Synthesis of 4,7-Difunctionalized Indoles via Imino Exchange and Sulfinyl Migration

Xiaohua Li, Lei Li, Weiyi Wang, Qiuqin He* and Renhua Fan*.

Department of Chemistry, Fudan University, 2005 Songhu Road, Shanghai 200438, China.

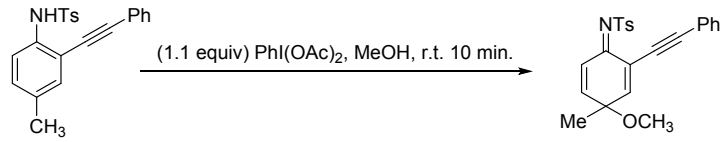
Supporting Information

General experimental methods

All reactions were performed in Schlenk tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 35–40 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. For reactions that require heating, oil bath is used as the heat source.

2. Representative procedure and characterization data

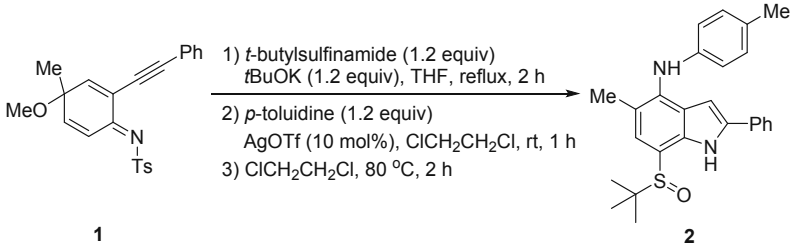
2.1 Synthesis of compounds 1



1

$PhI(OAc)_2$ (350 mg, 1.1 mmol) was added into the solution of 2-alkynyl aniline (360 mg, 1.0 mmol) in MeOH (20 mL) at 25 °C. After 10 min, the reaction mixture was quenched with saturated $NaHCO_3$ (20 mL), and extracted by ethyl acetate (50 mL x 3). The organic layer was dried over anhydrated Na_2SO_4, and concentrated in vacuo. The residue waspurified by flash column chromatography on silica gel (petroleum ether /ethyl acetate = 8:1) to afford 2-alkynycyclohexadienimine **1** (371 mg, 95% yield).

2.2 Representative procedure



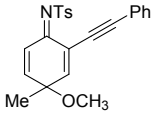
1 **2**

tert-Butanesulfinamide (0.12 mmol) and potassium t-butoxide (0.12 mmol) were added to a solution of 2-alkynylcyclohexadienimine **1** (0.1 mmol) in THF (2 mL). The reaction mixture was stirred at the refluxing temperature for 2 h. The crude product was purified by a short column chromatography on silica gel (eluent: petroleum ether/EtOAc 4:1). The isolated imino exchange intermediate was dissolved in dichloroethane (2 mL) and treated with *p*-toluidine (0.12 mmol) and AgOTf (0.01 mmol). The reaction mixture was stirred at room temperature for 1 h, then was filtered through a short silica gel column to remove AgOTf. The resulting filtrate was stirred at 80 °C. After the intermediate was completely consumed (monitored by TLC analysis), the mixture was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc 5:1) to furnish compound **2**, 30 mg, 72% yield.

2.3 Representative procedure in 1 mmol scale

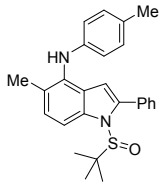
tert-Butanesulfinamide (1.2 mmol) and potassium *t*-butoxide (1.2 mmol) were added to a solution of 2-alkynylcyclohexadienimine **1** (1 mmol) in THF (10 mL). The reaction mixture was stirred at the refluxing temperature for 2 h. The crude product was purified by a short column chromatography on silica gel (eluent: petroleum ether/EtOAc 4:1). The isolated imino exchange intermediate was dissolved in dichloroethane (10 mL) and treated with *p*-toluidine (1.2 mmol) and AgOTf (0.1 mmol). The reaction mixture was stirred at room temperature for 1 h, then was filtered through a short silica gel column to remove AgOTf. The resulting filtrate was stirred at 80 °C. After the intermediate was completely consumed (monitored by TLC analysis), the mixture was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc 5:1) to furnish compound **2**, 287 mg, 69% yield.

2.3 Characterization data

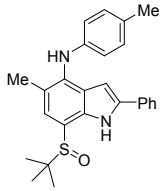


(Z)-*N*-(4-methoxy-4-methyl-2-(phenylethynyl)cyclohexa-2,5-dien-1-ylidene)-4-methylbenzenesulfonamide 1: (eluent: petroleum ether/EtOAc 8:1), 371 mg, 95%; colorless solid; m.p. 155-156 °C; ^{1}H NMR (400 MHz, CD_3CN) δ 7.94 (d, J = 8.3 Hz, 2H), 7.57 (d, J = 10.4 Hz, 1H), 7.44 (m, 7H), 7.16 (d, J = 2.6 Hz, 1H), 6.93 (dd, J =

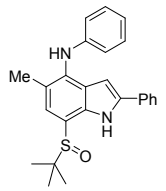
10.4 Hz, 2.6 Hz, 1H), 3.12 (s, 3H), 2.44 (s, 3H), 1.41 (s, 3H). (ref: Wang, L. F.; Fan, R. H. *Org. Lett.* **2012**, *14*, 3596-3599.)



1-(tert-butylsulfinyl)-5-methyl-2-phenyl-*N*-(p-tolyl)-1*H*-indol-4-amine int-2B: (eluent: petroleum ether/EtOAc 8:1), 38 mg, 92%; gray solid; m.p. 110-111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 7.0 Hz, 2H), 7.40 (m, 3H), 7.11 (d, J = 8.5 Hz, 1H), 7.00 (d, J = 8.2 Hz, 2H), 6.63 (d, J = 8.4 Hz, 2H), 6.38 (s, 1H), 5.51 (s, 1H), 2.32 (s, 3H), 2.26 (s, 3H), 1.07 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 141.2, 139.0, 132.0, 131.7, 130.0, 129.5, 128.2, 128.1, 126.6, 126.1, 125.8, 115.0, 113.0, 105.2, 64.4, 24.0, 20.4, 17.5. HRMS m/z calcd for $C_{26}H_{29}N_2OS$ ($[M+H]^+$): 417.1995, found 417.1995.

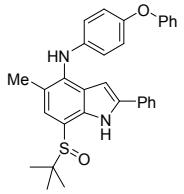


7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 2：(eluent: petroleum ether/EtOAc 5:1), 30 mg, 72%; gray solid; m.p. 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.57 (d, J = 7.7 Hz, 2H), 7.37 (t, J = 7.7 Hz, 2H), 7.27 (t, J = 7.2 Hz, 1H), 7.04 (d, J = 7.9 Hz, 2H), 6.88 (s, 1H), 6.77 (d, J = 8.2 Hz, 2H), 6.38 (d, J = 2.4 Hz, 1H), 2.30 (s, 6H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 137.9, 136.5, 135.7, 131.8, 129.8, 129.5, 128.8, 127.8, 125.3, 125.1, 124.3, 119. 1, 117.4, 112.8, 97.4, 58.2, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{29}N_2OS$ ($[M+H]^+$): 417.1995, found 417.1976.

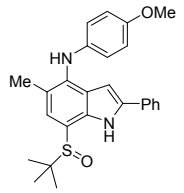


7-(*tert*-butylsulfinyl)-5-methyl-*N*,2-diphenyl-1*H*-indol-4-amine 3: (eluent: petroleum ether/EtOAc 5:1), 29 mg, 72%; brown solid; m.p. 159-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 7.57 (d, J = 7.4 Hz, 2H), 7.36 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 7.3 Hz, 1H), , 7.24-7.21 (m, 3H),, 6.89 (s, 1H), 6.83 (d, J = 7.7 Hz, 2H), 6.42 (d,

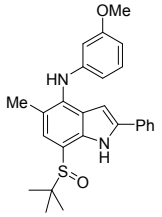
J = 2.3 Hz, 1H), 5.79 (s, 1H), 2.31 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 138.1, 136.4, 135.0, 131.7, 129.0, 128.9, 127.9, 125.7, 125.3, 124.2, 120.1, 120.1, 116.7, 113.6, 97.2, 58.2, 23.2, 17.8. HRMS m/z calcd for $C_{25}H_{27}N_2OS$ ($[M+H]^+$): 403.1839, found 403.1831.



7-(*tert*-butylsulfinyl)-5-methyl-*N*-(4-phenoxyphenyl)-2-phenyl-1*H*-indol-4-amine 4: (eluent: petroleum ether/EtOAc 5:1), 32 mg, 65%; gray solid; m.p. 112-113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51(s, 1H), 7.58 (d, J = 7.6 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.32-7.25 (m, 3H), 7.05-6.94 (m, 6H), 6.88-6.86 (m, 3H), 6.35(s, 1H), 2.33(s, 3H), 1.33(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 140.2, 137.9, 136.5, 135.78, 129.6, 128.9, 127.8, 125.3, 124.7, 124.4, 122.4, 120.4, 119.07, 118.8, 117.6, 112.7, 97.3, 58.2, 23.2, 17.8. HRMS m/z calcd for $C_{31}H_{31}N_2O_2S$ ($[M+H]^+$): 495.2101, found 495.2078.

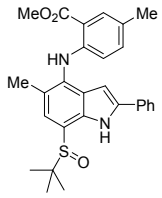


7-(*tert*-butylsulfinyl)-*N*-(4-methoxyphenyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 5: (eluent: petroleum ether/EtOAc 5:1), 29 mg, 68%; gray solid; m.p. 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.54 (d, J = 7.4 Hz, 2H), 7.36 (t, J = 7.6 Hz, 3H), 7.27 (t, J = 7.7 Hz, 1H), 6.90 (d, J = 8.9 Hz, 2H), 6.87 (s, 1H), 6.83 (d, J = 8.9 Hz, 2H), 6.23 (d, J = 2.4 Hz, 1H), 5.66 (s, 1H), 3.80 (s, 3H), 2.30 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) 154.7, 137.5, 137.2, 136.9, 136.7, 131.8, 128.8, 127.7, 125.2, 124.54, 123.5, 120.5, 117.1, 114.3, 111.3, 97.5, 58.1, 55.6, 23.2, 17.78. HRMS m/z calcd for $C_{26}H_{29}N_2O_2S$ ($[M+H]^+$): 433.1944, found 433.1944.

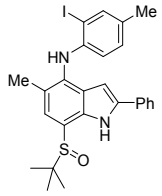


7-(*tert*-butylsulfinyl)-*N*-(3-methoxyphenyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 6: (eluent: petroleum ether/EtOAc 5:1), 26 mg, 60%; gray solid; m.p. 164-165 °C; ^{1}H

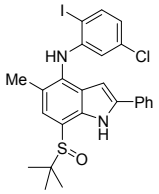
NMR (400 MHz, $CDCl_3$) δ 10.52 (s, 1H), 7.60 (d, J = 7.1 Hz, 2H), 7.38 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 7.1 Hz, 1H), 7.13 (t, J = 8.1 Hz, 1H), 6.90 (s, 1H), 6.49 (d, J = 2.5 Hz, 1H), 6.44 (td, J = 8.1, 2.3 Hz, 2H), 6.36 (t, J = 2.3 Hz, 1H), 5.75 (s, 1H), 3.73 (s, 3H), 2.32 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 145.9, 138.3, 136.3, 134.7, 131.8, 129.8, 128.9, 127.9, 126.3, 125.3, 124.1, 120.8, 114.2, 109.2, 105.3, 102.2, 97.2, 58.2, 55.1, 23.2, 17.8. HRMS m/z calcd for $C_{26}H_{29}N_2O_2S$ ([M+H]$^+$): 433.1944, found 433.1933.



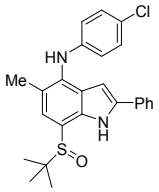
Methyl-2-((7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)amino)-5-methylbenzoate 7: (eluent: petroleum ether/EtOAc 5:1), 15 mg, 32%; gray solid; m.p. 117-118 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.53 (s, 1H), 7.59 (dt, J = 7.7 Hz, 1.7 Hz, 2H), 7.43 (t, J = 2.5 Hz, 1H), 7.38 (td, J = 7.7, 2.3 Hz, 2H), 7.30 (d, J = 7.4 Hz, 1H), 7.08 (dd, J = 8.3 Hz, 2.3 Hz, 1H), 6.90 (s, 1H), 6.81 (dt, J = 8.3, 2.5 Hz, 1H), 6.39 (d, J = 2.5 Hz, 1H), 5.76 (s, 1H), 3.85 (s, 3H), 2.52 (s, 3H), 2.31 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 138.3, 136.4, 134.7, 132.2, 131.7, 131.3, 130.0, 128.9, 127.9, 125.6, 125.3, 124.2, 120.1, 120.0, 118.7, 113.8, 97.1, 58.2, 51.8, 23.2, 20.8, 17.8. HRMS m/z calcd for $C_{28}H_{31}N_2O_3S$ ([M+H]$^+$): 475.2050, found 475.2030.



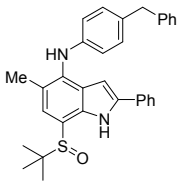
7-(*tert*-butylsulfinyl)-*N*-(2-iodo-4-methylphenyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 8: (eluent: petroleum ether/EtOAc 5:1), 28 mg, 52%; gray solid; m.p. 177-178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.64 (t, J = 7.8 Hz, 3H), 7.42 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.4 Hz, 1H), 6.94 (s, 1H), 6.44 (d, J = 8.2 Hz, 1H), 6.31 (s, 1H), 5.92 (s, 1H), 2.31 (s, 3H), 2.11 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 139.2, 138.8, 138.5, 136.1, 134.2, 131.6, 128.9, 128.0, 127.3, 125.4, 124.0, 122.5, 122.0, 115.5, 112.7, 96.9, 82.8, 58.2, 23.2, 21.3, 17.8. HRMS m/z calcd for $C_{26}H_{28}IN_2OS$ ([M+H]$^+$): 543.0962, found 543.0956.



7-(*tert*-butylsulfinyl)-*N*-(5-chloro-2-iodophenyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 9: (eluent: petroleum ether/EtOAc 5:1), 34 mg, 60%; gray solid; m.p. 176-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.59 (s, 1H), 7.62 (d, J = 7.5 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 7.3 Hz, 1H), 7.00 (t, J = 7.9 Hz, 1H), 6.96 – 6.91 (m, 2H), 6.47 (d, J = 2.4 Hz, 1H), 6.29 (d, J = 8.1 Hz, 1H), 6.23 (s, 1H), 2.32 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 139.2, 139.0, 136.2, 133.5, 131.5, 129.4, 128.9, 128.8, 128.2, 127.8, 125.4, 123.8, 119.5, 111.7, 96.7, 90.5, 58.3, 23.2, 17.7. HRMS m/z calcd for $C_{25}H_{25}ClIN_2OS$ ([M+H]$^+$): 563.0415, found 563.0410.

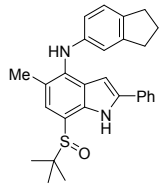


7-(*tert*-butylsulfinyl)-*N*-(4-chlorophenyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 10: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 58%; gray solid; m.p. 150-151 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.59 (d, J = 7.3 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.29 (t, J = 7.4 Hz, 1H), 7.17 (s, J = 8.8 Hz, 2 H), 6.89 (s, 1H), 6.73 (d, J = 8.8 Hz, 2H), 6.40 (d, J = 2.4 Hz, 1H), 5.75 (s, 1H), 2.30 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 138.5, 136.3, 134.3, 131.6, 128.9, 128.0, 125.9, 125.3, 124.5, 124.1, 120.6, 117.4, 114.3, 97.0, 58.2, 23.2, 17.8. HRMS m/z calcd for $C_{25}H_{26}ClN_2OS$, ([M+H]$^+$): 437.1449, found 437.1425.

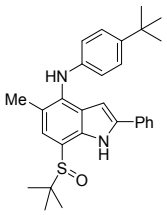


***N*-(4-benzylphenyl)-7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 11**: (eluent: petroleum ether/EtOAc 5:1), 32 mg, 65%; gray solid; m.p. 155-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.56 (d, J = 7.4 Hz, 2H), 7.37 (t, J = 7.3 Hz, 2H), 7.28 (t, J = 6.9 Hz, 3H), 7.20 (d, J = 7.5 Hz, 3H), 7.05 (d, J = 7.8 Hz, 2H), 6.88 (d, J = 2.3 Hz 1H), 6.78 (d, J = 7.7 Hz, 2H), 6.37 (s, 1H), 5.73 (s, 1H), 3.93 (s, 2H), 2.30 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.33, 141.5, 137.9, 136.4,

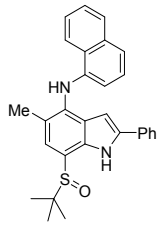
135.5, 133.1, 131.8, 129.4, 128.8, 128.8, 128.4, 127.8, 125.9, 125.3, 125.2, 124.3, 119.4, 117.4, 113.0, 97.4, 58.2, 41.2, 23.2, 17.8. HRMS m/z calcd for $C_{32}H_{33}N_2OS$ ($[M+H]^+$): 493.2308, found 493.2300.



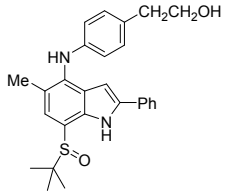
7-(*tert*-butylsulfinyl)-*N*-(2,3-dihydro-1*H*-inden-5-yl)-5-methyl-2-phenyl-1*H*-indol-4-amine 12: (eluent: petroleum ether/EtOAc 5:1), 30 mg, 68%; gray solid; m.p. 121-122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.49 (s, 1H), 7.58 (d, J = 7.7 Hz, 2H), 7.37 (t, J = 7.3 Hz, 2H), 7.31 (t, J = 7.4Hz, 2H), 7.08 (d, J = 8.1 Hz, 1H), 6.89 (d, J = 2.2 Hz, 1H), 6.75 (s, 1H), 6.66 (d, J = 8.3 Hz, 1H), 6.42 (s, 1H), 2.85 (q, J = 8.6 Hz, 4H), 2.31 (s, 3H), 2.12–2.03 (m, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 142.6, 137.9, 136.3, 135.9, 131.9, 128.8, 127.7, 125.3, 125.1, 124.5, 124.4, 119.2, 115.5, 113.5, 112.7, 97.4, 58.1, 33.0, 32.1, 25.7, 23.2, 17.8. HRMS m/z calcd for $C_{28}H_{31}N_2OS$ ($[M+H]^+$): 443.2152, found 443.2144.



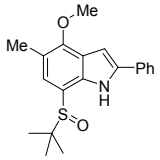
***N*-(4-(*tert*-butyl)phenyl)-7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indol-4-amine 13**: (eluent: petroleum ether/EtOAc 5:1), 21 mg, 45%; gray solid; m.p. 183-184 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.58 (d, J = 7.2 Hz, 2H,), 7.37 (t, J = 7.6 Hz, 2H), 7.30 – 7.23 (m, 4H), 6.89 (s, 1H), 6.81 (d, J = 8.6 Hz, 2H), 6.38 (d, J = 2.4 Hz, 1H), 5.71 (s, 1H), 2.31 (s, 3H), 1.31 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 141.7, 137.9, 136.5, 135.8, 131.9, 131.6, 128.8, 127.8, 125.8, 125.3, 124.3, 119.3, 117.0, 112.9, 97.4, 58.2, 34.1, 31.5, 23.2, 17.8. HRMS m/z calcd for $C_{29}H_{35}N_2OS$ ($[M+H]^+$): 459.2465, found 459.2441.



