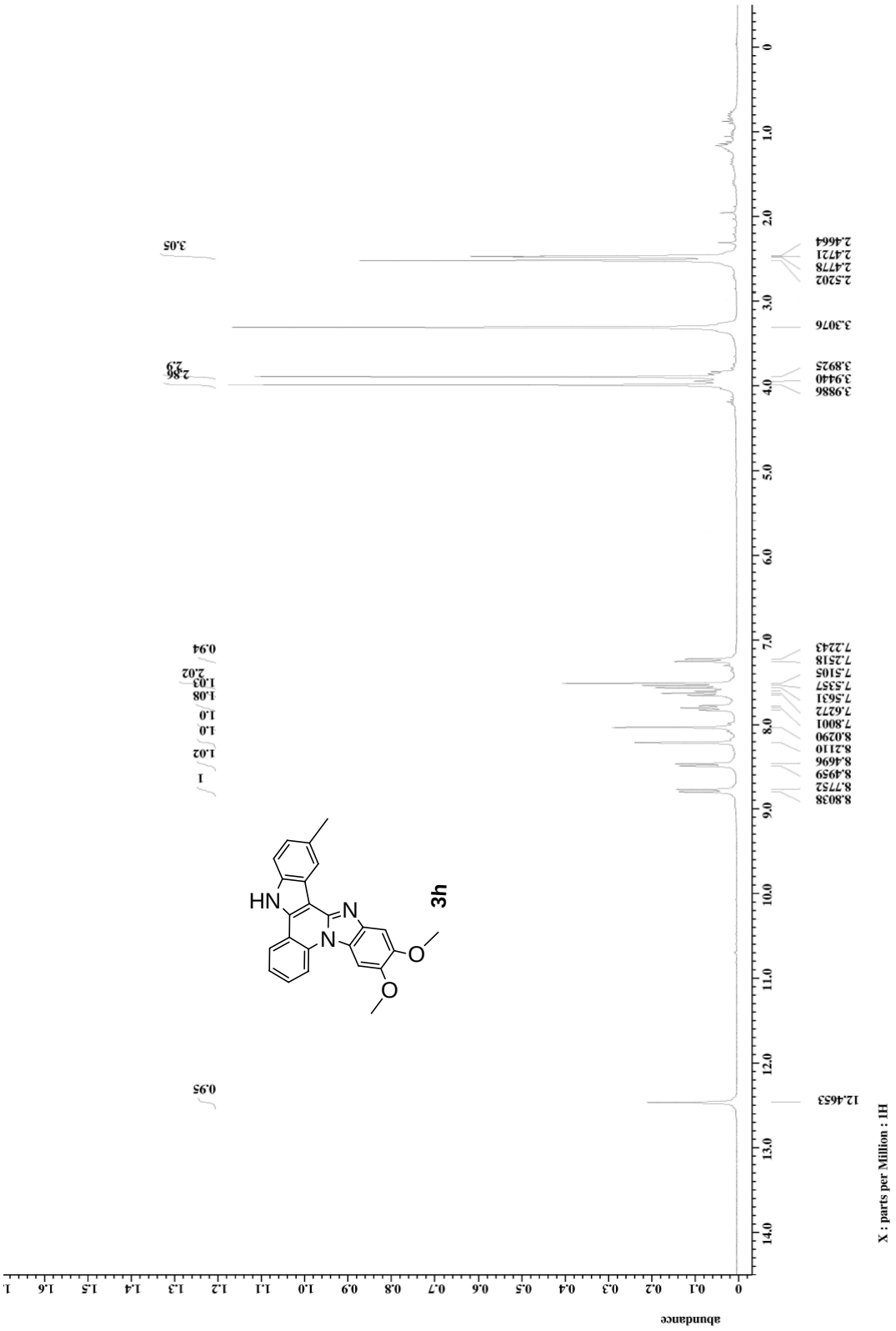
X : parts per Million : 13C
abundance







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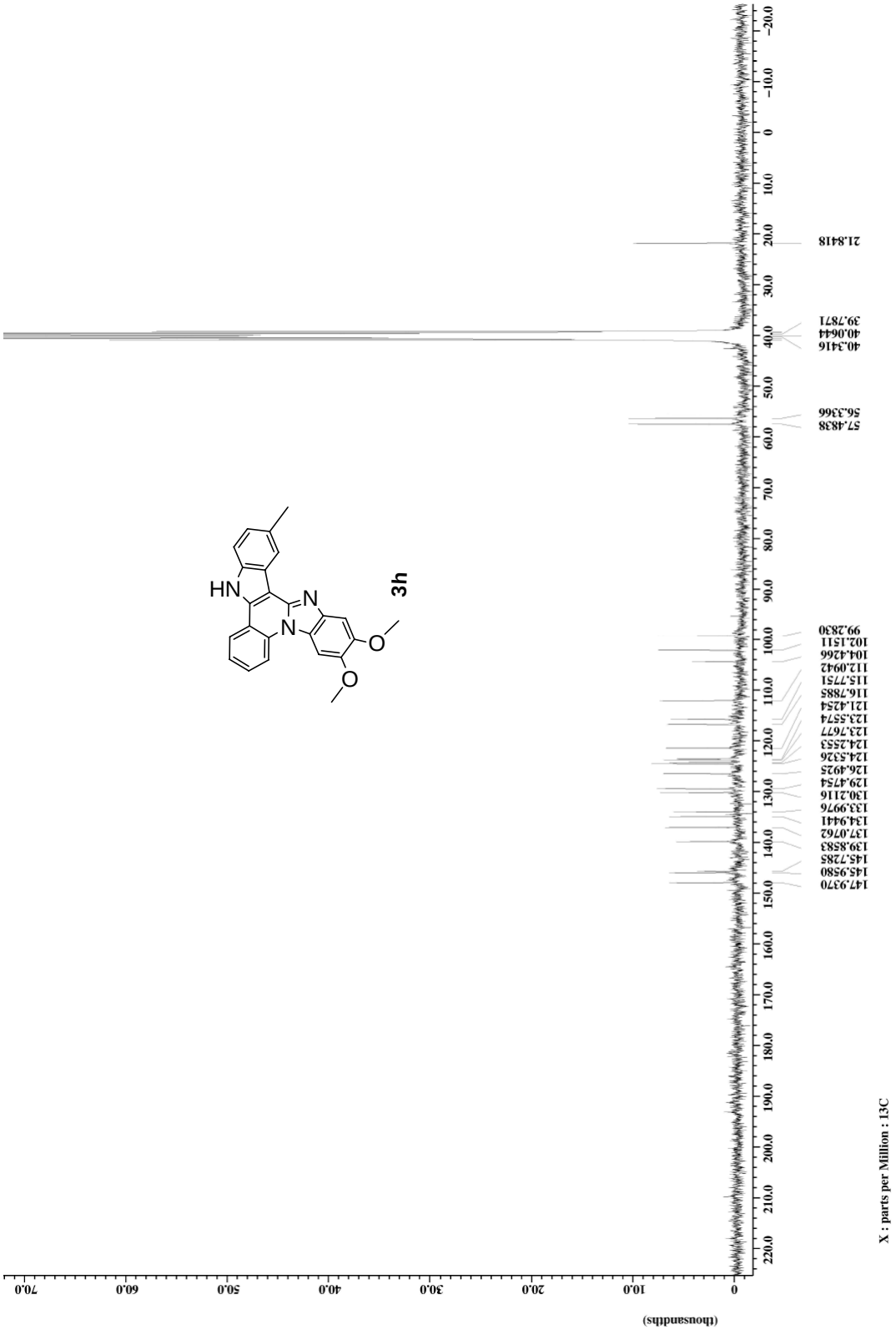
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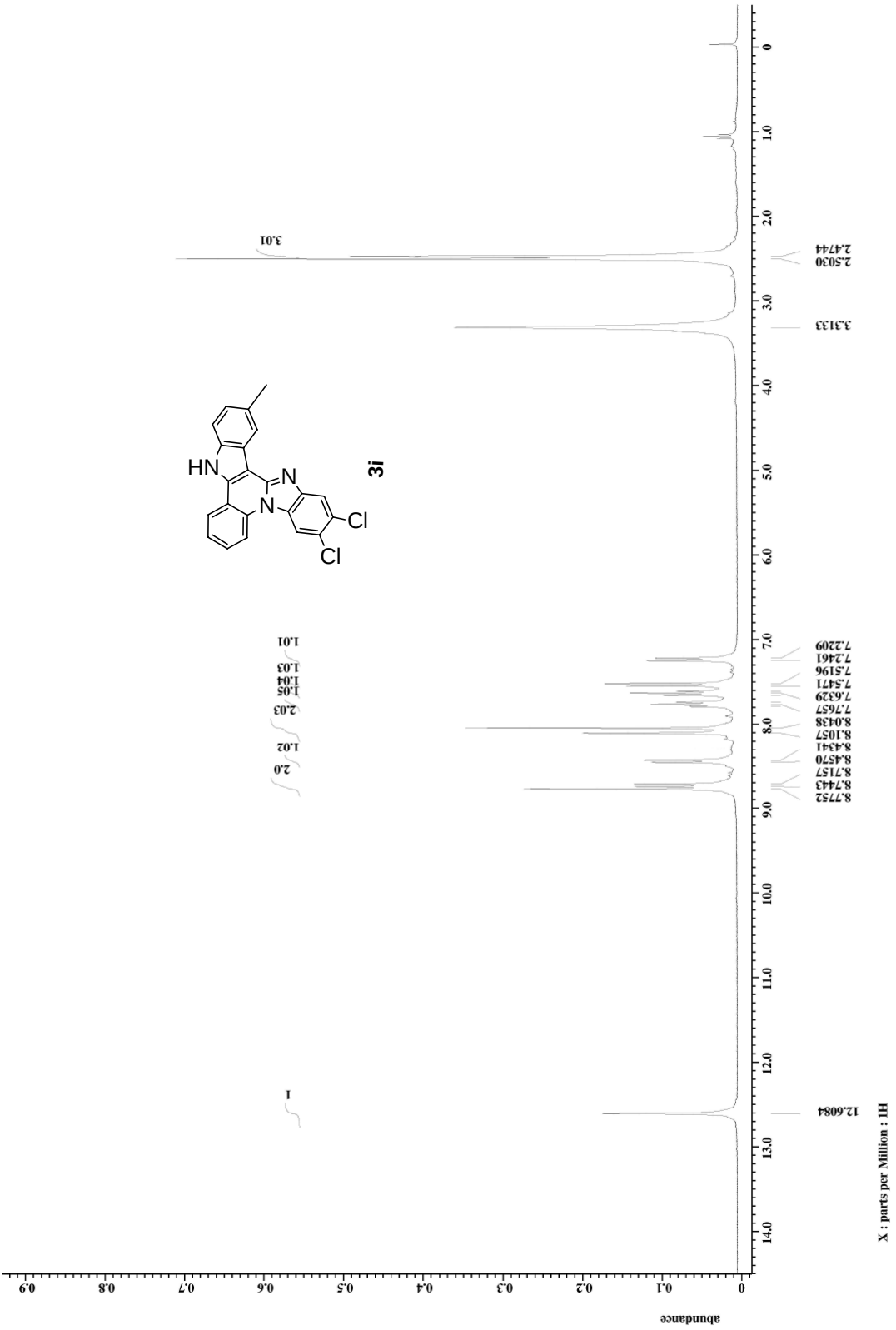
