SUPPORTING INFORMATION

Synthesis of 3-Iodoindoles by the Pd/Cu-Catalyzed Coupling of *N,N*-Dialkyl-2-iodoanilines and Terminal Acetylenes, Followed by Electrophilic Cyclization

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General. All ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75.5 MHz or 400 and 100 MHz. Thin-layer chromatography was performed using commercially prepared 60-mesh silica gel plates, and visualization was effected with short wavelength UV light (254 nm). All melting points are uncorrected. High resolution mass spectra were recorded on a double focusing magnetic sector mass spectrometer using EI at a voltage of 70 eV. All reagents were used directly as obtained commercially unless otherwise noted. **Preparation of 2-Iodoanilines.** 2-Iodo-4-nitroaniline,[1] 2-iodo-4-methylaniline,[1] 2-iodo-5-methoxyaniline[1], ethyl 4-(*n*-butylamino)-3-iodobenzoate[2] and methyl 3-iodo-4-(methylamino)benzoate[3] were prepared according to the literature procedures.

Ethyl 4-(*n*-butylamino)-3-iodobenzoate. The compound was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.98 (t, J = 7.2 Hz, 3H), 1.36 (t, J = 6.9 Hz, 3H), 1.40-1.52 (m, 2H), 1.63-1.72 (m, 2H), 3.18-3.22 (m, 2H), 4.31 (q, J = 7.2 Hz, 2H), 4.61 (s, 1H), 6.49 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.0, 14.6, 20.4, 31.2, 43.8, 60.7, 83.8, 108.9, 120.0, 131.7, 140.8, 150.7, 165.7; IR (neat, cm^{-1}) 3394, 2959, 2930, 2871, 1711. The product was used for the next step without further characterization.

General Procedure for Preparation of the *N,N*-Dialkyl-*o*-iodoanilines. These compounds were prepared by a procedure reported by Cadogan.[4] A solution of the corresponding aniline (2.0 mmol) and iodomethane (0.85 g, 6.0 mmol) in DMF (10 ml) containing K_2CO_3 (0.55 g, 4.0 mmol) was stirred for 48 h at room temperature. Water (10 ml) was then added, and the solution was extracted with

ethyl ether (3 x 10 ml). The organic extracts were washed with water (4 x 20 ml) to remove any remaining DMF, and then dried (Na_2SO_4) and the solvent was removed under reduced pressure to yield the crude product, which was further purified by flash chromatography on silica gel using ethyl acetate/hexane as the eluent.

***N,N*-Dialkyl-2-iodoanilines Prepared**

***N,N*-Dimethyl-2-iodoaniline (1)**. The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.76 (s, 6H), 6.76 (t, *J* = 8.2 Hz, 1H), 7.08 (d, *J* = 9.3 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 45.2, 97.3, 120.6, 125.2, 129.2, 140.4, 155.1; IR (neat, cm^{-1}) 3002, 1944, 2830, 2783; HRMS calcd for $C_8H_{10}IN$ 246.98580. Found 246.98605.

***N,N*-Dimethyl-2-iodo-4-nitroaniline (9)**. The compound was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.94 (s, 6H), 6.98 (d, *J* = 9.0 Hz, 1H), 8.16 (d, *J* = 9.0 Hz, 1H), 8.69 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 44.4, 90.6, 118.6, 124.8, 136.8, 160.7; IR (neat, cm^{-1}) 2947, 2871, 2843, 2794; HRMS calcd for $C_8H_9IN_2O_2$ 291.97088. Found 291.97104.

***N,N*-Dimethyl-2-iodo-4-methylaniline (13).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.72 (s, 6H), 6.99 (d, *J* = 9.0 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 7.68 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 20.4, 45.4, 97.6, 120.3, 130.0, 135.1, 140.7, 152.7; IR (neat, cm^{-1}) 3058, 2926, 2855, 2227, 1464, 1435, 749; HRMS calcd for $C_9H_{12}IN$ 261.00165. Found 261.00198.

***N,N*-Dimethyl-2-iodo-5-methoxyaniline (17).** The compound was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.75 (s, 6H), 3.78 (s, 3H), 6.38 (d, *J* =

10.4 Hz, 1H), 6.66 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 45.0, 55.5, 85.4, 107.8, 110.0, 140.3, 156.1, 160.9; IR (neat, cm^{-1}) 2293, 2829, 2780; HRMS calcd for $C_9H_{12}INO$ 276.99637. Found 276.99697.

Ethyl 4-(*n*-butylmethylamino)-3-iodobenzoate (21). The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.5 Hz, 3H), 1.30-1.40 (m, 5H), 2.78 (s, 3H), 3.03 (t, *J* = 9.0 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 1H), 7.96 (dd, *J* = 8.4, 2.1 Hz, 1H), 8.49 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 14.6, 20.4, 29.7, 41.9, 56.1, 61.2, 95.7, 120.7, 126.2, 130.5, 142.0, 158.9, 165.4; IR (neat, cm^{-1}) 3004, 2922, 1713; HRMS calcd for $C_{14}H_{20}INO_2$ 361.05388. Found 361.05433.

***N*-Cyclohexyl-*N*-methyl-2-iodoaniline (25).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08-1.13 (m, 4H), 1.32 (q, *J* = 12.0 Hz, 2H), 1.74-1.84 (m, 4H), 2.62 (s, 3H), 2.97-3.03 (m, 1H), 6.75 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 1H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 25.8, 26.3, 29.3, 35.6, 62.2, 100.2, 123.8, 125.1, 128.6, 140.2, 154.3; HRMS calcd for $C_{13}H_{18}IN$ 315.00637. Found 315.00684.

Procedure for the Preparation of Methyl 3-iodo-4-[methyl(phenyl)amino]benzoate (27). This compound was prepared by a procedure reported by Larock.[5] To a solution of MeCN (24 mL), methyl 3-iodo-4-(methylamino)benzoate (0.43 g, 1.5 mmol) and 2-(trimethylsilyl)phenyl triflate (1.5 equiv.) was added CsF (2.0 equiv.). The reaction mixture was allowed to stir at room temperature for 2 d and the resulting solution was washed by brine (40 mL) and extracted with diethyl ether (60 mL). The combined ether fractions were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was

purified by flash chromatography (silica gel, Hexane/EtOAc = 9:1), to afford the desired product (0.48 g, 87%) as a colorless solid: mp 78-79 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.25 (s, 3H), 3.93 (s, 3H), 6.61-6.64 (m, 2H), 6.84 (t, *J* = 7.2 Hz, 1H), 7.19-7.26 (m, 3H), 8.03 (dd, *J* = 8.4, 2.1 Hz, 1H), 8.61 (d, *J* = 1.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 39.8, 52.6, 99.8, 115.2, 119.2, 128.7, 129.2, 129.3, 131.4, 142.1, 148.3, 155.3, 165.5; IR (neat, cm^{-1}) 3088, 2949, 1724, 1586; HRMS *m/z* calcd for $C_{15}H_{14}INO_2$: 367.0069. Found: 367.0076.

General Procedure for Synthesis of the *N*,*N*-Dialkyl-2-(1-alkynyl)anilines. To a solution of Et_3N (12.5 ml), $PdCl_2(PPh_3)_2$ (0.070 g, 2 mol %), 5.0 mmol of *N,N*-dialkyl-*o*-iodoaniline and 6.0 mmol of terminal acetylene (stirring for 5 min beforehand), CuI (0.010 g, 1 mol %) was added and stirring was continued for another 2 min before flushing with Ar. The flask was then sealed. The mixture was allowed to stir at room temperature for the desired time and the resulting solution was filtered, washed with a satd aq NaCl solution and extracted with diethyl ether (2 x 10 ml). The combined ether fractions were dried over Na_2SO_4 and concentrated under vacuum to yield the crude product. The crude product was purified by flash chromatography on silica gel using ethyl acetate/hexane as the eluent.

***N,N*-Dialkyl-2-(1-alkynyl)anilines Prepared.**

***N,N*-Dimethyl-2-(phenylethynyl)aniline (2).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.01 (s, 6H), 6.88-6.94 (m, 2H), 7.25 (t, *J* = 6.3 Hz, 1H), 7.31-7.37 (m, 3H), 7.49 (d, *J* = 5.7 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.8, 89.1, 95.0, 115.3, 117.2, 120.7, 124.1,

128.2, 128.5, 129.5, 131.5, 134.6, 155.0; IR (neat, cm^{-1}) 3059, 2943, 2833, 2785, 2209; HRMS calcd for $C_{16}H_{15}N$ 221.12045. Found 221.12076.

***N,N*-Dimethyl-2-(3,3-dimethyl-1-butynyl)aniline (3).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.34 (s, 9H), 2.92 (s, 6H), 6.80-6.86 (m, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.5, 31.2, 43.6, 78.5, 104.0, 116.2, 116.9, 120.5, 128.5, 134.5, 154.6; IR (neat, cm^{-1}) 3004, 2923, 2147; HRMS calcd for $C_{14}H_{18}N$ 200.14392. Found 200.14417.

***N,N*-Dimethyl-2-(1-octynyl)aniline (4).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.90 (t, *J* = 6.9 Hz, 3H), 1.29-1.34 (m, 4 H), 1.46-1.49 (m, 2H), 1.62 (q, *J* = 3.8 Hz, 2H), 2.47 (t, *J* = 7.2 Hz, 2H), 2.91 (s, 3H), 6.83-6.90 (m, 2H), 7.18 (t, *J* = 5.0 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 20.1, 22.8, 28.9, 29.0, 31.6, 43.8, 79.7, 96.1, 116.8, 117.1, 120.9, 128.5, 134.5, 154.8; IR (neat, cm^{-1}) 2930, 2858, 2782, 2242; HRMS calcd for $C_{16}H_{23}N$ 229.18305. Found 229.18336.

***N,N*-Dimethyl-2-(cyclohex-1-enylethynyl)aniline (5).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.62-1.68 (m, 4H), 2.13-2.15 (m, 2H), 2.25-2.27 (m, 2H), 2.93 (s, 6H), 6.18-6.19 (m, 1H), 6.84-6.89 (m, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.8, 22.5, 25.9, 29.3, 43.6, 86.3, 96.8, 115.9, 117.0, 120.6, 121.3, 128.8, 134.2, 134.4, 154.6; IR (neat, cm^{-1}) 2932, 2859, 2832, 2196; HRMS calcd for $C_{16}H_{19}N$ 225.15175. Found 225.15209.

***N,N*-Dimethyl-2-(trimethylsilylethynyl)aniline (6).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.25 (s, 9H), 2.98 (s, 3H), 6.83 (dd,

J = 9.0, 6.0 Hz, 2H), 7.21 (t, *J* = 9.0 Hz, 1H), 7.41 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 0.2, 43.5, 99.7, 104.9, 114.9, 116.9, 120.3, 129.6, 135.1, 155.3; IR (neat, cm^{-1}) 3059, 2959, 2920, 2155, 1461, 1434, 1249, 843; HRMS calcd for $C_{13}H_{18}NSi$ 216.12085. Found 216.12100.

6-[2-(Dimethylamino)phenyl]-5-hexynenitrile (7). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (t, *J* = 7.2 Hz, 2H), 2.57 (t, *J* = 7.2 Hz, 2H), 2.67 (t, *J* = 6.8 Hz, 2H), 2.90 (s, 6H), 6.87 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 19.1, 24.9, 43.8, 81.6, 92.3, 115.9, 117.3, 119.4, 121.0, 129.1, 134.4, 155.0; IR (neat, cm^{-1}) 3061, 2942, 2834, 2785, 2247; HRMS calcd for $C_{14}H_{16}N_2$ 212.13135. Found 212.13172.

***N,N*-Dimethyl-2-(5-chloro-1-pentynyl)aniline (8).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.04-2.11 (m, 2H), 2.68 (t, *J* = 6.8 Hz, 2H), 2.91 (s, 6H), 3.74 (t, *J* = 6.3 Hz, 2H), 6.84-6.92 (m, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 17.6, 31.7, 43.8, 44.0, 80.8, 93.6, 116.3, 117.3, 121.0, 128.9, 134.5, 154.9; IR (neat, cm^{-1}) 2943, 2832, 2784, 2259; HRMS calcd for $C_{13}H_{16}ClN$ 221.69713. Found 221.69754.

***N,N*-Dimethyl-4-nitro-2-(phenylethynyl)aniline (10).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (s, 6H), 6.78 (d, *J* = 9.2 Hz, 1H), 7.36-7.38 (m, 3H), 7.50-7.52 (m, 2H), 8.06 (dd, *J* = 9.2, 2.4 Hz, 1H), 8.35 (d, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 42.7, 87.7, 95.3, 110.4, 114.7, 123.0, 125.1, 128.6, 128.7, 131.1, 131.4, 138.5, 157.5; IR (neat, cm^{-1}) 2954, 2917, 2849, 2133; HRMS calcd for $C_{16}H_{14}N_2O_2$ 266.10553. Found 266.10592.

***N,N*-Dimethyl-4-nitro-2-(1-octynyl)aniline (11).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (t, *J* = 6.8 Hz, 3H), 1.30-1.34 (m, 4H), 1.43-1.48 (m, 2H), 1.62 (q, *J* = 7.2 Hz, 2H), 2.45 (t, *J* = 7.1 Hz, 2H), 3.15 (s, 6H), 6.73 (d, *J* = 9.3 Hz, 1H), 7.99 (dd, *J* = 9.3, 2.7 Hz, 1H), 8.20 (d, *J* = 2.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 19.9, 22.7, 28.7, 28.9, 31.5, 42.8, 78.7, 97.3, 112.4, 114.9, 124.5, 131.4, 138.9, 158.0; IR (neat, cm^{-1}) 2930, 2857, 2806, 2224; HRMS calcd for $C_{16}H_{22}N_2O_2$ 274.16813. Found 274.16830.

***N,N*-Dimethyl-2-(cyclohex-1-enylethynyl)-4-nitroaniline (12).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.61-1.71 (m, 4H), 2.15-2.20 (m, 2H), 2.20-2.22 (m, 2H), 3.18 (s, 6H), 6.20-6.21 (m, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 12.0 Hz, 1H), 8.22 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 22.3, 25.8, 28.8, 42.7, 85.0, 97.5, 111.5, 114.6, 120.7, 124.6, 131.0, 135.4, 138.7, 157.5; IR (neat, cm^{-1}) 2924, 2853, 2354, 1454, 1432, 749; HRMS calcd for $C_{16}H_{18}N_2O_2$ 270.13683. Found 270.13735.

***N,N*-Dimethyl-4-methyl-2-(phenylethynyl)aniline (14)**. The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.95 (s, 6H), 6.83 (d, *J* = 8.1 Hz, 1H), 7.04 (d, *J* = 9.0 Hz, 1H), 7.22-7.33 (m, 4H), 7.52-7.55 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 44.0, 89.1, 94.7, 115.6, 117.3, 124.2, 128.2, 128.5, 130.3, 130.3, 131.6, 134.8, 152.8; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{17}H_{17}N$ 235.13610. Found 235.13582.

***N,N*-Dimethyl-4-methyl-2-(1-octynyl)aniline (15).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 6.0 Hz, 3H), 1.24-1.26 (m, 4H), 1.37-1.41 (m, 2H), 1.55 (q, *J* = 8.0 Hz, 2H), 2.16 (s, 3H), 2.40 (t, *J* = 8.0 Hz,

2H), 2.79 (s, 6H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 7.12 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 20.1, 20.4, 22.8, 28.9, 29.0, 31.6, 44.0, 79.6, 95.7, 116.9, 117.2, 129.2, 130.4, 134.9, 152.5; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{17}H_{25}N$ 243.19870. Found 243.19908.

***N,N*-Dimethyl-2-(cyclohex-1-enylethynyl)-4-methylaniline (16).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.52-1.63 (m, 4H), 2.05-2.06 (m, 2H), 2.15-2.17 (m, 5H), 2.81 (s, 3H), 6.09-6.11 (m, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 7.12 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 21.8, 22.6, 25.9, 29.3, 43.8, 86.2, 96.6, 116.1, 117.0, 121.3, 129.5, 130.1, 134.4, 134.5, 152.5; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{17}H_{21}N$ 239.16740. Found 239.16779.

***N,N*-Dimethyl-5-methoxy-2-(phenylethynyl)aniline (18).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.99 (s, 6H), 3.79 (s, 3H), 6.44 (d, *J* = 8.0 Hz, 2H), 7.23-7.34 (m, 3H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 43.5, 55.4, 89.2, 93.5, 103.8, 105.3, 107.6, 124.4, 127.8, 131.2, 135.6, 156.3, 160.8; IR (neat, cm^{-1}) 2924, 2853, 2354, 1454, 1432, 749; HRMS calcd for $C_{17}H_{17}NO$ 251.13101. Found 251.13132.

***N,N*-Dimethyl-5-methoxy-2-(1-octynyl)aniline (19).** The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.90 (t, *J* = 6.8 Hz, 3H), 1.30-1.33 (m, 4H), 1.42-1.49 (m, 2H), 1.62 (q, *J* = 7.6 Hz, 2H), 2.45 (t, *J* = 6.8 Hz, 2H), 2.90 (s, 6H), 3.77 (s, 3H), 6.36-6.42 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 20.0, 22.8, 28.9, 29.1, 31.6, 43.6, 55.3, 79.5, 94.2, 104.1,

105.3, 109.2, 135.4, 156.1, 160.0; IR (neat, cm^{-1}) 2924, 2853, 2354, 1454, 1432, 749; HRMS calcd for $C_{17}H_{25}NO$ 259.19361. Found 259.19389.

***N,N*-Dimethyl-2-(cyclohex-1-enylethynyl)-5-methoxyaniline (20).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.59-1.68 (m, 4H), 2.12-2.14 (m, 2H), 2.22-2.24 (m, 2H), 2.92 (s, 6H), 3.78 (s, 3H), 6.13-6.15 (m, 1H), 6.38-6.41 (m, 2H), 7.29 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8, 22.6, 25.9, 29.4, 43.4, 55.3, 86.2, 95.3, 103.8, 105.2, 108.3, 121.4, 133.6, 135.3, 156.0, 160.3; IR (neat, cm^{-1}) 2932, 2834, 2786, 2194; HRMS calcd for $C_{17}H_{21}NO$ 255.16231. Found 255.16270.

Ethyl 4-(*N*-*n*-butyl-*N*-methylamino)-3-(phenylethynyl)benzoate (22). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.87 (t, *J* = 7.4 Hz, 3H), 1.25-1.31 (m, 2H), 1.37 (t, *J* = 7.0 Hz, 3H), 1.63-1.69 (m, 2H), 3.02 (s, 3H), 3.54 (t, *J* = 7.8 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 1H), 7.31-7.35 (m, 3H), 7.49-7.51 (m, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 8.15 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 14.6, 20.4, 30.1, 39.8, 54.9, 60.7, 89.0, 94.2, 111.7, 115.8, 120.5, 123.8, 128.2, 128.5, 130.8, 131.3, 137.1, 156.6, 166.2; IR (neat, cm^{-1}) 2957, 2929, 2870, 2203; HRMS calcd for $C_{22}H_{25}NO_2$ 335.18853. Found 335.18887.

Ethyl 4-(*N*-*n*-butyl-*N*-methylamino)-3-(1-octynyl)benzoate (23). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.81-0.87 (m, 6H), 1.19-1.40 (m, 11H), 1.50-1.58 (m, 4H), 2.87 (s, 3H), 3.39 (q, *J* = 8.0 Hz, 2H) , 4.25 (q, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.94 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.3, 14.6, 20.1, 20.4, 22.8, 28.9, 28.9, 30.0, 31.6, 39.7, 54.9, 60.6, 79.6, 95.7, 113.4, 116.0, 120.8, 130.1, 137.0,

156.9, 166.4; IR (neat, cm^{-1}) 2924, 2853, 2354, 1454, 1432, 749; HRMS calcd for $C_{22}H_{33}NO_2$ 343.25113. Found 343.25150.

Ethyl 4-(*N*-*n*-butyl-*N*-methylamino)-3-(cyclohex-1-enylethynyl)benzoate (24). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 8.0 Hz, 3H), 1.20-1.28 (m, 5H), 1.54-1.59 (m, 6H), 2.06-2.15 (m, 4H), 2.89 (s, 3H), 3.39 (q, *J* = 8.0 Hz, 2H), 4.24 (t, *J* = 8.0 Hz, 2H), 6.09 (m, 1H), 6.69 (d, *J* = 8.0 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 14.6, 20.4, 21.7, 22.5, 25.9, 29.2, 30.0, 39.7, 54.8, 60.6, 86.1, 96.3, 112.6, 115.8, 120.5, 121.2, 130.3, 134.5, 136.8, 156.5, 166.3; IR (neat, cm^{-1}) 2924, 2853, 2354, 1454, 1432, 749; HRMS calcd for $C_{22}H_{29}NO_2$ 339.21983. Found 339.22025.

***N*-Cyclohexyl-*N*-methyl-2-(phenylethynyl)aniline (26).** The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07-1.28 (m, 4H), 1.51-1.62 (m, 2H), 1.78 (d, *J* = 13.2 Hz, 2H), 1.88 (d, *J* = 12.0 Hz, 2H), 2.77 (s, 3H), 3.80-3.85 (m, 1H), 6.87 (t, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.30-7.33 (m, 3H), 7.50 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.3, 26.4, 29.9, 32.8, 62.6, 89.2, 94.3, 116.0, 119.0, 120.3, 124.2, 128.0, 128.5, 129.1, 131.5, 134.7, 154.8; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{21}H_{23}N$ 289.0144. Found 289.0251.

Methyl 4-[methyl(phenyl)amino]-3-(phenylethynyl)benzoate (28). The product was obtained as a light yellow oil: H NMR (300 MHz, $CDCl_3$) δ 3.48 (s, 3H), 3.94 (s, 3H), 6.95-6.98 (m, 3H), 7.18-7.31 (m, 8H), 8.00 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.26 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 41.1, 52.4, 87.2, 96.4, 118.85, 118.9, 121.1, 123.3, 124.1, 125.0, 128.4, 128.5, 129.3, 130.9, 131.8,

136.2, 148.8, 154.3, 166.5; IR (neat, cm^{-1}) 3059, 2949, 2885, 1719, 1592; HRMS *m/z* calcd for $C_{23}H_{19}NO_2$: 341.1416. Found: 341.1416.

General Procedure for Iodocyclization. To a solution of 0.25 mmol of the *N,N*-dialkyl-2-(1-alkynyl)aniline and 3 ml of CH_2Cl_2, 2 equivs of I_2 dissolved in 2 ml of CH_2Cl_2 was added gradually. The reaction mixture was flushed with Ar and allowed to stir at room temperature for the desired time. The excess I_2 was removed by washing with a satd aq soln of $Na_2S_2O_3$. The aqueous solution was then extracted by diethyl ether (2 x 10 ml). The combined ether layers were dried over anhydrous Na_2SO_4 and concentrated under a vacuum to yield the crude product, which was purified by flash chromatography on silica gel using ethyl acetate/hexanes as the eluent.

3-Iodoindoles Prepared

3-Iodo-1-methyl-2-phenylindole (29). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 7.21-7.28 (m, 3H), 7.43-7.51 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.2, 59.0, 110.0, 120.9, 121.6, 123.1, 128.6, 129.0, 130.5, 131.1, 131.8, 137.9, 141.9; IR (neat, cm^{-1}) 3054, 2937; HRMS calcd for $C_{15}H_{12}IN$ 333.00145. Found 333.00194.

2-*t*-Butyl-3-iodo-1-methylindole (30). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.67 (s, 9H), 3.92 (s, 3H), 7.16-7.25 (m, 3H), 7.52 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.4, 32.4, 34.7, 54.5, 109.0, 120.5, 122.4, 122.8, 131.6, 138.6, 144.4; IR (neat, cm^{-1}) 3004, 2966, 2922; HRMS calcd for $C_{13}H_{16}IN$ 312.02492. Found 312.02515.

2-*n*-Hexyl-3-iodo-1-methylindole (31). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.0 Hz, 3H), 1.30-1.43 (m, 6H),

1.56-1.59 (m, 2H), 2.82 (t, *J* = 8.0 Hz, 2H), 3.70 (s, 3H), 7.12-7.20 (m, 3H), 7.37 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.8, 27.3, 29.2, 29.5, 30.8, 31.8, 57.9, 109.4, 120.4, 120.7, 122.1, 130.2, 137.6, 142.0; IR (neat, cm^{-1}) 3053, 2926, 2855; HRMS calcd for $C_{15}H_{20}IN$ 341.06405. Found 341.06452.

2-(Cyclohex-1-enyl)-3-iodo-1-methylindole (32). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.73-1.76 (m, 2H), 1.81-1.84 (m, 2H), 2.22-2.30 (m, 4H), 3.68 (s, 3H), 5.88-5.90 (m, 1H), 7.17-7.19 (m, 1H), 7.22-7.24 (m, 2H), 7.41 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.1, 22.9, 25.7, 29.4, 31.5, 57.0, 109.7, 120.5, 121.2, 122.4, 130.0, 130.3, 133.8, 137.3, 144.4; IR (neat, cm^{-1}) 2921, 2850; HRMS calcd for $C_{15}H_{16}IN$ 337.03275. Found 337.03300.

3-Iodo-1-methyl-2-(trimethylsilyl)indole (33). The product was obtained as an inseparable mixture of the desired product and decomposed product. Due to the compound's instability, we were unable to further characterize this compound,

4-(3-Iodo-1-methylindol-2-yl)butanenitrile (34). The product was obtained as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.99 (q, *J* = 7.4 Hz, 2H), 2.42 (t, *J* = 7.1 Hz, 2H), 3.02 (t, *J* = 7.5 Hz, 2H), 3.77 (s, 3H), 7.17-7.21 (m, 1H), 7.24-7.26 (m, 2H), 7.38 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.8, 25.4, 26.0, 30.9, 59.3, 109.6, 119.5, 120.8, 121.0, 122.8, 130.0, 137.8, 138.8; IR (neat, cm^{-1}) 2935, 2869, 2246; HRMS calcd for $C_{13}H_{13}IN_2$ 324.01235. Found 324.01269.

2-(3-Chloro-1-propyl)-3-iodo-1-methylindole (35). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04-2.11 (m, 2H), 3.02 (t, *J* = 7.6 Hz, 2H), 3.60 (t, *J* = 7.8 Hz, 2H), 3.76 (s, 3H), 7.14-7.18 (m, 1H), 7.22-7.23 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.6, 30.9, 32.3,

44.4, 58.6, 109.6, 120.6, 120.8, 122.5, 130.1, 137.7, 140.0; IR (neat, cm^{-1}) 2956, 2928, 2869; HRMS calcd for $C_{12}H_{13}ClIN$ 333.57813. Found 333.57851.

3-Iodo-1-methyl-5-nitro-2-phenylindole (36). The compound was obtained as pale yellow crystals: the compound decomposes at 125 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.74 (s, 3H), 7.36 (d, *J* = 9.0 Hz, 1H), 7.46-7.59 (m, 2H), 7.53-7.57 (m, 3H), 8.19 (dd, *J* = 9.0, 2.4 Hz, 1H), 8.45 (d, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.7, 61.3, 110.2, 118.6, 119.0, 128.9, 129.8, 130.2, 130.7, 130.9, 140.9, 142.7, 145.4; IR (neat, cm^{-1}) 2924, 2852; HRMS calcd for $C_{15}H_{11}IN_2O_2$ 378.01168. Found 378.01242.

2-*n*-Hexyl-3-iodo-1-methyl-5-nitroindole (37). The product was obtained as pale yellow crystals: the compound decomposes at 118 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.1 Hz, 3H), 1.31-1.37 (m, 4H), 1.39-1.46 (m, 2H), 1.57-1.64 (m, 2H), 2.87 (t, *J* = 7.5 Hz, 2H), 3.81 (s, 3H), 7.25 (d, *J* = 8.4 Hz, 1H), 8.09 (dd, *J* = 9.0, 2.4 Hz, 1H), 8.32 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 16.6, 22.8, 27.6, 29.3, 31.4, 31.7, 60.3, 109.5, 117.8, 118.0, 130.0, 140.8, 142.4, 145.9; IR (neat, cm^{-1}) 3004, 2964, 2923; HRMS calcd for $C_{15}H_{19}IN_2O_2$ 386.04913. Found 386.04988.