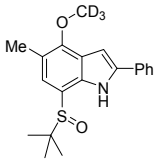
7-(*tert*-butylsulfinyl)-5-methyl-*N*-(naphthalen-1-yl)-2-phenyl-1*H*-indol-4-amine 14: (eluent: petroleum ether/EtOAc 5:1), 18 mg, 40%; gray solid; m.p. 147-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.53 (s, 1H), 8.22 (d, J = 7.7 Hz, 1H), 7.90 (d, J = 6.9 Hz, 2H), 7.54 (ddd, J = 10.5, 7.4, 2.7 Hz, 4H), 7.48 (d, J = 8.1 Hz, 1H), 7.34 (t, J = 7.4 Hz, 3H), 7.26 (q, J = 7.8 Hz, 3H), 6.94 (d, J = 2.3 Hz, 1H), 6.72 (d, J = 7.4 Hz, 2H), 6.32 (s, 1H), 6.15 (s, 1H), 2.34 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 138.2, 136.4, 135.9, 134.5, 131.7, 128.8, 128.6, 127.8, 126.1, 126.0, 125.9, 125.5, 125.2, 124.4, 121.1, 121.0, 119.5, 112.6, 113.3, 108.6, 97.0, 58.2, 23.2, 17.8. HRMS m/z calcd for $C_{29}H_{29}N_2OS$ ([M+H]$^+$): 453.1995, found 453.1982.



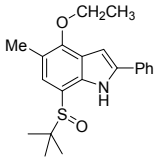
2-(4-((7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)amino)phenyl)ethan-1-ol 15: (eluent: petroleum ether/EtOAc 5:1), 27 mg, 60%; gray solid; m.p. 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.52 (s, 1H), 7.60 – 7.56 (m, 2H), 7.38 (t, J = 7.6 Hz, 2H), 7.29 (dt, J = 8.1, 1.6 Hz, 1H), 7.08 (d, J = 8.4 Hz, 2H), 6.90 (s, 1H), 6.79 (d, J = 8.5 Hz, 2H), 6.41 (d, J = 2.5 Hz, 1H), 5.73 (s, 1H), 3.84 (t, J = 6.6 Hz, 2H), 2.82 (t, J = 6.6 Hz, 2H), 2.31 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 138.1, 136.4, 135.2, 131.8, 129.9, 129.6, 128.9, 127.9, 125.6, 125.3, 124.3, 112.0, 117.0, 113.5, 97.2, 63.8, 58.2, 38.4, 23.2, 17.8. HRMS m/z calcd for $C_{27}H_{31}N_2O_2S$ ([M+H]$^+$): 447.2101, found 447.2100.



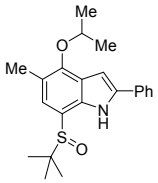
7-(*tert*-butylsulfinyl)-4-methoxy-5-methyl-2-phenyl-1*H*-indole 16: (eluent: petroleum ether/EtOAc 5:1), 29 mg, 85%; yellow solid; m.p. 138-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.68 (d, J = 7.2 Hz, 2H), 7.43 (t, J = 7.9 Hz, 2H), 7.32 (t, J = 7.4 Hz, 1H), 6.89 (d, J = 2.5 Hz, 1H), 6.82 (s, 1H), 4.14 (s, 3H), 2.32 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 138.3, 137.5, 131.7, 128.9, 127.9, 125.3, 124.3, 123.0, 118.4, 112.6, 95.8, 60.1, 58.1, 23.1, 15.7. HRMS m/z calcd for $C_{20}H_{24}NO_2S$ ([M+H]$^+$): 342.1522, found 342.1506.



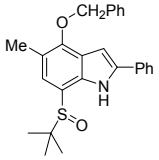
7-(*tert*-butylsulfinyl)-4-(methoxy-*d3*)-5-methyl-2-phenyl-1*H*-indole 17: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 72%; yellow solid; m.p. 131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.68 (d, J = 7.4 Hz, 3H), 7.43 (t, J = 7.7 Hz, 3H), 7.32 (t, J = 7.4 Hz, 1H), 6.89 (d, J = 2.4 Hz, 1H), 6.82 (s, 1H), 2.32 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 138.3, 137.5, 131.7, 128.9, 127.9, 125.3, 124.3, 122.9, 118.4, 112.5, 95.8, 58.1, 23.1, 15.8. HRMS m/z calcd for $C_{20}H_{21}D_3NO_2S$ ([M+H]$^+$): 345.1711, found 345.1700.



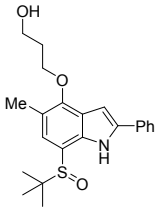
7-(*tert*-butylsulfinyl)-4-ethoxy-5-methyl-2-phenyl-1*H*-indole 18: (eluent: petroleum ether/EtOAc 5:1), 27 mg, 76%; yellow solid; m.p. 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 7.68 (d, J = 8.1 Hz, 2H), 7.43 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.9 Hz, 1H), 6.82 (s, 2H), 4.38 (q, J = 7.0 Hz, 2H), 2.33 (s, 3H), 1.48 (t, J = 7.0 Hz, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 137.3, 131.8, 128.9, 127.9, 125.3, 124.3, 123.7, 118.9, 112.7, 95.9, 68.3, 58.1, 23.1, 16.0, 15.9. HRMS m/z calcd for $C_{21}H_{26}NO_2S$ ([M+H]$^+$): 356.1679, found 356.1652.



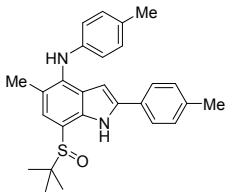
7-(*tert*-butylsulfinyl)-4-isopropoxy-5-methyl-2-phenyl-1*H*-indole 19: (eluent: petroleum ether/EtOAc 5:1), 24 mg, 65%; yellow solid; m.p. 165-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.68 (d, J = 6.9 Hz, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.32 (t, J = 7.4 Hz, 1H), 6.83 (s, 1H), 6.77 (d, J = 2.5 Hz, 1H), 4.79 (hept, J = 6.1 Hz, 1H), 2.33 (s, 3H), 1.40 (dd, J = 9.5, 6.1 Hz, 6H), 1.28 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 138.2, 137.1, 131.8, 128.9, 127.9, 125.3, 124.7, 124.3, 120.0, 113.0, 96.0, 74.7, 58.1, 23.1, 23.0, 22.9, 16.3. HRMS m/z calcd for $C_{22}H_{28}NO_2S$ ([M+H]$^+$): 370.1835, found 370.1847.



4-(benzyloxy)-7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indole 20: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 60%; yellow solid; m.p. 127-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.67 (d, J = 7.4 Hz, 2H), 7.50 (d, J = 7.1 Hz, 2H), 7.47 – 7.29 (m, 7H), 5.33 (s, 2H), 2.29 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 138.5, 137.7, 137.3, 131.7, 128.9, 128.5, 128.0, 128.0, 127.8, 125.4, 124.2, 123.8, 119.4, 113.3, 95.8, 74.5, 58.1, 23.1, 16.0. HRMS m/z calcd for $C_{26}H_{28}NO_2S$ ([M+H]$^+$): 418.1835, found 418.1820.

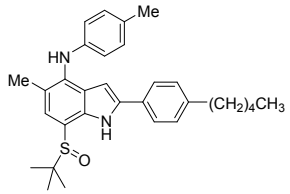


3-((7-(*tert*-butylsulfinyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)oxy)propan-1-ol 21: (eluent: petroleum ether/EtOAc 3:1), 26 mg, 68%; yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 7.69 (d, J = 7.3 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 6.86 (s, J = 2.4 Hz, 1H), 6.81 (s, 1H), 4.47 (t, J = 5.9 Hz, 2H), 4.01 (t, J = 5.9 Hz, 2H), 3.73 (s, 1H), 2.32 (s, 3H), 4.47 (t, J = 5.9 Hz, 2H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 138.5, 137.4, 131.6, 128.9, 128.0, , 125.3, 124.3, 123.4, 118.6, 112.9, 95.8, 70.7, 60.7, 58.2, 33.1, 23.1, 15.9. HRMS m/z calcd for $C_{22}H_{27}NNaO_3S$ ([M+Na]$^+$): 408.1604, found 408.1585.

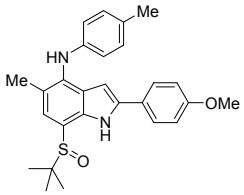


7-(*tert*-butylsulfinyl)-5-methyl-*N*,2-di-*p*-tolyl-1*H*-indol-4-amine 22: (eluent: petroleum ether/EtOAc 5:1), 32 mg, 75%; gray solid; m.p. 174-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.45 (s, 1H), 7.47 (d, J = 7.9 Hz, 2H), 7.18 (d, J = 7.9 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.87 (s, 1H), 6.76 (d, J = 8.2 Hz, 2H), 6.34 (d, J = 2.4 Hz, 1H), 5.68 (s, 1H), 2.35 (s, 3H), 2.31 (s, 3H), 2.30 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 138.1, 137.7, 136.3, 135.5, 133.8, 129.7, 129.5, 129.0, 125.2, 124.9,

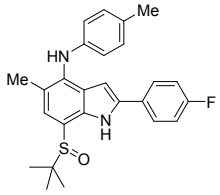
119.2, 117.3, 112.8, 96.8, 58.1, 23.2, 21.2, 20.6, 17.8. HRMS m/z calcd for $C_{27}H_{31}N_2OS$ ([M+H]$^+$): 431.2152, found 431.2131.



7-(*tert*-butylsulfinyl)-5-methyl-2-(4-pentylphenyl)-*N*-(*p*-tolyl)-1*H*-indol-4-amine 23: (eluent: petroleum ether/EtOAc 5:1), 23 mg, 48%; gray solid; m.p. 133-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.45 (s, 1H), 7.49 (d, J = 7.9 Hz, 2H), 7.18 (d, J = 7.9 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.87 (s, 1H), 6.77 (d, J = 8.3 Hz, 2H), 6.34 (d, J = 2.5 Hz, 1H), 5.68 (s, 1H), 2.60 (t, J = 7.7 Hz, 2H), 2.30 (s, 6H), 1.62 (q, J = 7.5 Hz, 2H), 1.32 – 1.30 (m, 4H), 1.30 (s, 9H), 0.89 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 141.8, 138.1, 136.3, 135.5, 135.0, 129.7, 129.5, 129.2, 128.9, 125.2, 124.1, 119.1, 117.3, 112.8, 96.8, 58.1, 35.6, 31.4, 31.0, 23.2, 22.5, 20.6, 17.8, 14.0. HRMS m/z calcd for $C_{31}H_{39}N_2OS$ ([M+H]$^+$): 487.2778, found 487.2758.

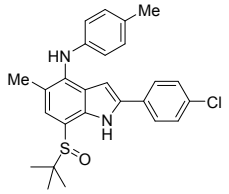


7-(*tert*-butylsulfinyl)-2-(4-methoxyphenyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 24: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 56%; gray solid; m.p. 159-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.40 (s, 1H), 7.51 (d, J = 8.8 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 6.86 (s, 1H), 6.77 (d, J = 8.4 Hz, 2H), 6.27 (d, J = 2.5 Hz, 2H), 5.67 (s, 1H), 3.83 (s, 3H), 2.30 (s, 3H), 2.30 (s, 3H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 141.7, 137.9, 136.2, 135.3, 129.5, 129.4, 126.6, 125.3, 124.6, 123.7, 119.2, 117.1, 114.2, 112.7, 96.1, 58.0, 55.2, 23.1, 20.5, 17.7. HRMS m/z calcd for $C_{27}H_{31}N_2O_2S$ ([M+H]$^+$): 447.2101, found 447.2103.



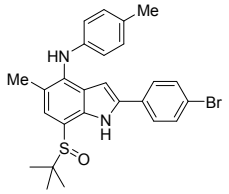
7-(*tert*-butylsulfinyl)-2-(4-fluorophenyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 25: (eluent: petroleum ether/EtOAc 5:1), 22 mg, 50%; gray solid; m.p. 172-173 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 7.57 – 7.49 (m, 2H), 7.10 – 7.01 (m, 4H), 6.88 (s, 1H), 6.80 – 6.75 (m, 2H), 6.30 (d, J = 2.5 Hz, 1H), 5.69 (s, 1H), 2.31 (s, 3H),2.30 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, J(C.F) = 247.7 Hz), 141.6, 137.0, 136.5, 135.7, 129.9, 129.5, 128.2 (d, J(C.F) = 2.7 Hz), 127.0 (d, J(C.F) = 8.1 Hz), 125.0, 124.4, 119.1, 117.5, 115.9 (d, J(C.F) = 21.9 Hz)., 112.7, 97.3, 58.2, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{28}FN_2OS$ ([M+H]$^+$): 435.1901, found 435.1908.



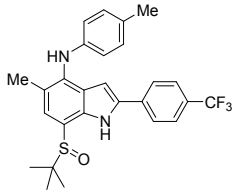
7-(*tert*-butylsulfinyl)-2-(4-chlorophenyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine

26: (eluent: petroleum ether/EtOAc 5:1), 31 mg, 68%; gray solid; m.p. 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.48 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.5 Hz, 2H)., 7.04 (d, J = 8.0 Hz, 2H), 6.89 (s, 1H), 6.77 (d, J = 8.3 Hz, 2H), 6.34 (d, J = 2.5 Hz, 1H), 5.70 (s, 1H), 2.30 (s, 6H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 136.6, 135.9, 133.4, 130.3, 130.0, 129.5, 129.1, 129.0, 126.4, 124.8, 124.6, 119.1, 117.5, 112.6, 97.9, 58.2, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{28}ClN_2OS$ ([M+H]$^+$): 451.1605, found 451.1597.

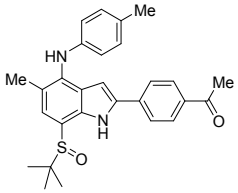


2-(4-bromophenyl)-7-(*tert*-butylsulfinyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine

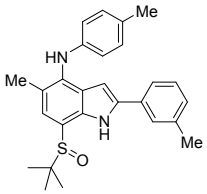
27: (eluent: petroleum ether/EtOAc 5:1), 27 mg, 55%; gray solid; m.p. 169-170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.41 (d, J = 8.5 Hz, 2H), 7.26 (s, 1H), 7.05 (d, J = 8.1 Hz, 2H), 6.89 (s, 1H), 6.77 (d, J = 8.2 Hz, 2H), 6.35 (d, J = 2.4 Hz, 1H), 5.70 (s, 1H), 2.31 (s, 6H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 136.6, 135.9, 131.9, 130.8, 130.0, 129.5, 127.4, 126.7, 124.8, 124.7, 121.6, 119.1, 117.6, 112.7, 97.9, 58.2, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{28}BrN_2OS$ ([M+H]$^+$): 495.1100, found 495.1077.



7-(*tert*-butylsulfinyl)-5-methyl-*N*-(*p*-tolyl)-2-(4-(trifluoromethyl)phenyl)-1*H*-indol-4-amine 28: (eluent: petroleum ether/EtOAc 5:1), 33 mg, 68%; gray solid; m.p. 161-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.62 (s, 1H), 7.62 (q, J = 8.5 Hz, 4H), 7.06 (d, J = 8.1 Hz, 2H), 6.92 (s, 1H), 6.80 (d, J = 8.3 Hz, 2H), 6.43 (d, J = 2.5 Hz, 1H), 5.73 (s, 1H), 2.31 (s, 6H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 136.9, 136.2, 136.0, 135.2, 130.3, 129.5, 129.3 (q, J(C,F) = 32.8 Hz), 129.1, 125.8, 125.8, 125.7, 125.3, 125.2, 124.5, 124.0 (q, J(C,F) = 272.00 Hz), 118.9, 117.8, 112.5, 99.1, 58.2, 23.1, 20.6, 17.8. HRMS m/z calcd for $C_{27}H_{28}F_3N_2OS$ ([M+H]$^+$): 485.1869, found 485.1860.

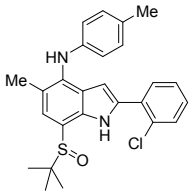


1-(4-(7-(*tert*-butylsulfinyl)-5-methyl-4-(*p*-tolylamino)-1*H*-indol-2-yl)phenyl)ethan-1-one 29: (eluent: petroleum ether/EtOAc 5:1), 21 mg, 45%; yellow solid; m.p. 85-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 7.96 (d, J = 8.6 Hz, 2H), 7.63 (d, J = 8.6 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 6.92 (s, 1H), 6.80 (d, J = 8.4 Hz, 2H), 6.48 (d, J = 2.5 Hz, 1H), 5.72 (s, 1H), 2.60 (s, 3H), 2.32 (s, 6H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 141.8, 138.1, 137.7, 136.3, 135.5, 133.8, 129.7, 129.5, 129.0, 125.2, 124.1, 119.2, 117.3, 112.8, 96.8, 58.1, 23.2, 21.2, 20.6, 17.8. HRMS m/z calcd for $C_{28}H_{31}N_2O_2S$ ([M+H]$^+$): 459.2101, found 459.2107.



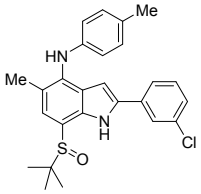
7-(*tert*-butylsulfinyl)-5-methyl-2-(*m*-tolyl)-*N*-(*p*-tolyl)-1*H*-indol-4-amine 30: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 58%; gray solid; m.p. 160-161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 7.41 – 7.36 (m, 2H), 7.26 (t, J = 7.9 Hz, 2H), 7.09 (d, J = 7.6 Hz, 1H), 7.04 (d, J = 8.1 Hz, 2H), 6.88 (s, 1H), 6.76 (d, J = 8.4 Hz, 2H), 6.38 (d, J = 2.5 Hz, 1H), 5.69 (s, 1H), 2.37 (s, 3H), 2.30 (s, 3H), 2.30 (s, 3H), 1.31 (s,

9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 138.5, 138.1, 136.4, 135.6, 131.8, 129.7, 129.5, 128.7, 128.6, 125.9, 125.2, 124.2, 122.6, 119.3, 117.2, 112.9, 97.3, 58.1, 23.2, 21.4, 20.6, 17.8. HRMS m/z calcd for $C_{27}H_{31}N_2OS$ ([M+H]$^+$): 431.2152, found 431.2151.