X : parts per Million : 13C
(thousandths)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Cl
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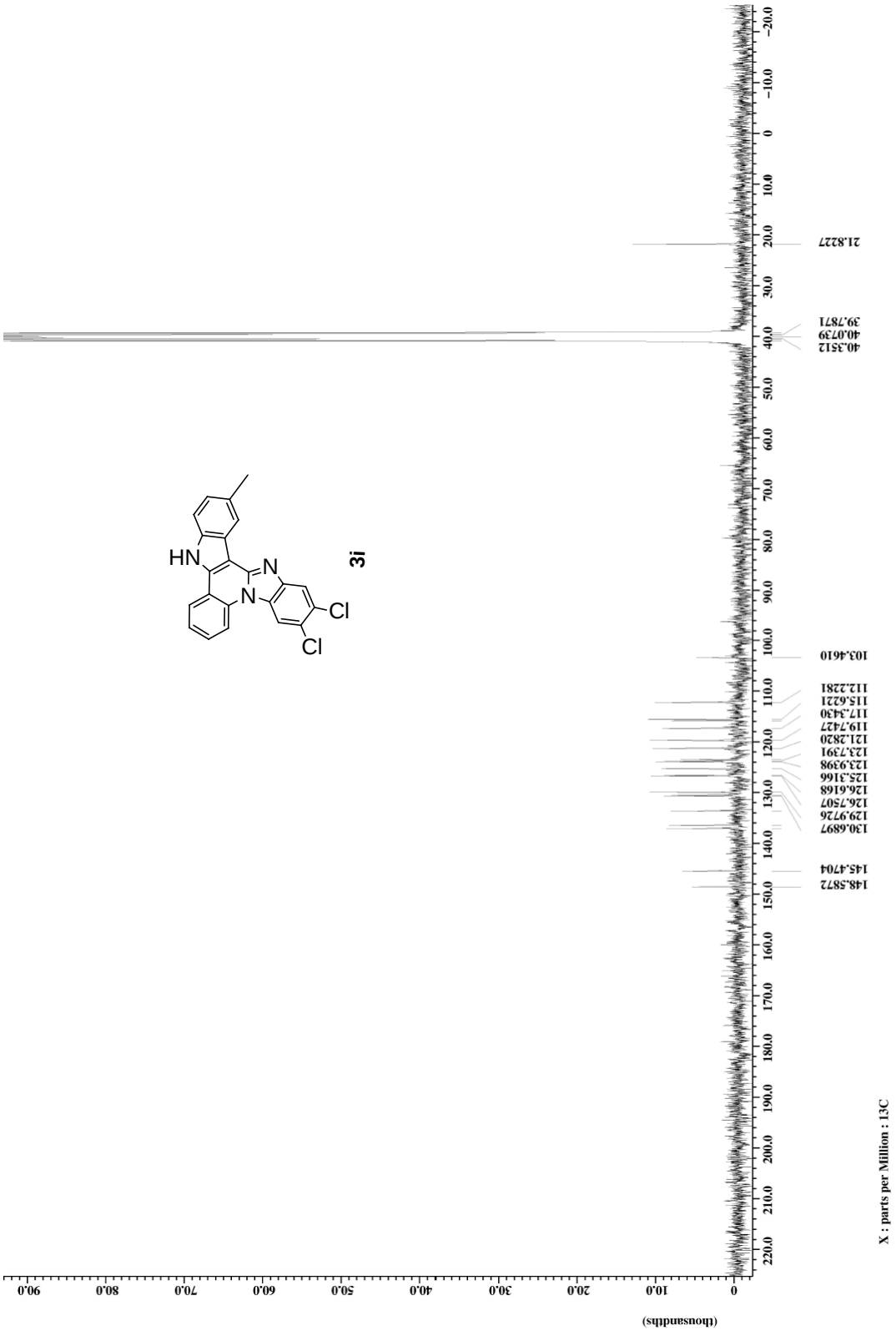
X : parts per Million : 1H