2-(Cyclohex-1-enyl)-3-iodo-1-methyl-5-nitroindole (38). The compound was obtained as pale yellow crystals: mp 112 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.76-1.85 (m, 4H), 2.22-2.32 (m, 4H), 3.74 (s, 3H), 5.95-5.96 (m, 1H), 7.24-7.27 (m, 1H), 8.08-8.12 (m, 1H), 8.34-8.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.0, 22.8, 25.7, 29.2, 32.0, 59.4, 109.9, 118.0, 118.5, 129.2, 130.0, 135.1, 140.5, 142.4, 147.9; IR (neat, cm^{-1}) 3095, 2920, 2849, 2249, 1735, 1577, 1513, 1338; HRMS calcd for $C_{15}H_{15}IN_2O_2$ 382.01783. Found 382.01837.

3-Iodo-1,5-dimethyl-2-phenylindole (39). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 3.54 (s, 3H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.20 (s, 1H), 7.37-7.41 (m, 5H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 21.6, 32.2, 58.4, 109.8, 121.2, 124.7, 128.6, 128.9, 130.4, 130.7, 131.1, 131.9, 136.4, 141.8; IR (neat, cm^{-1}) 3055, 2919, 2849, 1576, 1475; HRMS calcd for $C_{16}H_{14}IN$ 347.01710. Found 347.01747.

2-*n*-Hexyl-3-iodo-1,5-dimethylindole (40). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 6.8 Hz, 3H), 1.24-1.34 (m, 6H), 1.49 (q, *J* = 7.6 Hz, 2H), 2.39 (s, 3H), 2.73 (t, *J* = 8.0 Hz, 2H), 3.61 (s, 3H), 6.94 (d, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 7.08 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 14.3, 21.6, 22.8, 27.3, 29.2, 29.5, 30.8, 31.8, 57.3, 109.1, 120.4, 123.6, 129.8, 130.3, 136.0, 141.9; IR (neat, cm^{-1}) 3055, 2919, 2849, 1576, 1475; HRMS calcd for $C_{16}H_{22}IN$ 355.07970. Found 355.08037.

2-(Cyclohex-1-enyl)-3-iodo-1,5-dimethylindole (41). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64-1.74 (m, 4H), 2.15-2.19 (m, 4H), 2.39 (s, 3H), 3.56 (s, 3H), 5.79 (m, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 7.11 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 21.6, 22.1, 22.9, 25.7, 29.4, 31.5, 56.4, 109.5, 120.8, 124.0, 129.9, 130.0, 130.4, 133.6, 135.7, 144.4; IR (neat, cm^{-1}) 3055, 2919, 2849, 1576, 1475; HRMS calcd for $C_{16}H_{18}IN$ 351.04840. Found 351.04879.

3-Iodo-6-methoxy-1-methyl-2-phenylindole (42). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.60 (s, 3H), 3.89 (s, 3H), 6.77 (s, 1H), 6.89 (d, *J* = 12.0 Hz, 1H), 7.37 (d, *J* = 12.0 Hz, 1H), 7.40-7.51 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.2, 56.0, 58.7, 93.5, 110.7, 122.3, 125.0, 128.6, 128.8,

131.1, 131.9, 138.5, 140.9, 157.4; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{16}H_{14}INO$ 363.01202. Found 363.01270.

2-*n*-Hexyl-3-iodo-6-methoxy-1-methylindole (43). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* = 6.8 Hz, 3H), 1.31-1.33 (m, 4H), 1.40-1.42 (m, 2H), 1.56 (q, *J* = 7.6 Hz, 2H), 2.79 (t, *J* = 8.0 Hz, 2H), 3.66 (s, 3H), 3.86 (s, 3H), 6.70 (s, 1H), 6.81 (d, *J* = 8.8 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.8, 27.3, 29.2, 29.6, 30.8, 31.8, 56.1, 57.4, 93.4, 109.8, 121.3, 124.5, 138.1, 140.9, 156.8; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{16}H_{22}INO$ 371.07462. Found 371.07537.

2-(1-Cyclohexenyl)-3-iodo-6-methoxy-1-methylindole (44). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.72-1.75 (m, 2H), 1.79-1.82 (m, 2H), 2.22-2.26 (m, 4H), 3.61 (s, 3H), 3.86 (s, 3H), 5.87 (s, 1H), 6.70 (d, *J* = 2.0 Hz, 1H), 6.82 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.27 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.1, 22.9, 25.7, 29.5, 31.5, 56.0, 56.5, 93.4, 110.1, 121.8, 124.6, 130.0, 133.7, 137.8, 143.5, 157.0; IR (neat, cm^{-1}) 2925, 2855; HRMS calcd for $C_{16}H_{18}INO$ 367.06332. Found 367.06396.

Ethyl 1-*n*-butyl-3-iodo-2-phenylindole-5-carboxylate (45). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.67 (t, *J* = 7.2 Hz, 3H), 1.02-1.07 (m, 2H), 1.36 (t, *J* = 7.0 Hz, 3H), 1.47-1.51 (m, 2H), 4.00 (t, *J* = 7.2 Hz, 2H), 4.34 (t, *J* = 7.0 Hz, 2H), 7.25 (d, *J* = 8.8 Hz, 1H), 7.34-7.43 (m, 5H), 7.91 (d, *J* = 8.4 Hz, 1H), 8.17 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 14.7, 20.0, 32.2, 45.2, 60.9, 61.2, 110.1, 123.2, 124.2, 124.5, 128.7, 129.3, 130.3, 130.9,

131.7, 139.6, 143.3, 167.6; IR (neat, cm^{-1}) 3058, 2959, 2932, 2872, 1709; HRMS calcd for $C_{21}H_{22}INO_2$ 447.06953. Found 447.07000.

Ethyl 3-iodo-1-methyl-2-phenylindole-5-carboxylate (46). The product was obtained as a pale yellow solid: mp 103-105 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 1.38 (t, *J* = 7.2 Hz, 3H), 3.62 (s, 3H), 4.36 (q, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.38-7.48 (m, 5H), 7.94 (d, *J* = 8.8 Hz, 1H), 8.18 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.7, 32.4, 60.6, 61.0, 109.8, 123.3, 124.4, 124.5, 128.7, 129.3, 130.2, 131.0, 131.3, 140.5, 143.4, 167.6; IR (neat, cm^{-1}) 2978, 2933, 1705; HRMS calcd for $C_{18}H_{16}INO_2$ 405.02258. Found 405.02306.

Ethyl 1-*n*-butyl-2-*n*-hexyl-3-iodoindole-5-carboxylate (47). The product was obtained as a yellow oil: ^1H NMR (400 MHz, $CDCl_3$) δ 0.83-0.90 (m, 6H), 1.26-1.37 (m, 11H), 1.52-1.55 (m, 2H), 1.64-1.67 (m, 2H), 2.76 (t, *J* = 8.0 Hz, 2H), 4.06 (t, *J* = 8.0 Hz, 2H), 4.34 (q, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 12.0 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 8.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 14.3, 14.7, 20.5, 22.8, 27.4, 29.4, 29.6, 31.7, 32.7, 44.7, 59.8, 60.8, 109.4, 122.7, 123.4, 123.5, 130.0, 139.5, 143.2, 167.7; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{21}H_{30}INO_2$ 455.13213. Found 455.13262.

Ethyl 2-*n*-hexyl-3-iodo-1-methylindole-5-carboxylate (48). The product was obtained as a yellow oil: ^1H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 6.0 Hz, 3H), 1.25-1.26 (m, 4H), 1.34-1.38 (m, 5H), 1.53 (q, *J* = 8.0 Hz, 2H), 2.78 (t, *J* = 8.0 Hz, 2H), 3.70 (s, 3H), 4.34 (q, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 8.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.7, 22.8, 27.4, 29.2, 29.4, 31.1, 31.8, 59.5, 60.9, 109.1, 122.8, 123.5, 123.6, 129.9, 140.3,

143.7, 167.7; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{18}H_{24}INO_2$ 413.08518. Found 413.08573.

Ethyl 1-*n*-butyl-2-(cyclohex-1-enyl)-3-iodoindole-5-carboxylate (49). The product was obtained as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.85 (t, *J* = 8.0 Hz, 3H), 1.21-1.27 (m, 2H), 1.35 (t, *J* = 8.0 Hz, 3H), 1.58-1.75 (m, 6H), 2.18-2.19 (m, 4H), 4.00 (q, *J* = 8.0 Hz, 2H), 4.33 (q, *J* = 8.0 Hz, 2H), 5.83 (m, 1H), 7.18 (d, *J* = 12.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 14.7, 20.3, 22.0, 22.9, 25.7, 29.6, 32.6, 45.1, 59.0, 60.8, 109.8, 122.7, 123.7, 124.0, 129.8, 130.1, 134.2, 139.2, 145.6, 167.7; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{21}H_{26}INO_2$ 451.10083. Found 451.10169.

Ethyl 2-(cyclohex-1-enyl)-3-iodo-1-methylindole-5-carboxylate (50). The product was obtained as a pale yellow solid: mp. 121-122 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.36 (t, *J* = 8.0 Hz, 3H), 1.68-1.77 (m, 4H), 2.17-2.22 (m, 4H), 3.64 (s, 3H), 4.34 (q, *J* = 8.0 Hz, 2H), 5.85 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 14.7, 20.0, 32.2, 45.2, 60.9, 61.2, 110.1, 123.2, 124.2, 124.5, 128.7, 134.2, 139.6, 139.6, 143.3, 167.6; IR (neat, cm^{-1}) 3378, 3057, 2925, 2853, 1453, 1433, 750; HRMS calcd for $C_{18}H_{20}INO_2$ 409.05388. Found 409.05434.

Methyl 3-iodo-1,2-diphenylindole-5-carboxylate (52). The product was obtained as a colorless solid: mp 185-186 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.97 (s, 3H), 7.14-7.18 (m, 2H), 7.21-7.26 (m, 1H), 7.30-7.38 (m, 8H), 7.94 (dd, *J* = 8.7, 1.8 Hz, 1H), 8.33 (d, *J* = 1.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 52.3, 63.4, 111.0, 123.8, 124.8, 125.1, 128.1, 128.2, 128.3, 128.8, 129.6, 130.7, 131.16,

131.19, 137.8, 141.0, 142.7, 167.9; IR (neat, cm^{-1}) 3057, 2949, 2849, 1712, 1596; HRMS *m/z* calcd for $C_{22}H_{16}INO_2$: 453.0226. Found: 453.0233.

1-Methyl-2-phenyl-3-(phenylethynyl)indole (53). This indole was prepared by the following procedure. Into a well mixed Et_3N solution (5 ml) containing 5.0 mmol of 3-iodo-1-methyl-2-phenylindole, 6.0 mmol of phenylacetylene and $PdCl_2(PPh_3)_2$ (5 mol %), CuI (2.5 mol %) was added and the flask was flushed with Ar, sealed and allowed to stir at room temperature for 2 h. The resulting precipitate was filtered off and washed with ethyl ether (10 ml). The combined ether layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum to afford a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.69 (s, 3H), 7.21-7.32 (m, 6H), 7.41-7.44 (m, 3H), 7.49 (t, *J* = 7.2 Hz, 2H), 7.65 (dd, *J* = 10.8, 2.0 Hz, 2H), 7.85 (dd, *J* = 10.4, 2.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 31.8, 84.5, 91.9, 110.0, 120.2, 121.0, 123.1, 124.7, 127.4, 128.1, 128.4, 128.5, 128.7, 129.0, 130.4, 131.0, 131.3, 137.4, 144.0; IR (neat, cm^{-1}) 3004, 2962, 2923, 2204; HRMS calcd for $C_{23}H_{17}N$ 307.13610. Found 307.13698.

1-Methyl-2,3-diphenylindole (54). This indole was prepared according to a literature procedure.[7] Into 10 ml of a 2:1 DMF/H_2O solution containing 5.0 mmol of 3-iodo-1-methyl-2-phenylindole, 5.0 mmol of Na_2CO_3 and 1.25 mmol of $NaBPh_4$ were added and the reaction mixture was stirred for 2 min. $Pd(OAc)_2$ (5 mol %) was then added and the flask was flushed with Ar, sealed and allowed to stir at 100 ^{o}C for 2 h. The resulting reaction mixture was extracted with ethyl ether (2 x 10 ml). The combined ether layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum to afford a white solid. Recrystallization afforded a 92 % yield of a crystalline solid. The product was obtained as white

needles: mp 113-114 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.67 (s, 3H), 7.16-7.39 (m, 13H), 7.80 (d, *J* = 10.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 31.1, 109.8, 115.3, 119.8, 120.4, 122.4, 125.7, 127.2, 128.2, 128.4, 128.6, 130.1, 131.4, 132.1, 135.4, 137.5, 137.9; IR (neat, cm^{-1}) 3058, 2923, 2849; HRMS calcd for $C_{21}H_{17}N$ 283.13610. Found 283.13690.

***n*-Butyl (*E*)-3-[1-methyl-2-phenylindol-3-yl]propenoate (55).** This indole was prepared by the following procedure. Into 1 ml of DMF containing 0.25 mmol of 3-iodo-1-methyl-2-phenylindole, 0.25 mmol of Na_2CO_3, 0.25 mmol of *n*-Bu_4NCl and 0.525 mmol of *n*-butyl acrylate were added and the reaction mixture was stirred for 2 min. $Pd(OAc)_2$ (5 mol %) was then added and the flask was flushed with Ar, sealed and allowed to stir at 80 ^{o}C for 24 h.[8] The resulting reaction mixture was extracted with ethyl ether (2 x 10 ml). The combined ether layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum to afford a pale yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.94 (t, *J* = 7.5 Hz, 3H), 1.37-1.44 (m, 2H), 1.62-1.67 (m, 2H), 3.61 (s, 3H), 4.15 (t, *J* = 6.6 Hz, 2H), 6.48 (d, *J* = 15.9 Hz, 1H), 7.32-7.40 (m, 5H), 7.50-7.53 (m, 3H), 7.72 (d, *J* = 16.2 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.0, 19.4, 31.1, 31.3, 64.0, 110.2, 110.6, 113.1, 120.9, 121.9, 123.2, 125.8, 128.8, 129.4, 130.2, 131.1, 138.1, 139.0, 145.6, 168.8; IR (neat, cm^{-1}) 3004, 2963, 2925, 1711; HRMS calcd for $C_{22}H_{23}NO_2$ 333.17288. Found 333.17370.