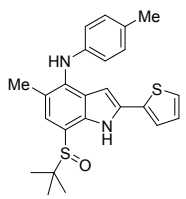
7-(*tert*-butylsulfinyl)-2-(2-chlorophenyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine

31: (eluent: petroleum ether/EtOAc 5:1), 23 mg, 50%; gray solid; m.p. 179-180 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.70 (s, 1H), 7.51 (dd, J = 7.5, 2.0 Hz, 1H), 7.43 (dd, J = 7.6, 1.7 Hz, 1H), 7.30 – 7.17 (m, 2H), 7.04 (d, J = 8.2 Hz, 2H), 6.93 (s, 1H), 6.80 (d, J = 8.3 Hz, 2H), 6.41 (d, J = 2.5 Hz, 1H), 5.73 (s, 1H), 2.31 (s, 3H), 2.30 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 136.1, 135.7, 134.9, 131.6, 130.7, 130.6, 130.1, 129.5, 128.8, 127.0, 124.9, 123.8, 120.7, 118.6, 117.8, 101.2 , 58.0, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{28}ClN_2OS$ ([M+H]$^+$): 451.1605, found 451.1602.

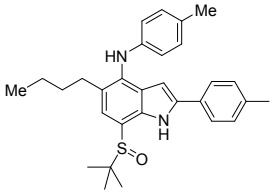


7-(*tert*-butylsulfinyl)-2-(3-chlorophenyl)-5-methyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine

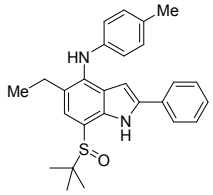
32: (eluent: petroleum ether/EtOAc 5:1), 16 mg, 35%; gray solid; m.p. 164-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 7.44 – 7.36 (m, 2H), 7.26 (t, J = 7.7 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 7.04 (d, J = 8.2 Hz, 2H), 6.88 (s, 1H), 6.76 (d, J = 8.4 Hz, 2H), 6.38 (d, J = 2.5 Hz, 1H), 5.69 (s, 1H), 2.37 (s, 3H), 2.30 (s, 3H), 2.30 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 136.7, 136.3, 136.0, 134.8, 133.7, 130.1, 129.6, 127.6, 125.3, 124.8, 124.7, 123.3, 120.9, 119.1, 117.6, 112.7, 98.4, 58.2, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{26}H_{28}ClN_2OS$ ([M+H]$^+$): 451.1605, found 451.1602.



7-(*tert*-butylsulfinyl)-5-methyl-2-(thiophen-2-yl)-*N*-(*p*-tolyl)-1*H*-indol-4-amine 33: (eluent: petroleum ether/EtOAc 5:1), 22 mg, 51%; gray solid; m.p. 180-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.24 – 7.19 (m, 2H), 7.06 – 7.01 (m, 3H), 6.87 (s, 1H), 6.75 (d, J = 8.4 Hz, 2H), 6.28 (d, J = 2.4 Hz, 1H), 5.68 (s, 1H), 2.30 (s, 3H), 2.29 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 136.1, 135.6, 135.2, 132.4, 129.8, 129.5, 127.8, 125.0, 124.8, 124.4, 123.4, 119.5, 117.3, 112.8, 97.8, 58.1, 23.2, 20.6, 17.8. HRMS m/z calcd for $C_{24}H_{27}N_2OS_2$ ([M+H]$^+$): 423.1559, found 423.1550.

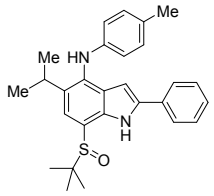


5-butyl-7-(*tert*-butylsulfinyl)-*N*,2-di-*p*-tolyl-1*H*-indol-4-amine 34: (eluent: petroleum ether/EtOAc 5:1), 26 mg, 56%; gray solid; m.p. 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.43 (s, 1H), 7.46 (d, J = 7.9 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 8.1 Hz, 1H), 6.87 (s, 1H), 6.74 (d, J = 8.3 Hz, 2H), 6.31 (d, J = 2.0 Hz, 1H), 5.69 (s, 1H), 2.66 (td, J = 7.4, 2.9 Hz, 2H), 2.35 (s, 3H), 2.29 (s, 3H), 1.57 (t, J = 7.6 Hz, 2H), 1.38 – 1.33 (m, 2H), 1.30 (s, 9H), 0.89 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 138.1, 137.7, 136.1, 135.0, 129.5, 129.1, 125.8, 125.3, 124.6, 123.3, 117.0, 113.3, 97.2, 58.2, 32.8, 31.0, 23.2, 22.4, 21.2, 20.6, 13.9. HRMS m/z calcd for $C_{30}H_{37}N_2OS$ ([M+H]$^+$): 473.2621, found 473.2616.

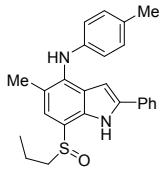


7-(*tert*-butylsulfinyl)-5-ethyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 35: (eluent: petroleum ether/EtOAc 5:1), 30 mg, 69%; gray solid; m.p. 165-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.51 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 7.03 (d, J = 8.1 Hz, 2H), 6.91(s, 1H), 6.77 (d, J = 8.4 Hz, 2H), 6.38 (d, J = 2.5 Hz, 1H), 5.71 (s, 1H), 2.72 (q, J = 7.5 Hz, 2H), 2.29 (s, 3H), 1.31 (s, 9H), 1.24 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 138.0, 136.3, 135.0, 131.9, 129.5, 129.1, 128.8, 127.8, 126.1, 125.8, 125.3, 122.7, 117.0, 113.5, 97.7, 58.2,

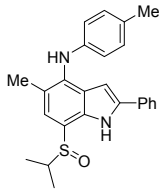
24.3, 23.2, 20.6, 15.0. HRMS m/z calcd for $C_{27}H_{31}N_2OS$ ([M+H]$^+$): 431.2152, found 431.2147.



7-(*tert*-butylsulfinyl)-5-isopropyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 36: (eluent: petroleum ether/EtOAc 5:1), 18 mg, 41%; gray solid; m.p. 167-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.59 (d, J = 8.5 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 8.3 Hz, 2H), 7.02 (d, J = 8.2 Hz, 2H), 6.97(s, 1H), 6.72 (d, J = 8.4 Hz, 1H), 6.41 (d, J = 2.5 Hz, 1H), 5.67 (s, 1H), 3.33 (hept, J = 6.8 Hz, 1H), 2.28 (s, 3H), 1.30 (s, 9H), 1.24 (d, J = 3.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 138.2, 135.9, 133.9, 131.9, 129.9, 129.6, 129.0, 128.8, 126.6, 125.4, 119.6, 116.3, 114.6, 97.7, 58.1, 27.5, 27.2, 23.8, 23.7, 23.2. HRMS m/z calcd for $C_{28}H_{33}N_2OS$ ([M+H]$^+$): 445.2308, found 445.2251.

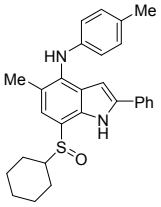


5-methyl-2-phenyl-7-(propylsulfinyl)-*N*-(*p*-tolyl)-1*H*-indol-4-amine 37: (eluent: petroleum ether/EtOAc 5:1), 18 mg, 45%; gray oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.61 (d, J = 7.6 Hz, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.30 (t, J = 7.5 Hz, 1H), 7.05 (d, J = 7.3 Hz, 2H), 6.94 (s, 1H), 6.79 (d, J = 7.3 Hz, 2H), 6.42 (s, 1H), 5.71 (s, 1H), 3.24 (m, 1H), 3.02 (m, 1H), 2.30 (s, 3H), 2.30 (s, 3H), 1.86 (m, 2H), 1.10 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 138.1, 135.9, 135.1, 131.8, 129.9, 129.5, 128.9, 127.8, 125.4, 125.8, 129.7, 117.5, 116.7, 98.0, 58.2, 20.6, 17.7, 16.5, 13.2. HRMS m/z calcd for $C_{25}H_{26}N_2NaOS$ ([M+Na]$^+$): 425.1658, found 425.1694.

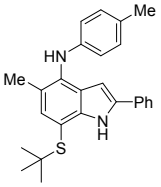


7-(isopropylsulfinyl)-5-methyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 38: (eluent: petroleum ether/EtOAc 5:1), 22 mg, 55%; gray oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.59 (d, J = 7.6 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 7.4 Hz, 1H),

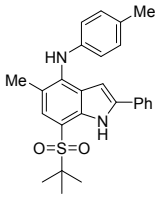
7.05 (d, *J* = 7.9 Hz, 2H), 6.91 (s, 1H), 6.78 (d, *J* = 7.9 Hz, 2H), 6.41 (d, *J* = 2.4 Hz, 1H), 5.70 (s, 1H), 3.2 (p, *J* = 6.9 Hz, 1H), 2.30 (s, 6H), 1.38 (d, *J* = 6.9 Hz, 3H), 1.26 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 138.0, 135.8, 135.8, 131.8, 129.9, 129.5, 128.8, 127.8, 125.4, 125.2, 122.9, 119.5, 117.4, 114.7, 97.8, 55.0, 20.6, 17.7, 16.3, 15.3. HRMS m/z calcd for $C_{25}H_{27}N_2OS$ ([M+H]$^+$): 403.1839, found 403.1832.



7-(cyclohexylsulfinyl)-5-methyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 39: (eluent: petroleum ether/EtOAc 5:1)， 23 mg, 51%; gray oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 10.34 (s, 1H), 7.60 (d, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.90 (s, 1H), 6.79 (d, *J* = 7.9 Hz, 2H), 6.41 (d, *J* = 2.4 Hz, 1H), 5.71(s, 1H), 2.97 (m, 1H), 2.31 (s, 3H), 2.30 (s, 3H), 2.11 (m, 2H), 1.92 (m, 3H), 1.67 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 141.8, 138.0, 135.8, 135.8, 131.8, 129.9, 129.5, 128.8, 127.8, 125.4, 125.1, 122.8, 119.5, 117.5, 114.7, 97.8, 63.1, 26.4, 25.5, 25.3, 25.2, 20.6, 17.8. HRMS m/z calcd for $C_{28}H_{31}N_2OS$ ([M+H]$^+$): 443.2152, found 443.2080.

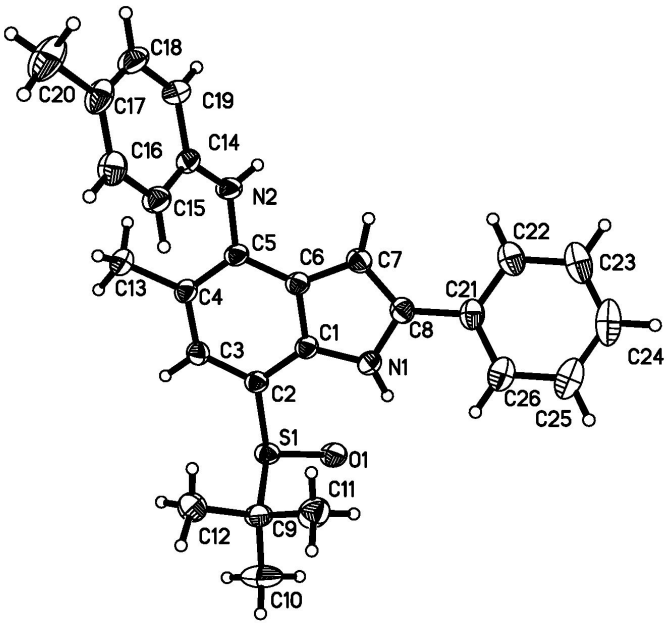


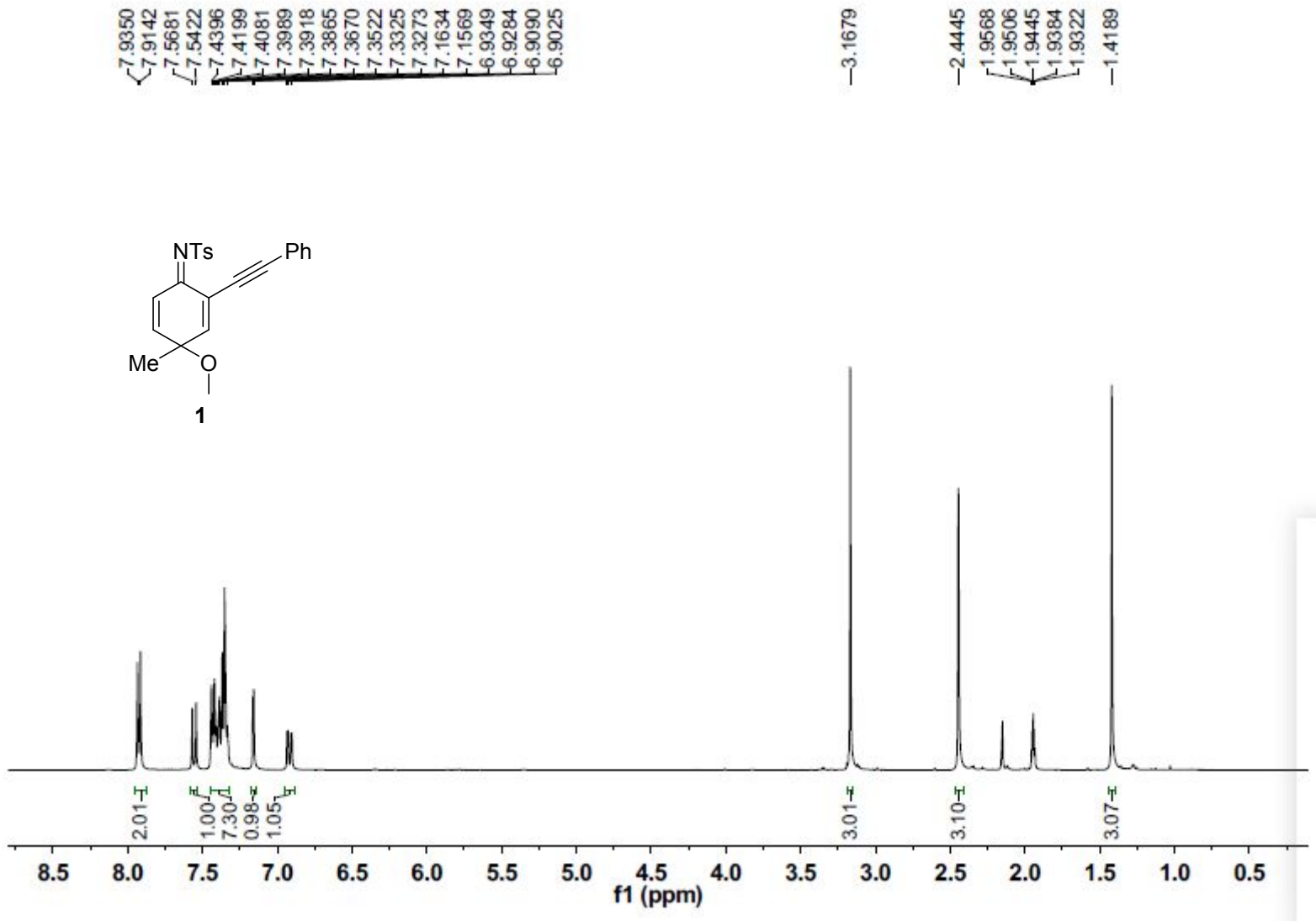
7-(*tert*-butylthio)-5-methyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 41: (eluent: petroleum ether/EtOAc 5:1), 25 mg, 62%; yellow solid; m.p. 133-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.70 (s, 1H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.21 (s, 1H), 7.02 (d, *J* = 8.2 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.49 (d, *J* = 2.4 Hz, 1H), 5.60 (s, 1H), 2.31 (s, 3H), 2.28 (s, 3H), 1.37 (s, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 142.5, 140.6, 136.5, 135.2, 133.8, 132.2, 129.5, 128.5, 127.6, 125.1, 123.8, 121.6, 116.4, 108.4, 99.3, 47.5, 31.3, 20.6, 17.7. HRMS m/z calcd for $C_{26}H_{29}N_2S$ ([M+H]$^+$): 401.2046, found 401.2038.



7-(*tert*-butylsulfonyl)-5-methyl-2-phenyl-*N*-(*p*-tolyl)-1*H*-indol-4-amine 42: (eluent: petroleum ether/EtOAc 5:1), 40 mg, 93%; yellow solid; m.p. 163-164 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (s, 1H), 7.51 (d, J = 7.3 Hz, 2H), 7.41 (s, 1H), 7.38 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 7.3 Hz, 1H), 7.09 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.3 Hz, 2H), 6.25 (d, J = 2.4 Hz, 1H), 5.91 (s, 1H), 2.34 (s, 6H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 139.6, 137.3, 136.0, 131.7, 131.5, 129.5, 128.9, 128.0, 125.2, 121.7, 119.9, 117.2, 108.3, 99.0, 61.3, 23.5, 20.8, 17.8. HRMS m/z calcd for $C_{26}H_{29}N_2O_2S$ ($[M+H]^+$): 433.1944, found 433.1922.