abundance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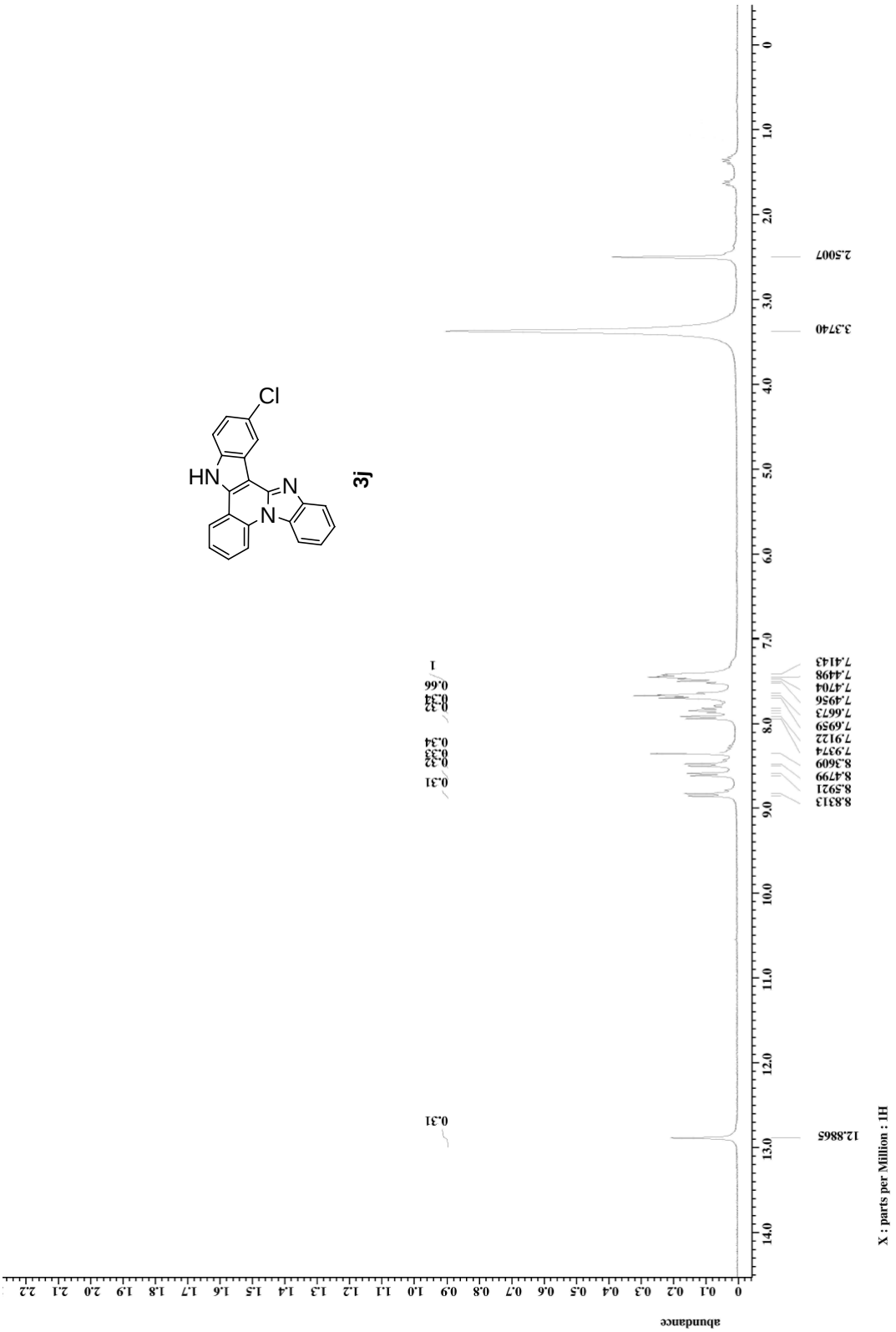
(thousandths)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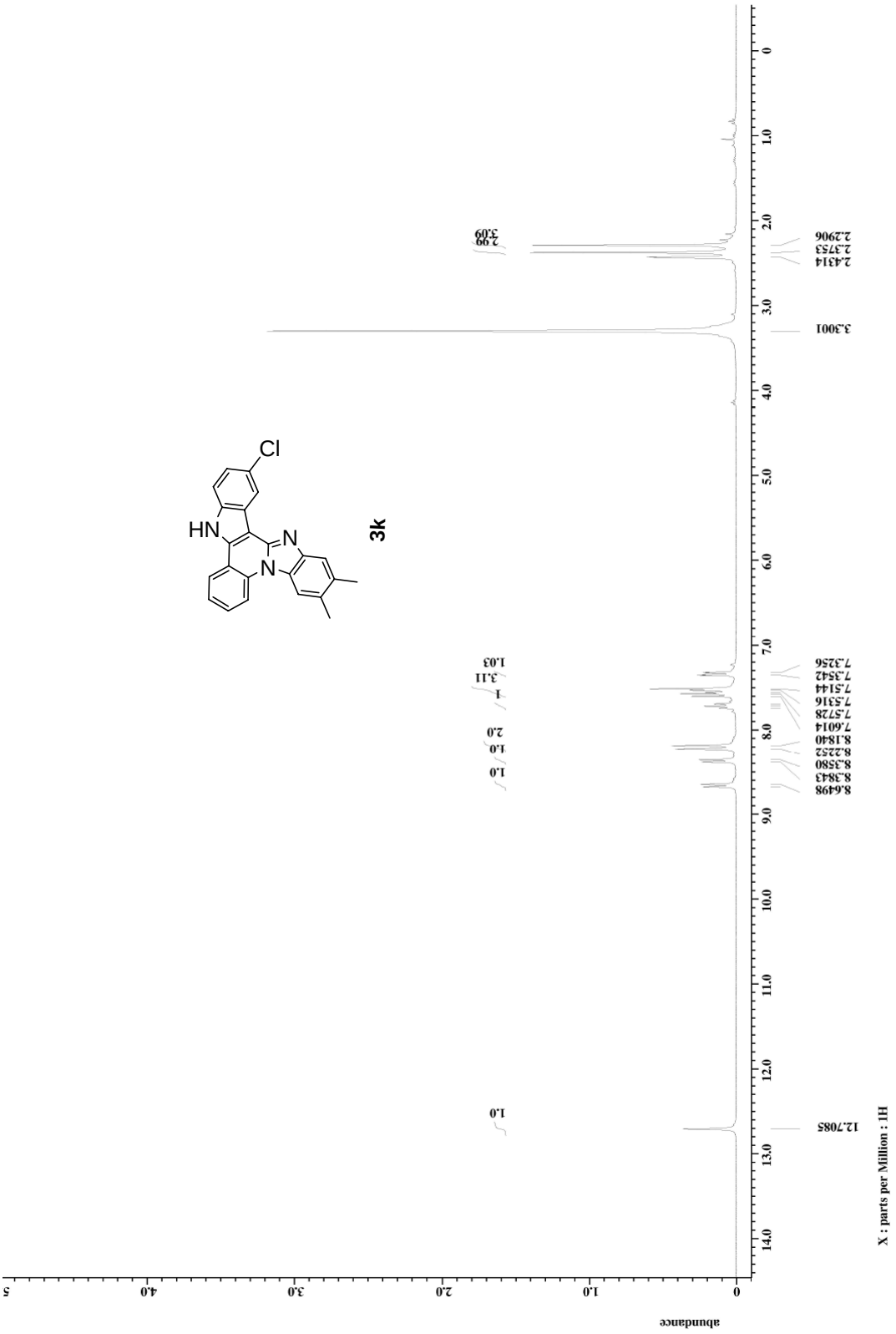