References

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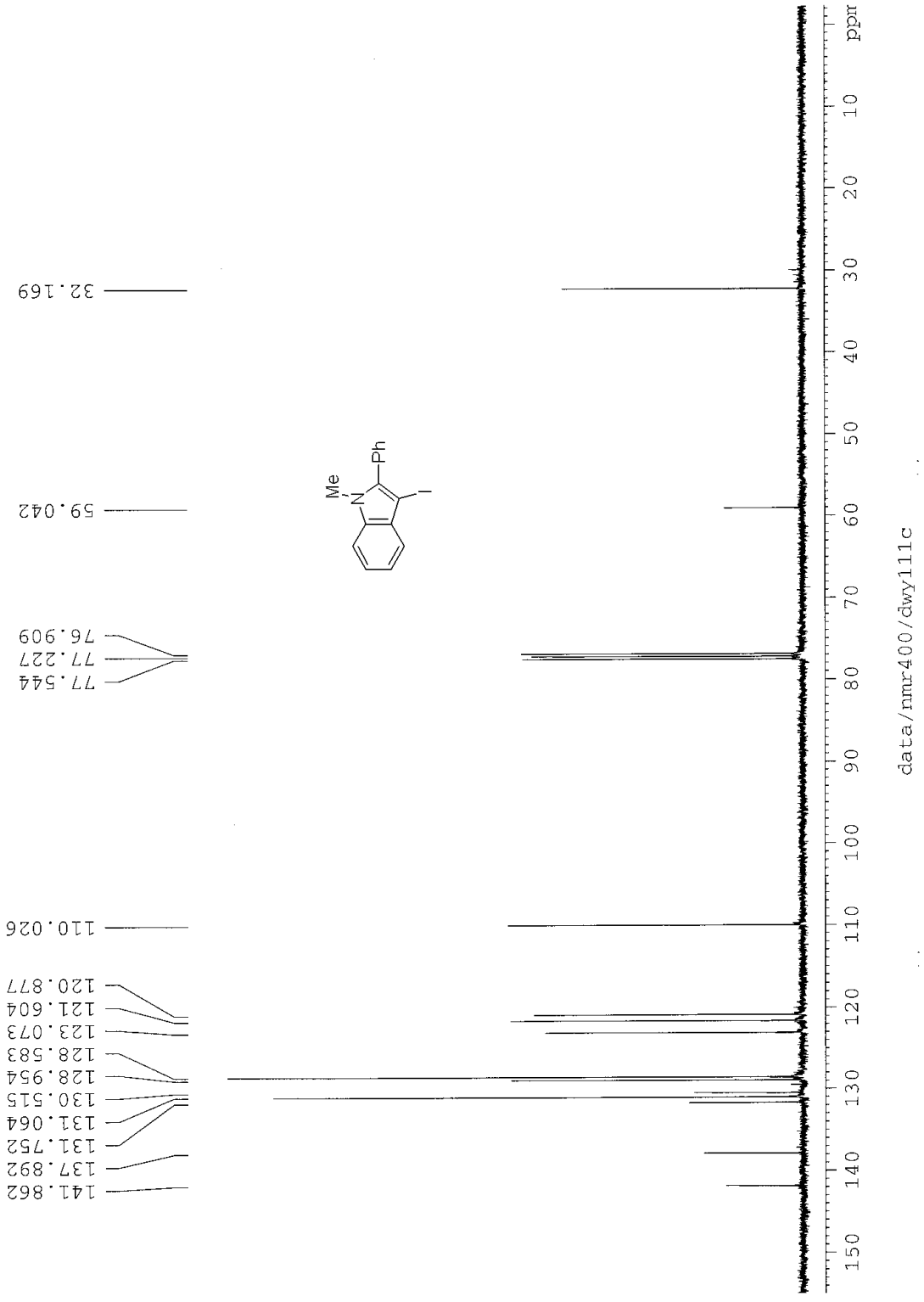
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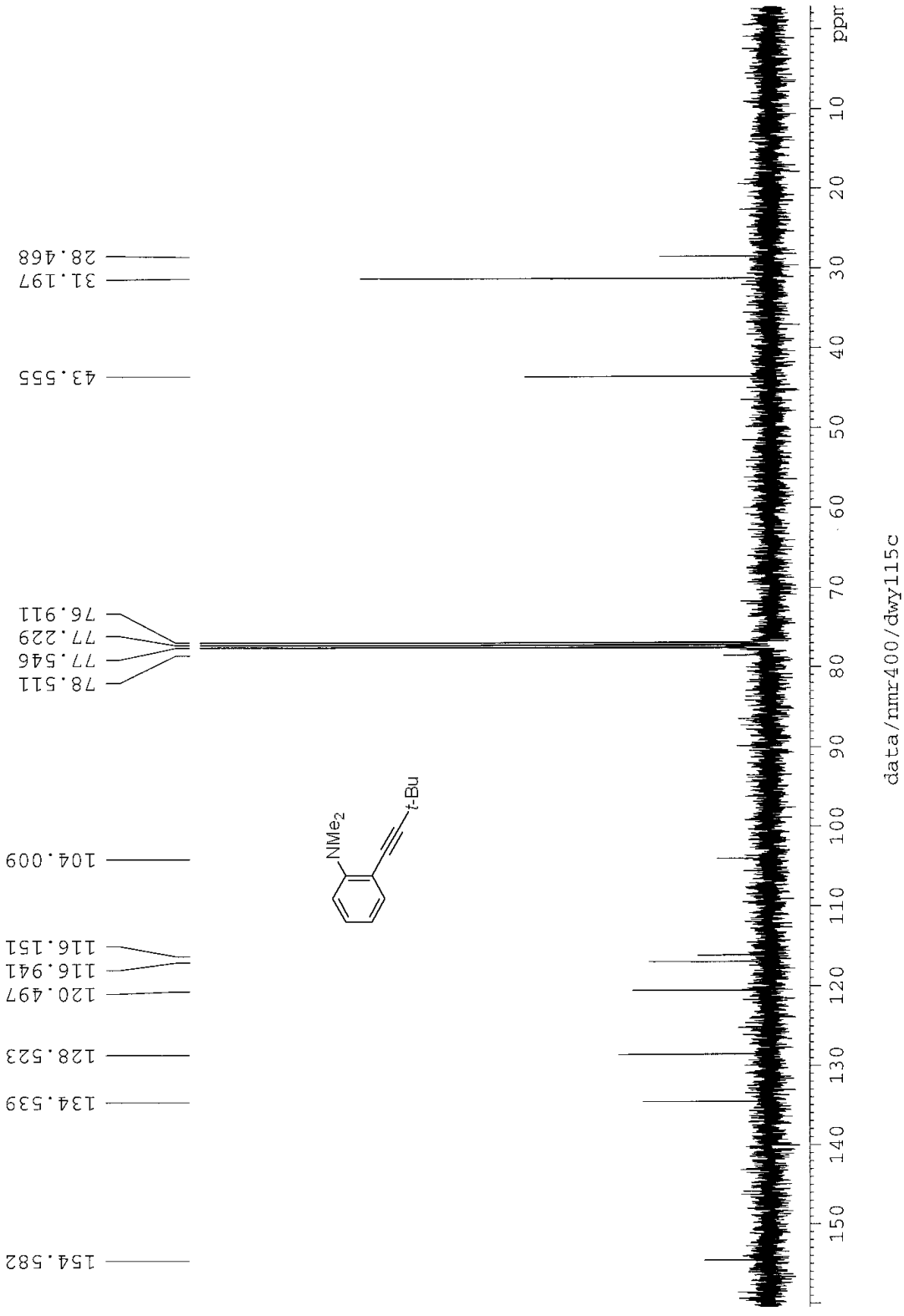
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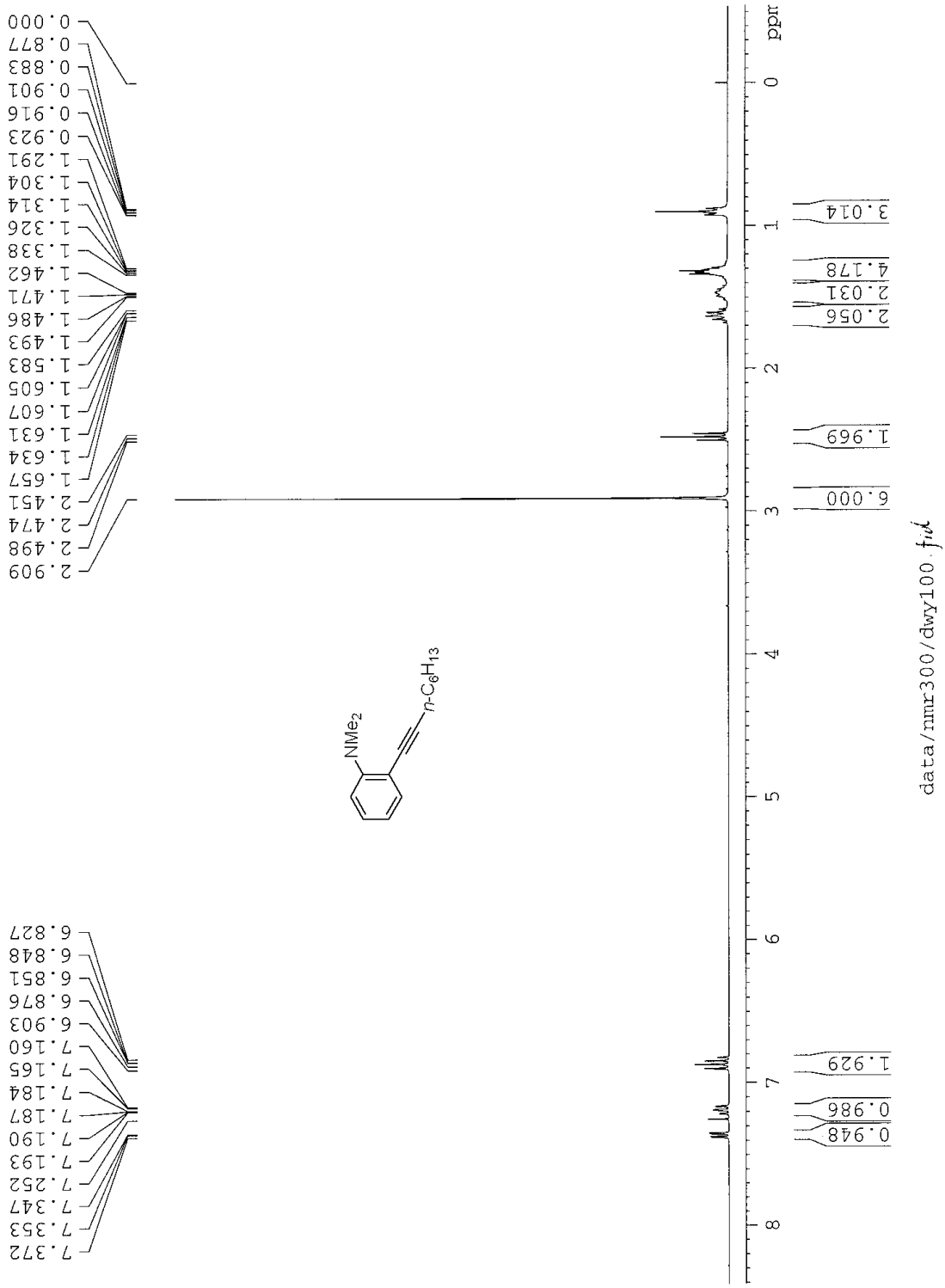
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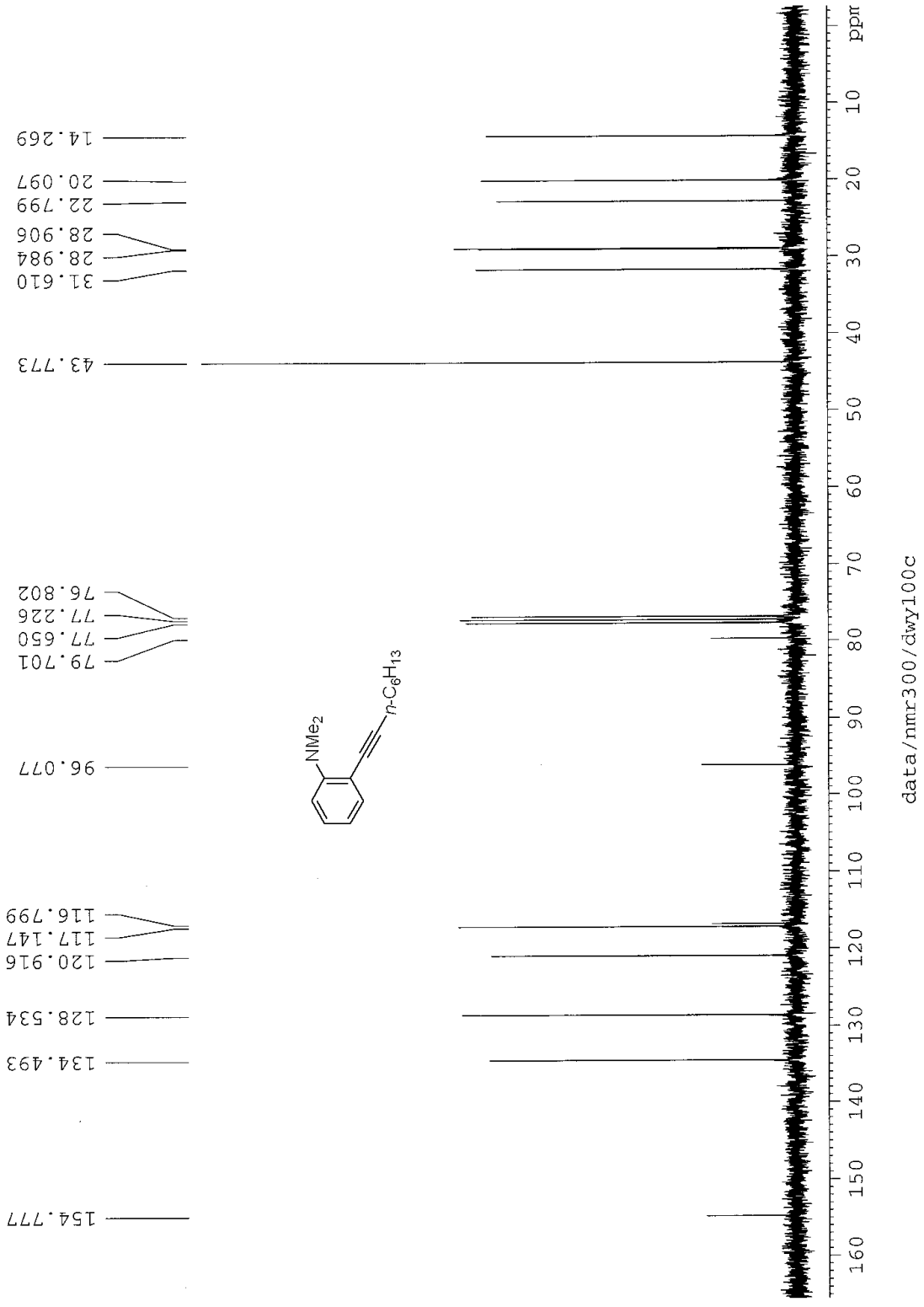
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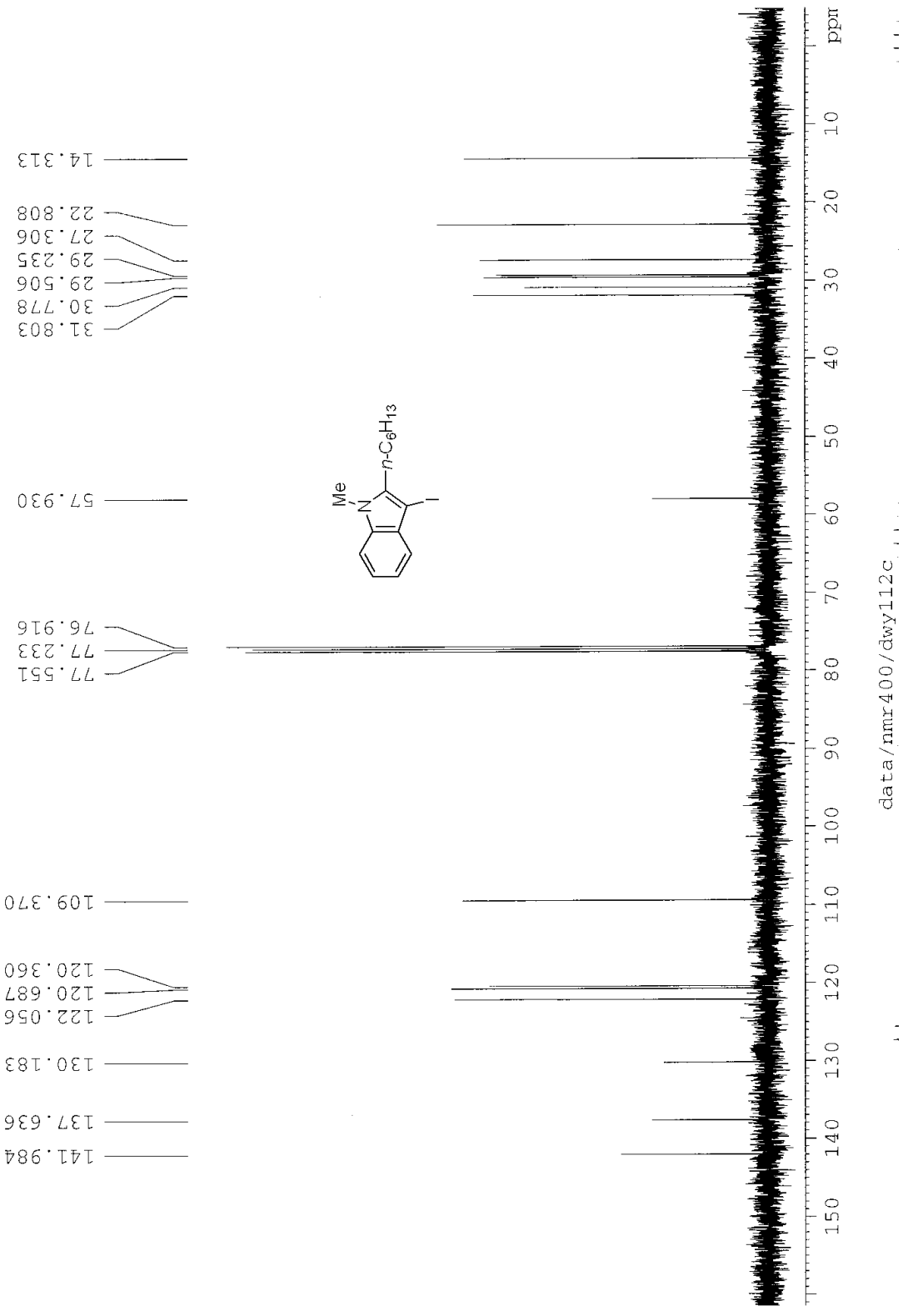
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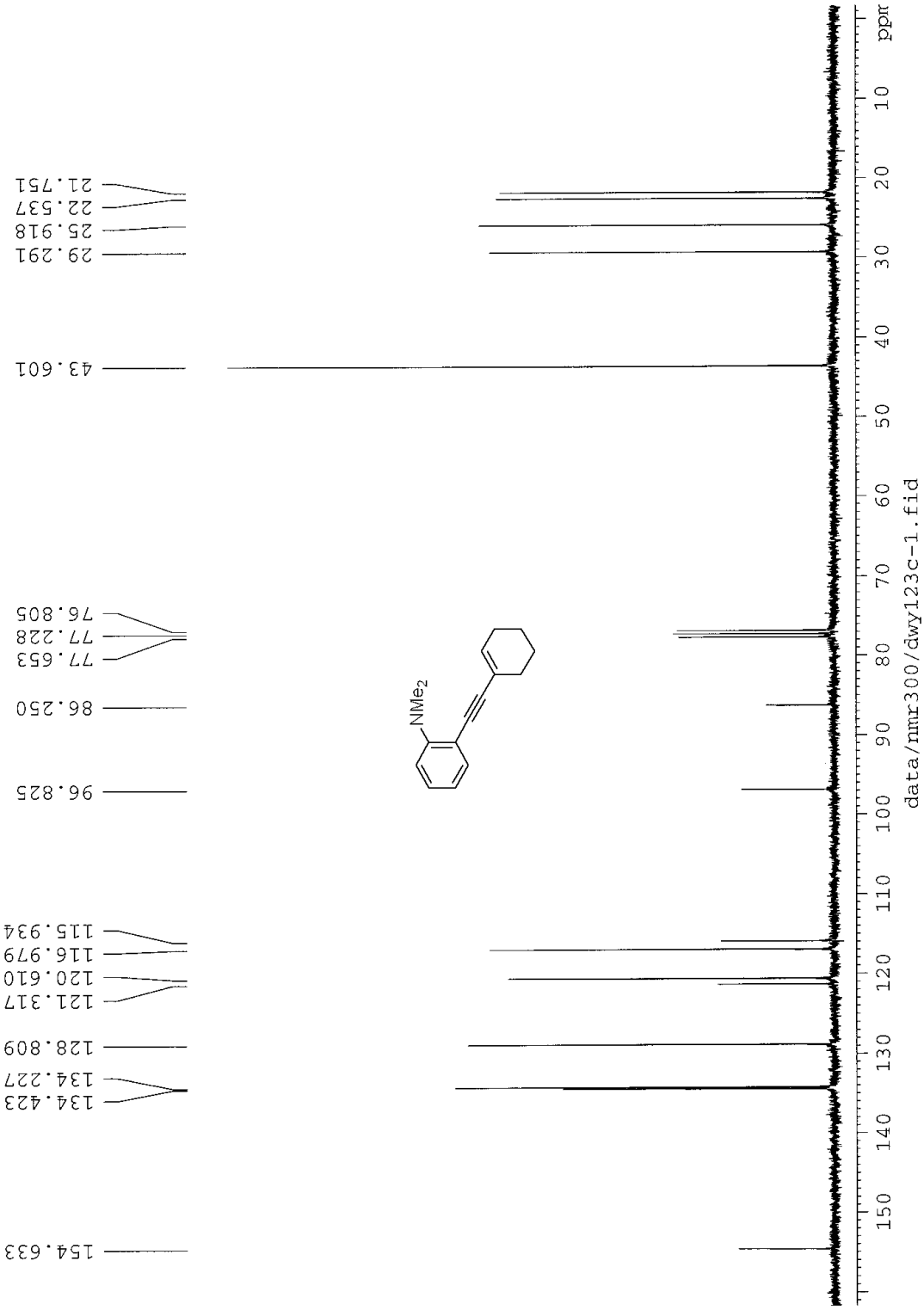
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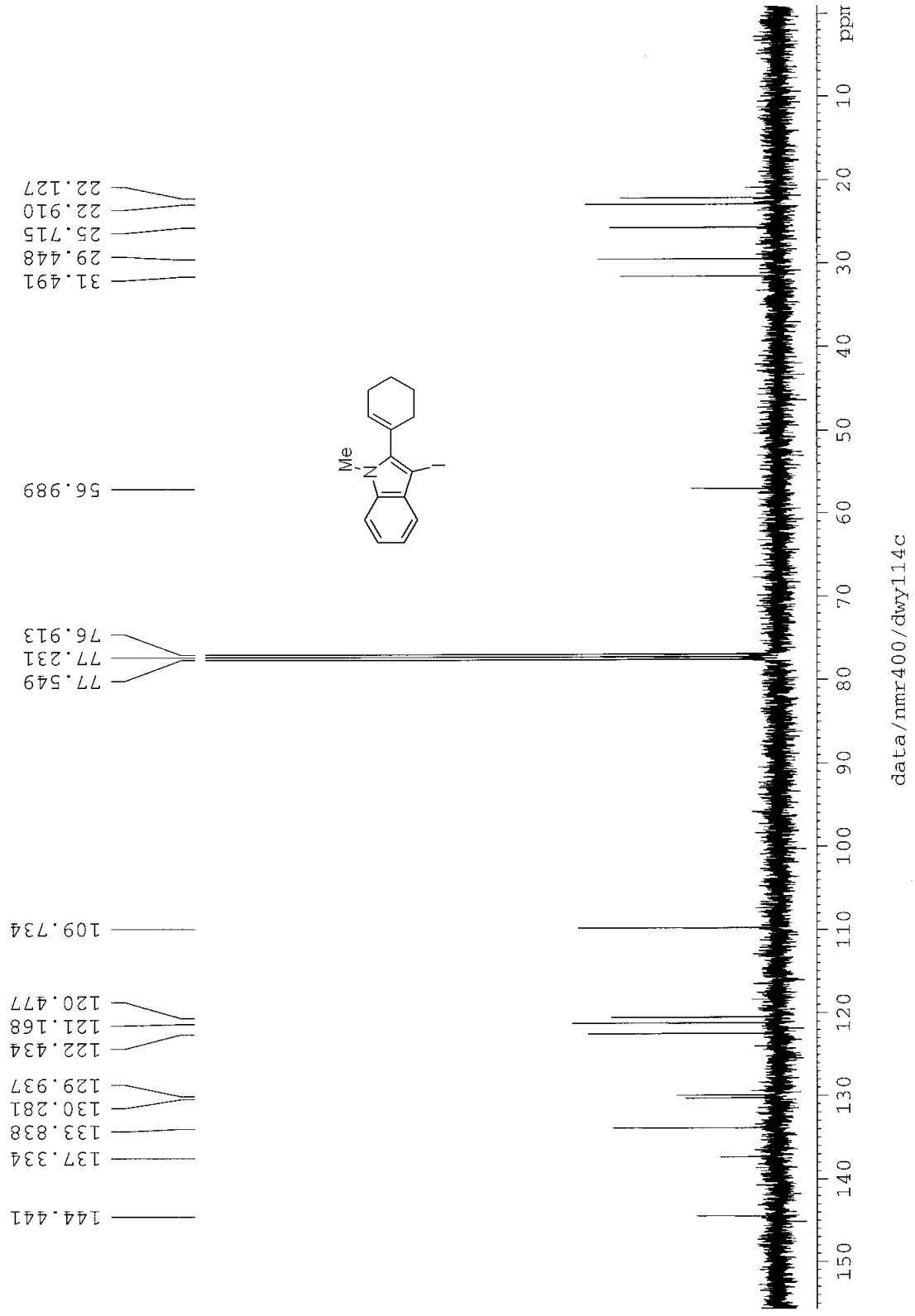
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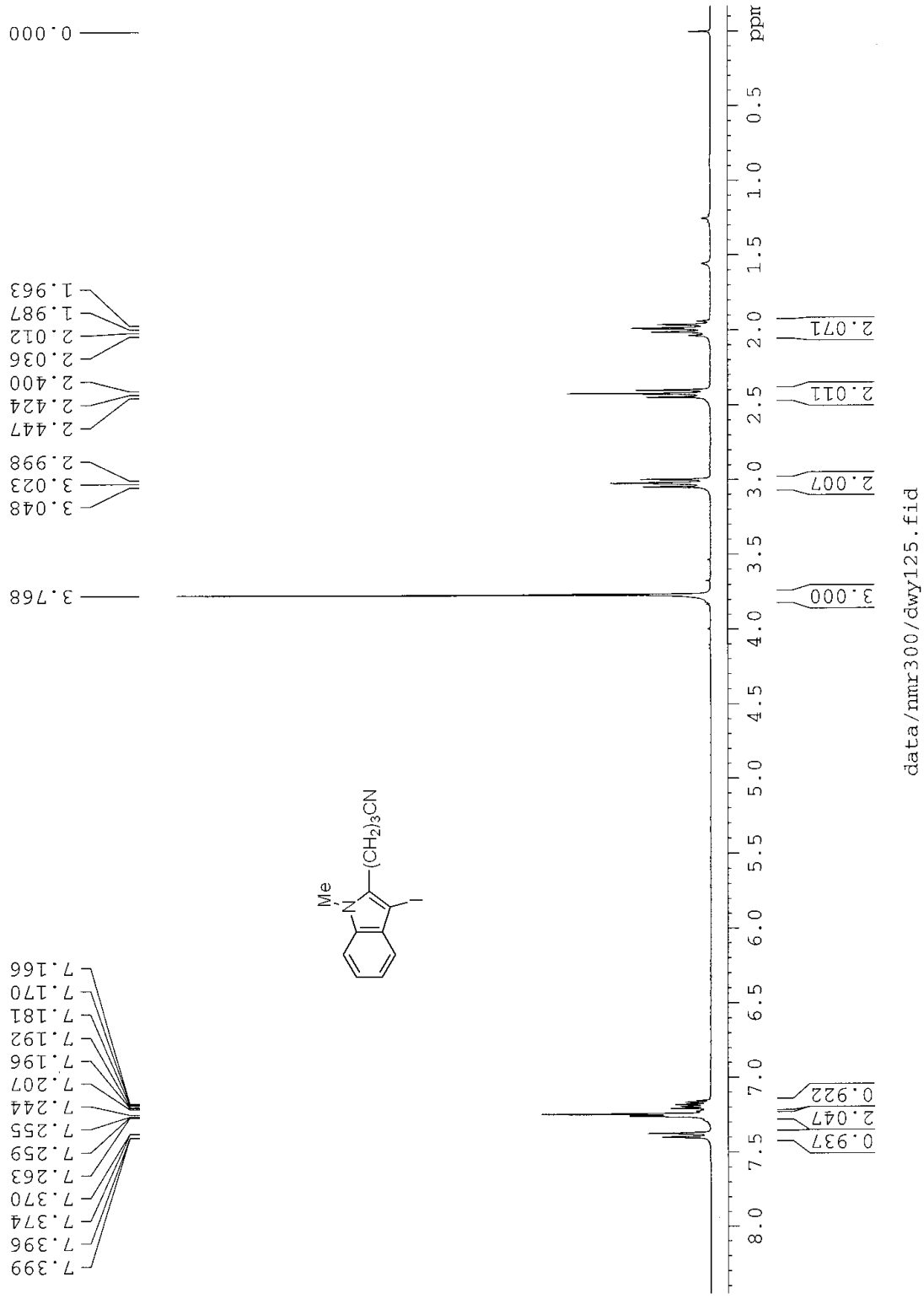
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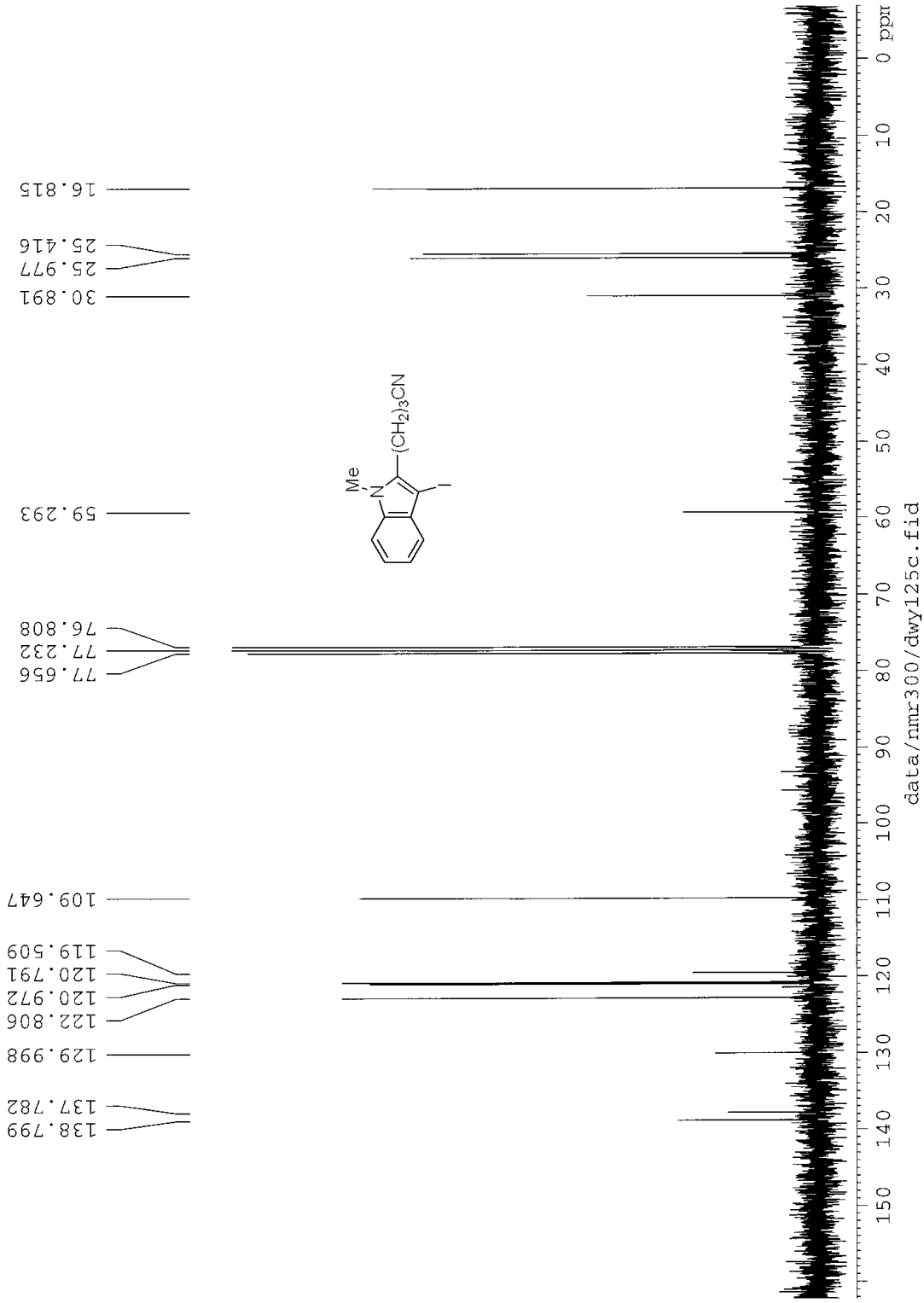
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76.808
77.232
77.656
109.647
119.509
120.791
120.972
122.806
129.998
137.782
138.799
Me
N
(CH2)3CN
I
0 ppm
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60
70
80
90
100
110
120
130
140
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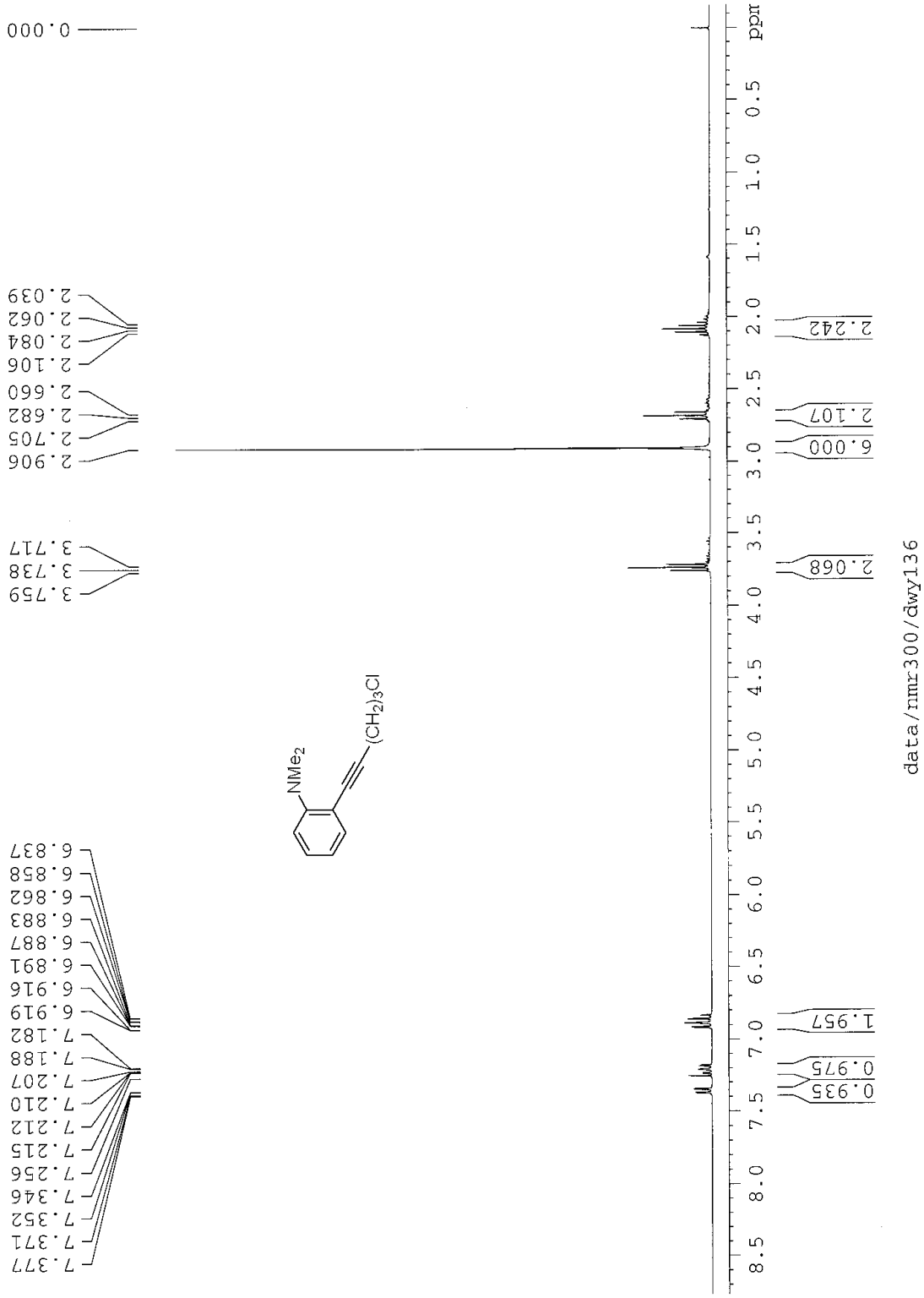
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6.837
6.858
6.862
6.883
6.887
6.891
6.916
6.919
7.182
7.188
7.207
7.210
7.212
7.215
7.256
7.346
7.352
7.371
7.377
NMe2
(CH2)3Cl
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.935
0.975
1.957
2.068
6.000
2.107
2.242
data/nmr300/dwy136

17.553
31.718
43.801
44.041
76.806
77.230
77.654
80.788
93.550
116.277
117.263
120.977
128.897
134.522
154.944
NMe2
(CH2)3Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
data/nmr300/dwy136c

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2.092
2.075
2.072
2.054
2.038
3.004
3.023
3.042
3.583
3.599
3.614
3.628
3.664
3.755
7.145
7.155
7.165
7.175
7.184
7.224
7.232
7.368
7.388
Me
N
(CH2)3Cl
I
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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2.101
0.965
3.000
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2.007
2.338
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24.602
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32.308
44.382
58.558
76.916
77.233
77.551
109.559
120.612
120.810
122.485
130.114
137.698
140.005
Me
N
(CH2)3Cl
I
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr400/dwy129c