3. X-ray diffraction structure of compound 2

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7.3918
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7.3325
7.3273
7.1634
7.1569
6.9349
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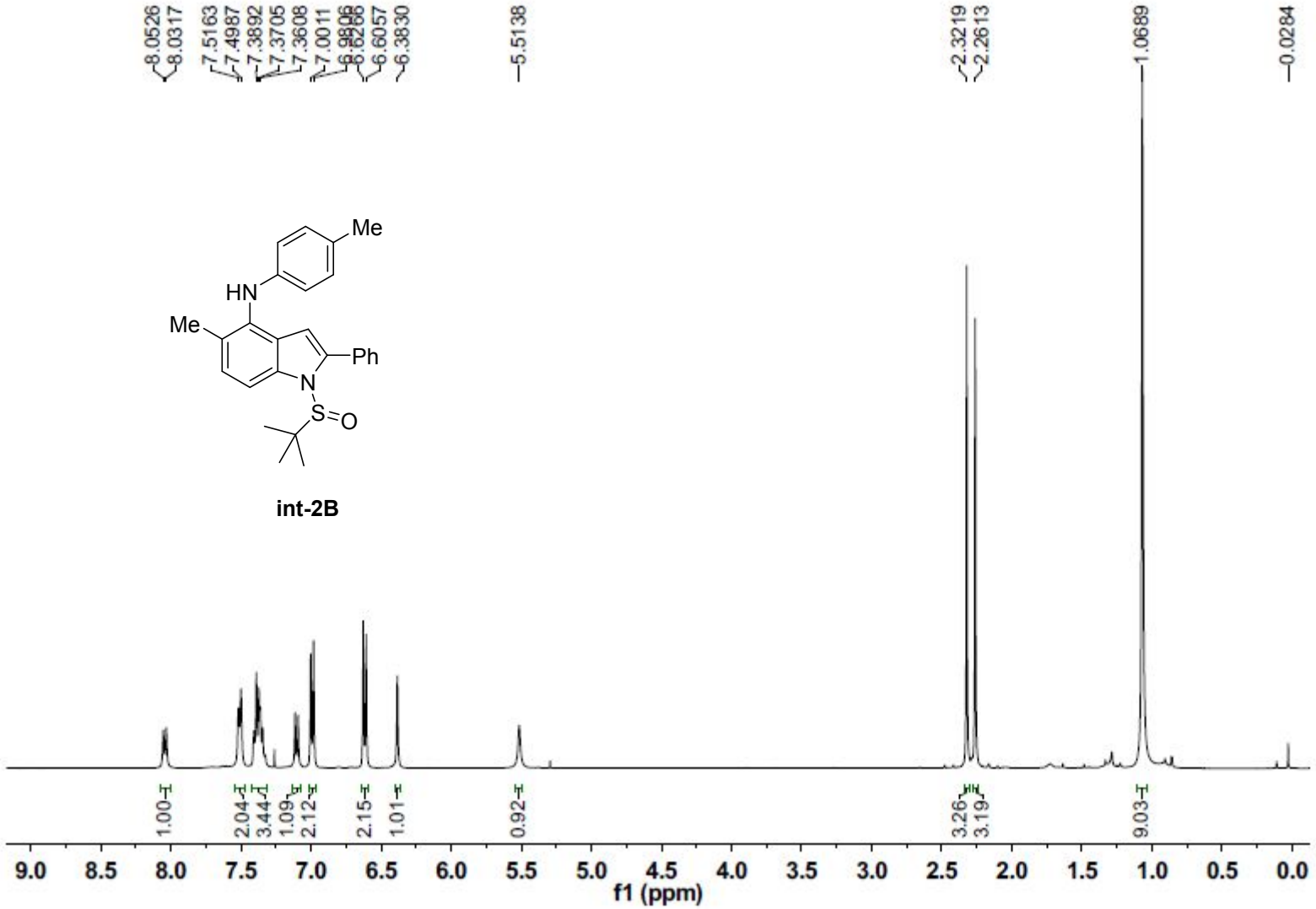
3.1679
2.4445
1.9568
1.9506
1.9445
1.9384
1.9322
1.4189
NTs
Ph
Me
O
1
2.01
1.00
7.30
0.98
1.05
3.01
3.10
3.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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6.3830
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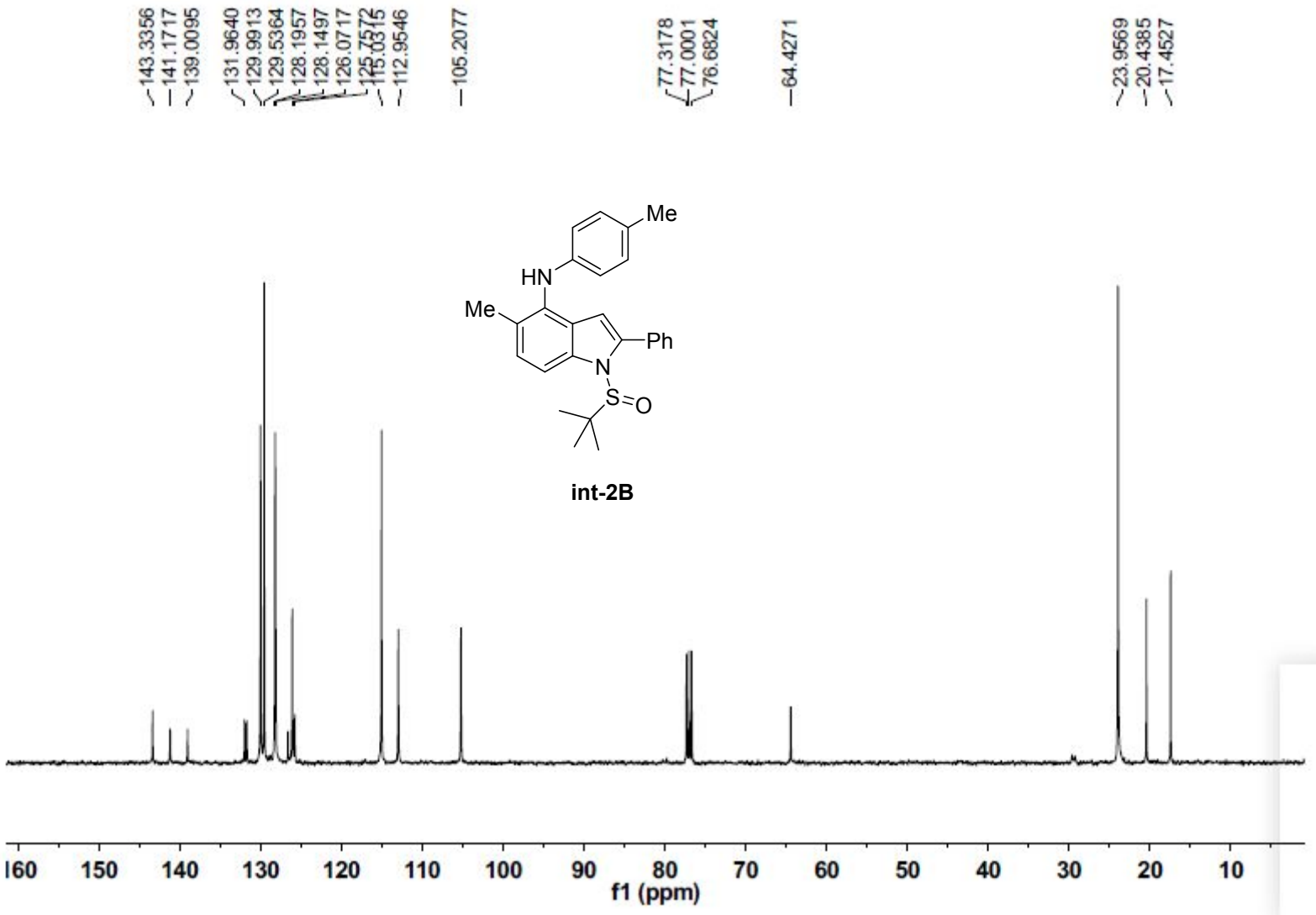
2.2613
1.0689
0.0284
Me
HN
Me
Ph
N
S
O
1.00
2.04
3.44
1.09
2.12
2.15
1.01
0.92
3.26
3.19
9.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

int-2B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128.1957
128.1497
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125.7572
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112.9546
105.2077
77.3178
77.0001
76.6824
64.4271
23.9569
20.4385
17.4527
Me
HN
Me
Ph
N
S
O
160
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120
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100
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80
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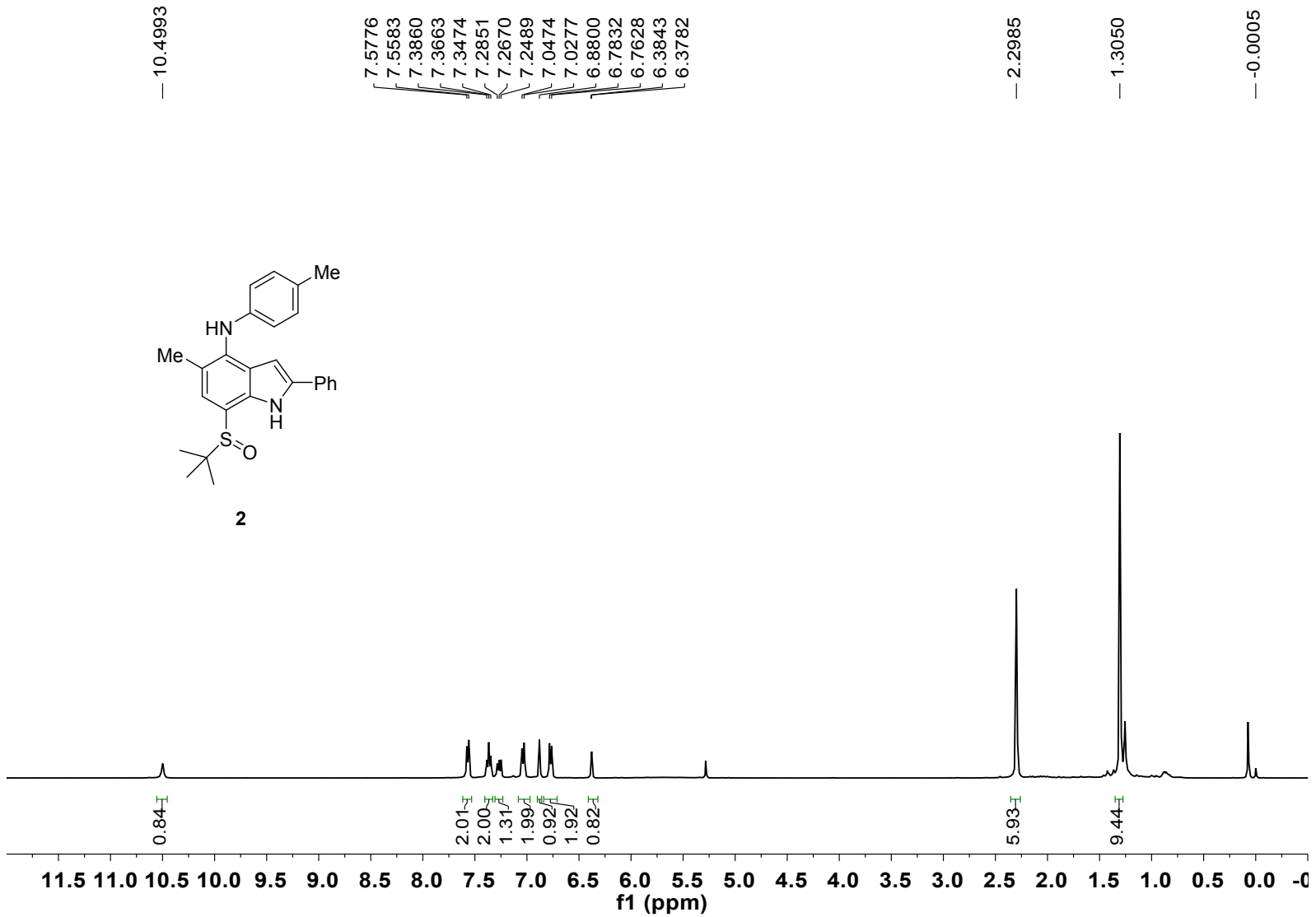
60
50
40
30
20
10
f1 (ppm)