abundance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abundance
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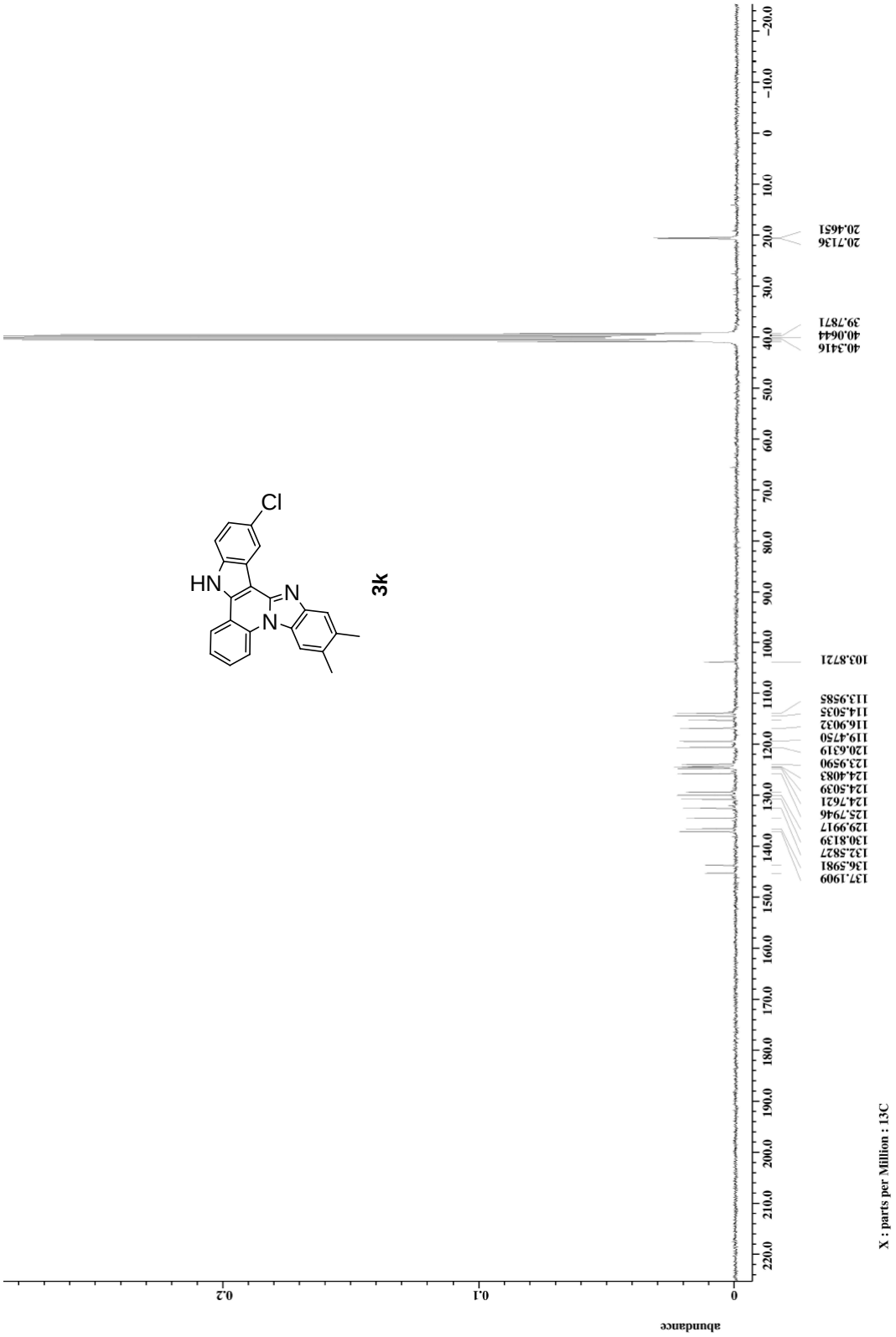

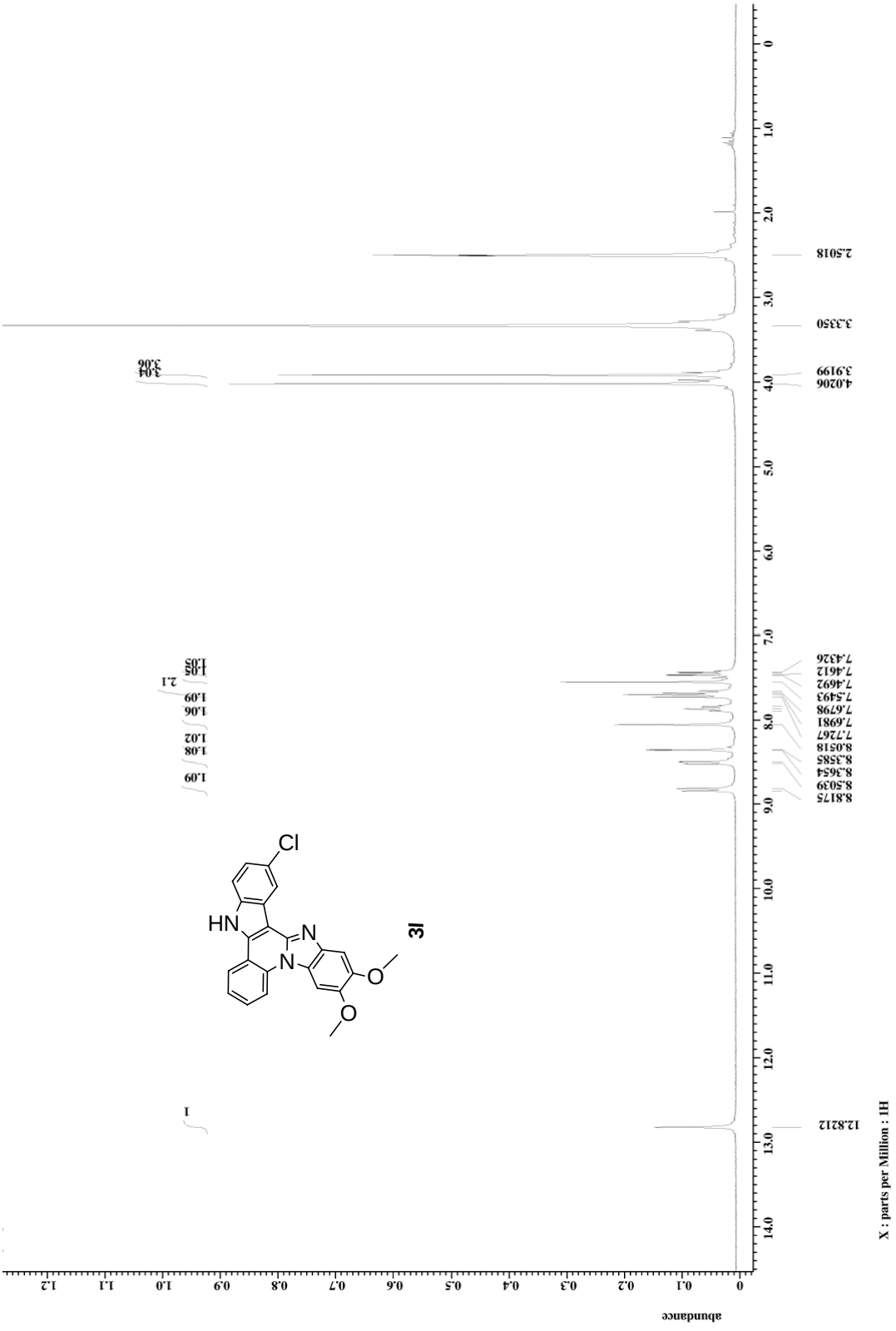

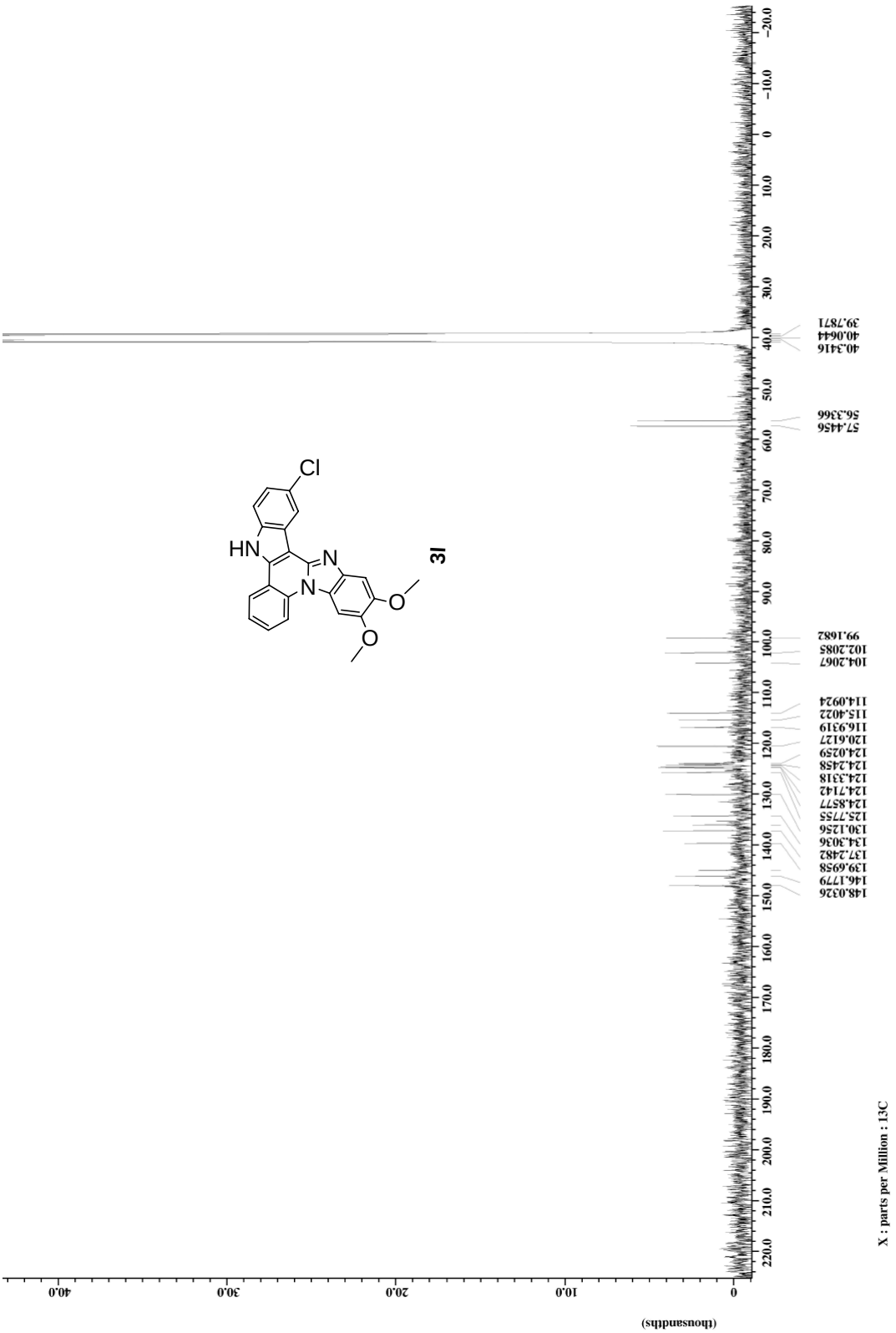