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6.961
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I
O2N
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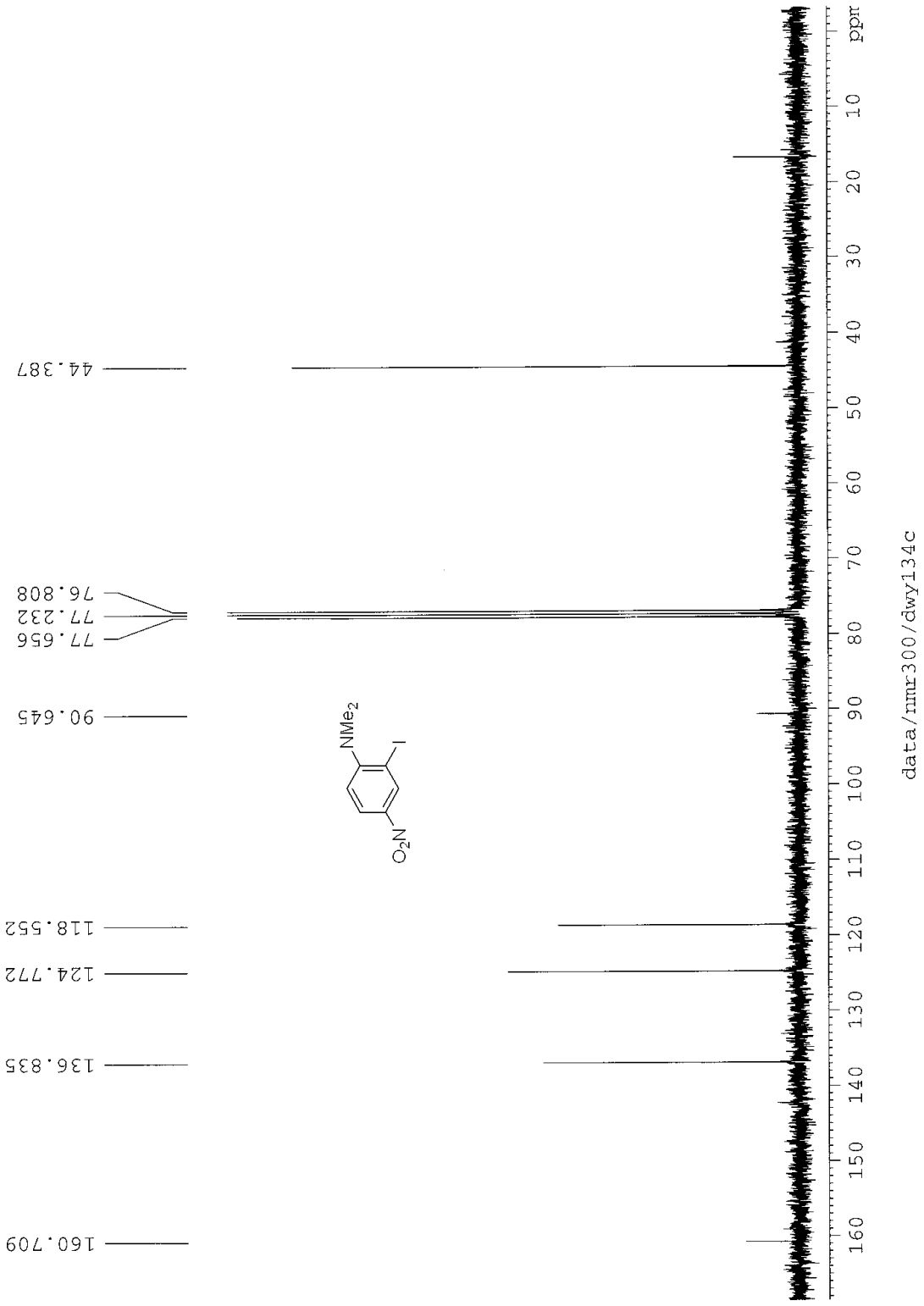
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76.808
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I
O2N
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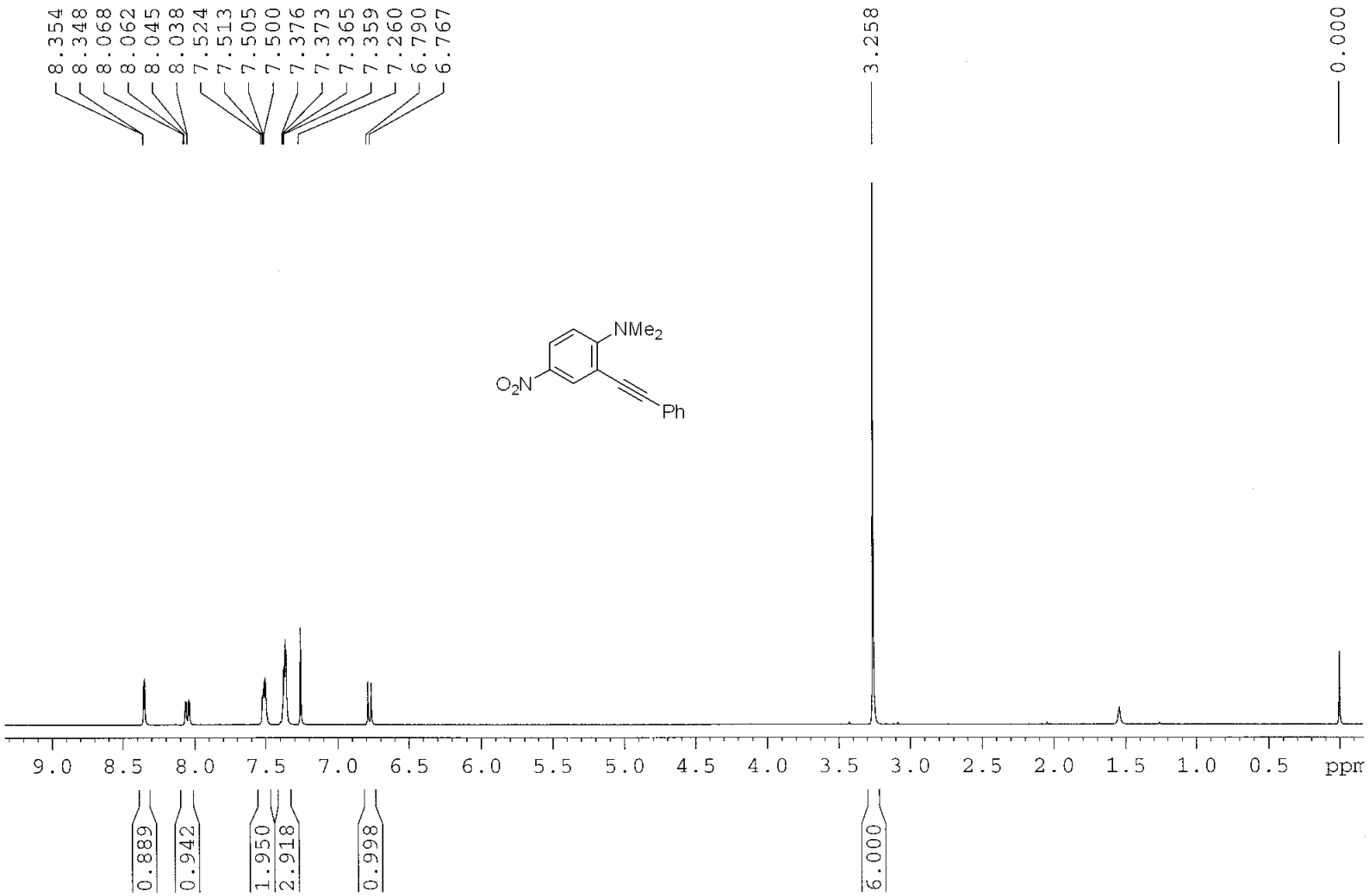
ppm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7.524
7.513
7.505
7.500
7.376
7.373
7.365
7.359
7.260
6.790
6.767
3.258
0.000
NMe2
O2N
Ph
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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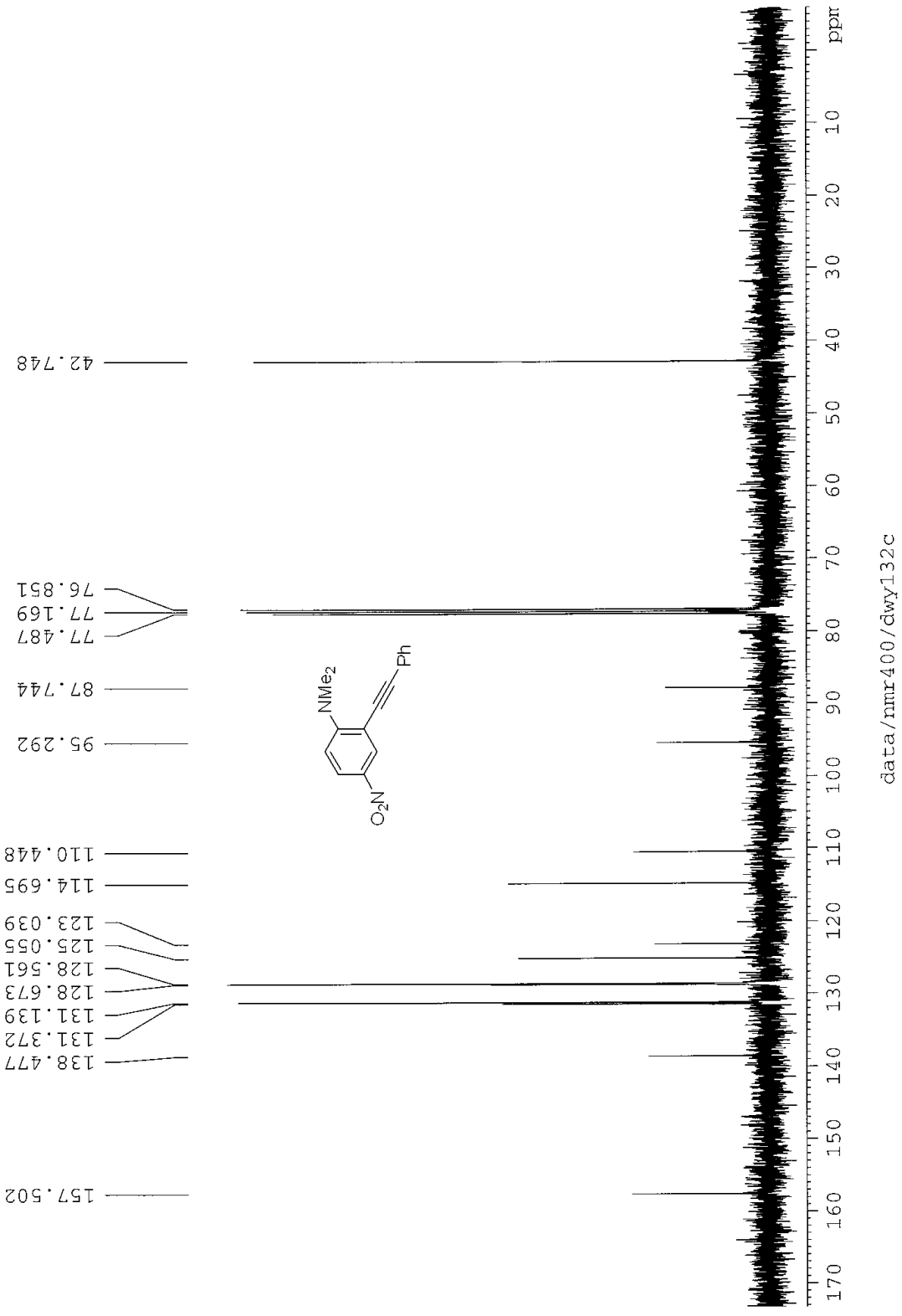
2.918
0.998
6.000
data/nmr400/dwy132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77.169
77.487
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110.448
114.695
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125.055
128.561
128.673
131.139
131.372
138.477
157.502
NMe2
Ph
O2N
data/nmr400/dwy132c
ppm

8.474
8.473
8.466
8.465
8.218
8.210
8.188
8.180
7.569
7.568
7.565
7.554
7.551
7.547
7.545
7.543
7.539
7.487
7.479
7.478
7.461
7.455
7.381
7.380
7.351
7.350
0.000
3.741
Me
N
Ph
I
O2N
ppm
1
2
3
4
5
6
7
8
9
10
3.000
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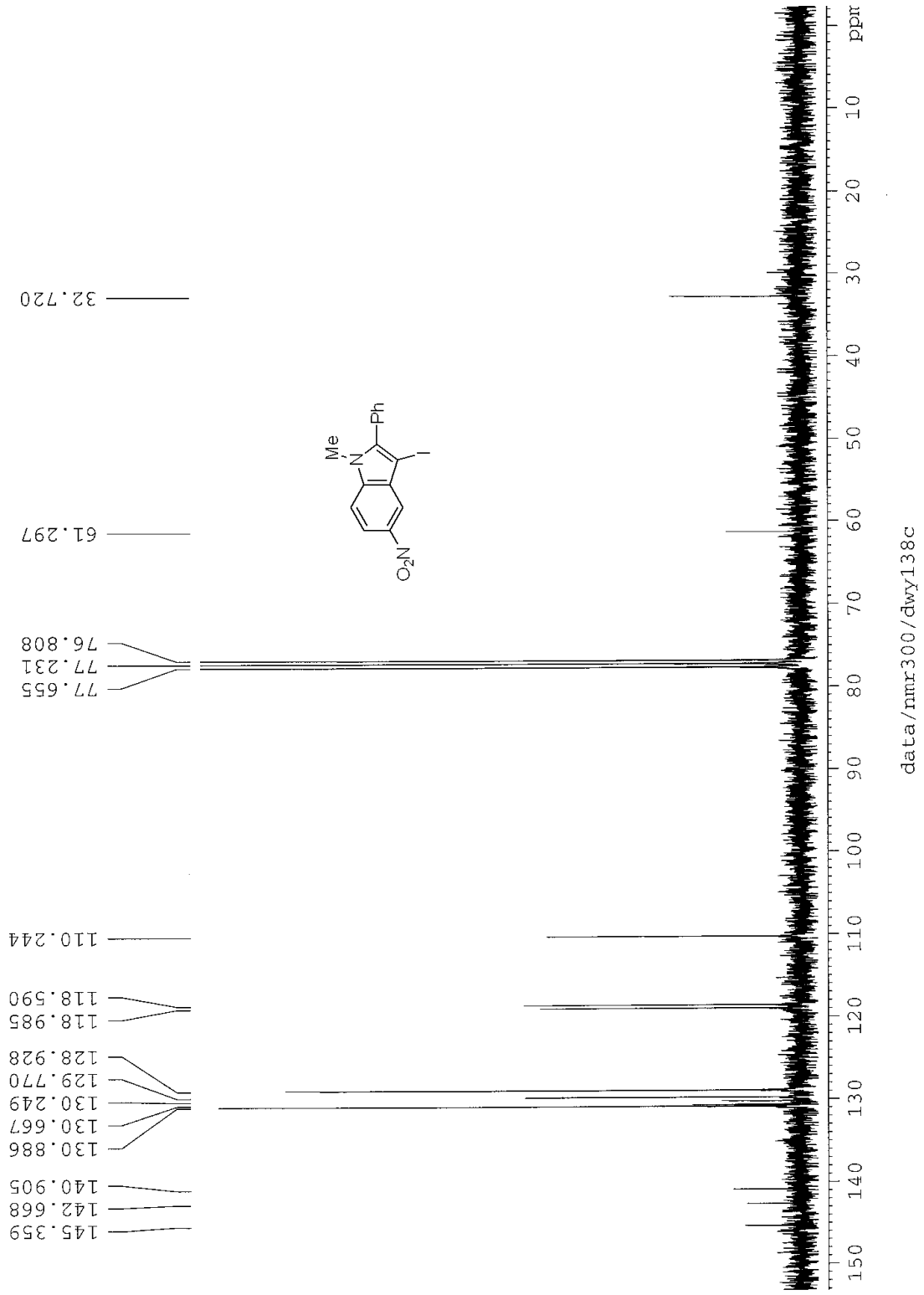
2.978
0.956
0.879
data/nmr300/dwy138-1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140.905
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129.770
128.928
118.985
118.590
110.244
77.655
77.231
76.808
61.297
32.720
Me
N
Ph
I
O2N
ppm
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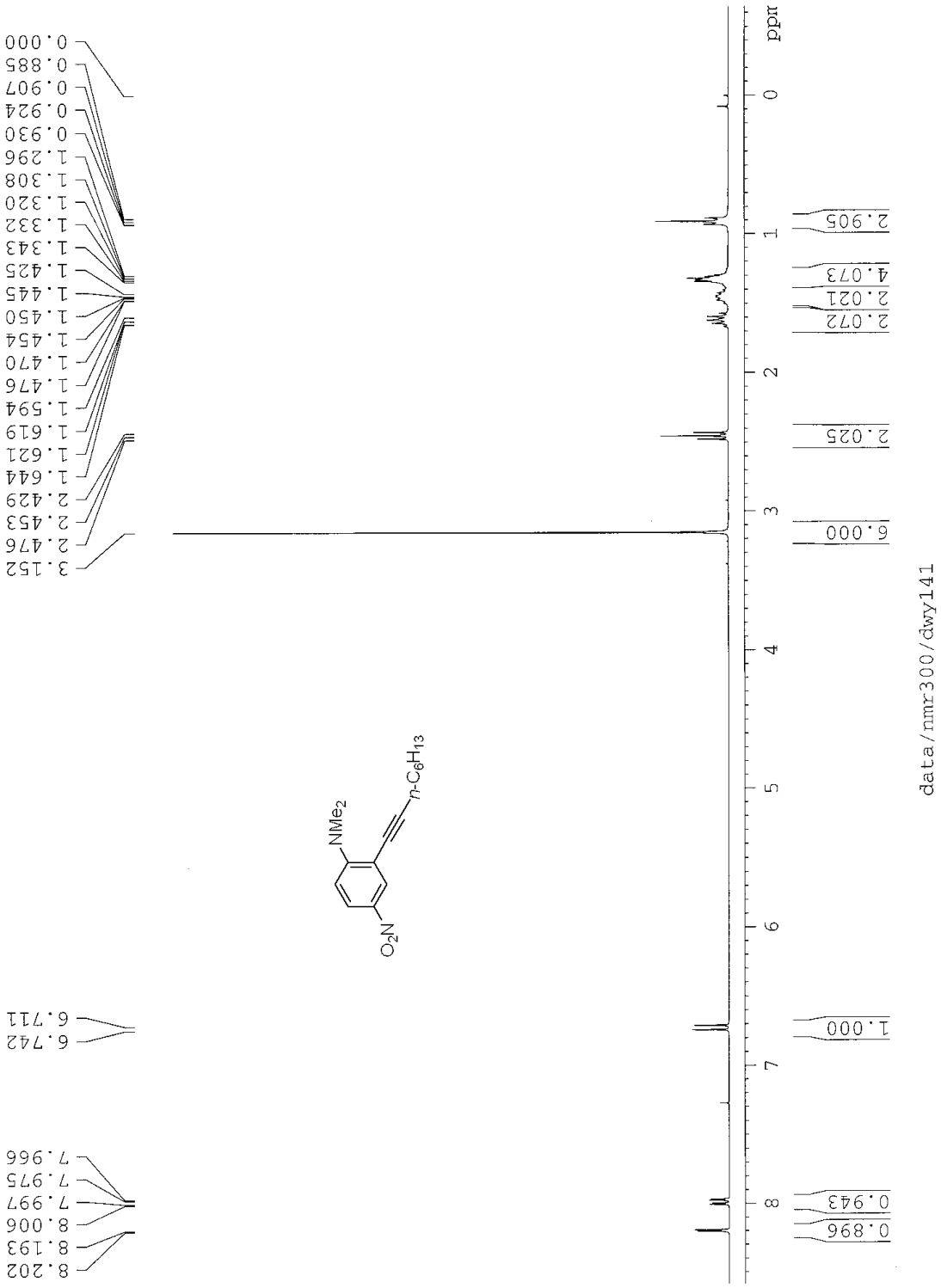
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr300/dwy138c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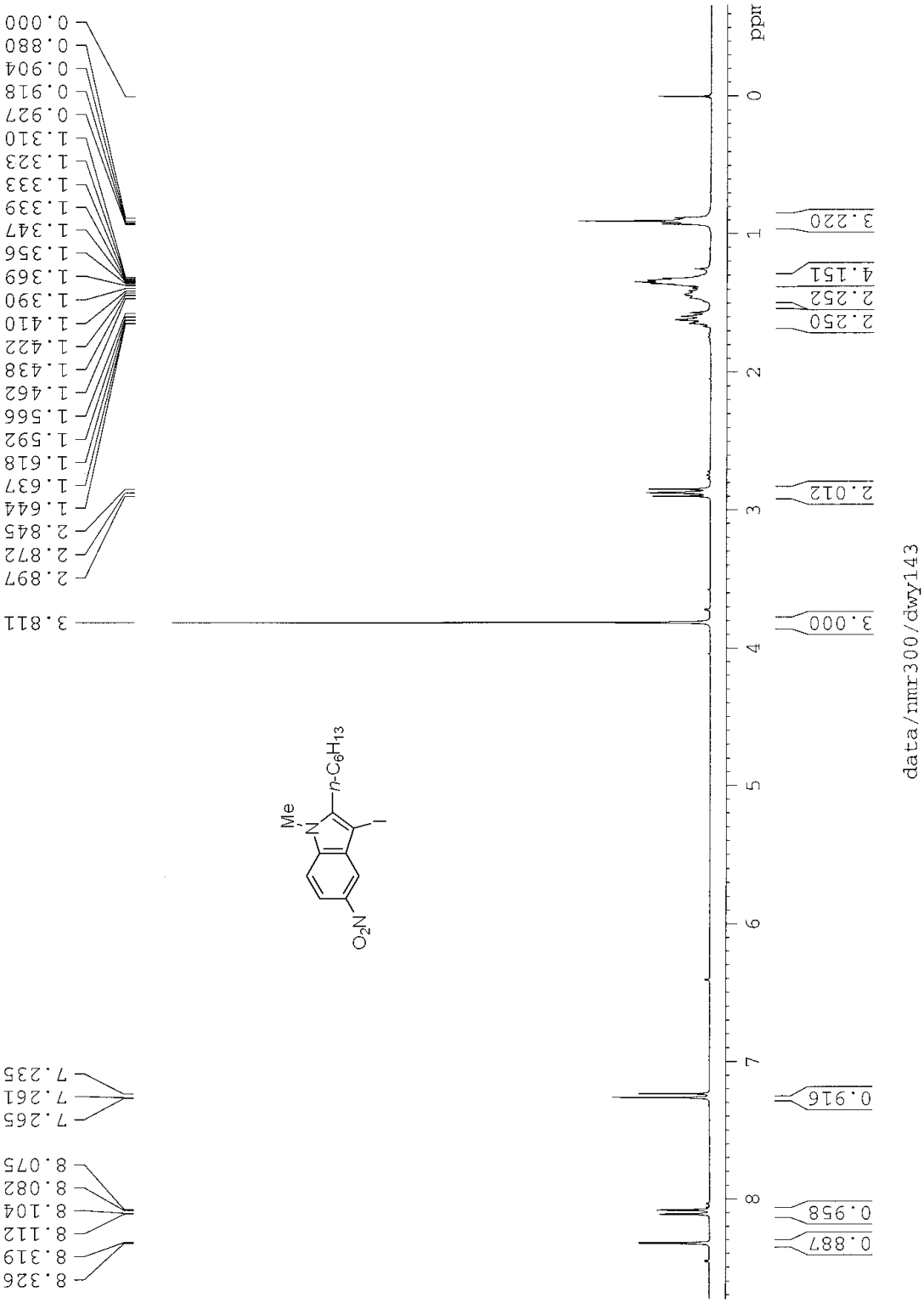
8.193
8.006
7.997
7.975
7.966
6.742
6.711
3.152
2.476
2.453
2.429
1.644
1.621
1.619
1.594
1.476
1.470
1.454
1.450
1.445
1.425
1.343
1.332
1.320
1.308
1.296
0.930
0.924
0.907
0.885
0.000
NMe2
n-C6H13
O2N
ppm
0
1
2
3
4
5
6
7
8
0.896
0.943
1.000
2.905
4.073
2.021
2.072
2.025
6.000
data/nmr300/dwy141

14.219
19.891
22.725
28.652
28.894
31.508
42.784
76.806
77.229
77.653
78.735
97.280
112.361
114.897
124.477
131.381
138.890
158.034
NMe2
n-C6H13
O2N
ppm
data/nmr300/dwy141c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1.333
1.339
1.347
1.356
1.369
1.390
1.410
1.422
1.438
1.462
1.566
1.592
1.618
1.637
1.644
2.845
2.872
2.897
3.811
7.235
7.261
7.265
8.075
8.082
8.104
8.112
8.319
8.326
Me
N
n-C6H13
I
O2N
ppm
0
1
2
3
4
5
6
7
8
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0.916
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2.252
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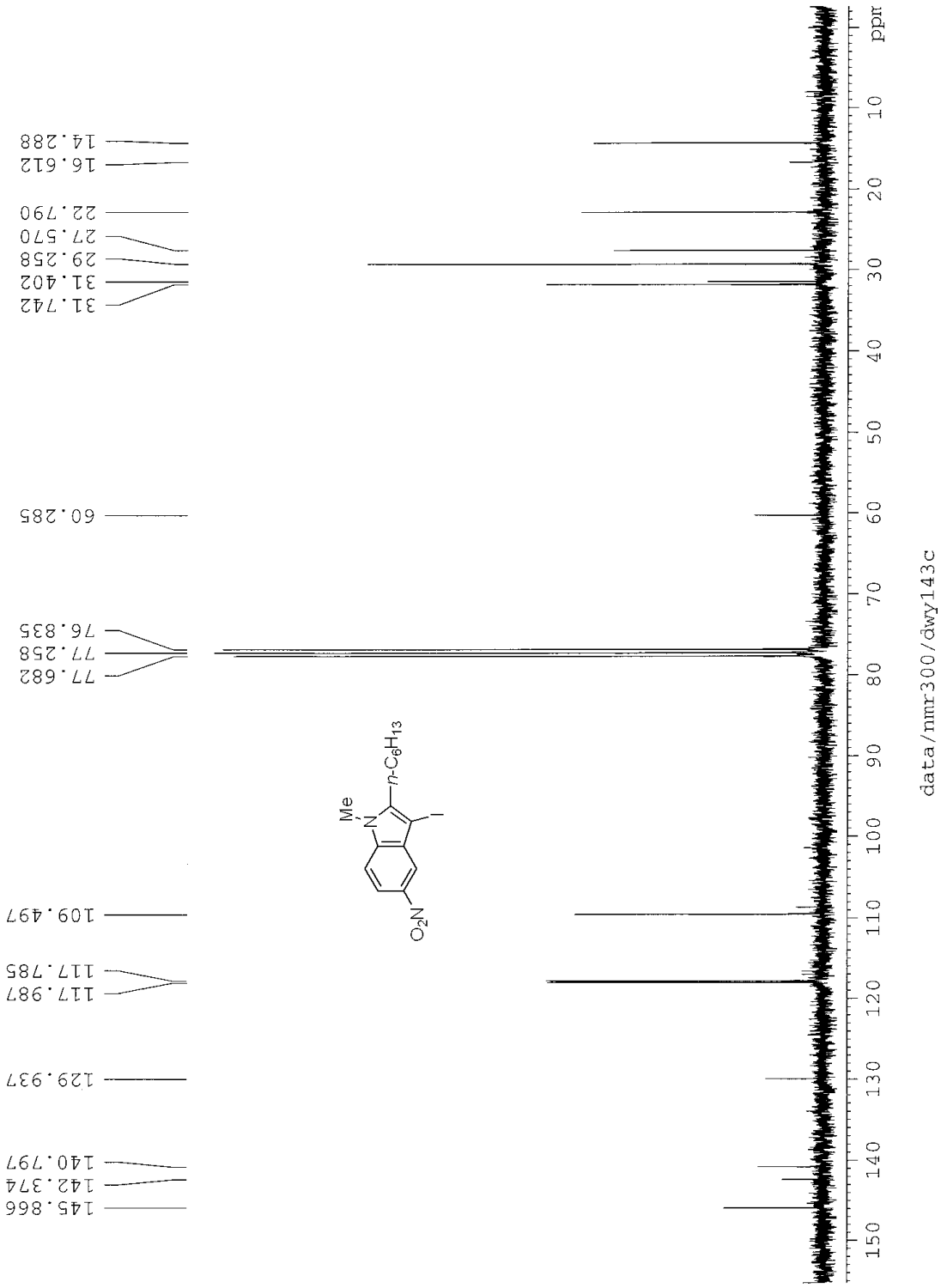
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31.402
31.742
60.285
76.835
77.258
77.682
109.497
117.785
117.987
129.937
140.797
142.374
145.866
Me
N
n-C6H13
I
O2N
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr300/dwy143c

0.002
2.745
3.775
7.695
7.673
6.664
6.658
6.388
6.384
6.369
6.366
6.362
NMe2
I
MeO
6.000
3.031
0.936
0.946
0.915
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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45.032
55.540
76.911
77.231
77.550
85.424
107.781
110.008
140.345
156.120
160.920
NMe2
I
MeO
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
data/nmr400/dwy160c

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1.597
1.602
1.611
1.616
1.626
1.631
1.641
1.646
1.656
1.660
1.671
1.675
1.684
2.123
2.133
2.138
2.221
2.236
2.240
2.924
3.779
6.132
6.138
6.142
6.146
6.152
6.380
6.386
6.407
7.283
7.304
NMe2
MeO
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.921
1.904
0.960
3.060
6.000
2.007
2.020
4.060
data/nmr400/dwy166

21.781
22.564
25.879
29.356
43.434
55.335
76.912
77.230
77.547
86.228
95.306
103.825
105.191
108.341
121.431
133.583
135.276
156.036
160.299
NMe2
MeO
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
data/nmr400/dwy166c