int-2B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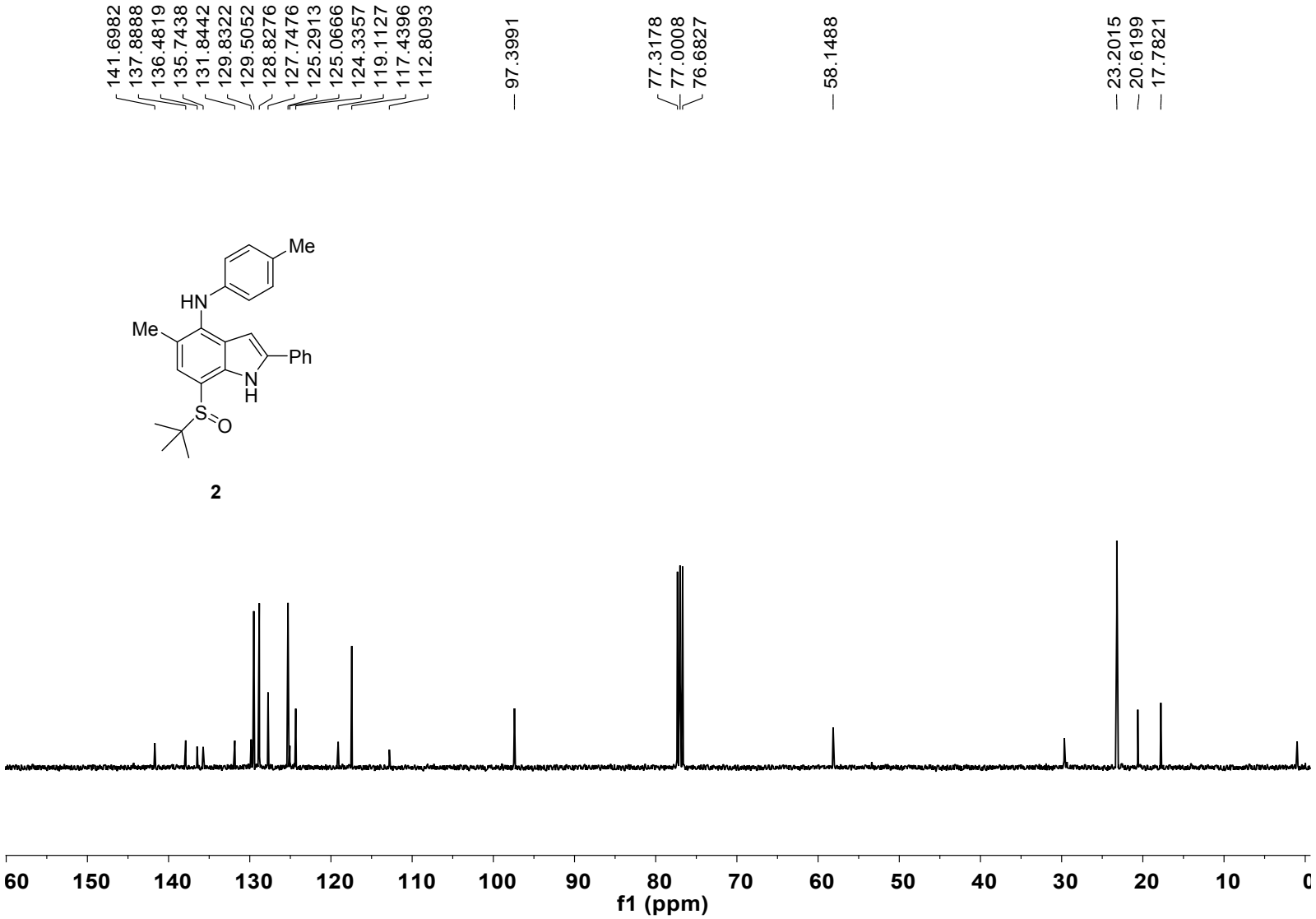
6.7832
6.7628
6.3843
6.3782
2.2985
1.3050
-0.0005
Me
HN
Me
Ph
N
H
S
O
2
0.84
2.01
2.00
1.31
1.99
0.92
1.92
0.82
5.93
9.44
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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97.3991
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23.2015
20.6199
17.7821
Me
HN
Me
Ph
N
H
S
O
2
60
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110
100
90
80
70
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50
40
30
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10
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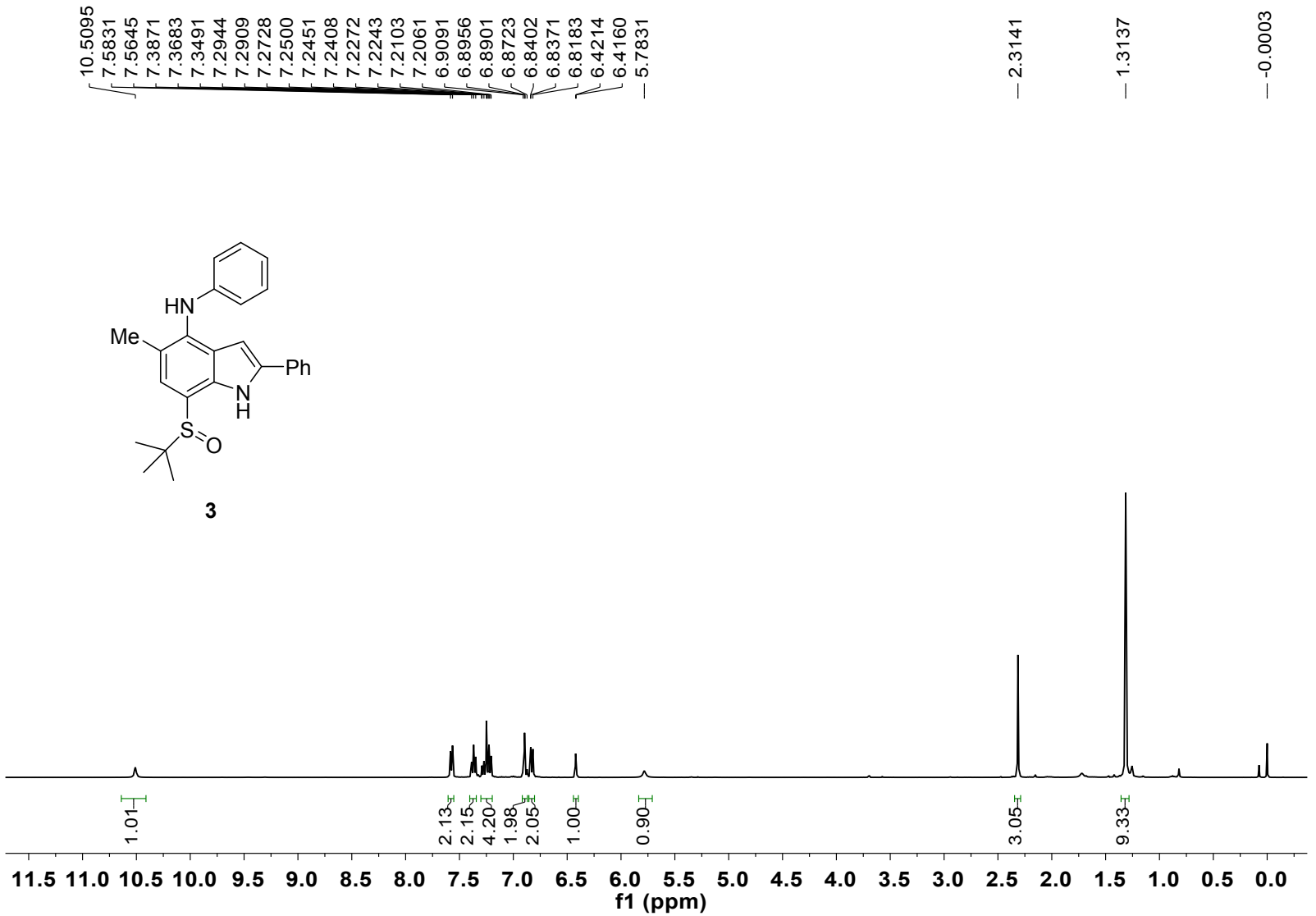
f1 (ppm)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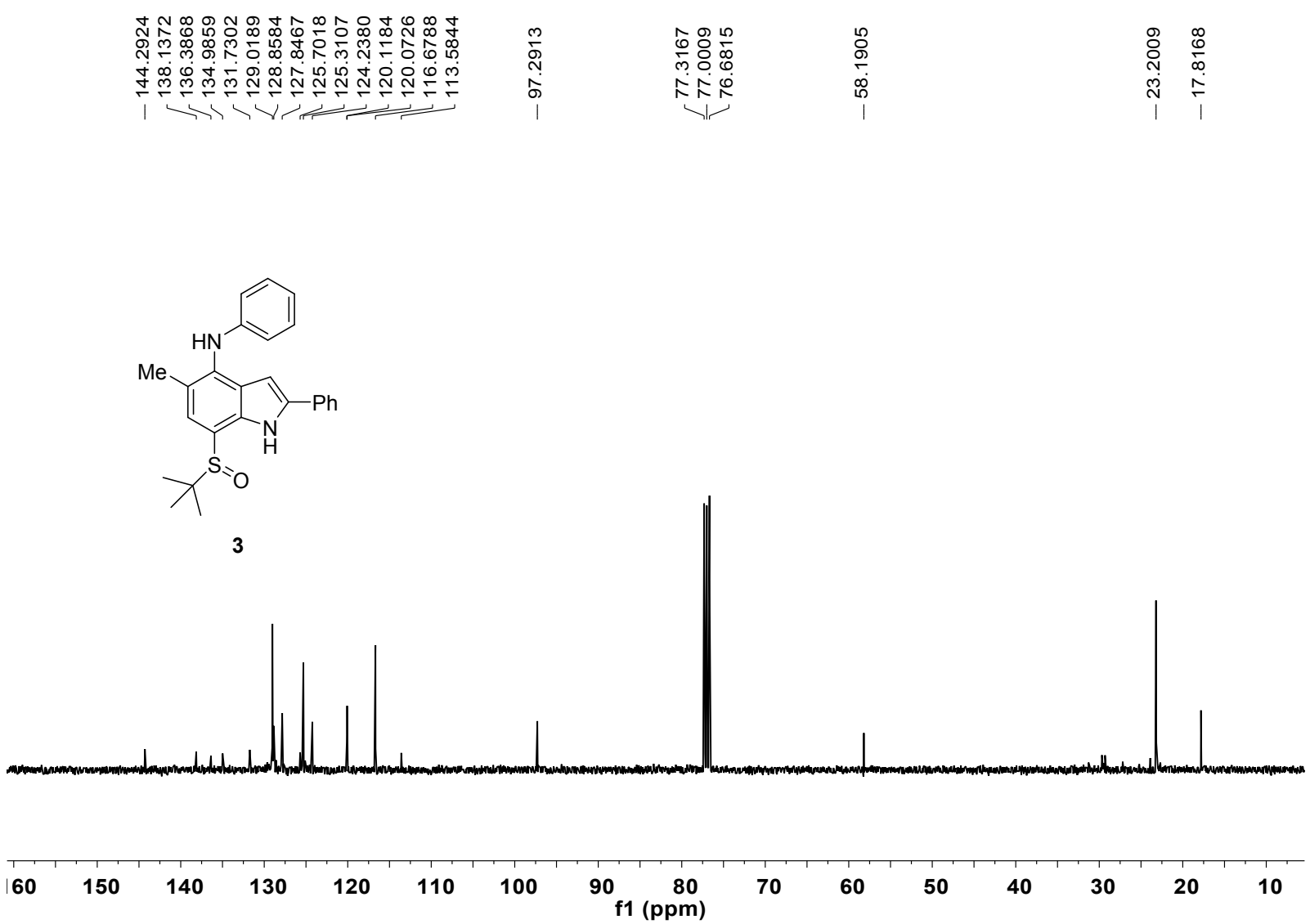
7.3491
7.2944
7.2909
7.2728
7.2500
7.2451
7.2408
7.2272
7.2243
7.2103
7.2061
6.9091
6.8956
6.8901
6.8723
6.8402
6.8371
6.8183
6.4214
6.4160
5.7831
2.3141
1.3137
-0.0003
HN
Me
Ph
N
H
S
O
3
1.01
2.13
2.15
4.20
1.98
2.05
1.00
0.90
3.05
9.33
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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120.0726
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113.5844
97.2913
77.3167
77.0009
76.6815
58.1905
23.2009
17.8168
HN
Me
Ph
N
H
S
O
3
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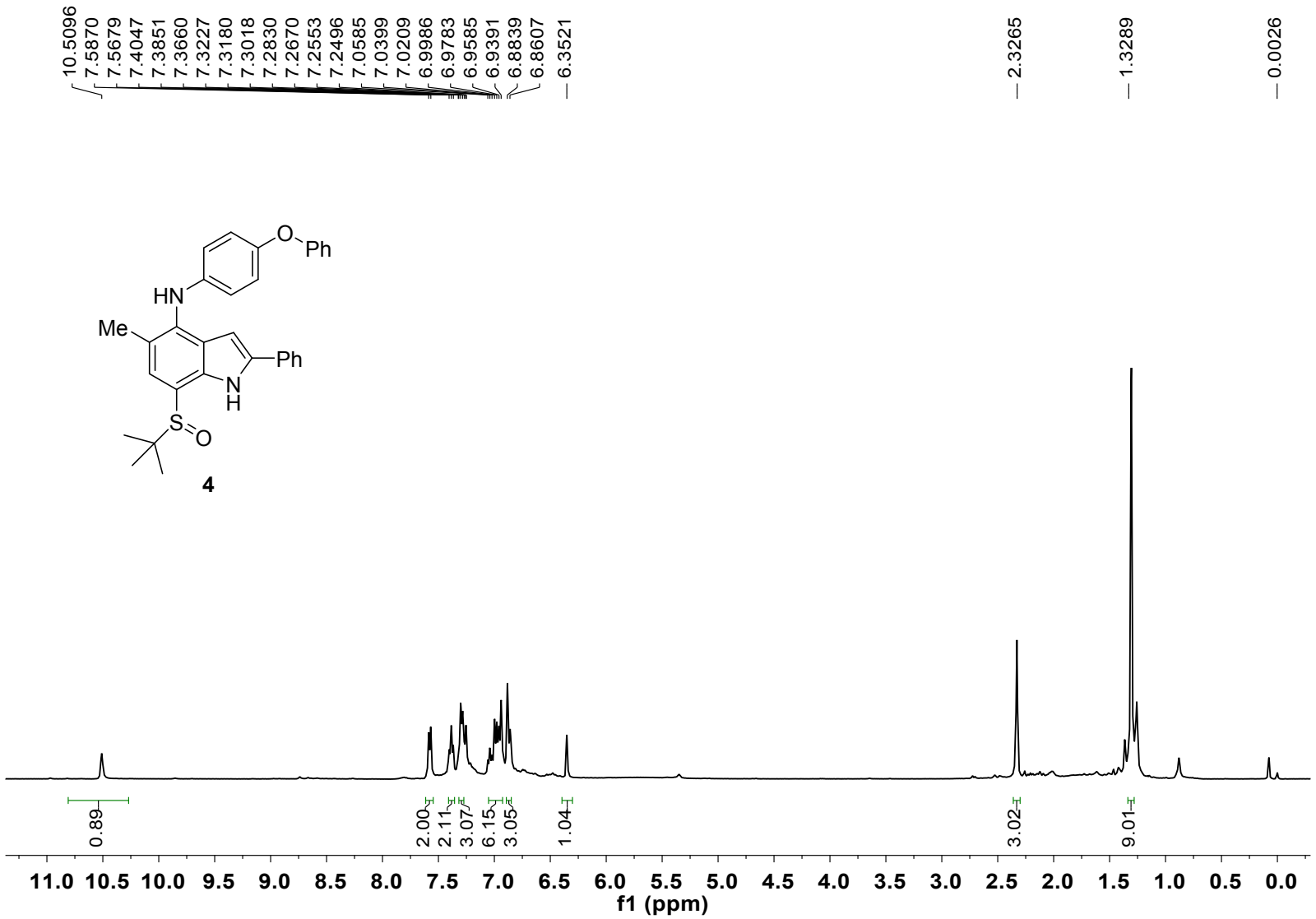
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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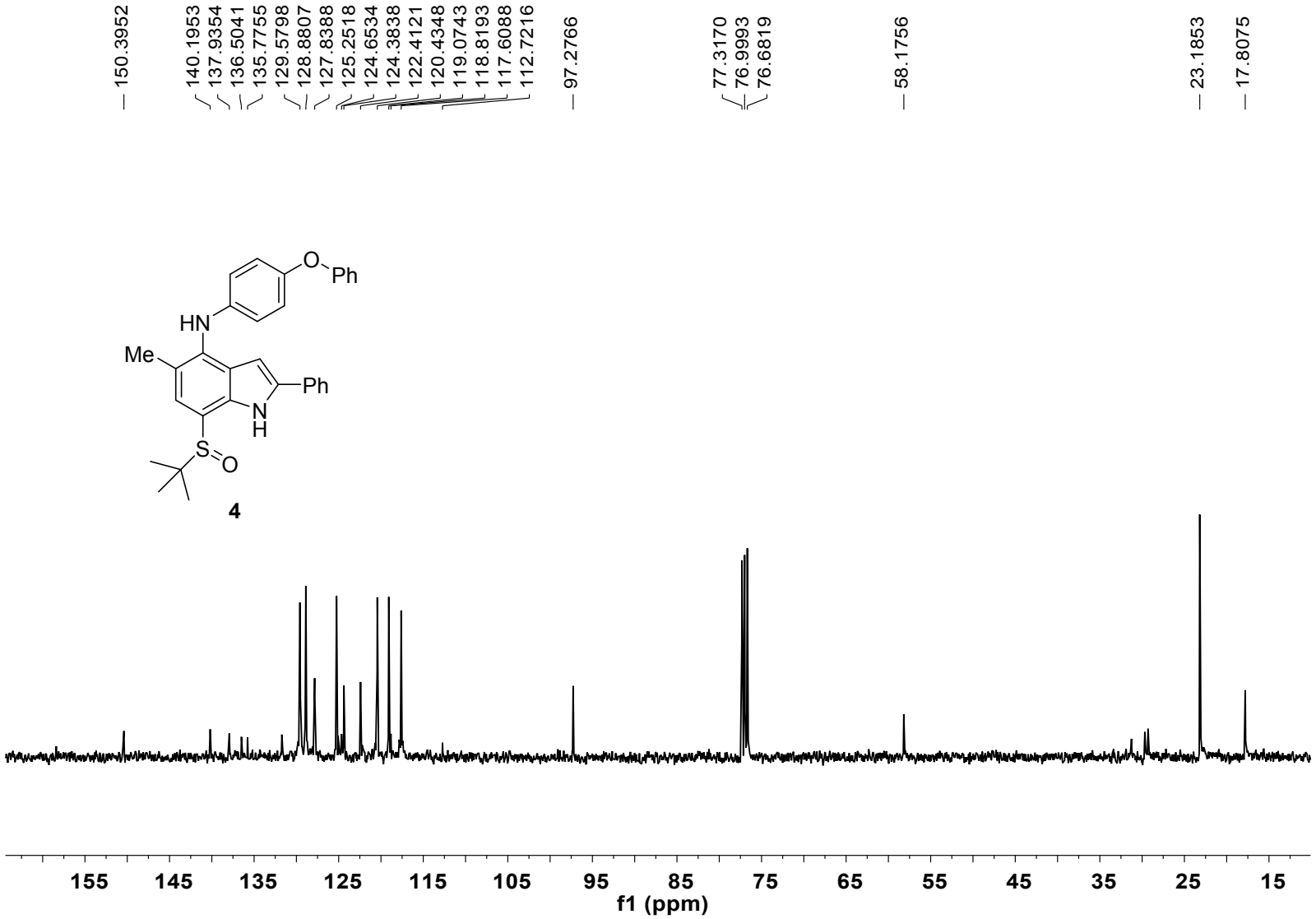
7.3660
7.3227
7.3180
7.3018
7.2830
7.2670
7.2553
7.2496
7.0585
7.0399
7.0209
6.9986
6.9783
6.9585
6.9391
6.8839
6.8607
6.3521
2.3265
1.3289
0.0026
O
Ph
HN
Me
Ph
N
H
S
O
4
0.89
2.00
2.11
3.07
6.15
3.05
1.04
3.02
9.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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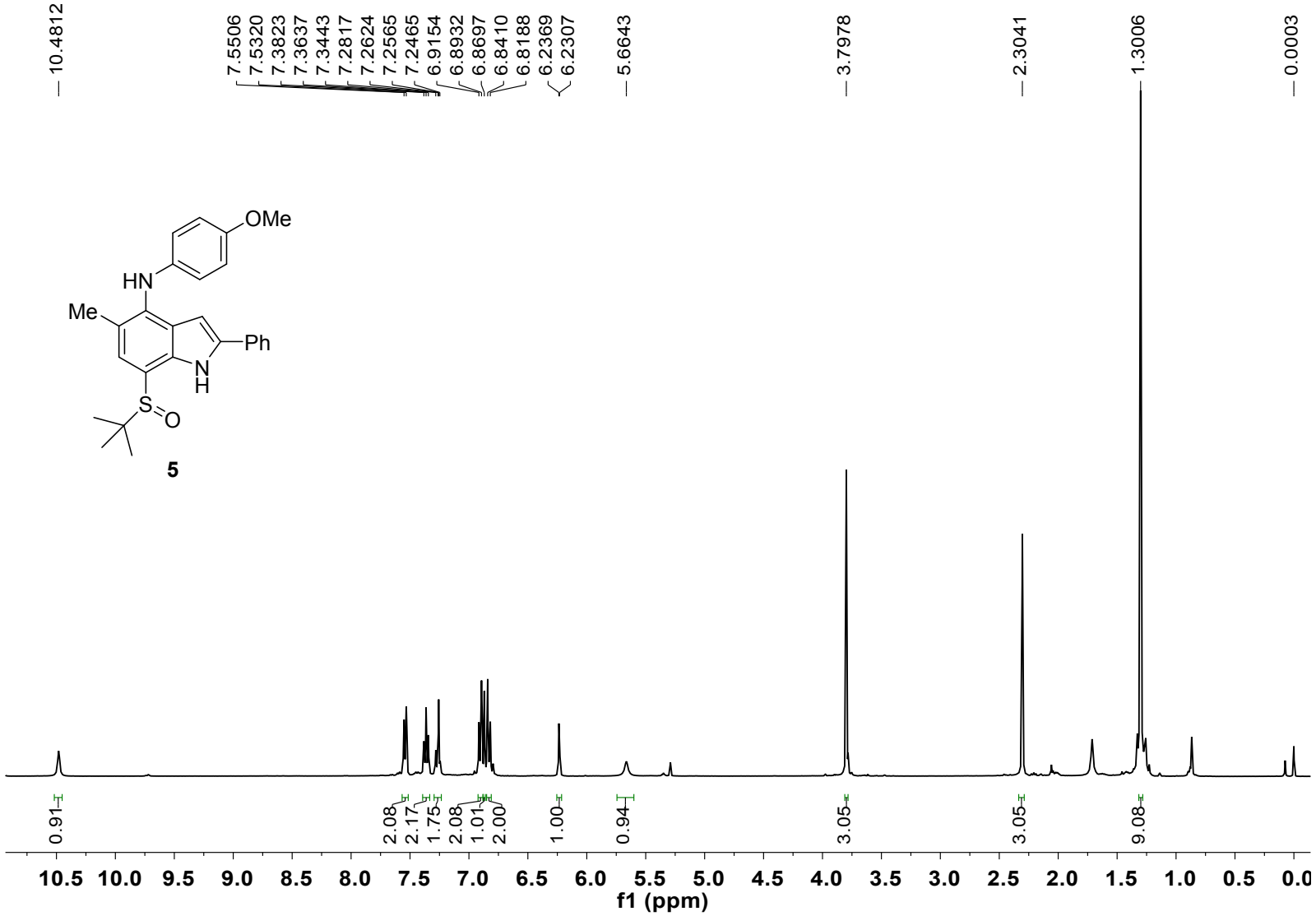
125.2518
124.6534
124.3838
122.4121
120.4348
119.0743
118.8193
117.6088
112.7216
97.2766
77.3170
76.9993