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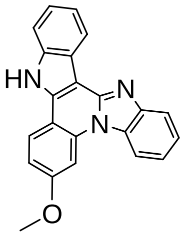
X : parts per Million : 13C
(thousandths)



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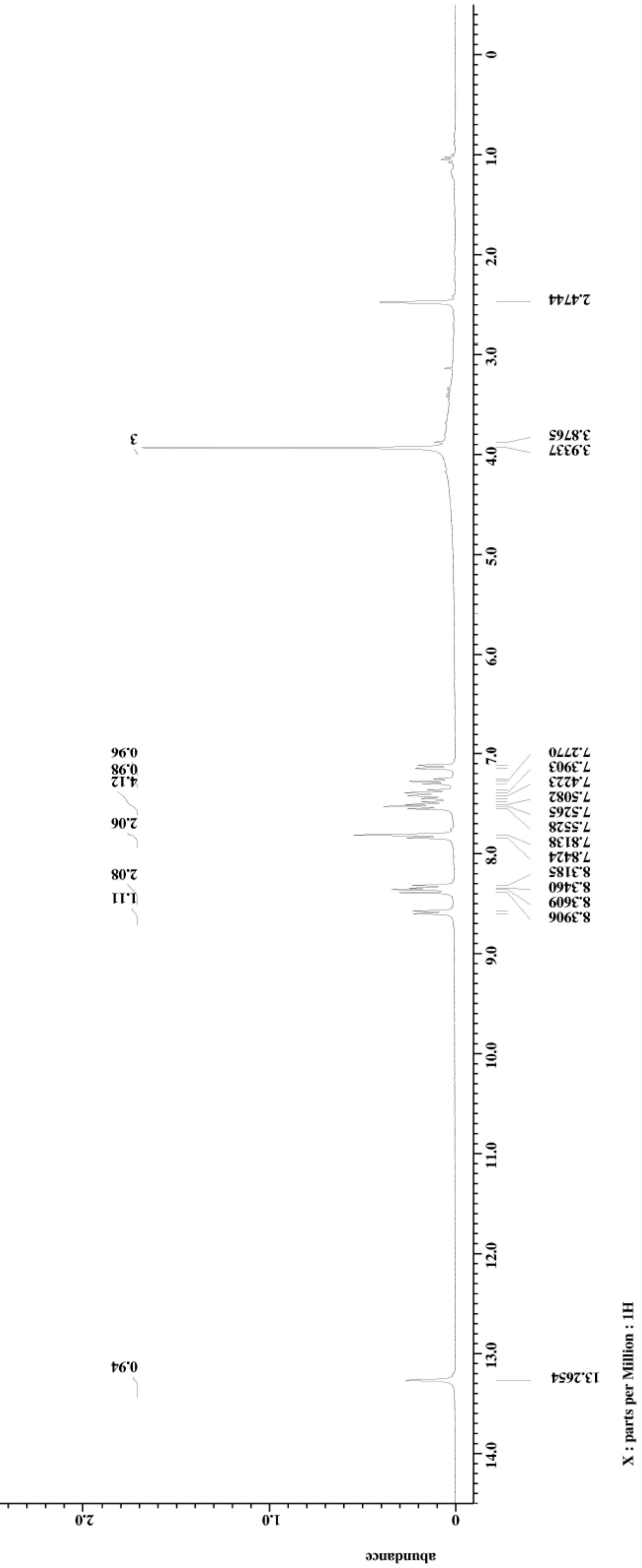

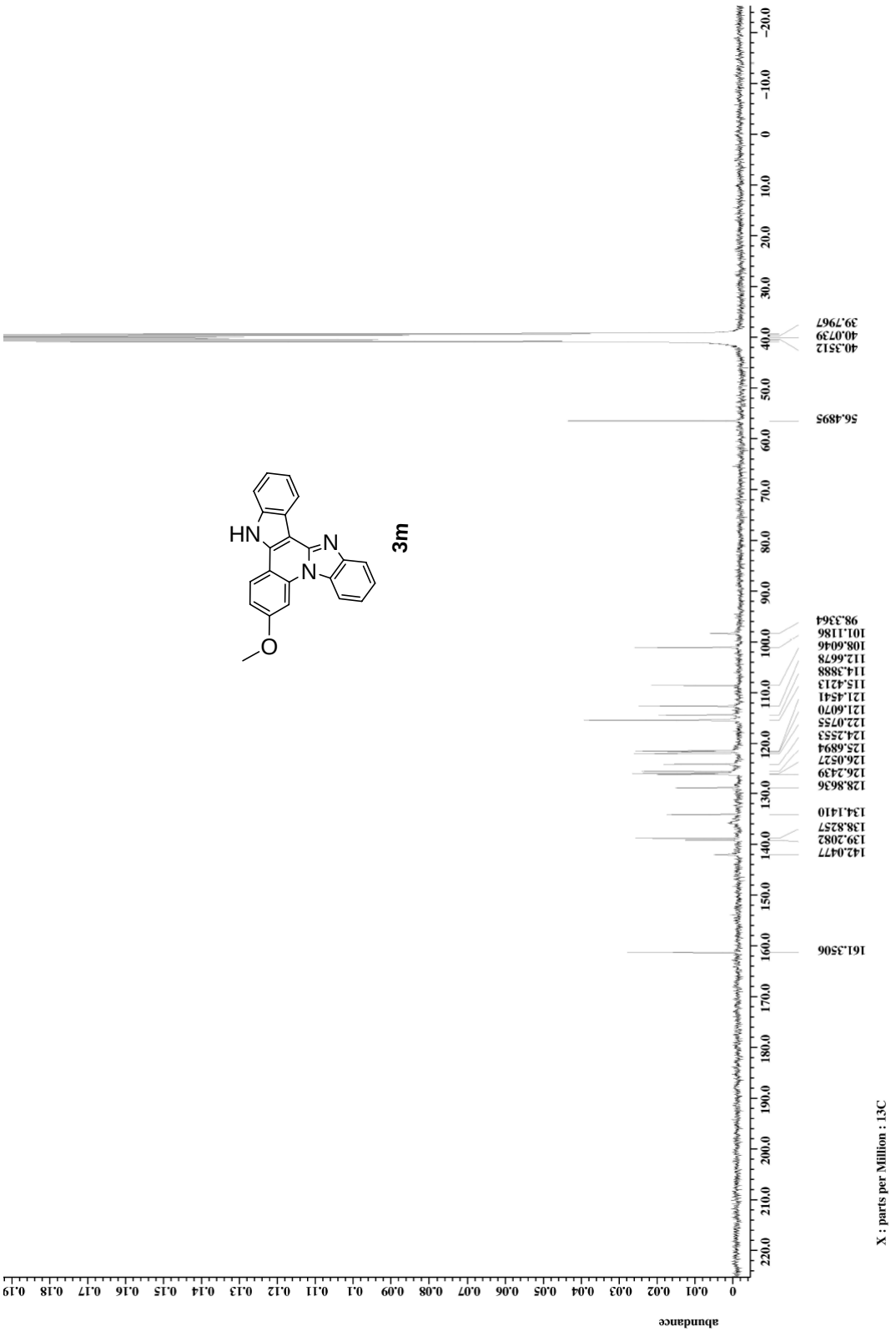