0.000
1.718
1.731
1.745
1.793
1.804
1.817
2.223
2.237
2.249
2.256
2.264
3.612
3.859
5.868
6.699
6.704
6.807
6.812
6.828
6.833
7.260
7.282
Me
N
I
MeO
ppm
0.950
0.972
1.002
1.017
3.000
3.186
4.202
4.311
data/nmr400/dwy167

22.121
22.917
25.702
29.510
31.527
56.044
56.530
76.915
77.232
77.550
93.440
110.084
121.768
124.622
129.967
133.672
137.826
143.454
157.000
Me
N
I
MeO
ppm
10
20
30
40
50
60
70
80
90
100
110
120
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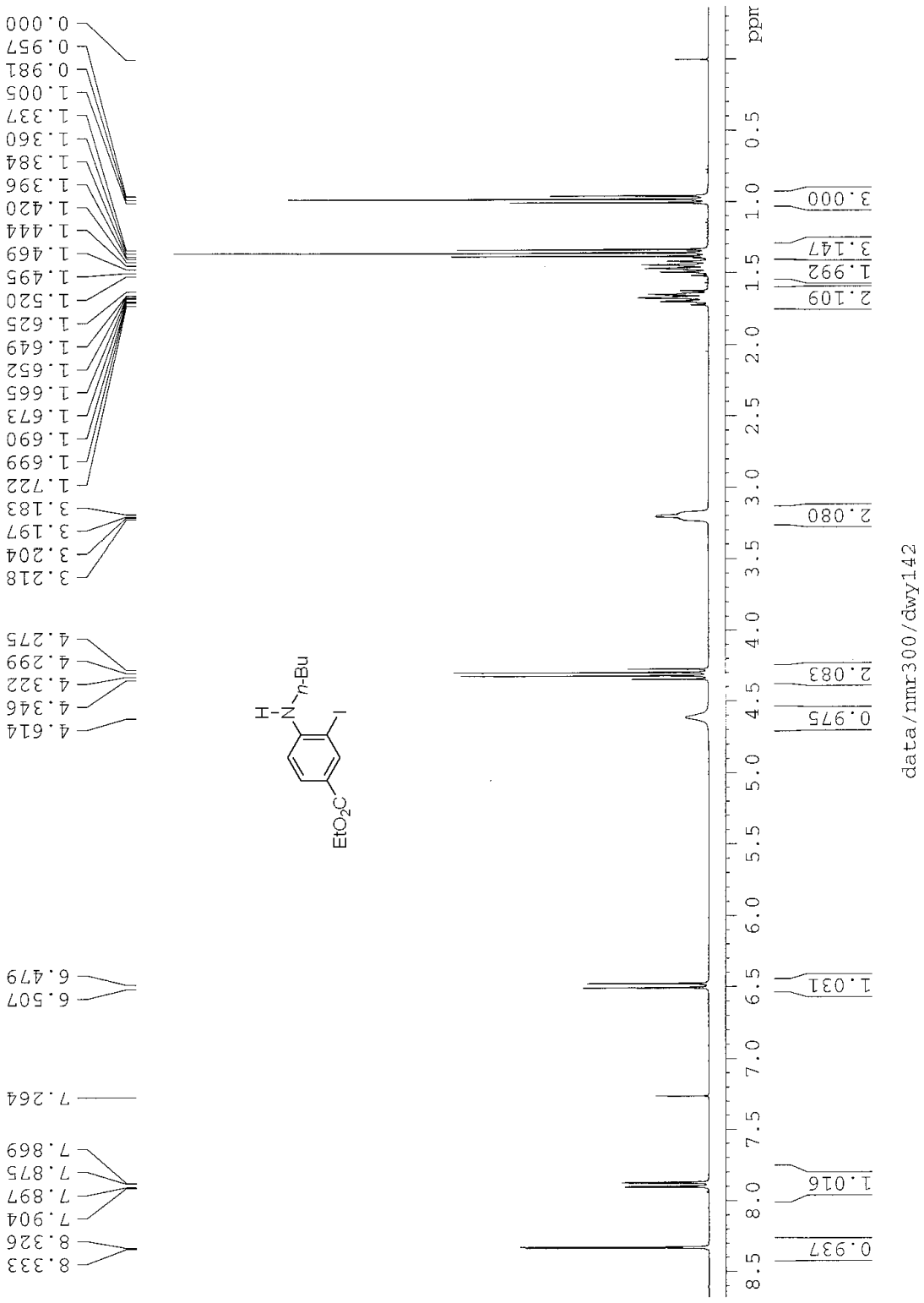
140
150
160
170
data/nmr400/dwy167c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4.299
4.275
3.218
3.204
3.197
3.183
1.722
1.699
1.690
1.673
1.665
1.652
1.649
1.625
1.520
1.495
1.469
1.444
1.420
1.396
1.384
1.360
1.337
1.005
0.981
0.957
0.000
0.937
1.016
1.031
0.975
2.083
2.080
2.109
1.992
3.147
3.000
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H-N
n-Bu
I
EtO2C

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20.412
31.233
43.777
60.666
76.807
77.231
77.654
83.768
108.873
119.955
131.663
140.836
150.695
165.747
H
N
n-Bu
I
EtO2C
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
data/nmr300/dwy142c

8.499
8.492
7.974
7.967
7.946
7.939
7.034
7.006
4.381
4.357
4.334
4.310
3.054
3.030
3.004
2.780
1.589
1.563
1.538
1.531
1.401
1.377
1.353
1.348
1.321
1.297
0.932
0.908
0.883
0.000
0.916
0.979
1.015
2.050
2.065
3.078
2.198
5.102
3.000
ppm
Me
N
n-Bu
I
EtO2C
data/nmr300/dwy145

14.155
14.573
20.418
29.686
41.942
56.127
61.160
76.806
77.229
77.653
95.739
120.697
126.228
130.519
142.002
158.882
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Me
N
n-Bu
I
EtO2C
ppm
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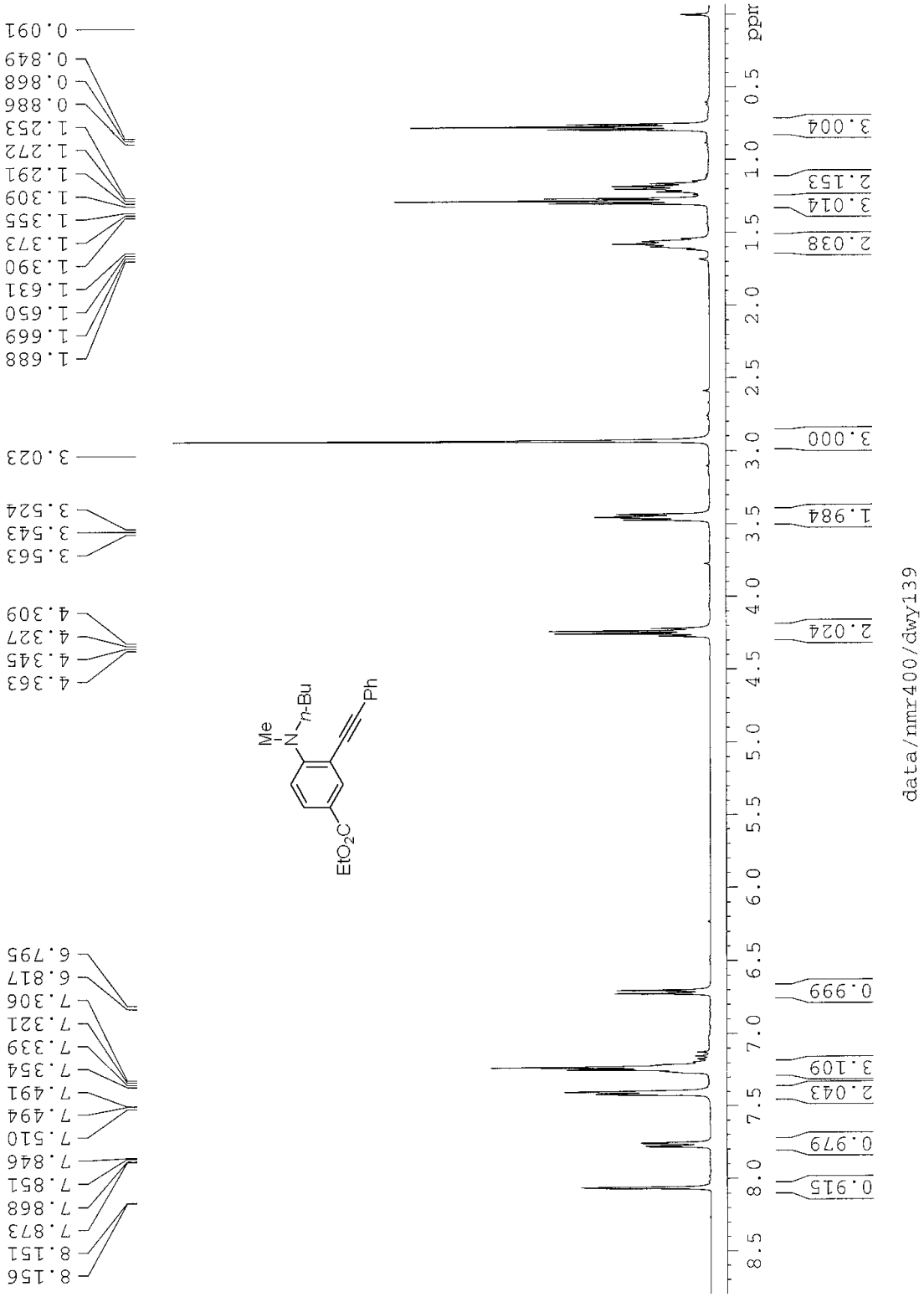
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7.491
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7.339
7.321
7.306
6.817
6.795
4.363
4.345
4.327
4.309
3.563
3.543
3.524
3.023
1.688
1.669
1.650
1.631
1.390
1.373
1.355
1.309
1.291
1.272
1.253
0.886
0.868
0.849
0.091
Me
N
n-Bu
Ph
EtO2C
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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0.999
2.024
1.984
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3.014
2.153
3.004
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54.925
60.665
76.914
77.231
77.549
88.952
94.224
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115.847
120.495
123.813
128.249
128.507
130.831
131.279
137.137
156.630
166.249
Me
N
n-Bu
Ph
EtO2C
ppm
data/nmr400/dwy139c

8.165
7.917
7.896
7.433
7.418
7.353
7.338
7.261
7.239
4.354
4.337
4.319
4.021
4.003
3.985
1.506
1.489
1.471
1.375
1.358
1.340
1.069
1.051
1.033
1.015
0.686
0.668
0.650
0.000
Bu-n
N
Ph
I
EtO2C
0.917
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1.986
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2.018
3.000
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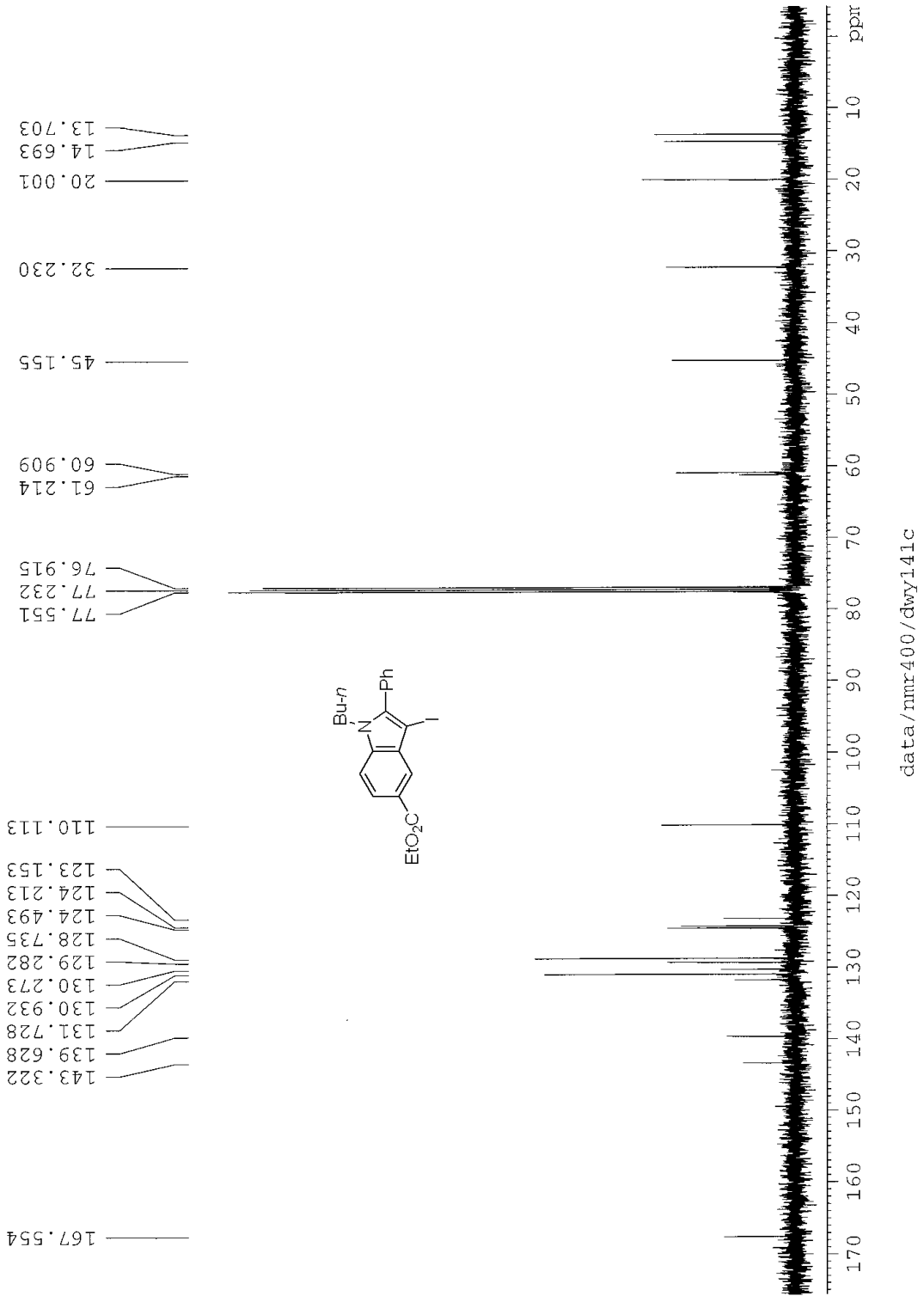
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77.551
110.113
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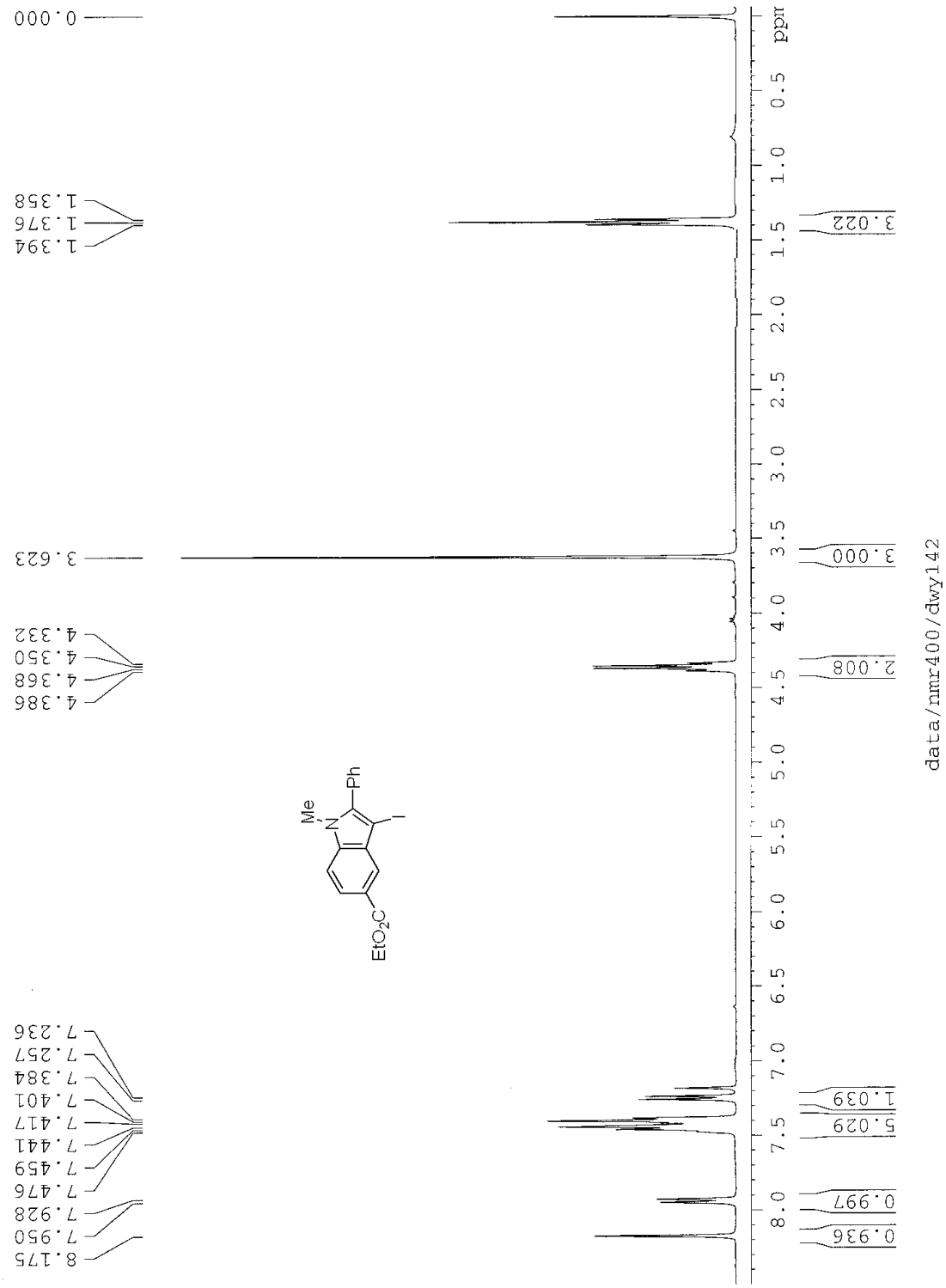
124.213
124.493
128.735
129.282
130.273
130.932
131.728
139.628
143.322
167.554
Bu-n
Ph
I
EtO2C
ppm
data/nmr400/dwy141c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7.441
7.417
7.401
7.384
7.257
7.236
4.386
4.368
4.350
4.332
3.623
1.394
1.376
1.358
0.000
Me
N
Ph
I
EtO2C
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3.000
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ppm
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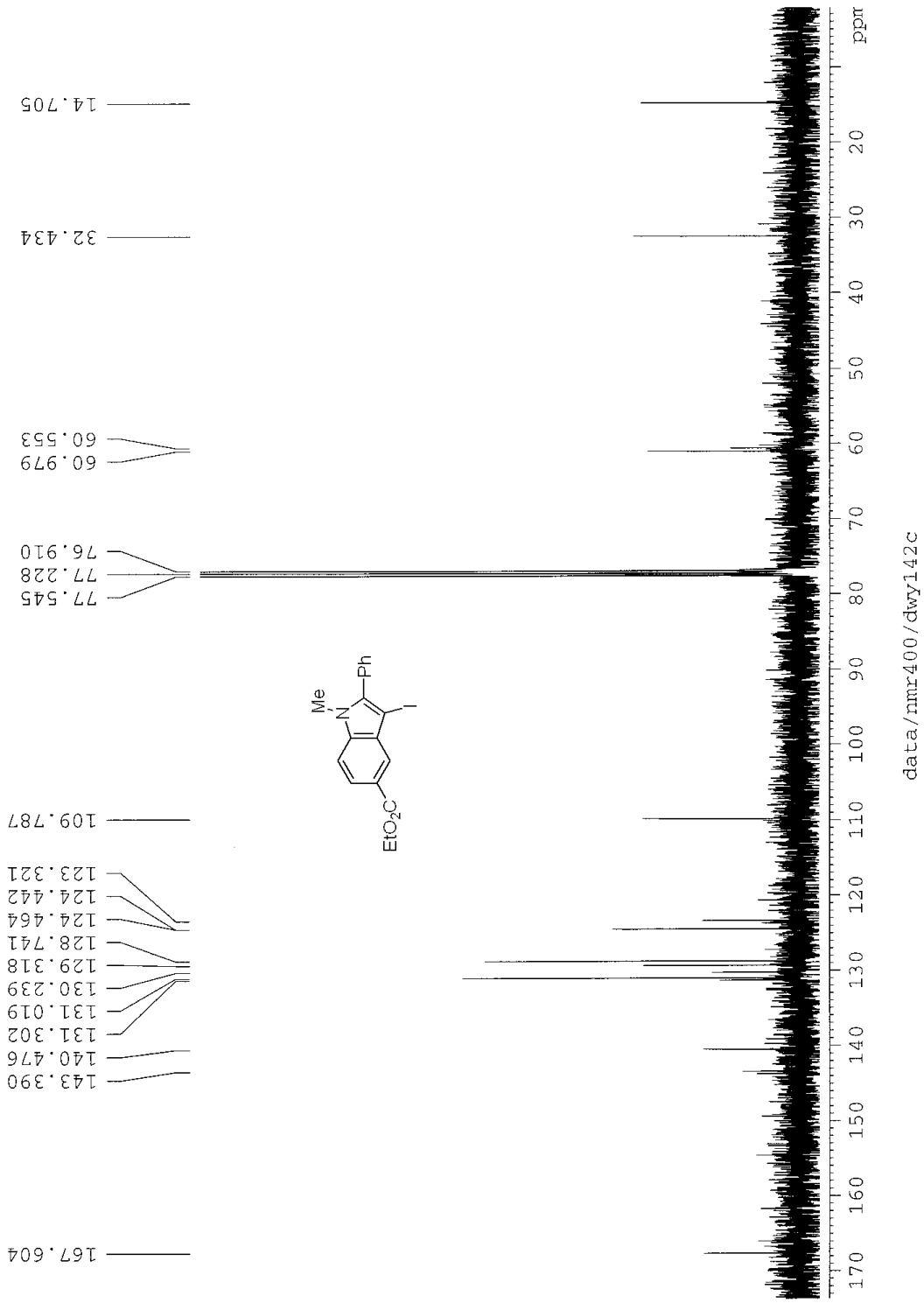
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77.545
109.787
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129.318
130.239
131.019
131.302
140.476
143.390
167.604
Me
N
Ph
I
EtO2C
ppm
data/nmr400/dwy142c

0.000
3.678
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7.210
7.232
7.234
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7.258
7.262
7.266
7.282
7.287
7.309
7.406
7.411
7.433
7.435
7.438
7.467
7.492
7.516
7.520
7.631
7.635
7.640
7.658
7.663
7.834
7.836
7.841
7.863
7.866
Me
N
Ph
Ph
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6
7
8
9
10
1.000
2.067
2.205
3.035
6.492
data/nmr300/dwy161

31.775
76.808
77.232
77.656
84.463
91.924
96.940
110.037
120.198
120.987
123.076
124.718
127.368
128.375
128.530
128.664
128.942
130.422
130.943
131.247
137.357
144.000
Me
N
Ph
Ph
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr300/dwy161c

0.000
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7.190
7.259
7.261
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7.285
7.288
7.293
7.301
7.322
7.325
7.329
7.335
7.357
7.359
7.364
7.394
7.783
7.784
7.807
7.809
7.811
7.813
Me
N
Ph
Ph
3.000
13.188
0.984
ppm
data/nmr300/dwy163

31.149
77.655
77.231
76.808
109.779
115.306
119.821
120.399
122.381
125.701
127.178
128.232
128.375
128.593
130.080
131.365
132.113
135.423
137.527
137.934
Me
N
Ph
Ph
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
data/nmr300/dwy163c

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0.936
0.960
1.365
1.389
1.397
1.415
1.440
1.621
1.638
1.647
1.648
1.669
1.671
3.614
4.123
4.145
4.167
6.450
6.503
7.324
7.341
7.346
7.368
7.374
7.377
7.379
7.383
7.387
7.390
7.400
7.500
7.505
7.508
7.514
7.518
7.521
7.525
7.694
7.748
7.994
7.998
8.022
Me
N
Ph
CO2-n-Bu
ppm
1
2
3
4
5
6
7
8
9
2.973
2.021
2.045
2.910
2.000
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1.596
3.137
2.912
0.970
0.984
data/nmr300/dwyl1g2l

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19.423
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31.340
64.016
76.804
77.228
77.652
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110.567
113.061
120.948
121.874
123.209
125.751
128.823
129.359
130.190
131.105
138.135
138.991
145.571
168.766
Me
N
Ph
CO2-n-Bu
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
ppm
data/nmr300/dwy162c

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1.621
1.626
1.636
1.641
1.655
1.662
1.669
1.679
1.683
1.694
1.698
1.706
2.154
2.164
2.170
2.203
2.218
2.223
3.179
6.198
6.204
6.208
6.213
6.716
6.739
7.264
7.982
7.989
8.005
8.012
8.220
8.227
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O2N
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0.941
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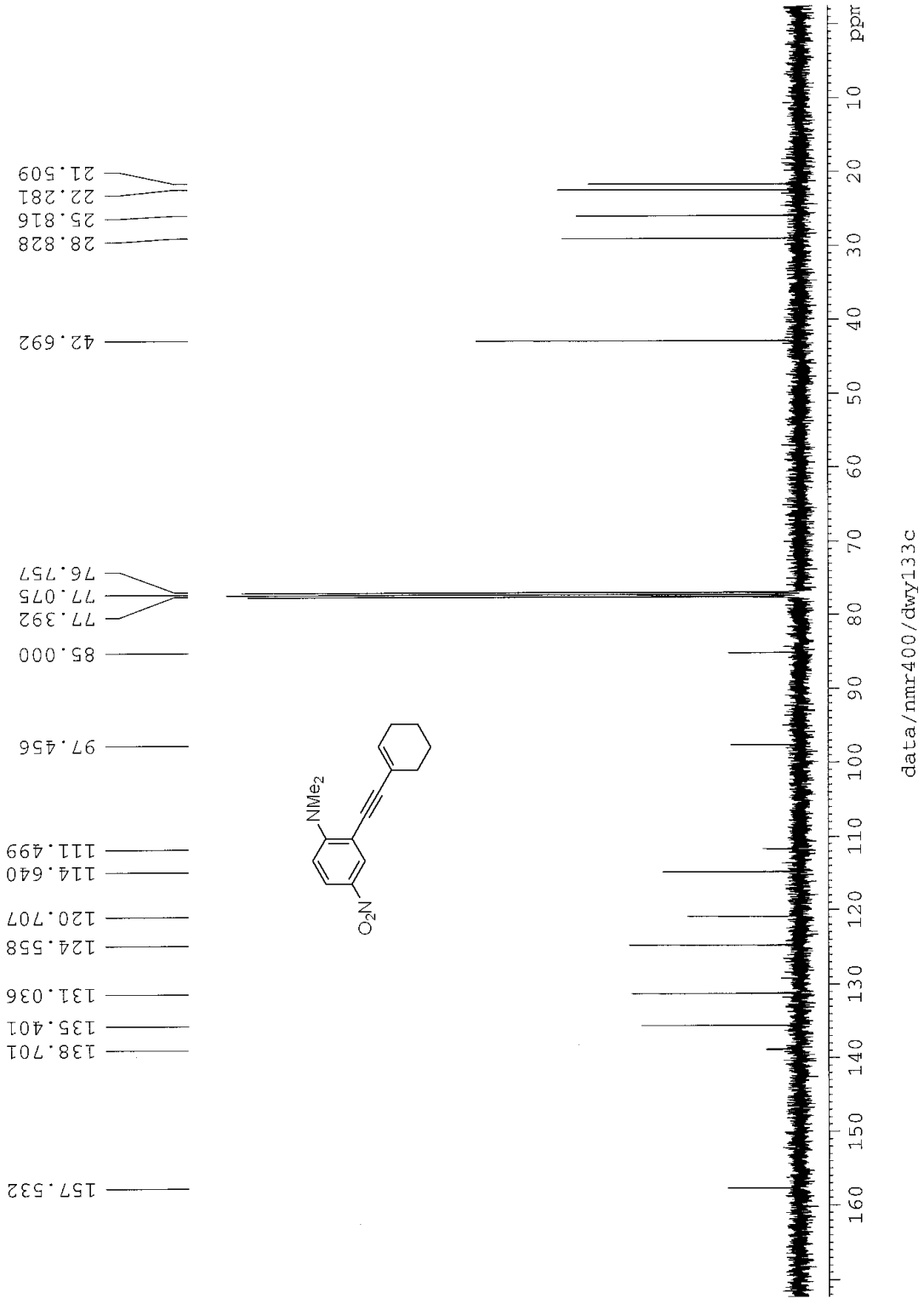
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76.757
77.075
77.392
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114.640
120.707
124.558
131.036
135.401
138.701
157.532
NMe2
O2N
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
data/nmr400/dwy133c