76.6819
58.1756
23.1853
17.8075
O
Ph
HN
Me
Ph
N
H
S
O
4
155
145
135
125
115
105
95
85
75
65
55
45
35
25
15
f1 (ppm)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7.3823
7.3637
7.3443
7.2817
7.2624
7.2565
7.2465
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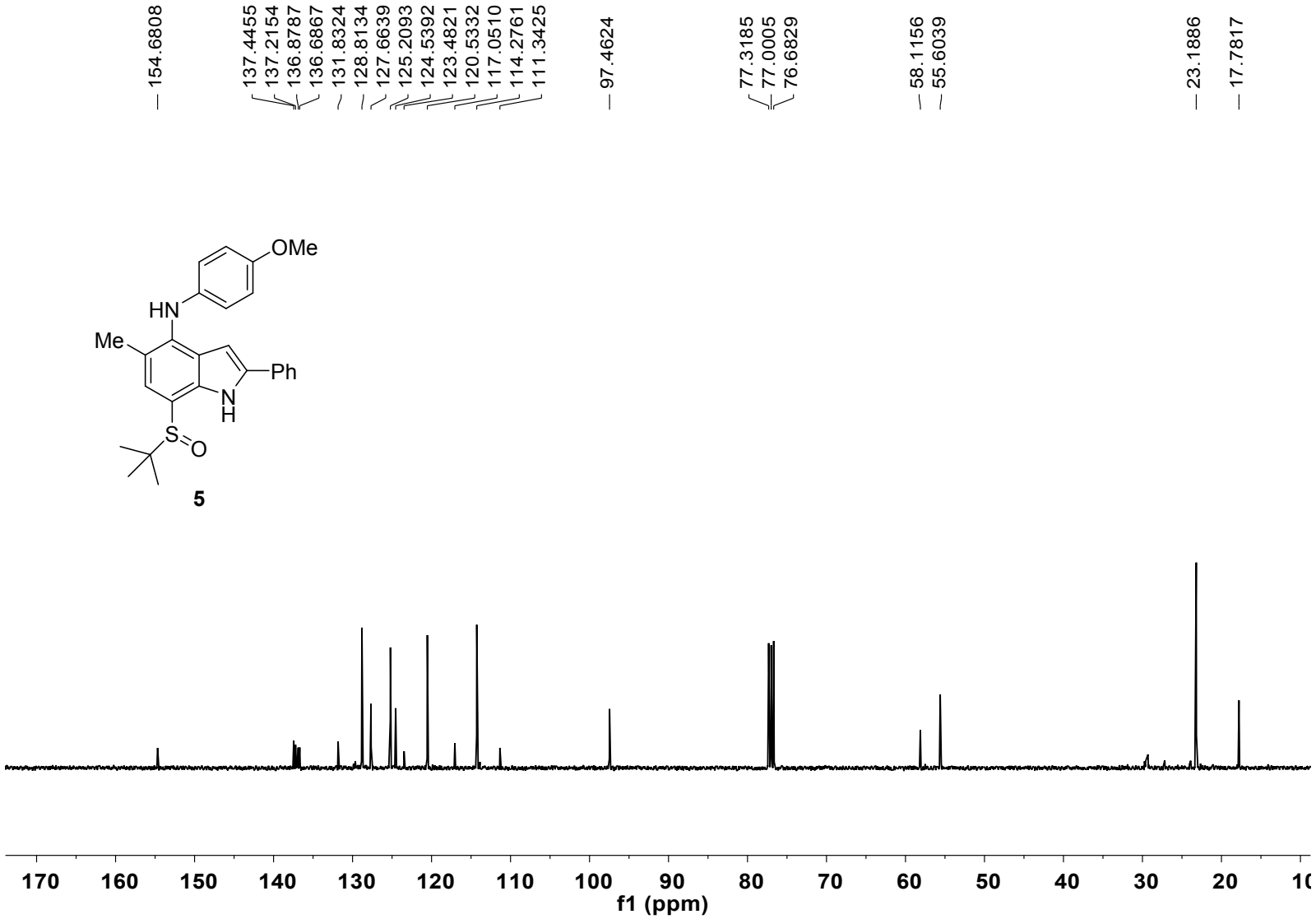
6.8932
6.8697
6.8410
6.8188
6.2369
6.2307
5.6643
3.7978
2.3041
1.3006
0.0003
OMe
HN
Me
Ph
N
H
S
O
5
0.91
2.08
2.17
1.75
2.08
1.01
2.00
1.00
0.94
3.05
3.05
9.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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120.5332
117.0510
114.2761
111.3425
97.4624
77.3185
77.0005
76.6829
58.1156
55.6039
23.1886
17.7817
OMe
HN
Me
Ph
N
H
S
O
5
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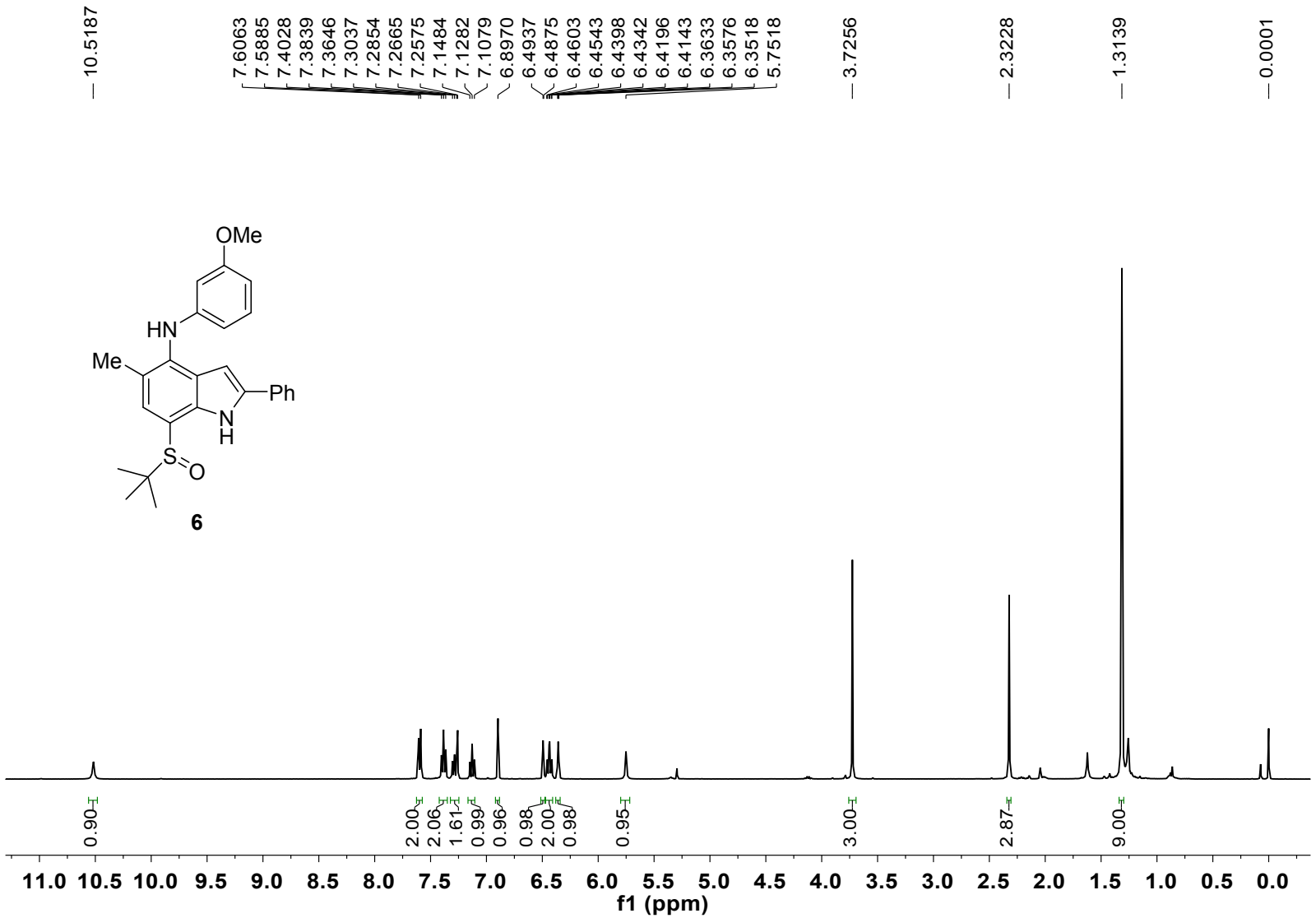
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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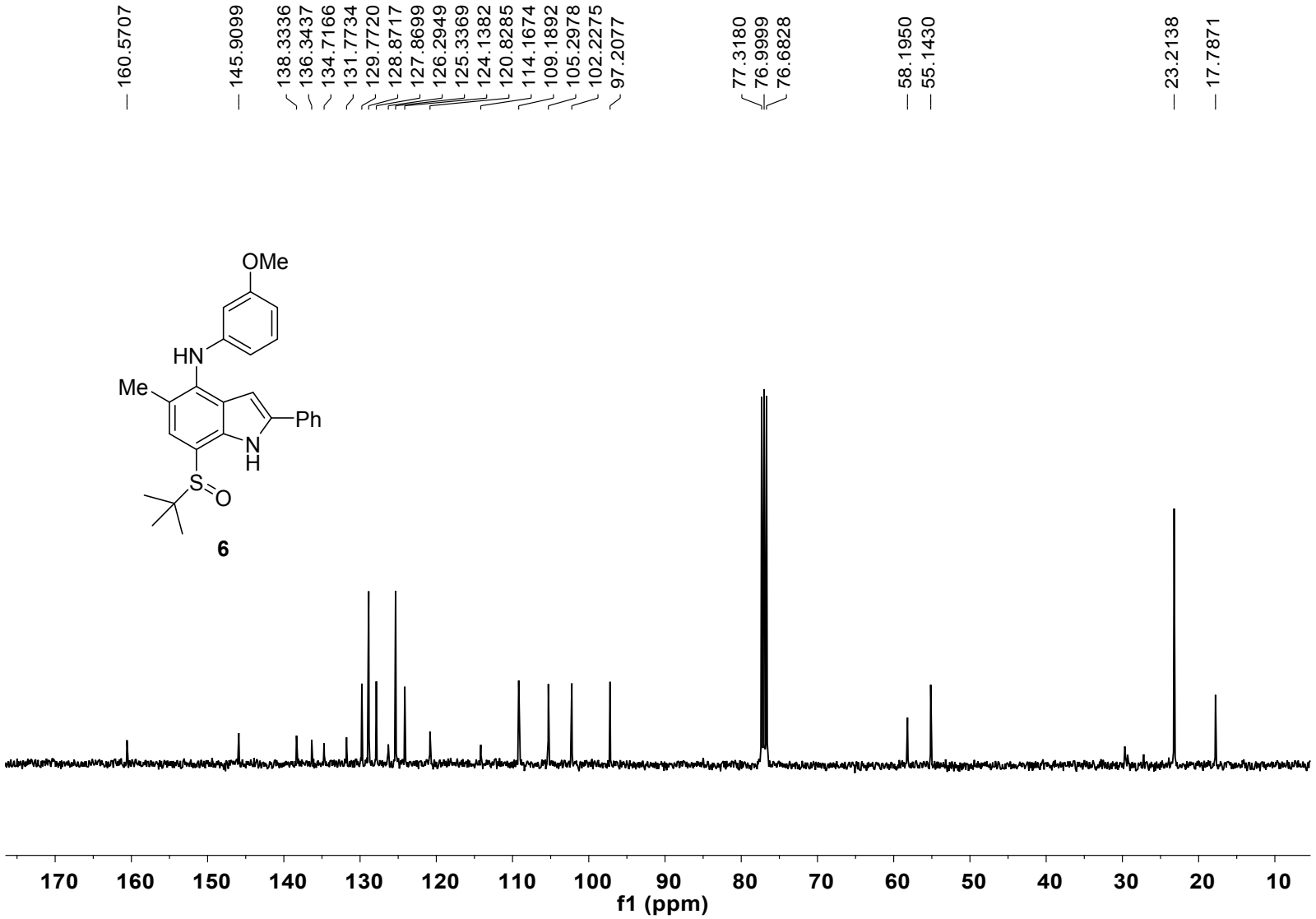
7.3037
7.2854
7.2665
7.2575
7.1484
7.1282
7.1079
6.8970
6.4937
6.4875
6.4603
6.4543
6.4398
6.4342
6.4196
6.4143
6.3633
6.3576
6.3518
5.7518
3.7256
2.3228
1.3139
0.0001
OMe
HN
Me
Ph
N
H
S
O
6
0.90
2.00
2.06
1.61
0.99
0.96
0.98
2.00
0.98
0.95
3.00
2.87
9.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.1382
120.8285
114.1674
109.1892
105.2978
102.2275
97.2077
77.3180
76.9999
76.6828
58.1950
55.1430
23.2138
17.7871
OMe
HN
Me
Ph
N
H
S
O
6
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140
130
120
110
100
90
80
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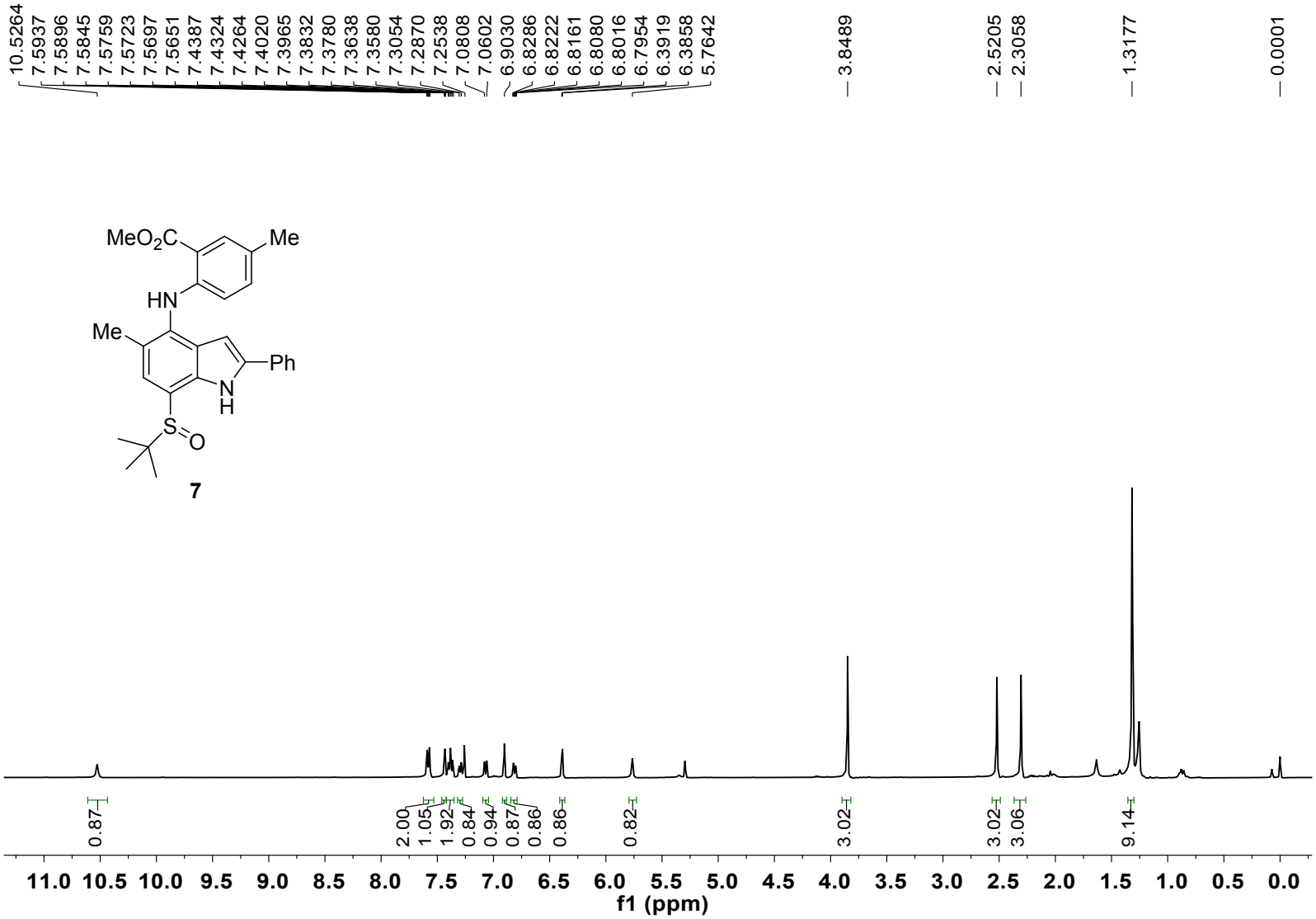
60
50
40
30
20
10
f1 (ppm)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7.4264
7.4020
7.3965
7.3832
7.3780
7.3638
7.3580
7.3054
7.2870
7.2538
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6.8222
6.8161
6.8080
6.8016
6.7954
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6.3858
5.7642
3.8489
2.5205
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1.3177
0.0001
MeO2C
Me
HN
Me
Ph
N
H
S
O
7