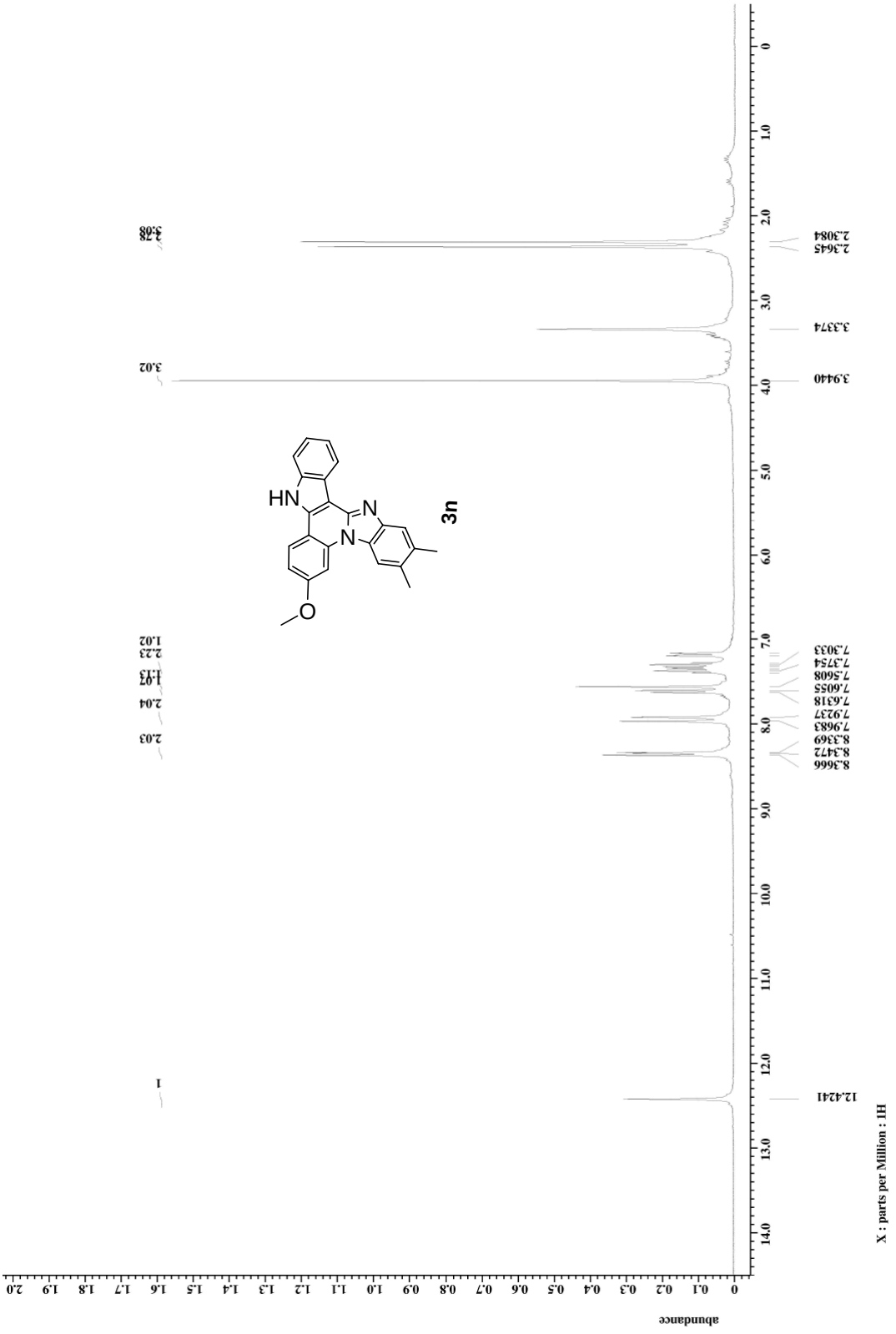

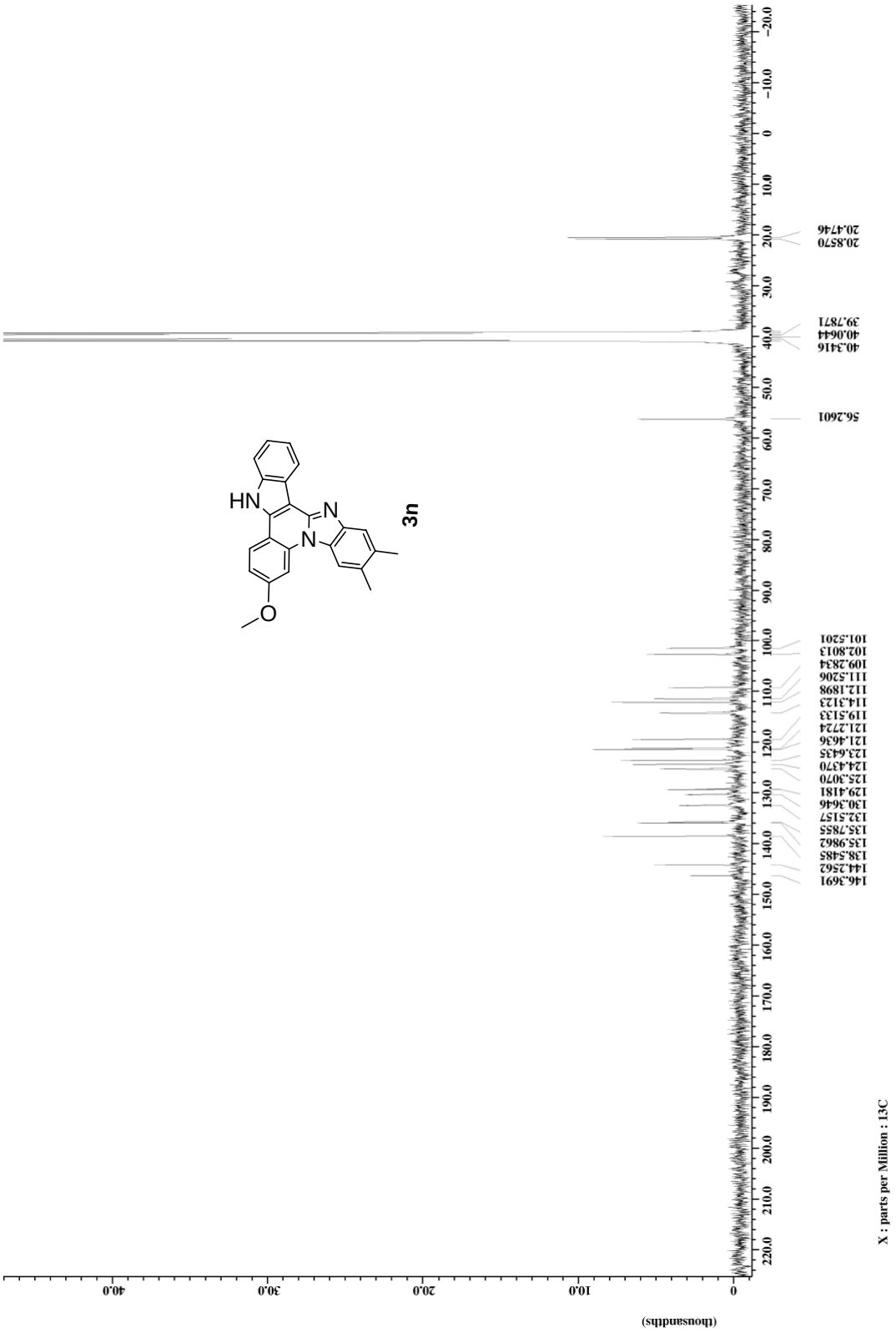

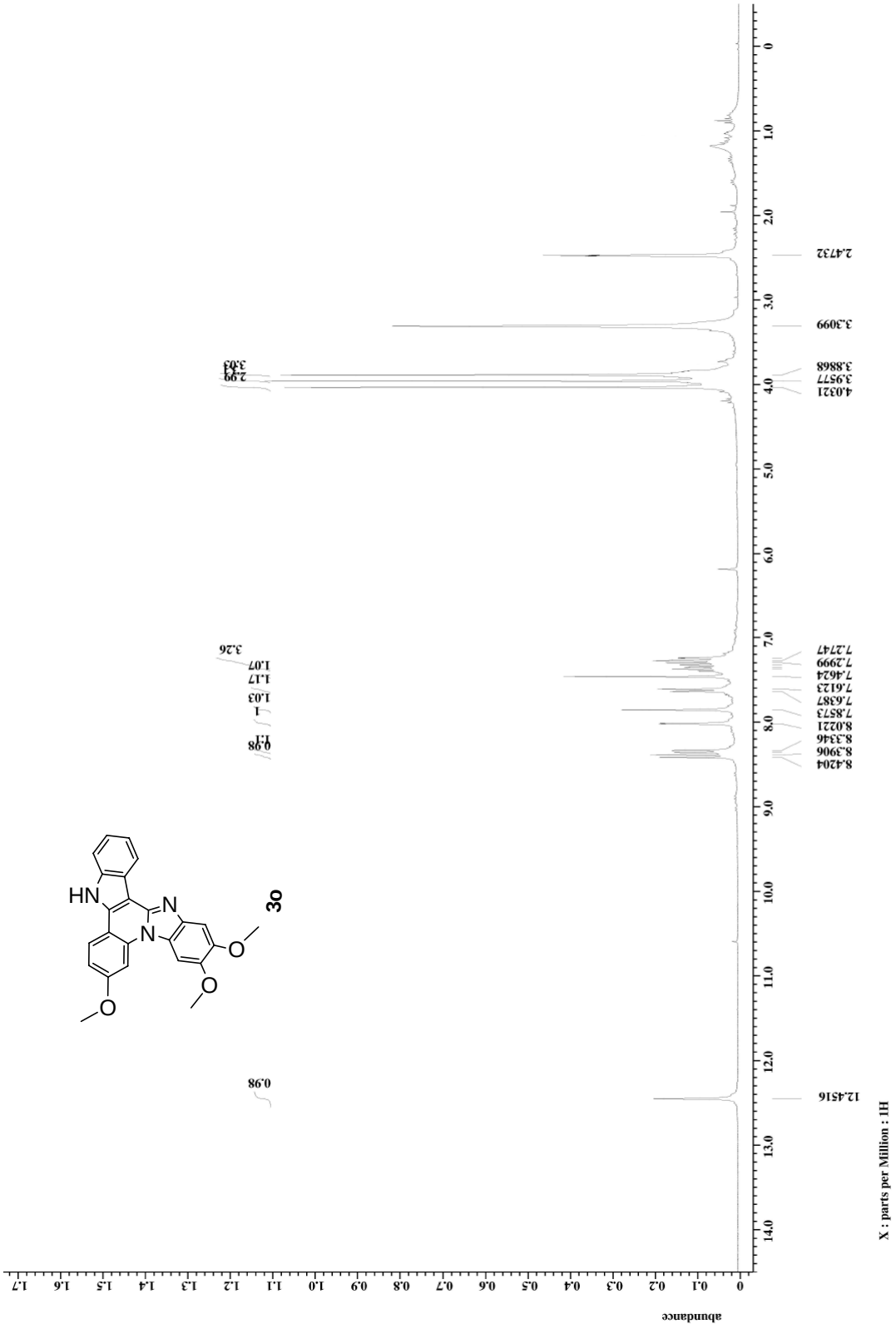

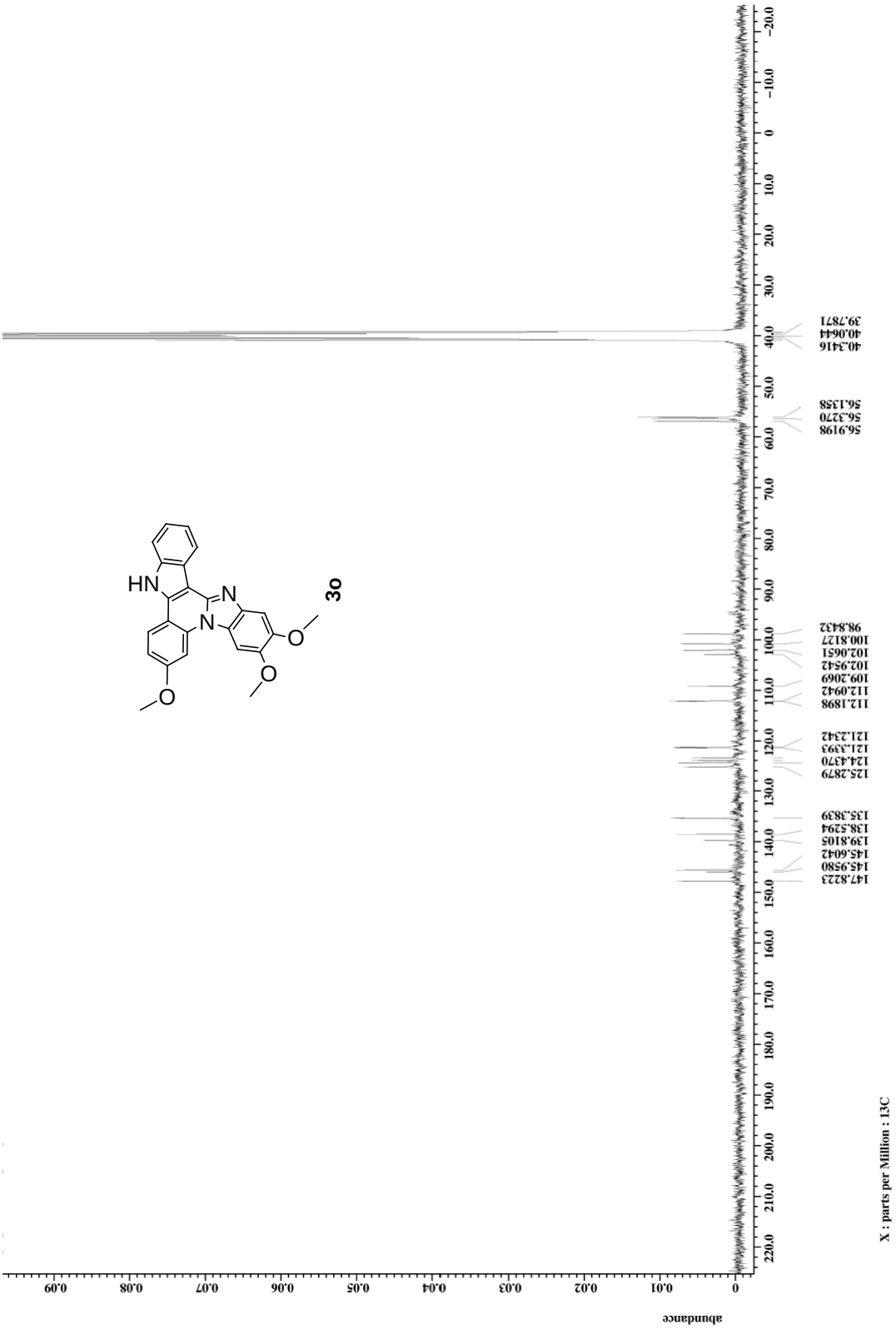
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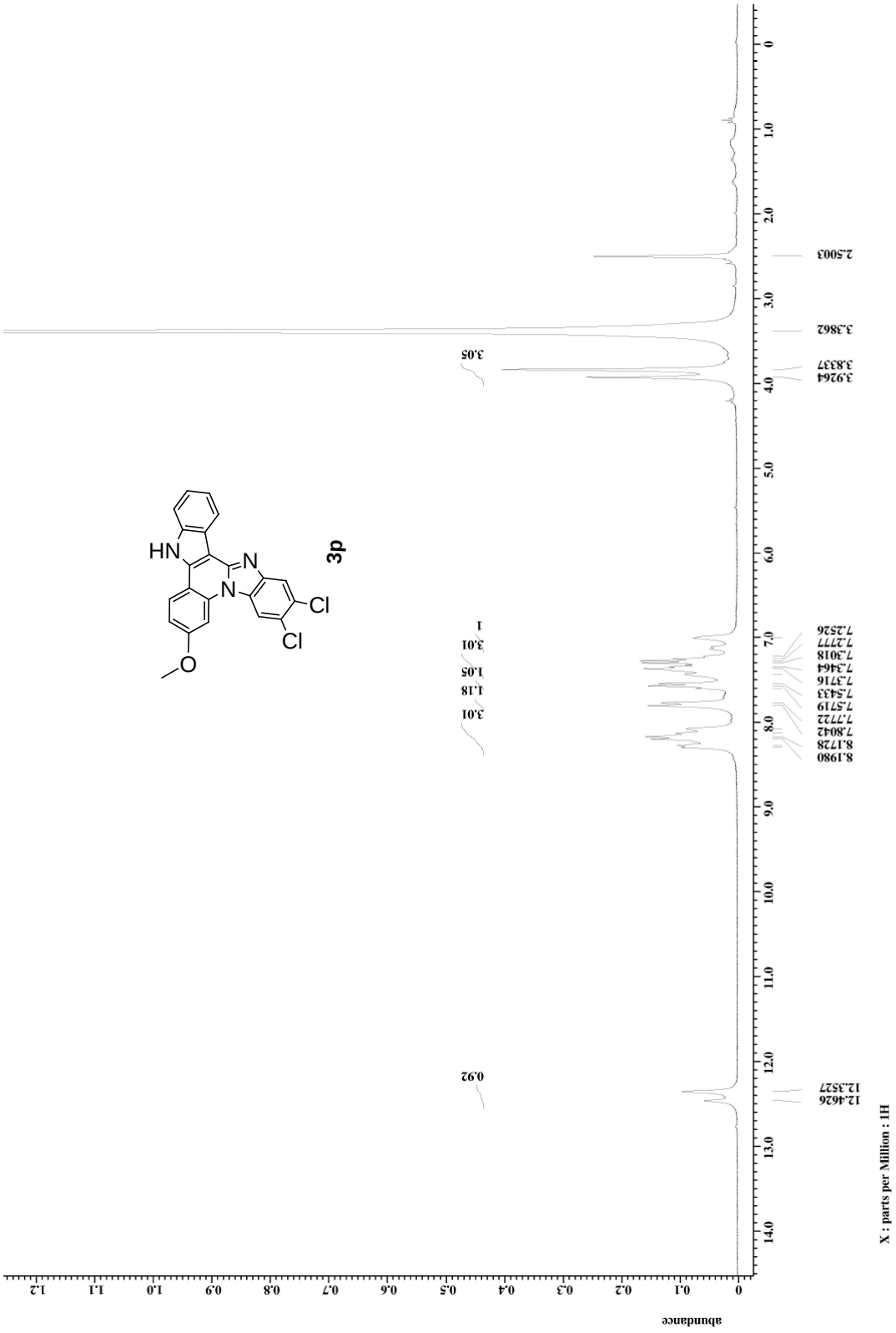