0.000
2.256
2.724
7.683
7.678
7.129
7.124
7.102
7.097
6.999
6.972
NMe2
I
Me
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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0.5
ppm
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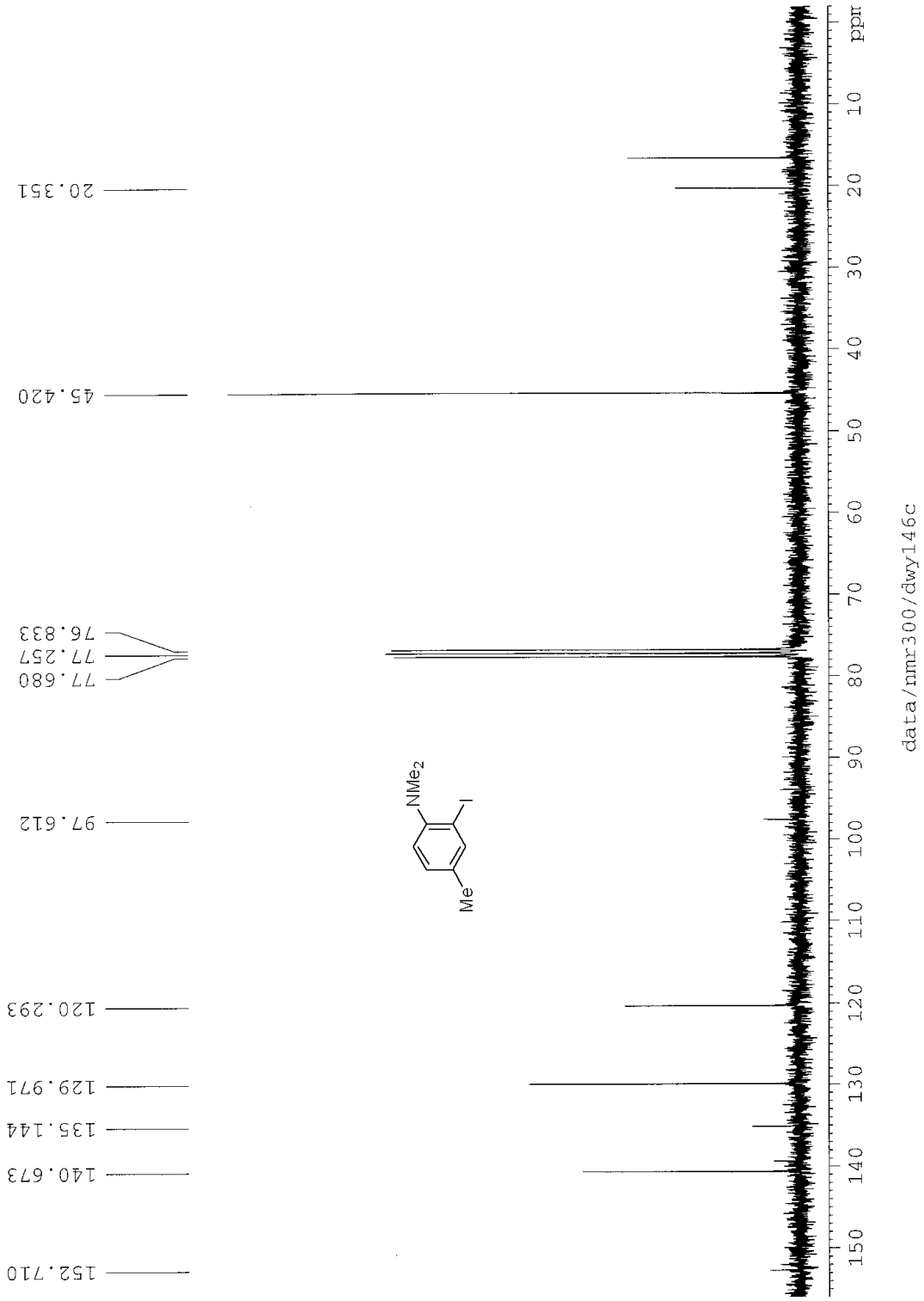
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77.257
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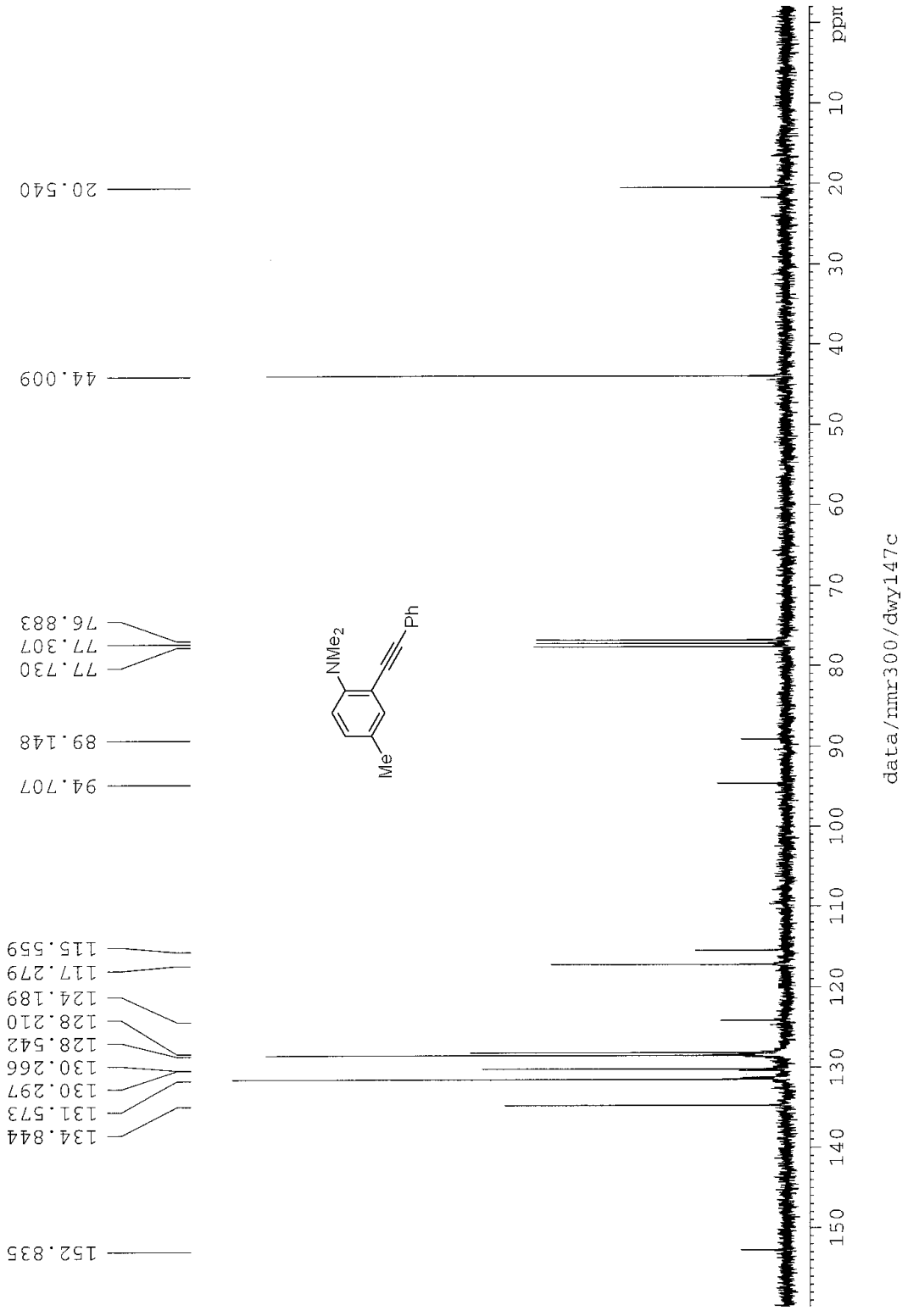
97.612
120.293
129.971
135.144
140.673
152.710
NMe2
I
Me
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr300/dwy146c

0.000
2.263
2.947
6.821
6.848
7.033
7.035
7.040
7.042
7.061
7.063
7.220
7.268
7.286
7.302
7.306
7.308
7.313
7.316
7.320
7.323
7.324
7.328
7.330
7.332
7.515
7.521
7.527
7.534
7.535
7.538
7.541
7.547
NMe2
Ph
Me
ppm
1
2
3
4
5
6
7
8
9
10
3.000
6.128
2.336
3.718
1.255
1.173
1.055
data/nmr300/dwy147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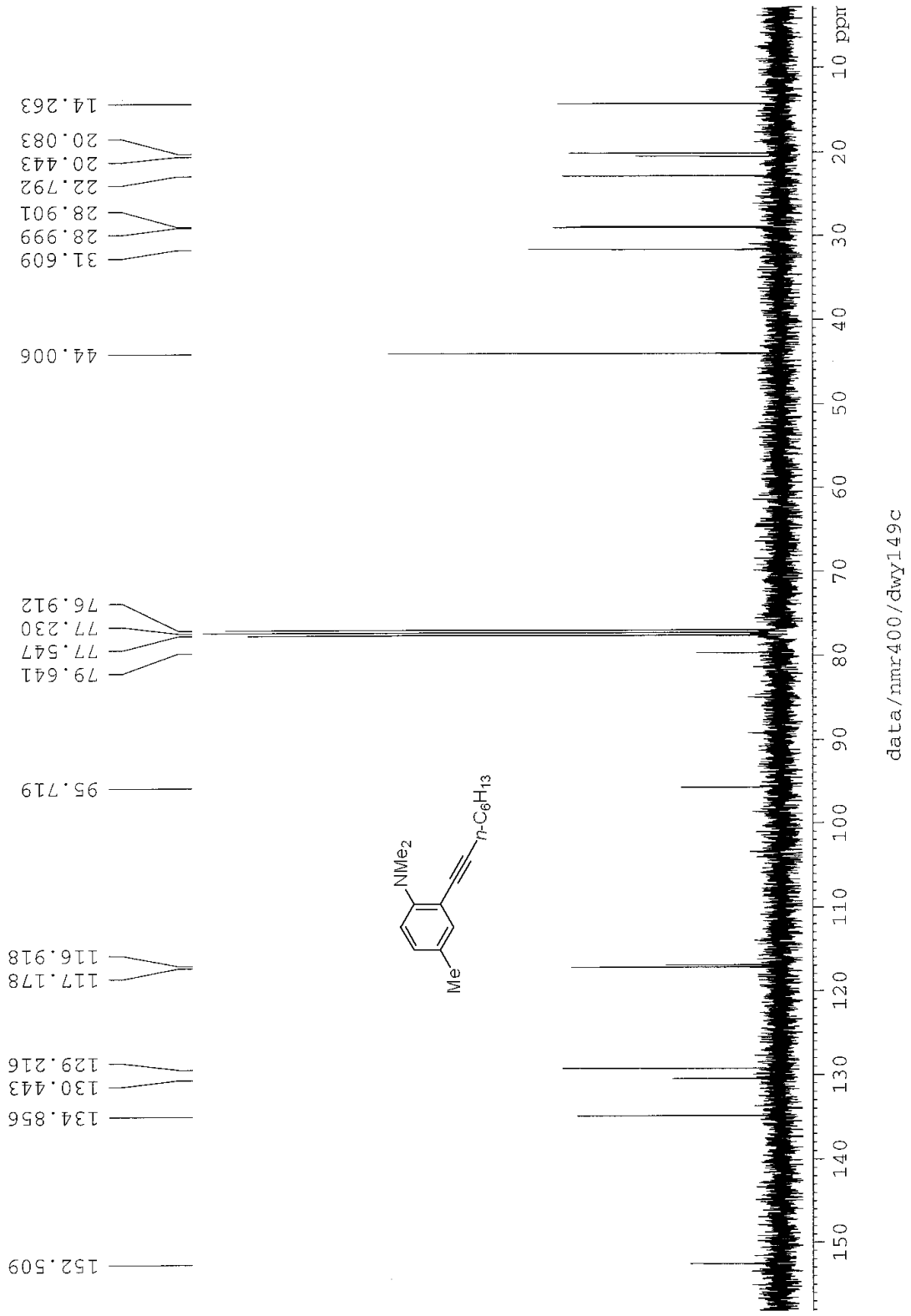
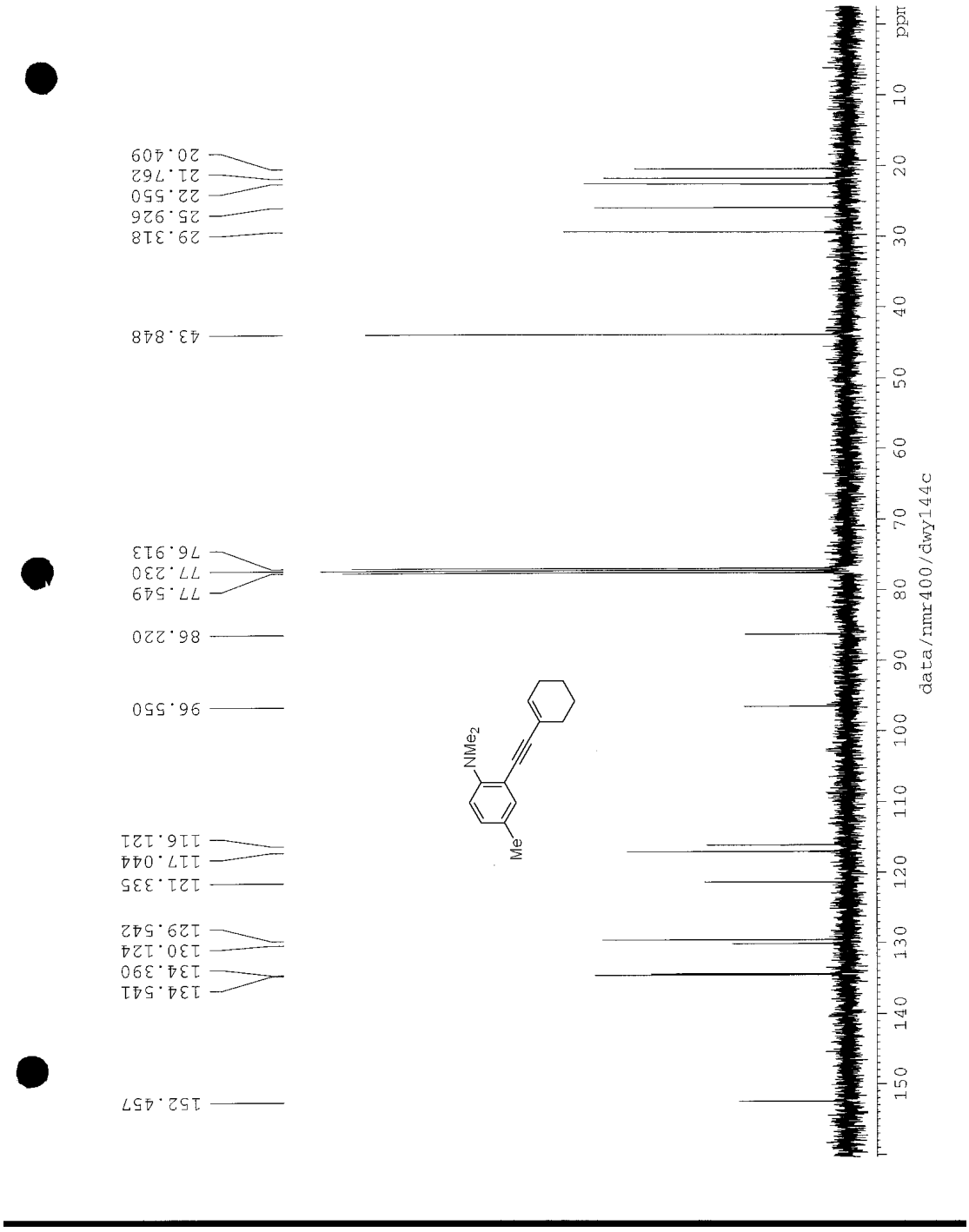
76.883
77.307
77.730
89.148
94.707
115.559
117.279
124.189
128.210
128.542
130.266
130.297
131.573
134.844
152.835
NMe2
Ph
Me
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
data/nmr300/dwy147c

0.000
0.809
0.826
0.842
1.241
1.249
1.258
1.373
1.390
1.407
1.515
1.533
1.552
1.570
2.157
2.376
2.393
2.411
2.790
6.719
6.740
6.910
6.930
7.117
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.909
0.958
0.957
6.000
1.987
2.953
2.005
2.056
4.364
3.229
NMe2
n-C6H13
Me
data/nmr400/dwy149


152.509
134.856
130.443
129.216
117.178
116.918
95.719
79.641
77.547
77.230
76.912
44.006
31.609
28.999
28.901
22.792
20.443
20.083
14.263
NMe2
n-C6H13
Me
10 ppm
data/nmr400/dwy149c

0.000
1.516
1.528
1.543
1.558
1.567
1.584
1.598
1.610
1.625
2.054
2.061
2.153
2.169
2.806
3.983
2.035
4.875
5.943
0.923
0.945
0.950
0.902
6.106
6.703
6.724
6.909
6.930
7.123
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
NMe2
Me
data/nmr400/dwy144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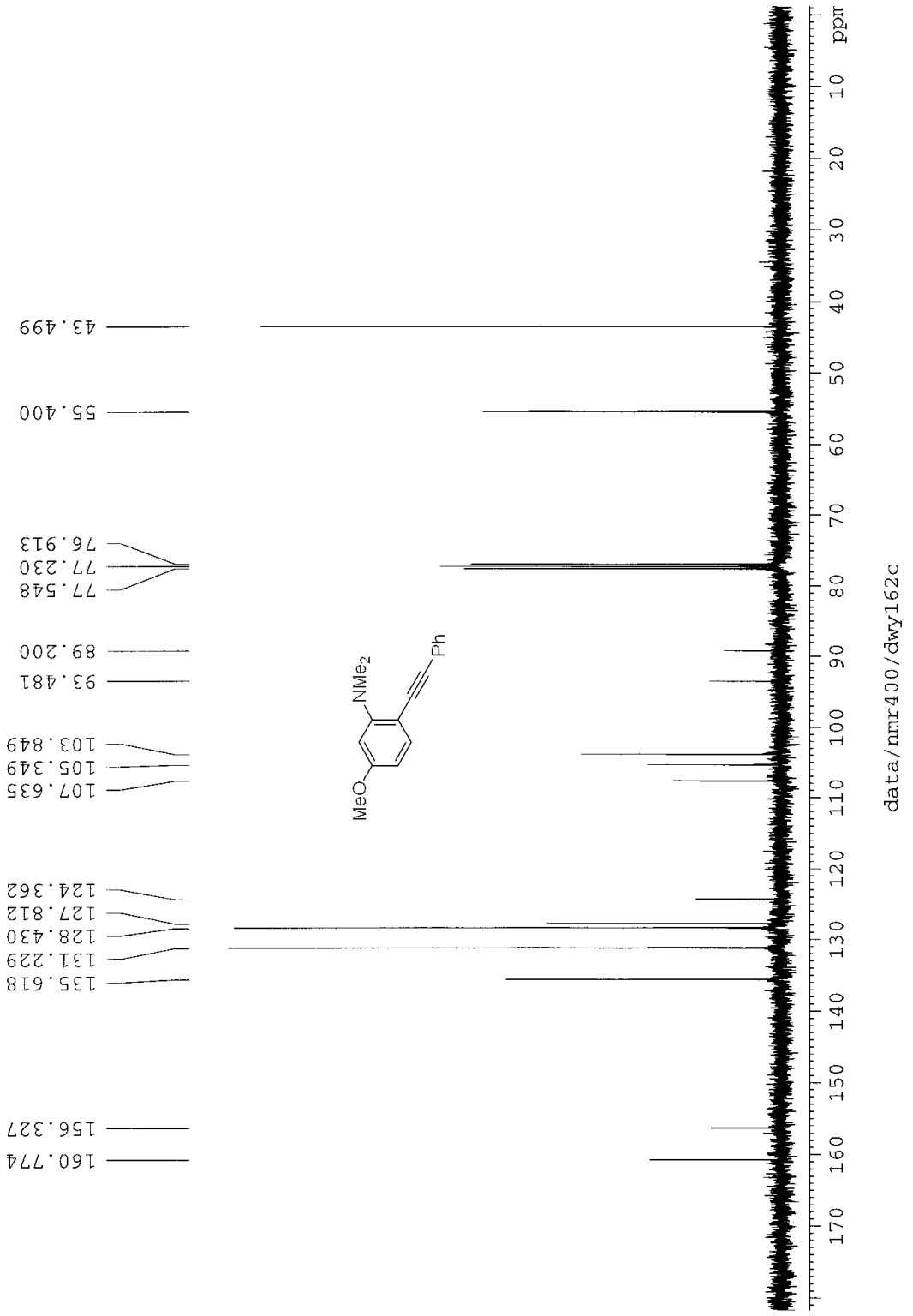
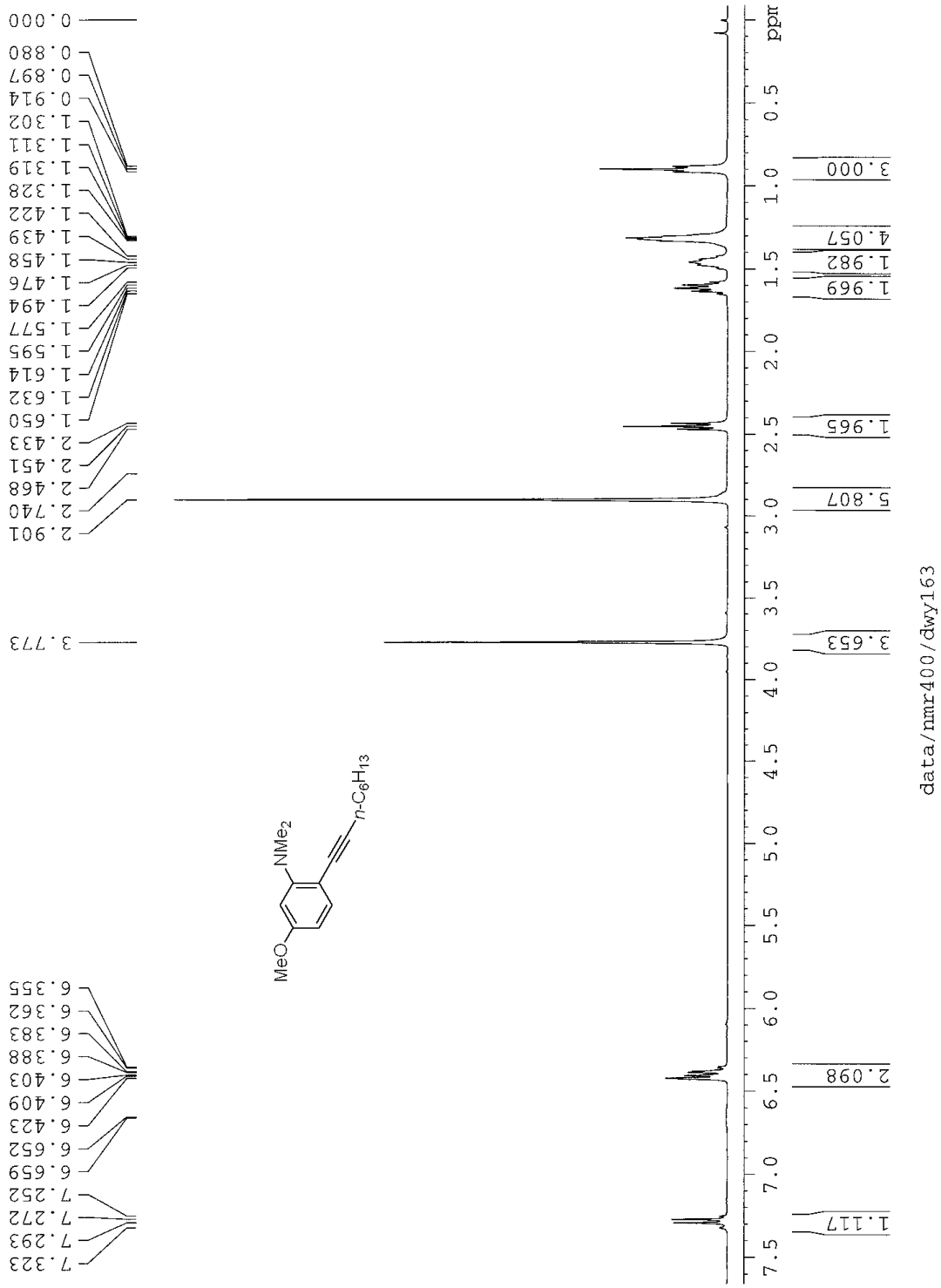
21.762
22.550
25.926
29.318
43.848
76.913
77.230
77.549
86.220
96.550
116.121
117.044
121.335
129.542
130.124
134.390
134.541
152.457
NMe2
Me
data/nmr400/dwy144c
ppm

0.000
2.988
3.792
7.517
7.513
7.497
7.422
7.400
7.337
7.332
7.327
7.315
7.297
7.292
7.288
7.277
7.270
7.261
7.255
7.252
7.227
6.446
6.428
6.422
NMe2
Ph
MeO
6.000
3.056
1.953
3.183
0.978
1.994
ppm
data/nmr400/dwy162