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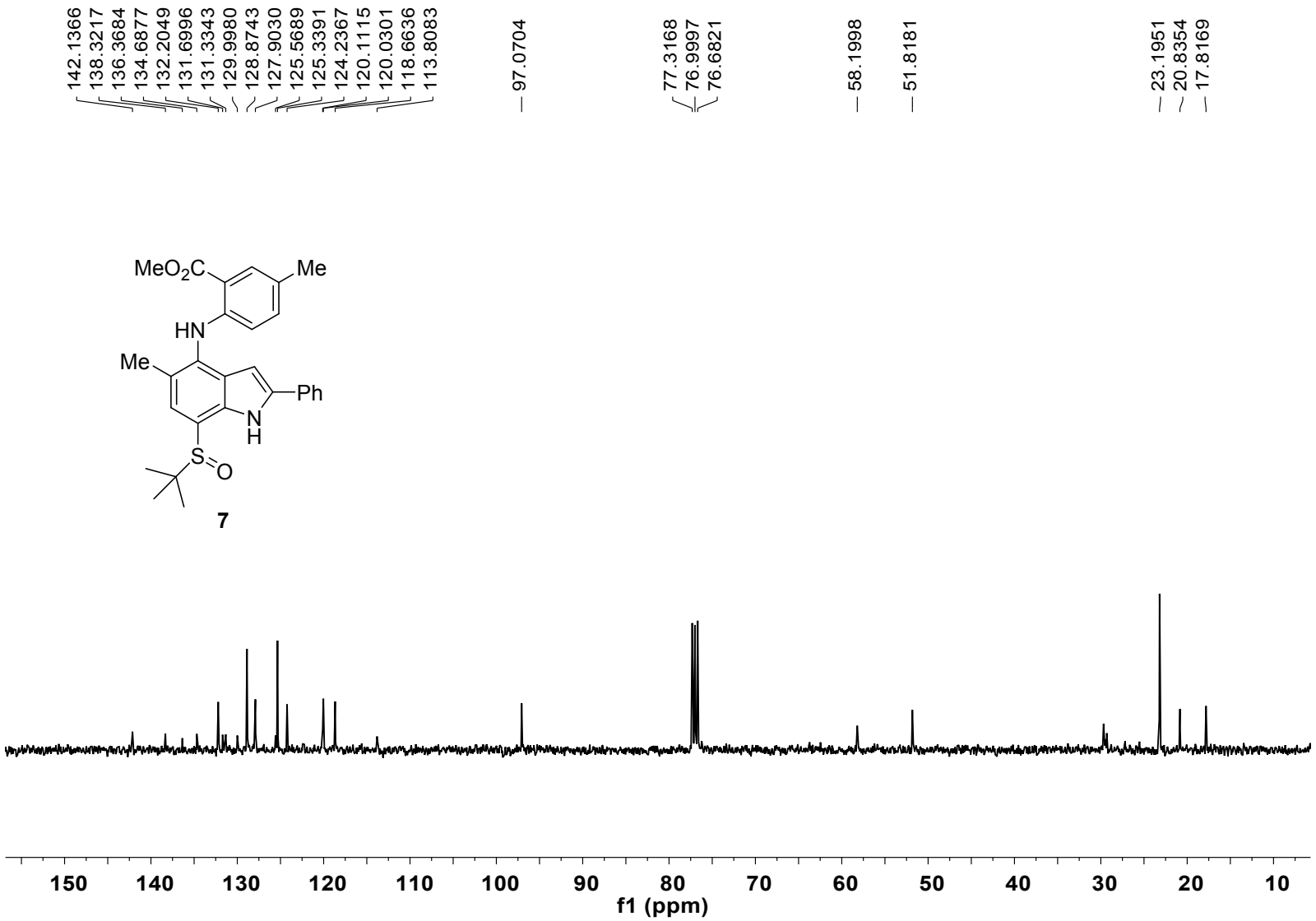
2.00
1.05
1.92
0.84
0.94
0.87
0.86
0.86
0.82
3.02
3.02
3.06
9.14
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.9030
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125.3391
124.2367
120.1115
120.0301
118.6636
113.8083
97.0704
77.3168
76.9997
76.6821
58.1998
51.8181
23.1951
20.8354
17.8169
MeO2C
Me
HN
Me
Ph
N
H
S
O
7
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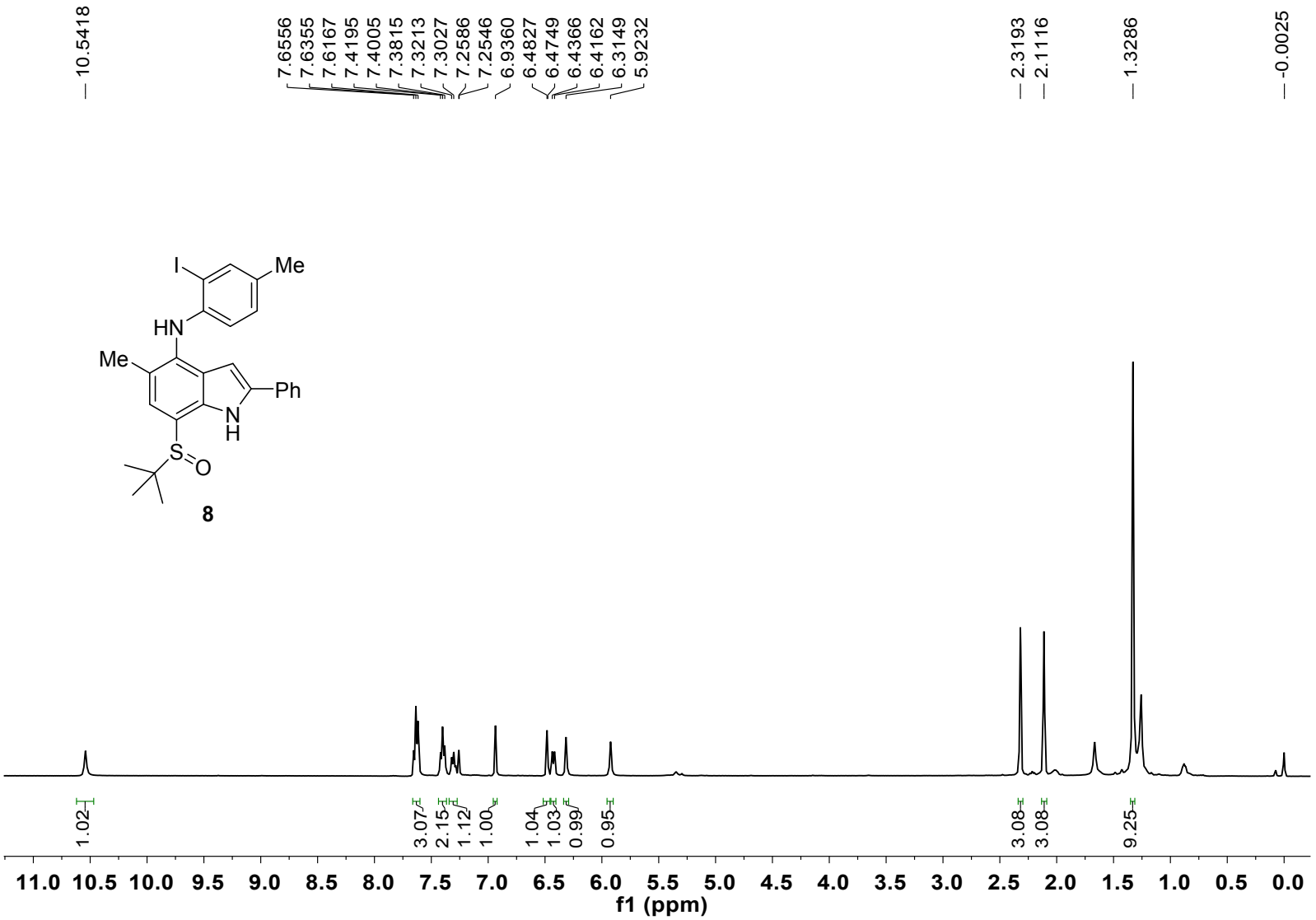
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.4005
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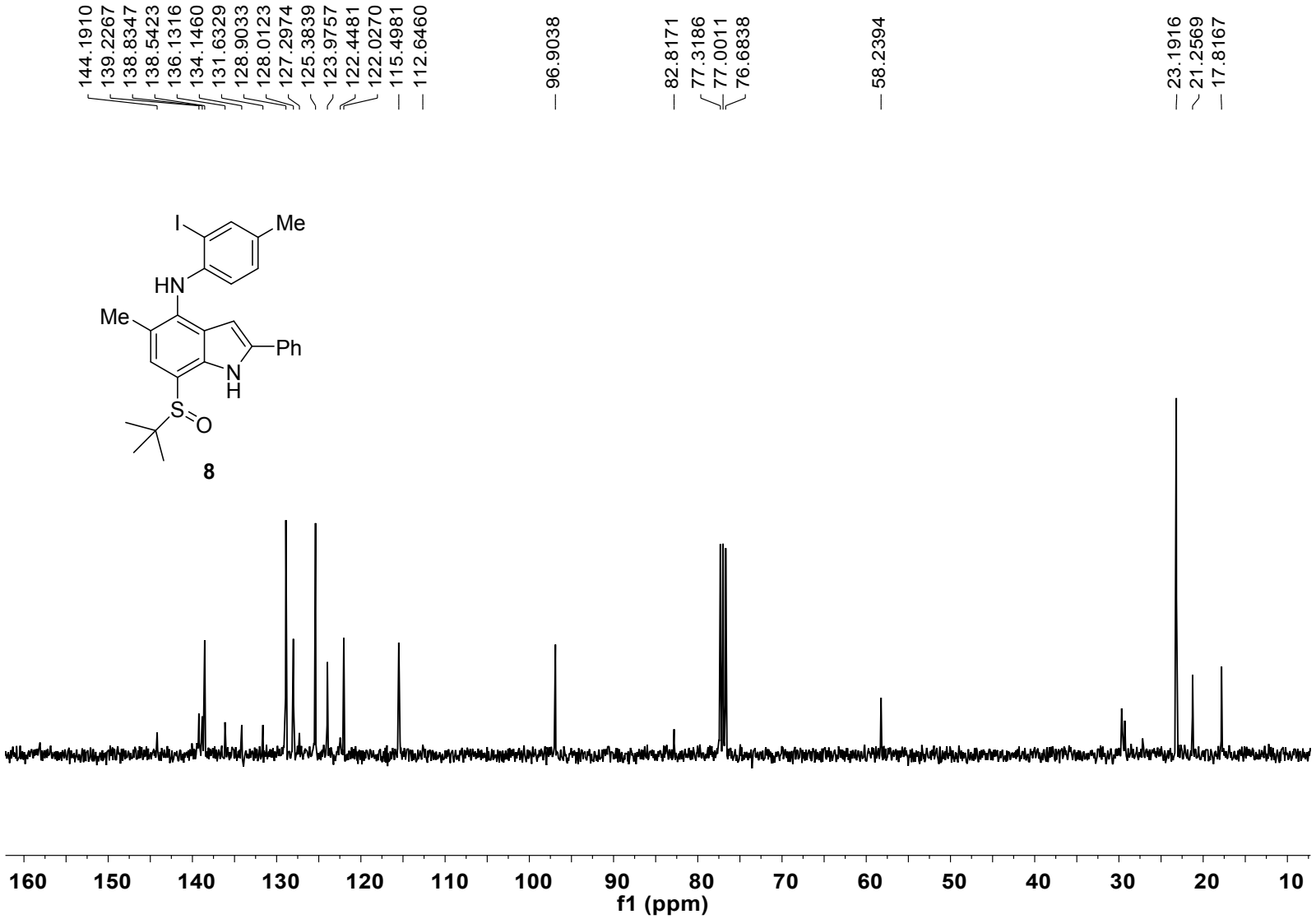
7.3213
7.3027
7.2586
7.2546
6.9360
6.4827
6.4749
6.4366
6.4162
6.3149
5.9232
2.3193
2.1116
1.3286
-0.0025
I
Me
HN
Me
Ph
N
H
S
O
8
1.02
3.07
2.15
1.12
1.00
1.04
1.03
0.99
0.95
3.08
3.08
9.25
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.3839
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122.0270
115.4981
112.6460
96.9038
82.8171
77.3186
77.0011
76.6838
58.2394
23.1916
21.2569
17.8167
I
Me
HN
Me
Ph
N
H
S
O
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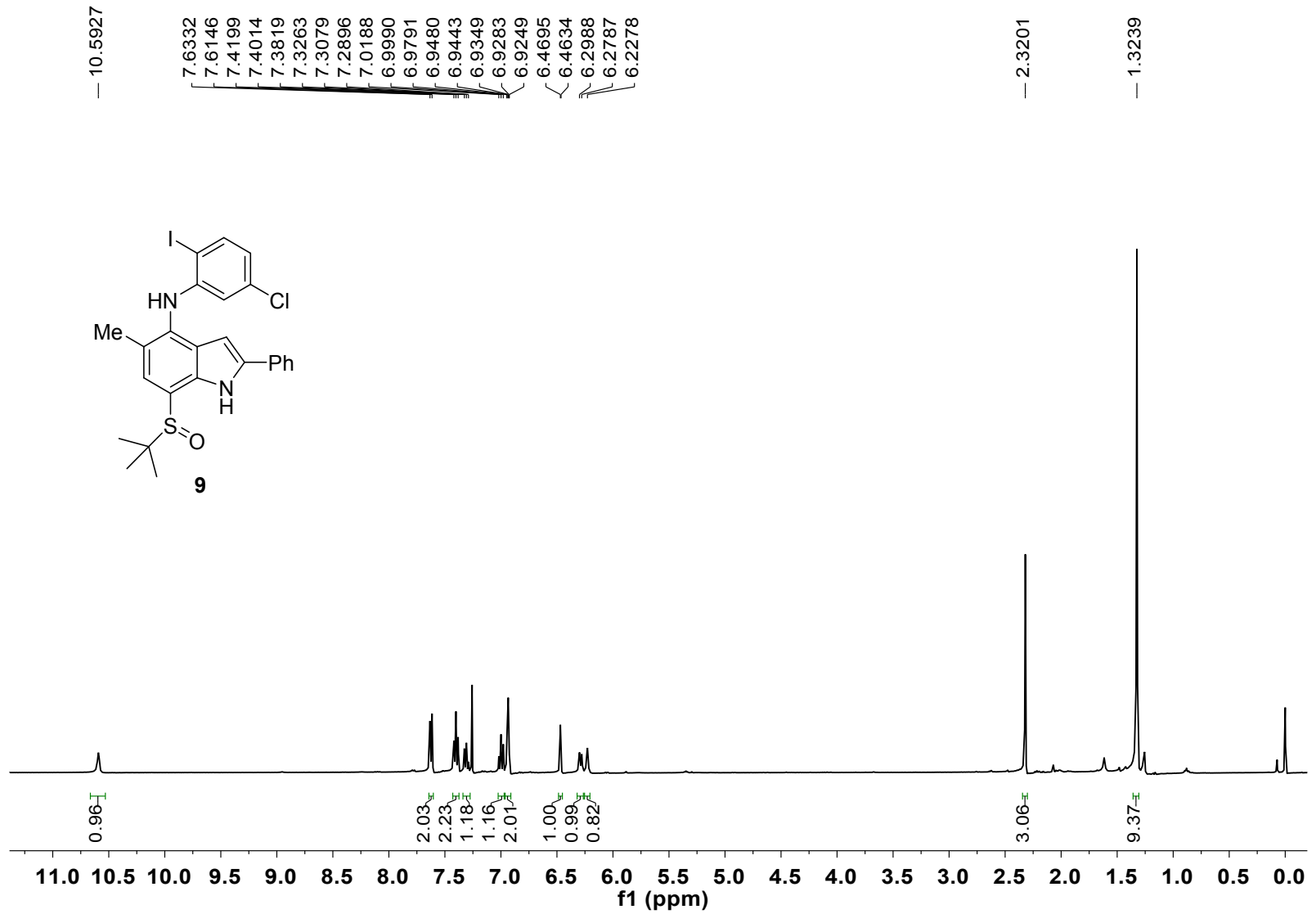
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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I
HN
Cl
Me
Ph
N
H
S
O
9
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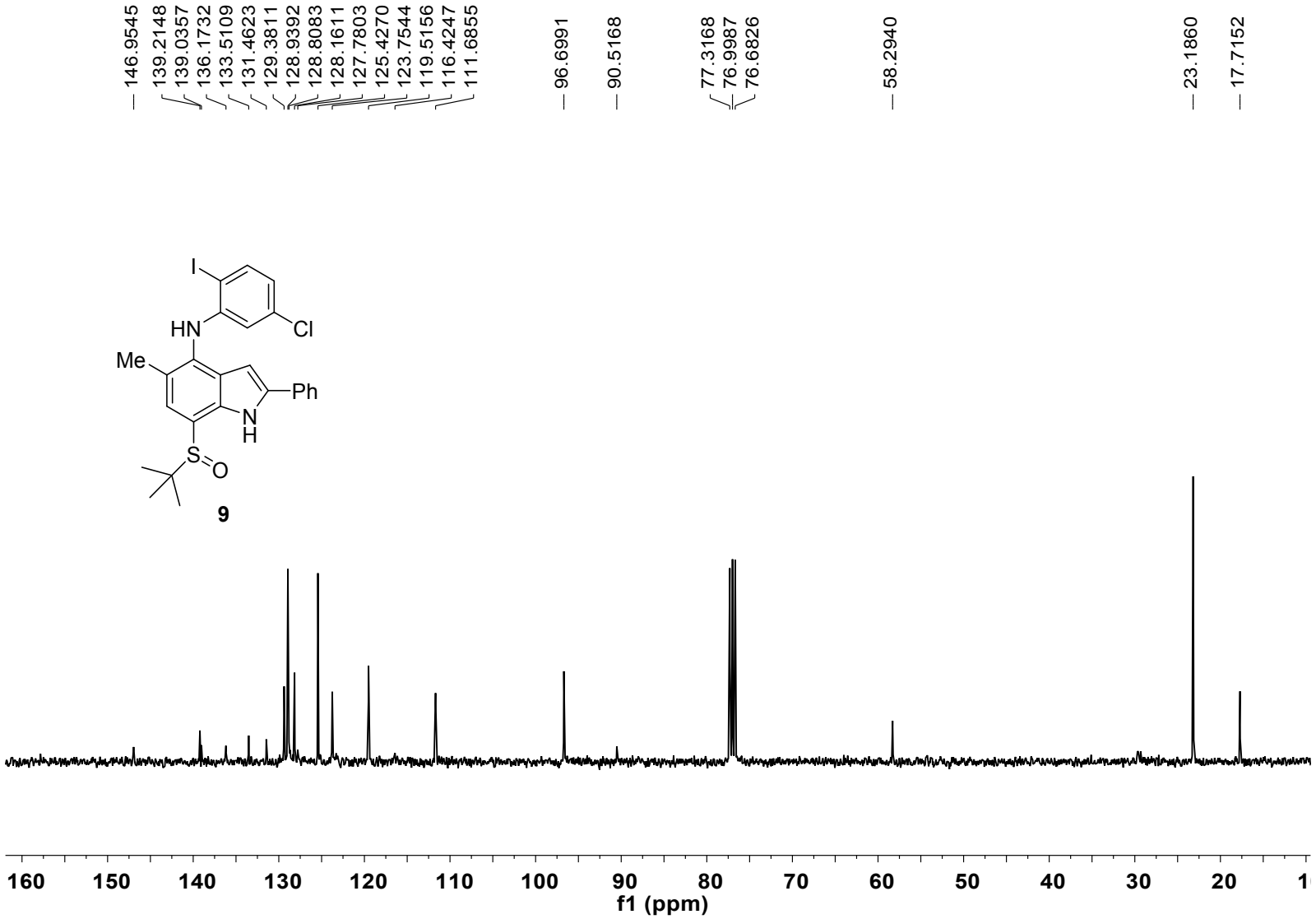
1.18
1.16
2.01
1.00
0.99
0.82
3.06
9.37
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.4270
123.7544
119.5156
116.4247
111.6855
96.6991
90.5168
77.3168
76.9987
76.6826
58.2940
23.1860
17.7152
I
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Cl
Me
Ph
N
H
S
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80
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60
50
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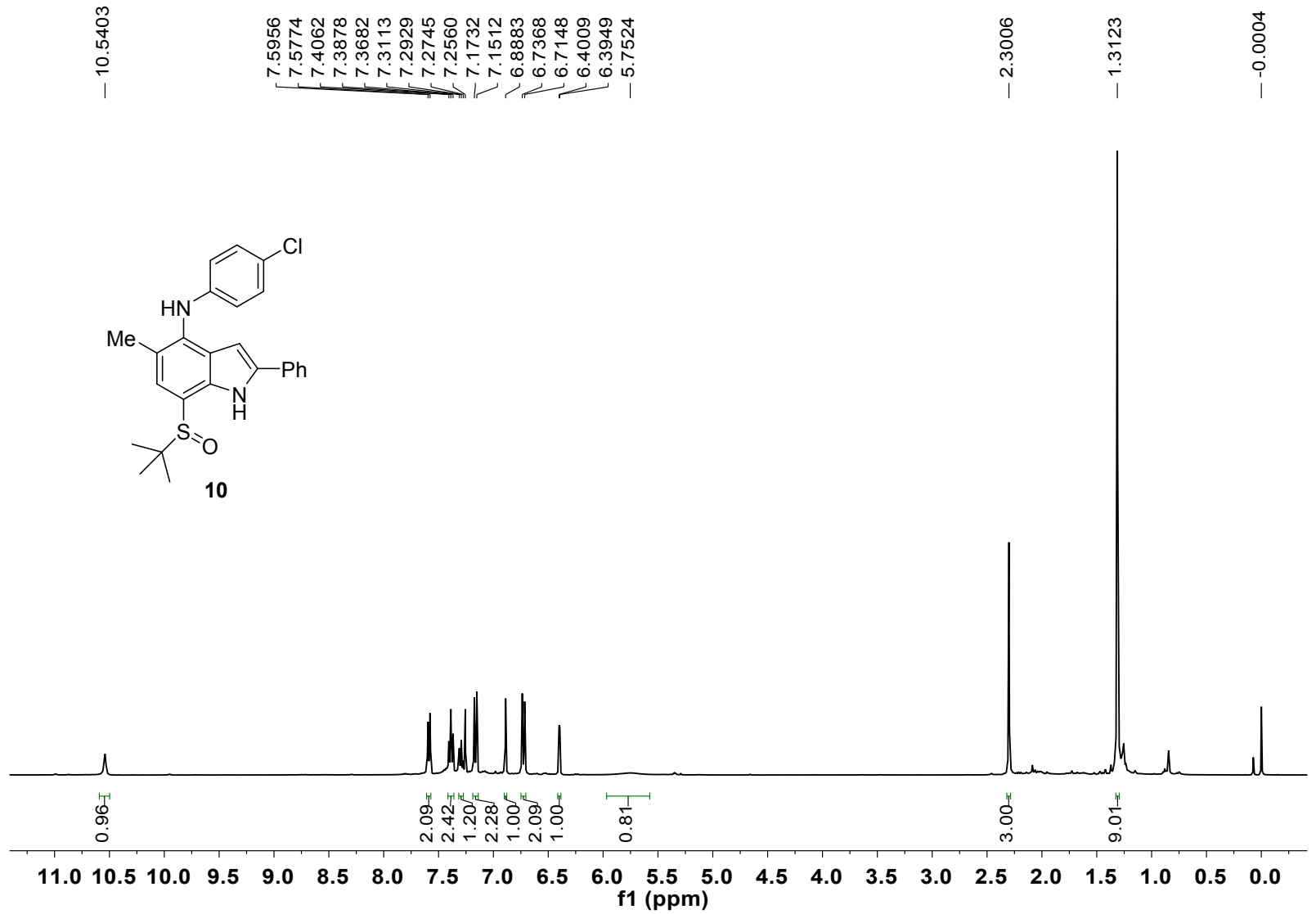
30
20
1
f1 (ppm)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7.1732
7.1512
6.8883
6.7368
6.7148
6.4009
6.3949
5.7524
2.3006
1.3123
-0.0004