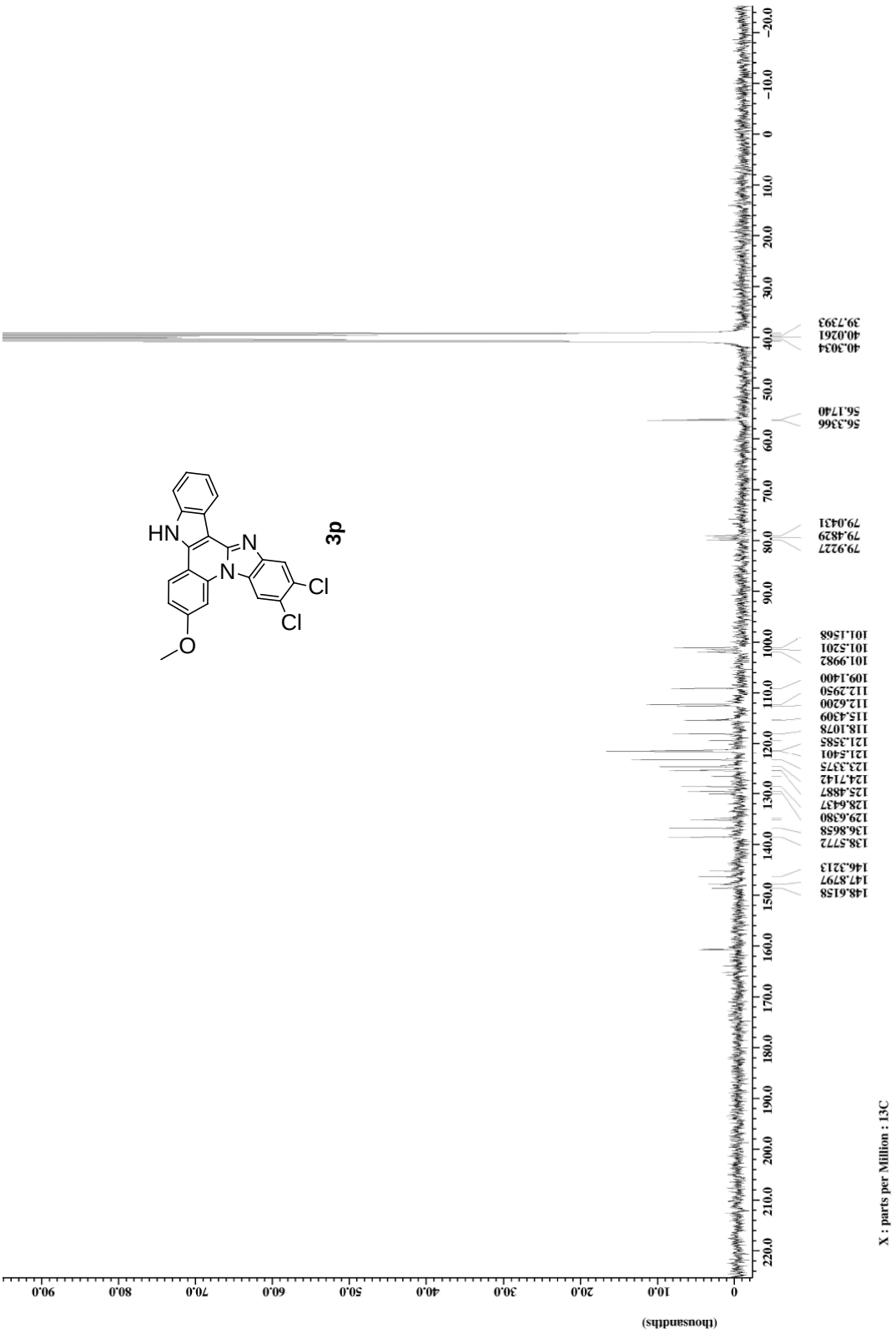
X : parts per Million : 13C
abundance

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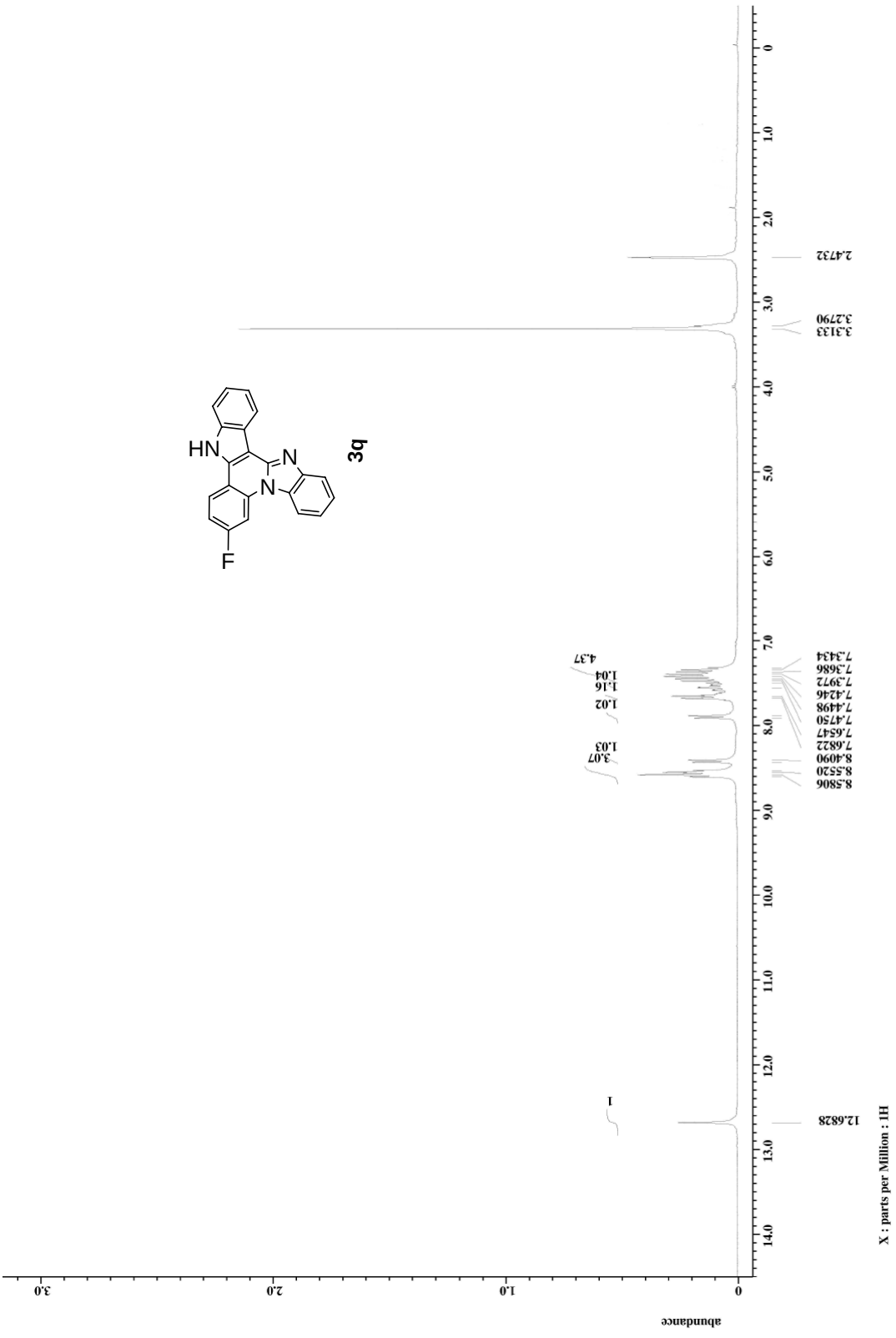
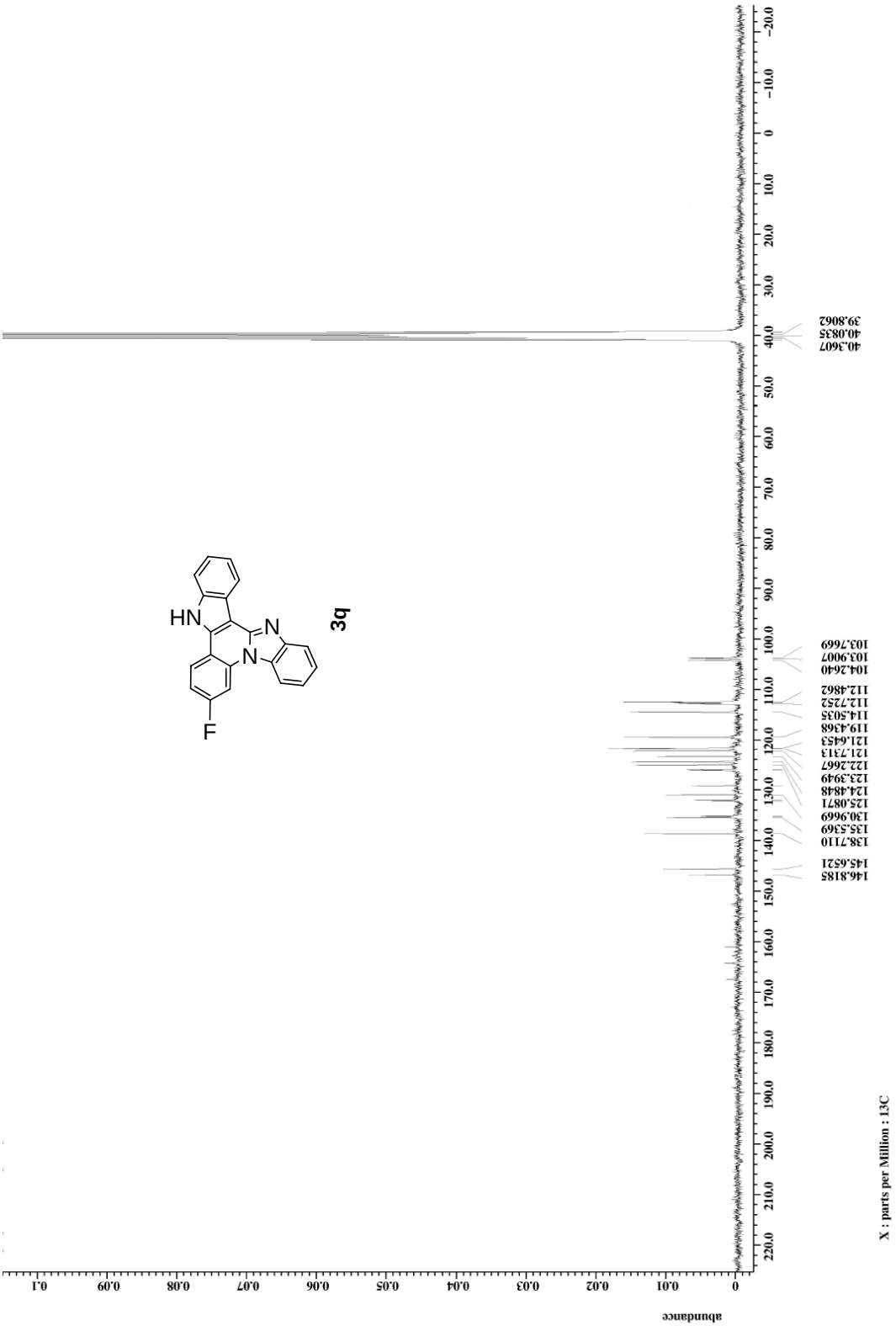
(thousandths)




HN
N
N
F
3q
39.8062
40.0835
40.3607
103.7669
103.9007
104.2640
112.4862
112.7252
114.5035
119.4368
121.6453
121.7313
122.2667
123.3949
124.4848
125.0871
130.9669
135.5369
138.7110
145.6521
146.8185
abundance
X : parts per Million : 13C