160.774
156.327
135.618
131.229
128.430
127.812
124.362
107.635
105.349
103.849
93.481
89.200
77.548
77.230
76.913
55.400
43.499
NMe2
Ph
MeO
data/nmr400/dwy162c
ppm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0.897
0.914
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1.311
1.319
1.328
1.422
1.439
1.458
1.476
1.494
1.577
1.595
1.614
1.632
1.650
2.433
2.451
2.468
2.740
2.901
3.773
6.355
6.362
6.383
6.388
6.403
6.409
6.423
6.652
6.659
7.252
7.272
7.293
7.323
NMe2
n-C6H13
MeO
ppm
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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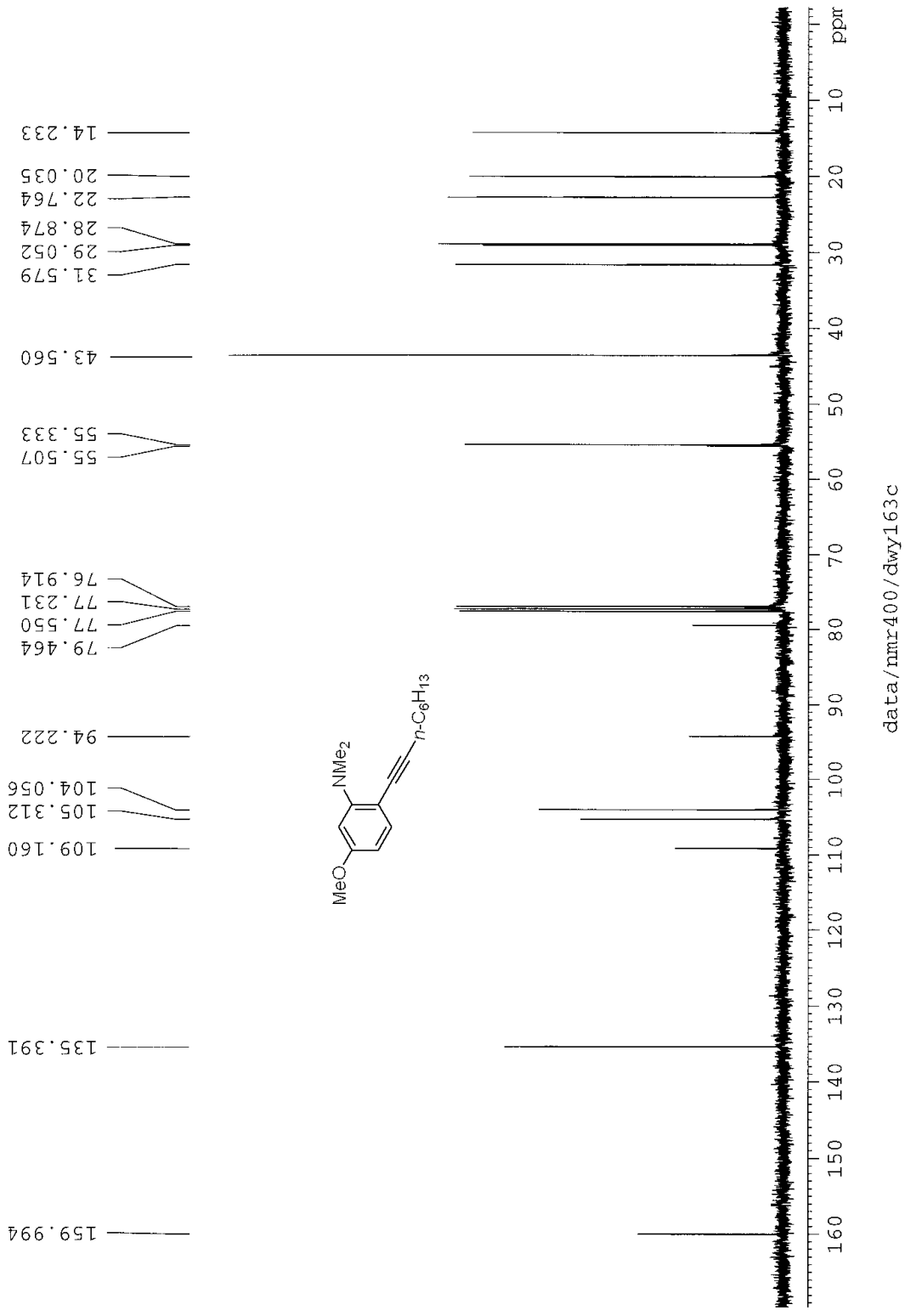
3.653
5.807
1.965
1.969
1.982
4.057
3.000
data/nmr400/dwy163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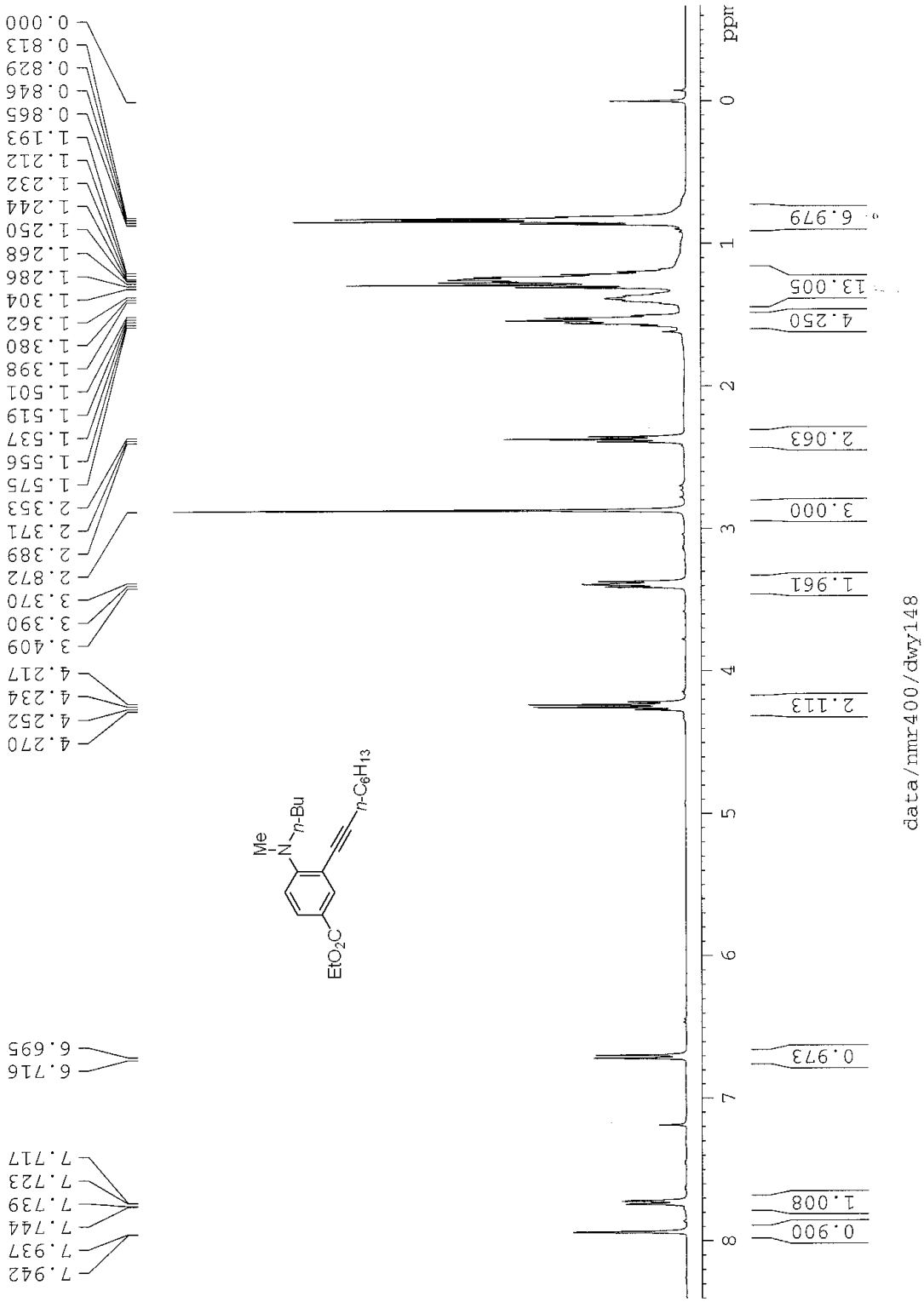
20.035
22.764
28.874
29.052
31.579
43.560
55.333
55.507
76.914
77.231
77.550
79.464
94.222
104.056
105.312
109.160
135.391
159.994
MeO
NMe2
n-C6H13
ppm
data/nmr400/dwy163c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7.937
7.744
7.739
7.723
7.717
6.716
6.695
4.270
4.252
4.234
4.217
3.409
3.390
3.370
2.872
2.389
2.371
2.353
1.575
1.556
1.537
1.519
1.501
1.398
1.380
1.362
1.304
1.286
1.268
1.250
1.244
1.232
1.212
1.193
0.865
0.846
0.829
0.813
0.000
Me
N
n-Bu
n-C6H13
EtO2C
ppm
0.900
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2.113
1.961
3.000
2.063
4.250
13.005
6.979
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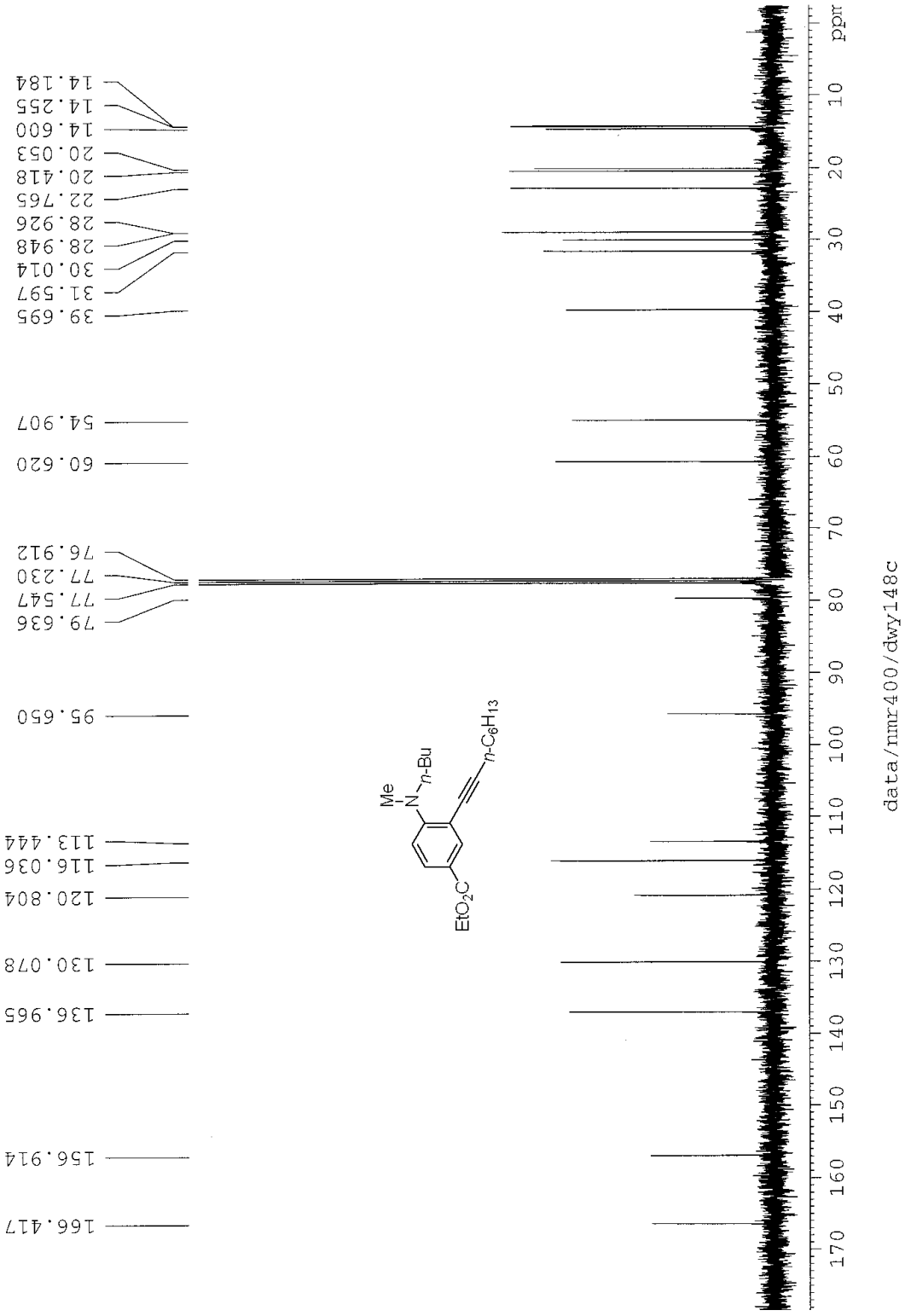
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14.255
14.600
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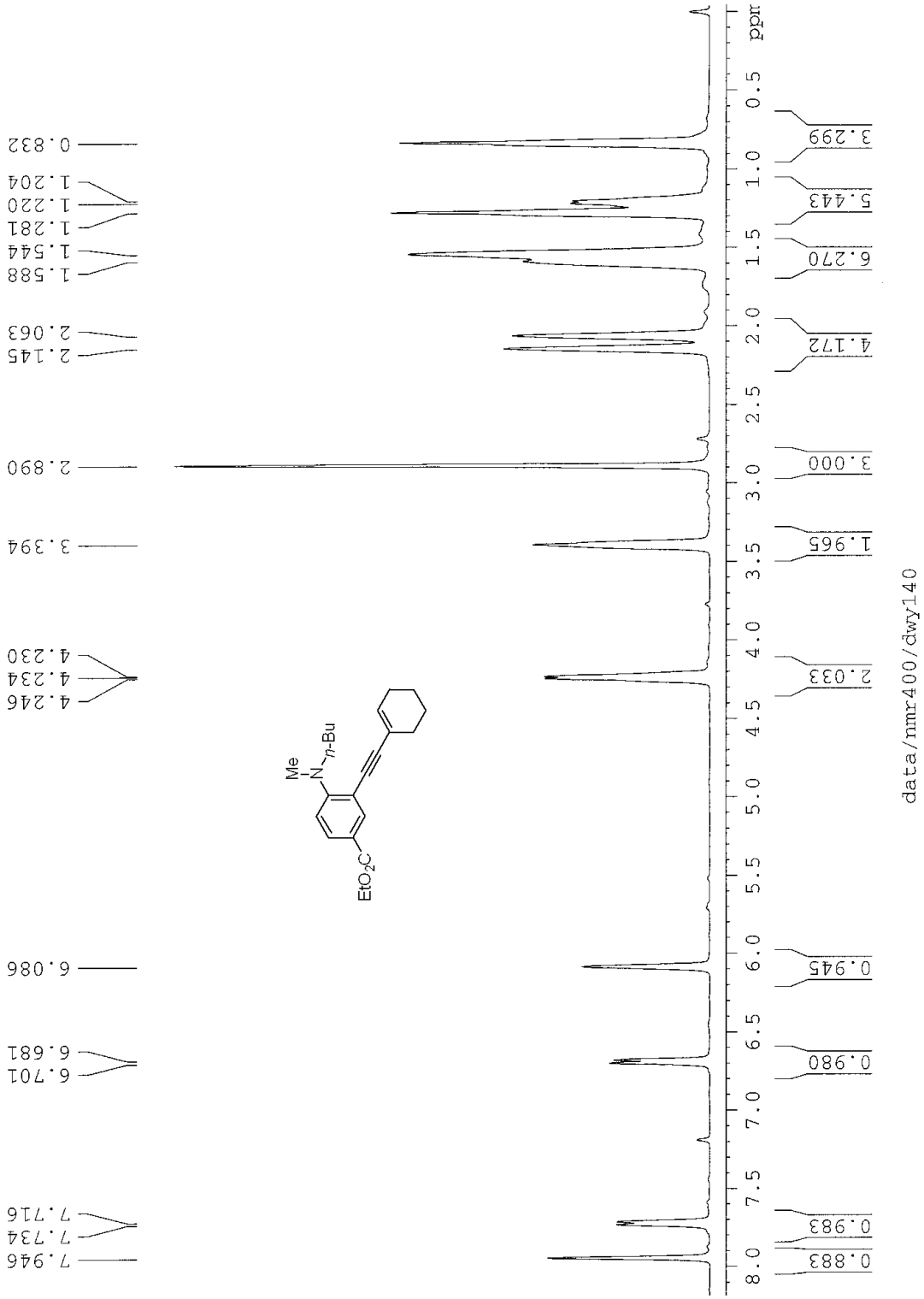
20.418
22.765
28.926
28.948
30.014
31.597
39.695
54.907
60.620
76.912
77.230
77.547
79.636
95.650
113.444
116.036
120.804
130.078
136.965
156.914
166.417
Me
N
n-Bu
n-C6H13
EtO2C
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
data/nmr400/dwy148c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7.716
6.701
6.681
6.086
4.246
4.234
4.230
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2.145
2.063
1.588
1.544
1.281
1.220
1.204
0.832
0.883
0.983
0.945
0.980
2.033
1.965
3.000
4.172
6.270
5.443
3.299
ppm
Me
N
n-Bu
EtO2C
data/nmr400/dwy140

14.104
14.575
20.379
21.713
22.506
25.910
29.223
30.046
39.701
54.815
60.592
76.911
77.230
77.548
86.113
96.260
112.564
115.815
120.525
121.205
130.309
134.539
136.844
156.546
166.335
Me
N
n-Bu
EtO2C
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ppm

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1.769
1.780
1.787
1.807
1.828
1.834
1.847
1.853
2.223
2.231
2.243
2.250
2.270
2.277
2.290
2.298
2.310
2.319
3.748
5.950
5.956
5.962
7.241
7.263
7.271
8.082
8.090
8.112
8.120
8.345
8.352
Me
N
I
O2N
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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1.209
0.980
3.000
4.160
4.076
data/nmr300/dwy137

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25.712
29.182
32.042
59.410
76.848
77.272
77.696
109.899
118.048
118.516
129.192
130.019
135.085
140.467
142.373
147.875
Me
N
I
O2N
ppm
data/nmr300/dwy137c

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2.422
3.543
7.023
7.043
7.091
7.112
7.126
7.199
7.371
7.393
7.407
3.000
2.993
5.022
0.979
1.120
0.978
ppm
data/nmr400/dwy143
Me
N
Ph
I
Me

21.636
32.206
58.447
76.914
77.231
77.549
109.785
121.203
124.713
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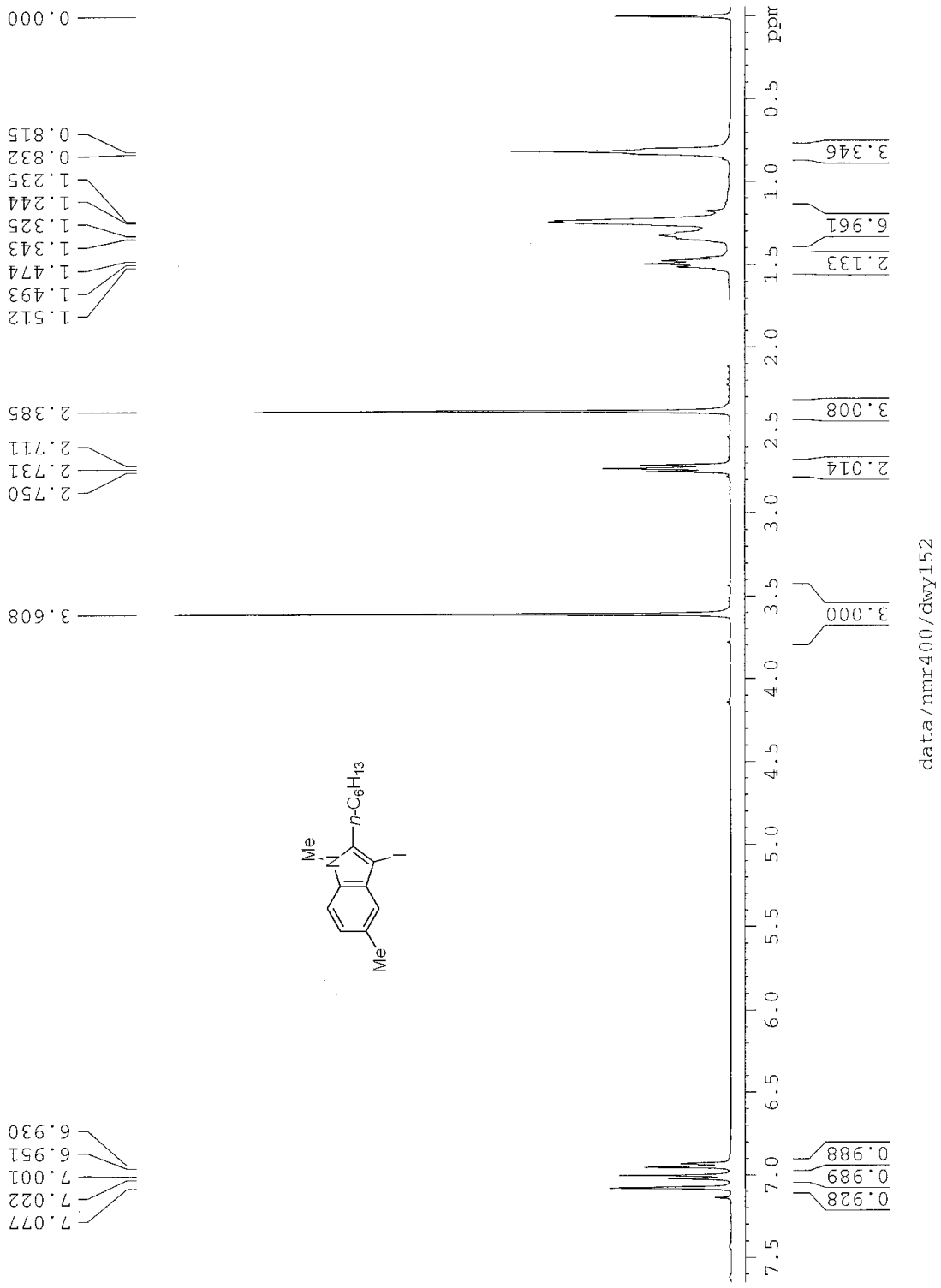
128.882
130.366
130.679
131.083
131.910
136.367
141.849
Me
N
Ph
I
Me
ppm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1.474
1.493
1.512
2.385
2.711
2.731
2.750
3.608
6.930
6.951
7.001
7.022
7.077
ppm
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
3.346
6.961
2.133
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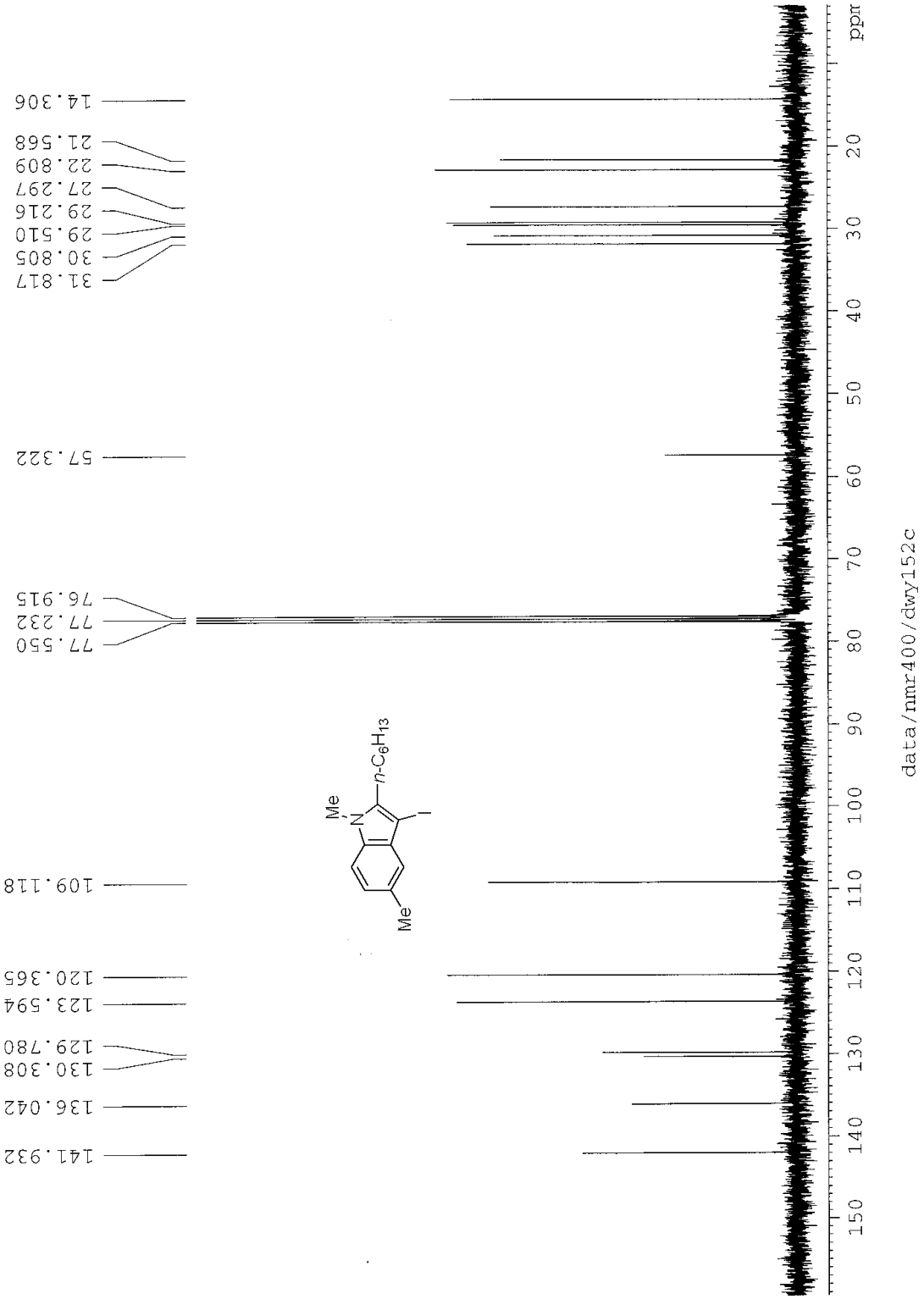
2.014
3.000
0.928
0.989
0.988
Me
N
n-C6H13
I
Me
data/nmr400/dwy152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21.568
22.809
27.297
29.216
29.510
30.805
31.817
57.322
76.915
77.232
77.550
109.118
120.365
123.594
129.780
130.308
136.042
141.932
Me
N
n-C6H13
I
Me
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
data/nmr400/dwy152c

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1.643
1.656
1.667
1.716
1.730
1.742
2.150
2.171
2.179
2.187
2.387
3.557
5.792
6.949
6.969
7.011
7.032
7.110
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1.009
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3.000
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3.980
3.982
Me
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I
Me
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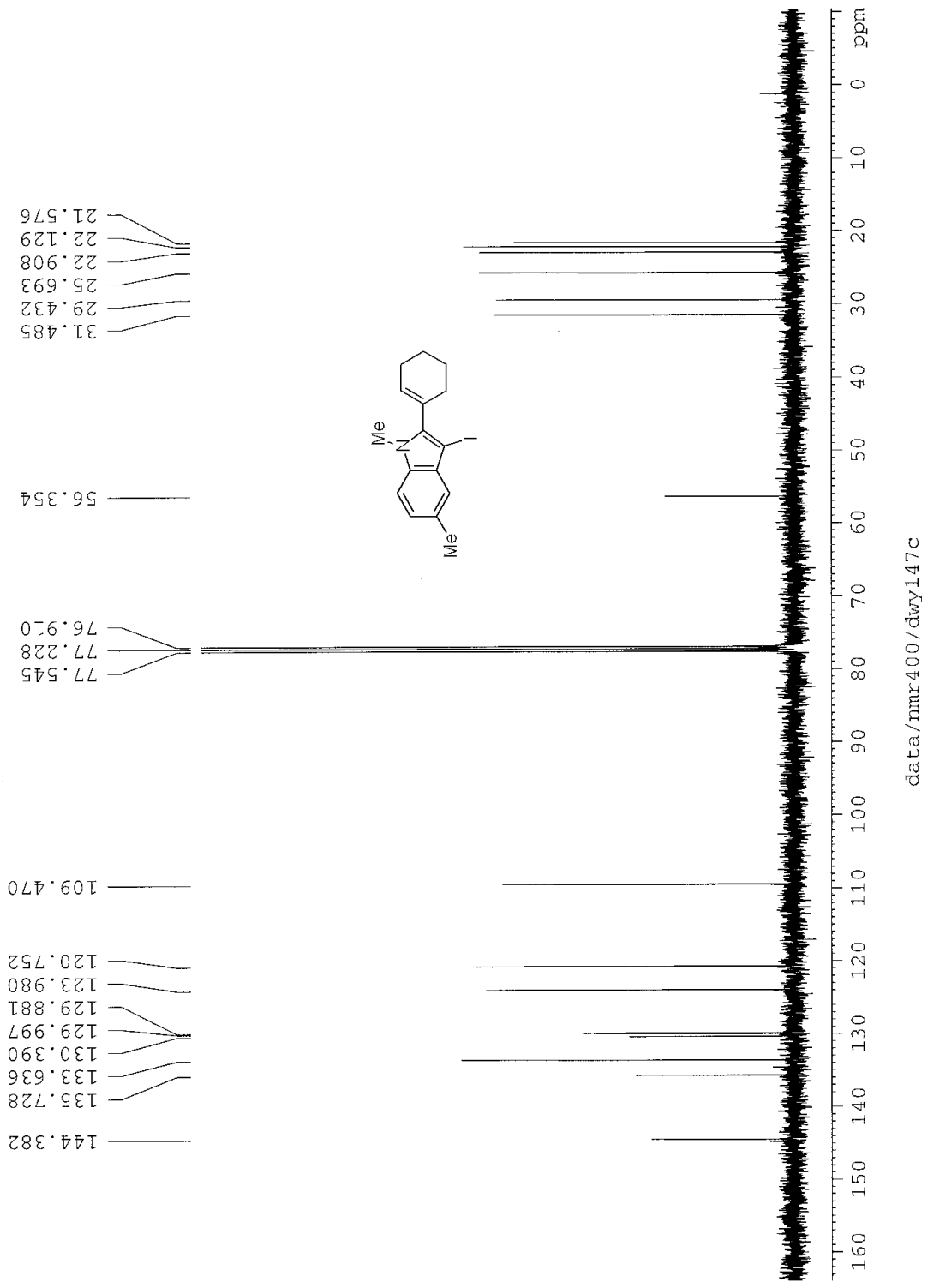
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76.910
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77.545
109.470
120.752
123.980
129.881
129.997
130.390
133.636
135.728
144.382
Me
N
I
Me
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
data/nmr400/dwy147c

0.000
3.604
3.887
7.506
7.501
7.496
7.485
7.470
7.447
7.438
7.430
7.419
7.413
7.375
7.354
6.900
6.894
6.878
6.873
6.769
6.763
Me
N
Ph
I
MeO
2.931
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0.951
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ppm
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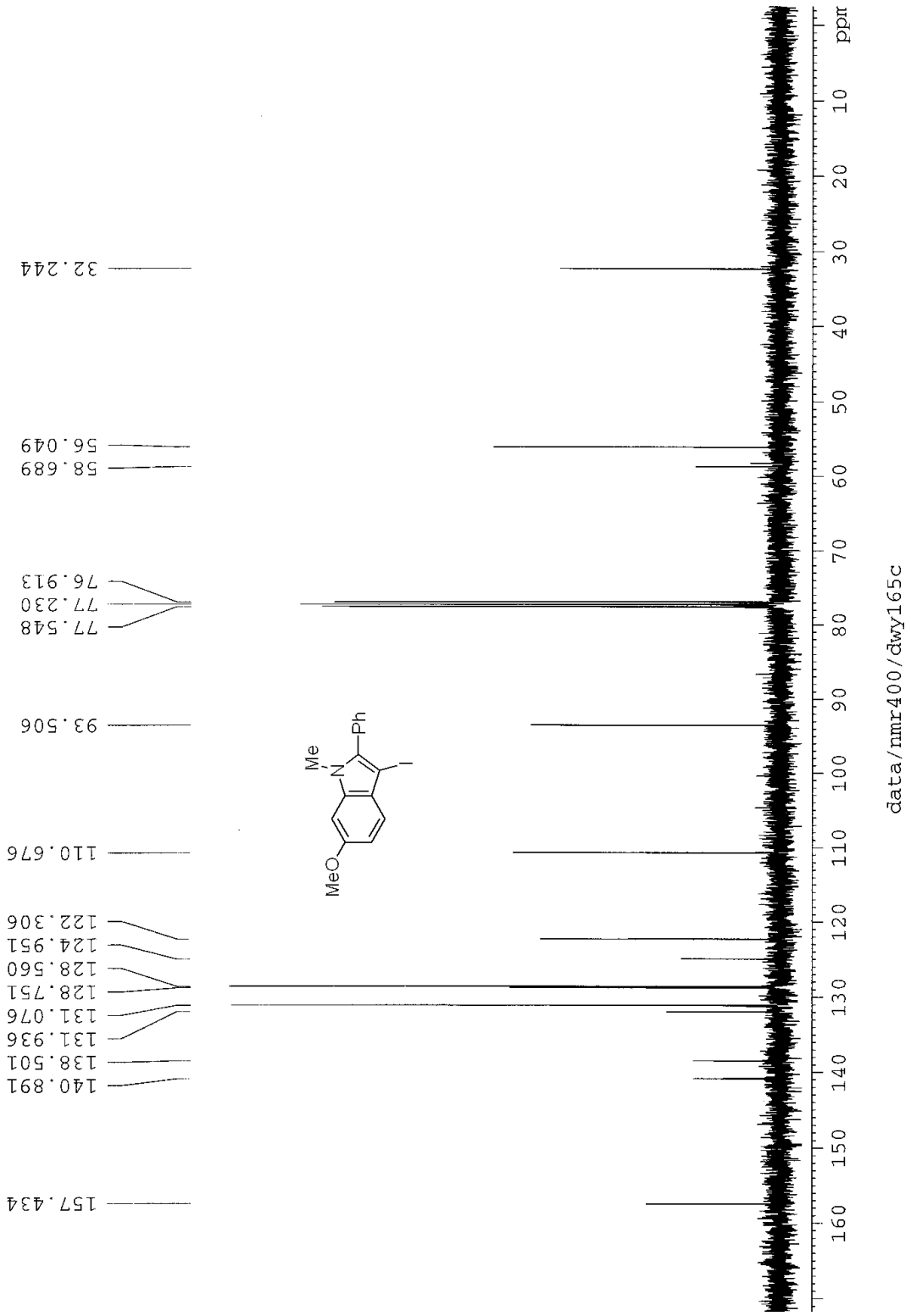
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77.548
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110.676
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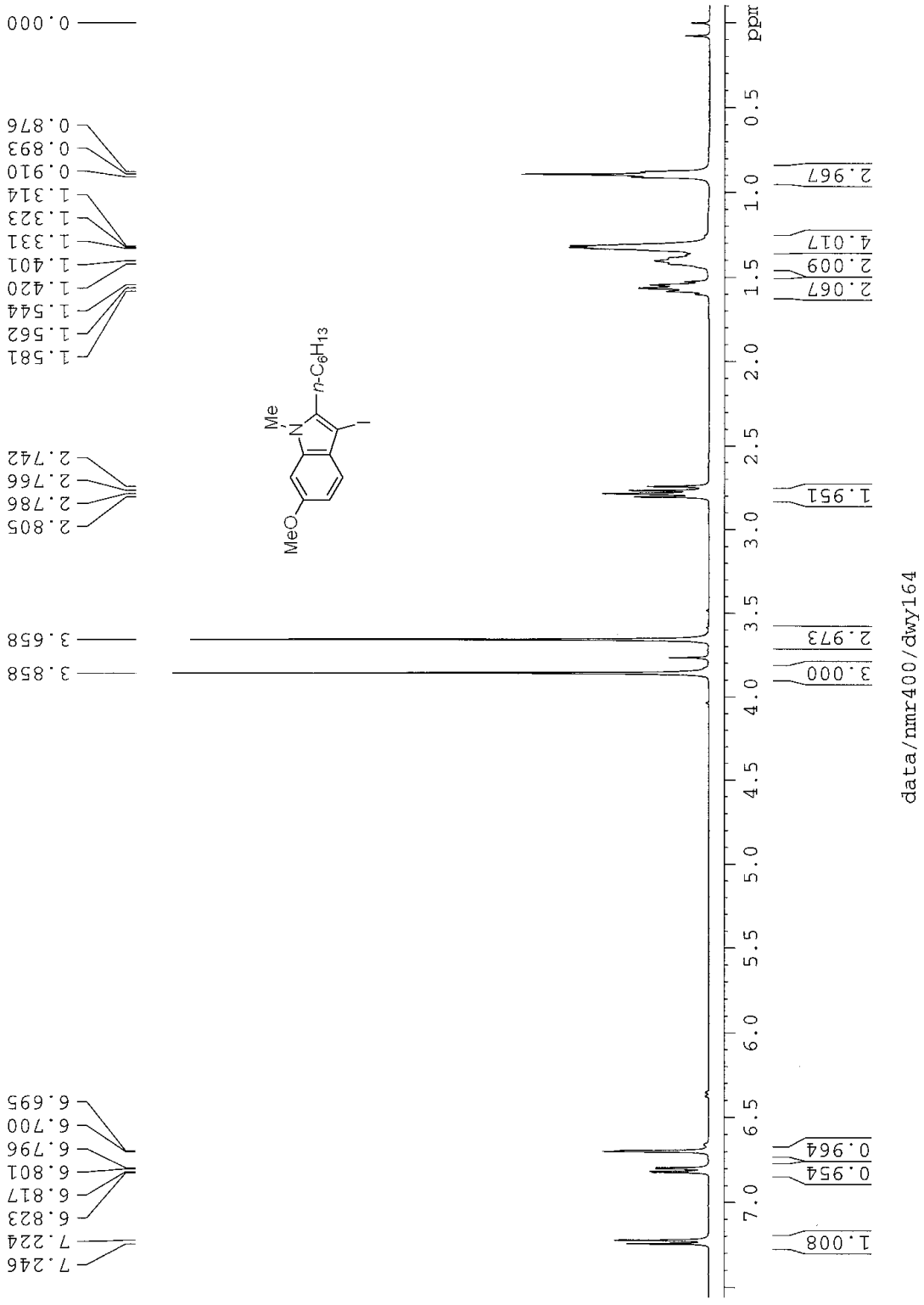
124.951
128.560
128.751
131.076
131.936
138.501
140.891
157.434
Me
N
Ph
I
MeO
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
data/nmr400/dwy165c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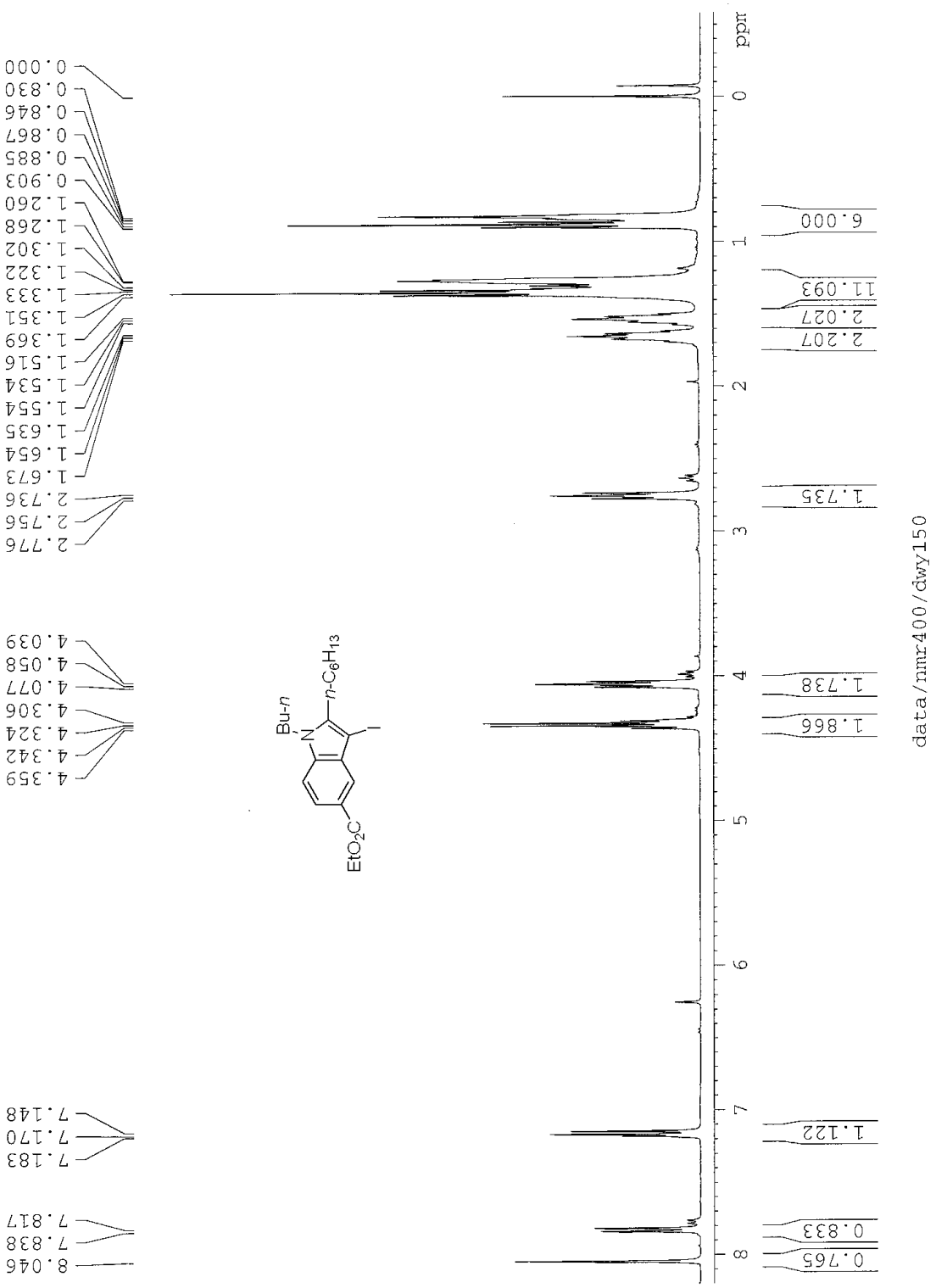
1.323
1.331
1.401
1.420
1.544
1.562
1.581
2.742
2.766
2.786
2.805
3.658
3.858
6.695
6.700
6.796
6.801
6.817
6.823
7.224
7.246
Me
N
n-C6H13
I
MeO
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.008
0.954
0.964
1.951
2.973
3.000
2.967
4.017
2.009
2.067
data/nmr400/dwy164

14.295
22.802
27.349
29.193
29.612
30.823
31.804
56.066
57.449
76.910
77.228
77.545
93.424
109.763
121.254
124.535
138.097
140.885
156.785
Me
N
n-C6H13
I
MeO
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
data/nmr400/dwy164c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7.838
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7.183
7.170
7.148
4.359
4.342
4.324
4.306
4.077
4.058
4.039
2.776
2.756
2.736
1.673
1.654
1.635
1.554
1.534
1.516
1.369
1.351
1.333
1.322
1.302
1.268
1.260
0.903
0.885
0.867
0.846
0.830
0.000
Bu-n
n-C6H13
I
EtO2C
0.765
0.833
1.122
1.738
1.866
1.735
2.207
2.027
11.093
6.000
ppm
data/nmr400/dwy150

13.997
14.272
14.707
20.452
22.776
27.414
29.368
29.648
31.726
32.714
44.656
59.761
60.830
76.915
77.233
77.550
109.444
122.726
123.434
123.501
130.040
139.549
143.212
167.702
Bu-n
n-C6H13
I
EtO2C
ppm
data/nmr400/dwy150c

8.047
7.859
7.837
7.185
7.163
7.141
4.363
4.346
4.328
4.310
3.695
2.799
2.780
2.760
1.548
1.528
1.510
1.376
1.359
1.341
1.264
1.255
1.247
0.843
0.827
0.809
0.000
ppm
0.902
0.971
0.988
2.000
2.966
1.991
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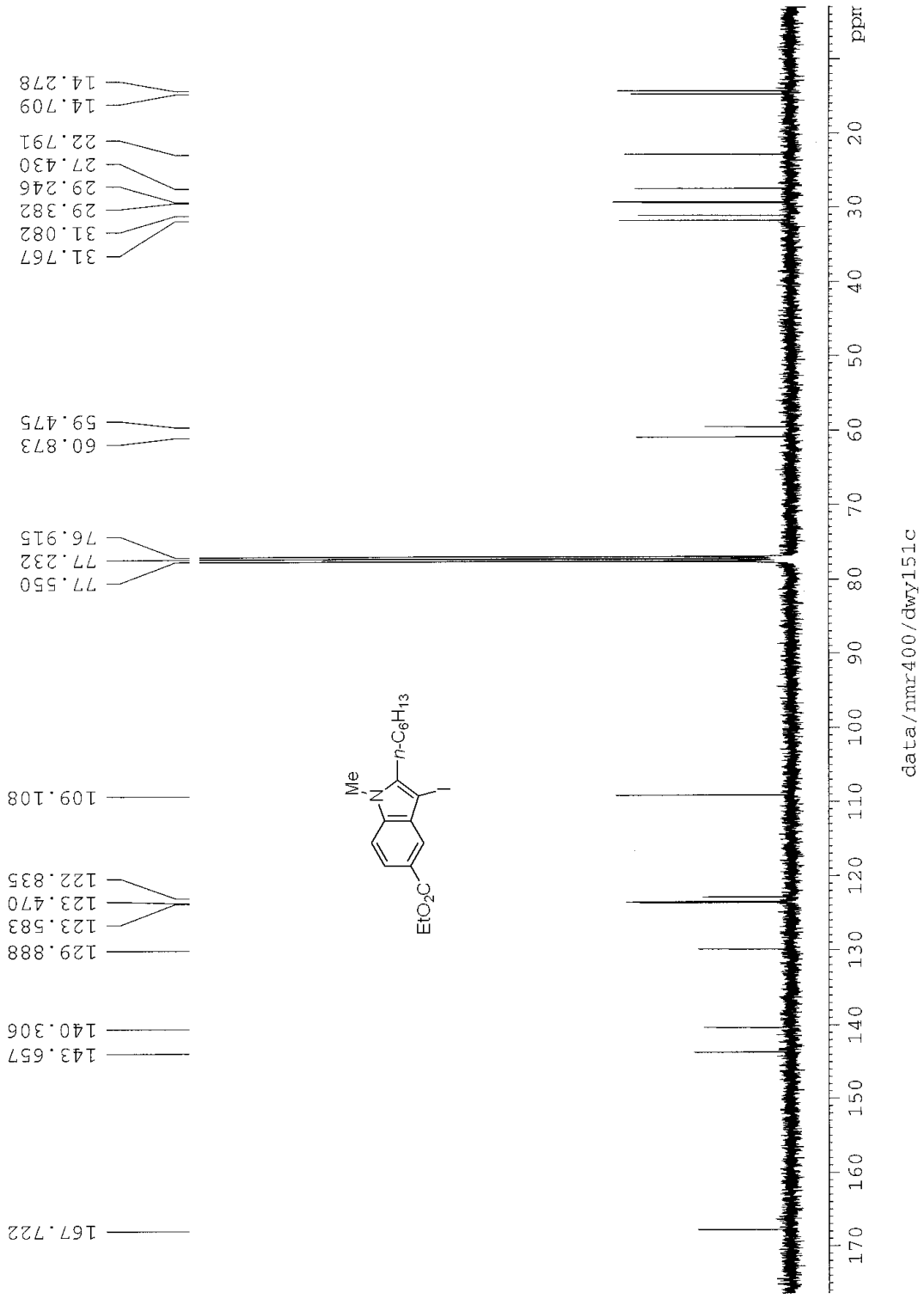
5.100
4.104
3.058
Me
N
n-C6H13
I
EtO2C
data/nmr400/dwy151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14.709
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29.382
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31.767
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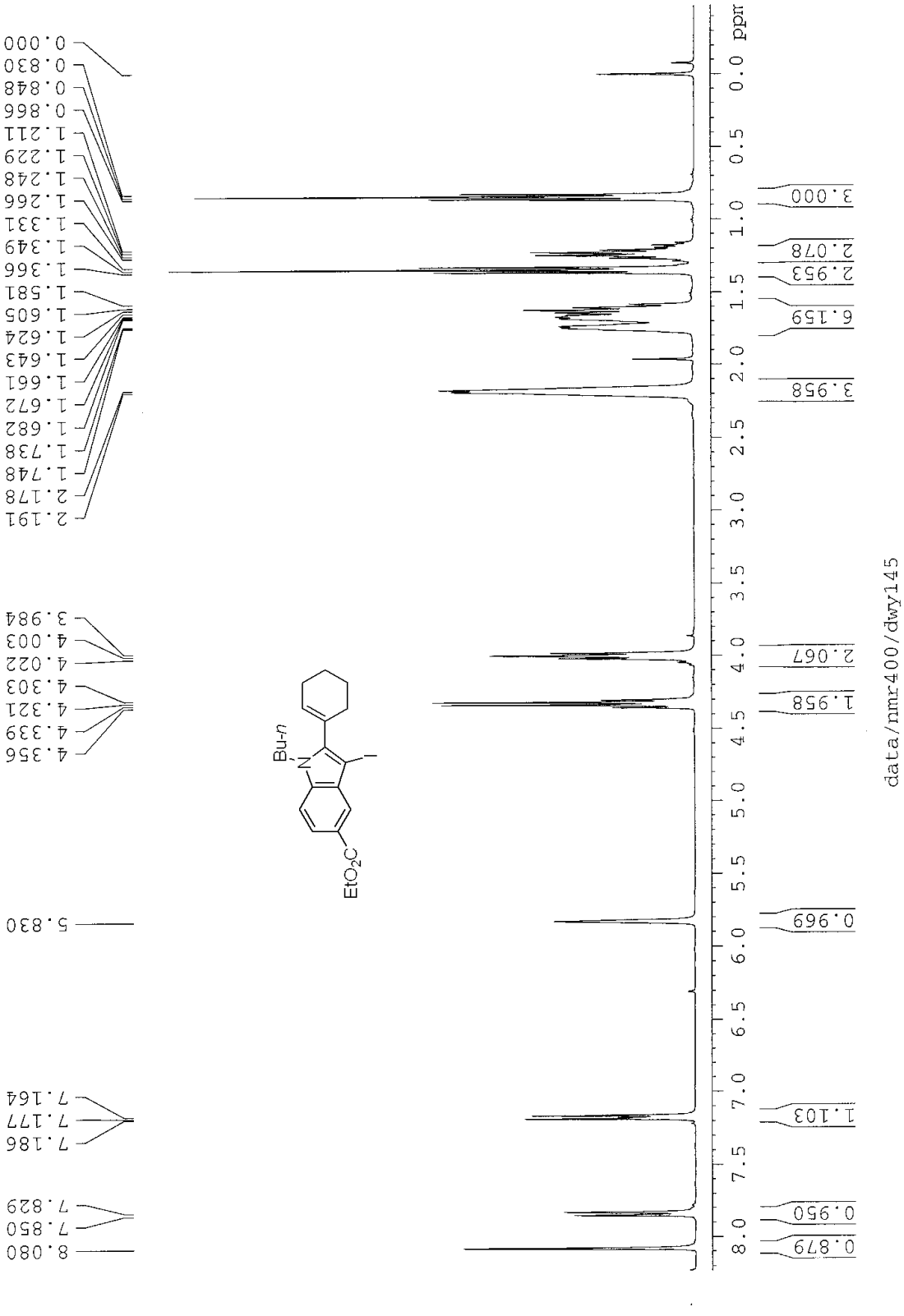
60.873
76.915
77.232
77.550
109.108
122.835
123.470
123.583
129.888
140.306
143.657
167.722
Me
N
n-C6H13
I
EtO2C
ppm
data/nmr400/dwy151c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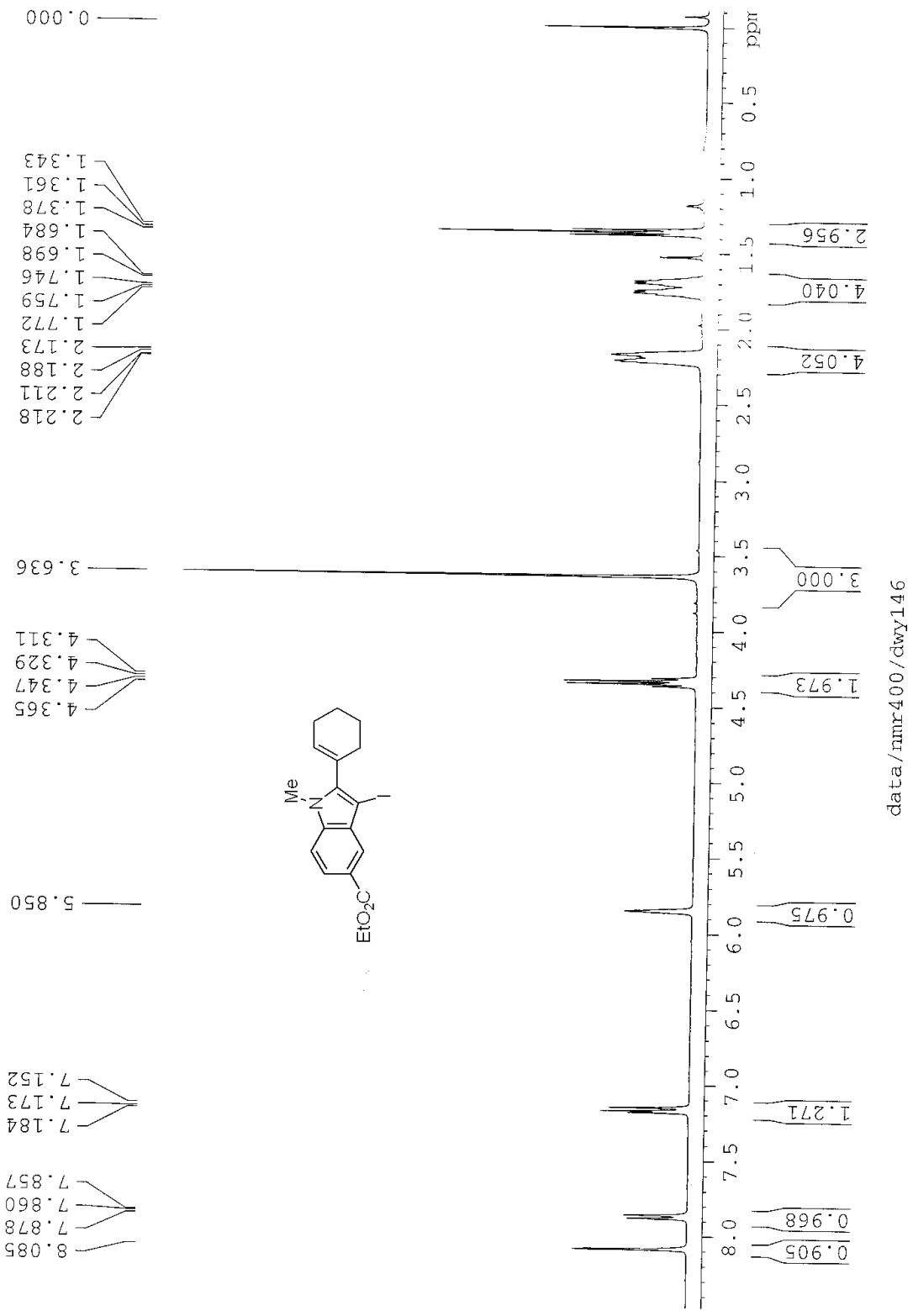
7.850
7.829
7.186
7.177
7.164
5.830
4.356
4.339
4.321
4.303
4.022
4.003
3.984
2.191
2.178
1.748
1.738
1.682
1.672
1.661
1.643
1.624
1.605
1.581
1.366
1.349
1.331
1.266
1.248
1.229
1.211
0.866
0.848
0.830
0.000
Bu-n
I
EtO2C
0.879
0.950
1.103
0.969
1.958
2.067
3.958
6.159
2.953
2.078
3.000
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
data/nmr400/dwy145

13.913
14.684
20.264
22.031
22.897
25.696
29.580
32.584
45.085
59.008
60.814
76.909
77.228
77.545
109.821
122.731
123.656
124.005
129.828
130.056
134.169
139.163
145.565
167.652
Bu-n
N
I
EtO2C
data/nmr400/dwy145c
ppm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1.759
1.772
2.173
2.188
2.211
2.218
3.636
4.311
4.329
4.347
4.365
5.850
7.152
7.173
7.184
7.857
7.860
7.878
8.085
Me
N
I
EtO2C
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.905
0.968
1.271
0.975
1.973
3.000
4.052
4.040
2.956
data/nmr400/dwy146

13.713
14.684
20.004
29.580
32.224
45.185
60.908
61.184
76.888
77.225
77.544
110.121
123.231
124.156
124.505
128.658
129.256
134.239
139.563
143.255
167.632
Me
N
I
EtO2C
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
ppm
data/nmr400/dwy146