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Me
Ph
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H
S
O
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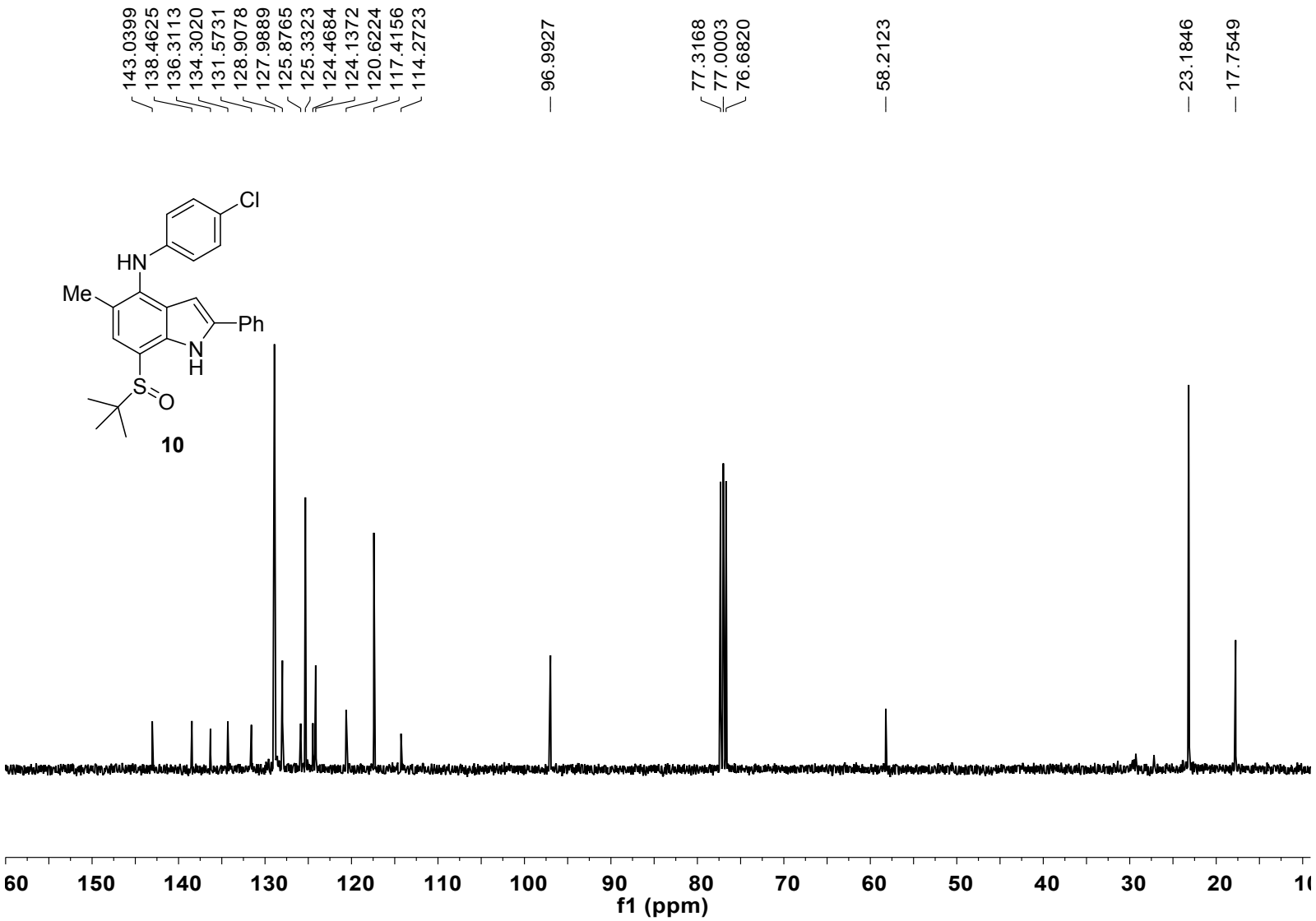
2.42
1.20
2.28
1.00
2.09
1.00
0.81
3.00
9.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.1372
120.6224
117.4156
114.2723
96.9927
77.3168
77.0003
76.6820
58.2123
23.1846
17.7549
Cl
HN
Me
Ph
N
H
S
O
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130
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110
100
90
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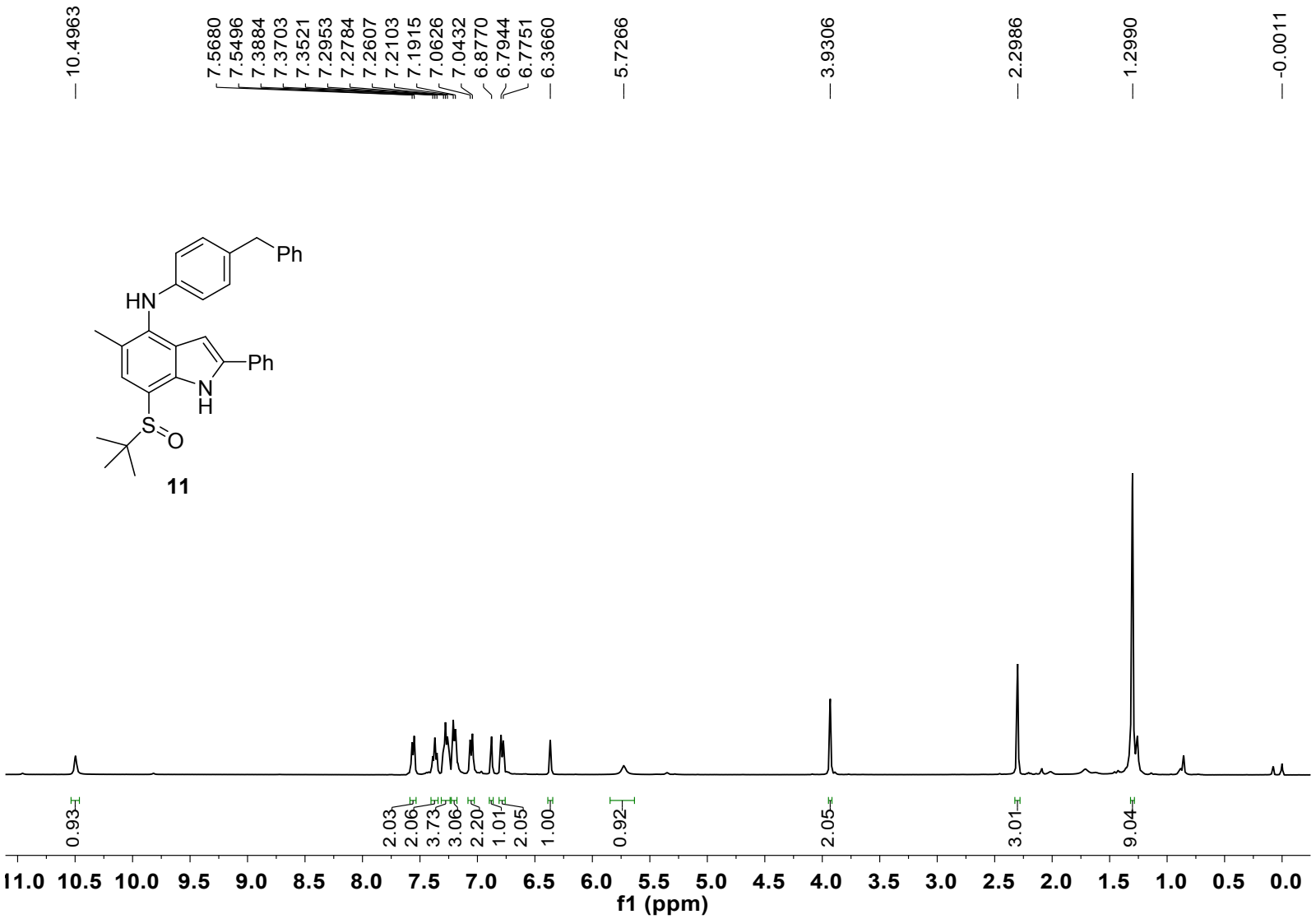
70
60
50
40
30
20
f1 (ppm)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7.0626
7.0432
6.8770
6.7944
6.7751
6.3660
5.7266
3.9306
2.2986
1.2990
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Ph
N
H
S
O
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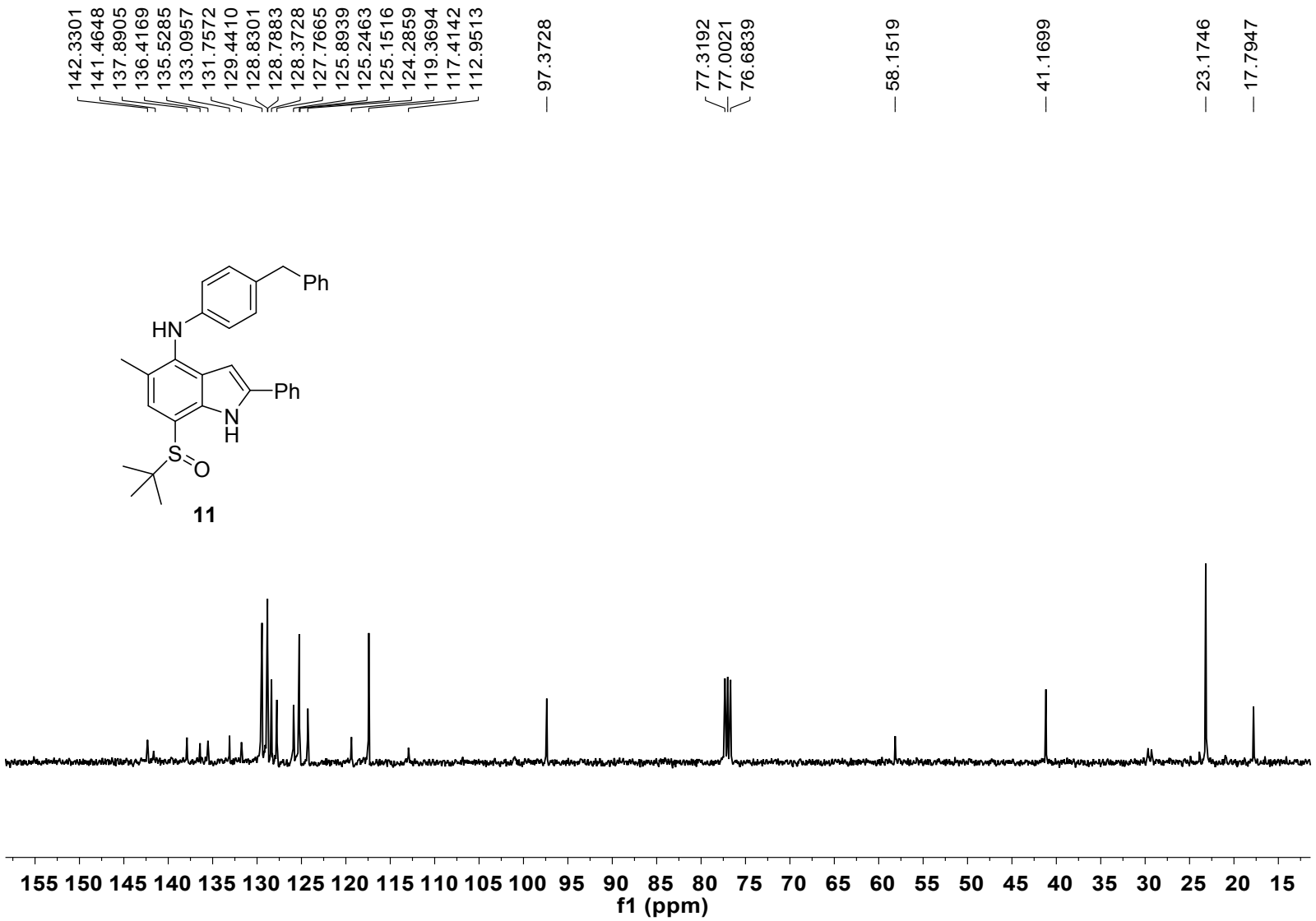
9.04
f1 (ppm)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124.2859
119.3694
117.4142
112.9513
97.3728
77.3192
77.0021
76.6839
58.1519
41.1699
23.1746
17.7947
HN
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Ph
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S
O
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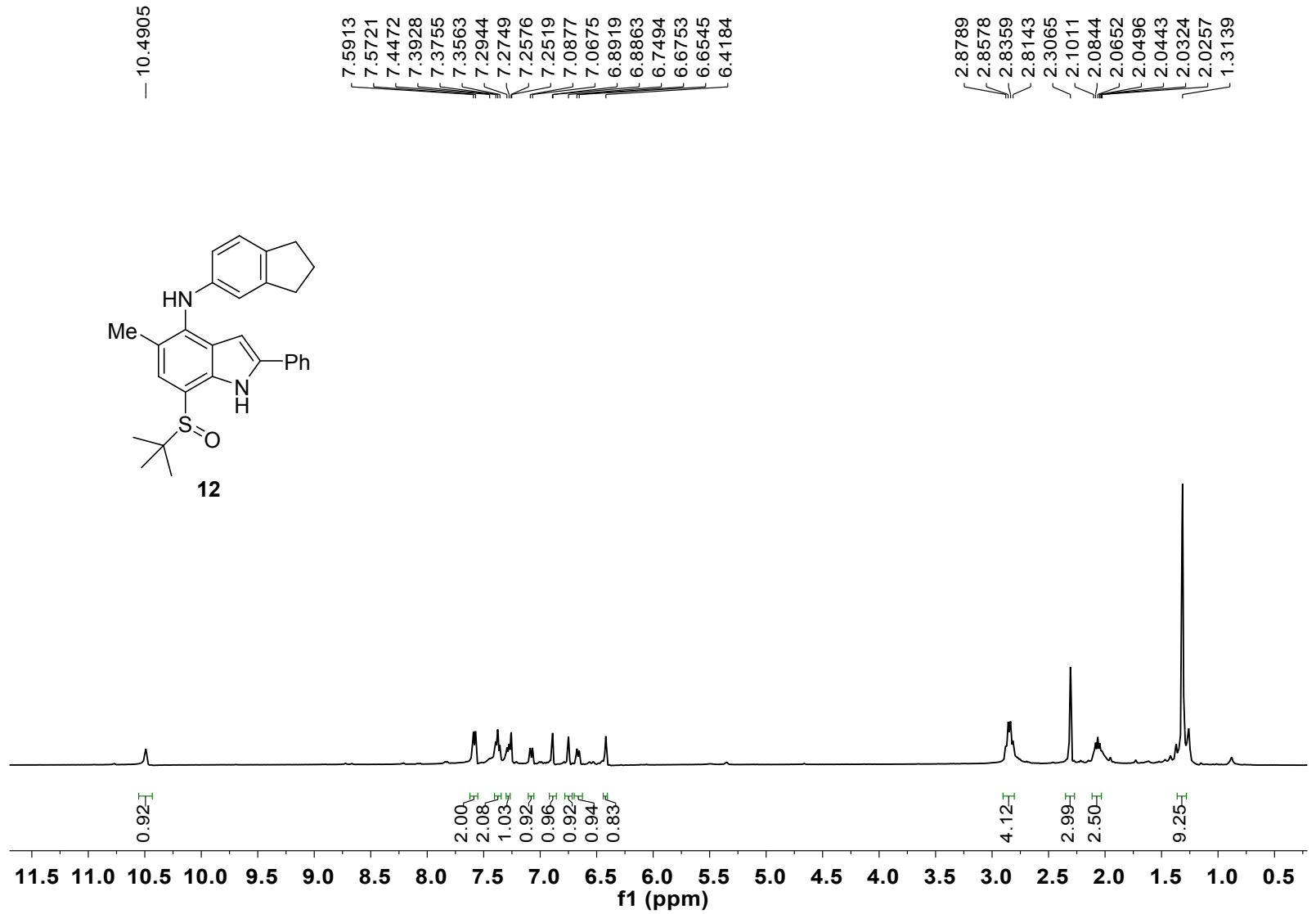
f1 (ppm)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7.0675
6.8919
6.8863
6.7494
6.6753
6.6545
6.4184
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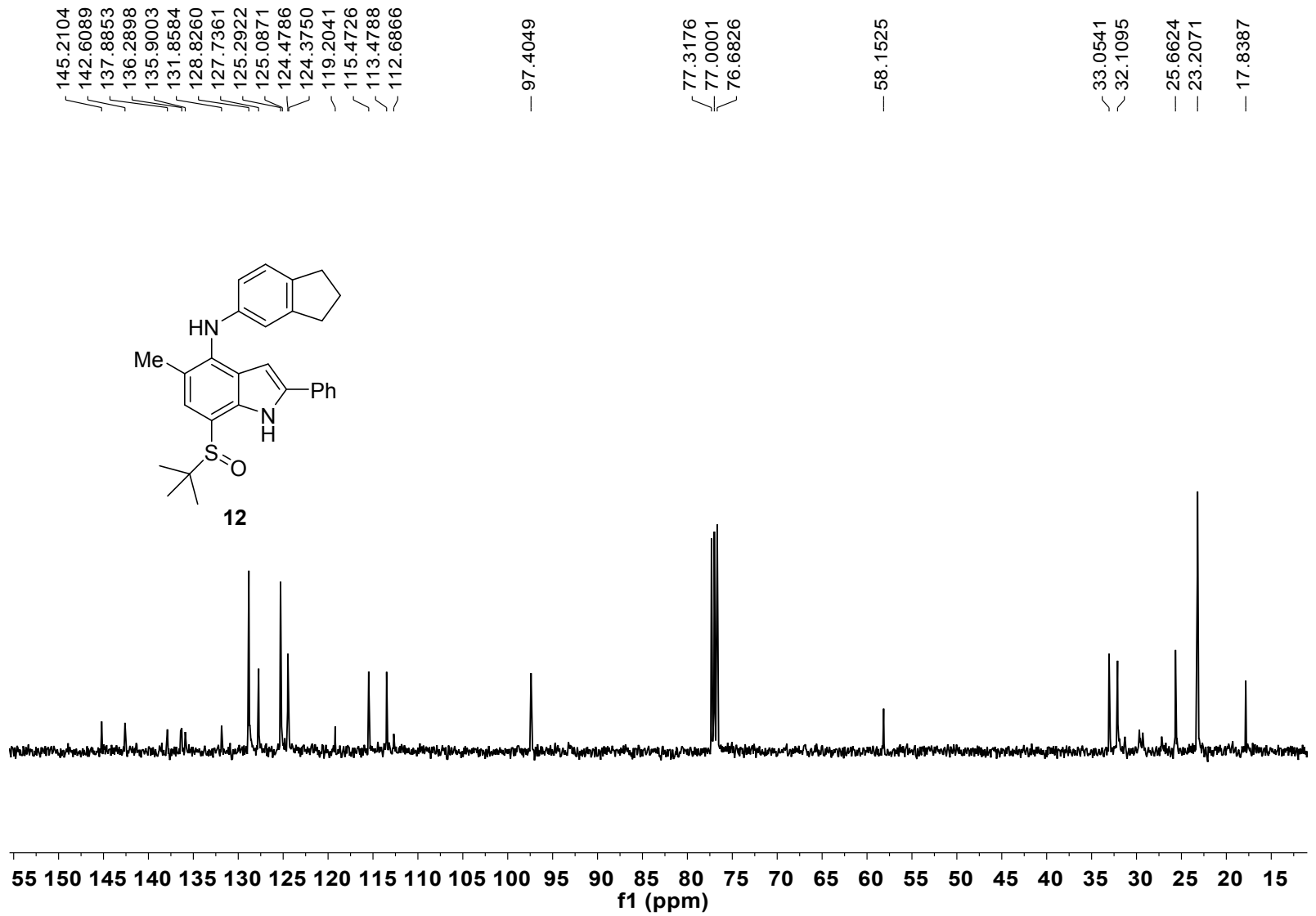
2.8578
2.8359
2.8143
2.3065
2.1011
2.0844
2.0652
2.0496
2.0443
2.0324
2.0257
1.3139
HN
Me
Ph
N
H
S
O
12
0.92
2.00
2.08
1.03
0.92
0.96
0.92
0.94
0.83
4.12
2.99
2.50
9.25
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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124.3750
119.2041
115.4726
113.4788
112.6866
97.4049
77.3176
77.0001
76.6826
58.1525
33.0541
32.1095
25.6624
23.2071
17.8387
HN
Me
Ph
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H
S
O
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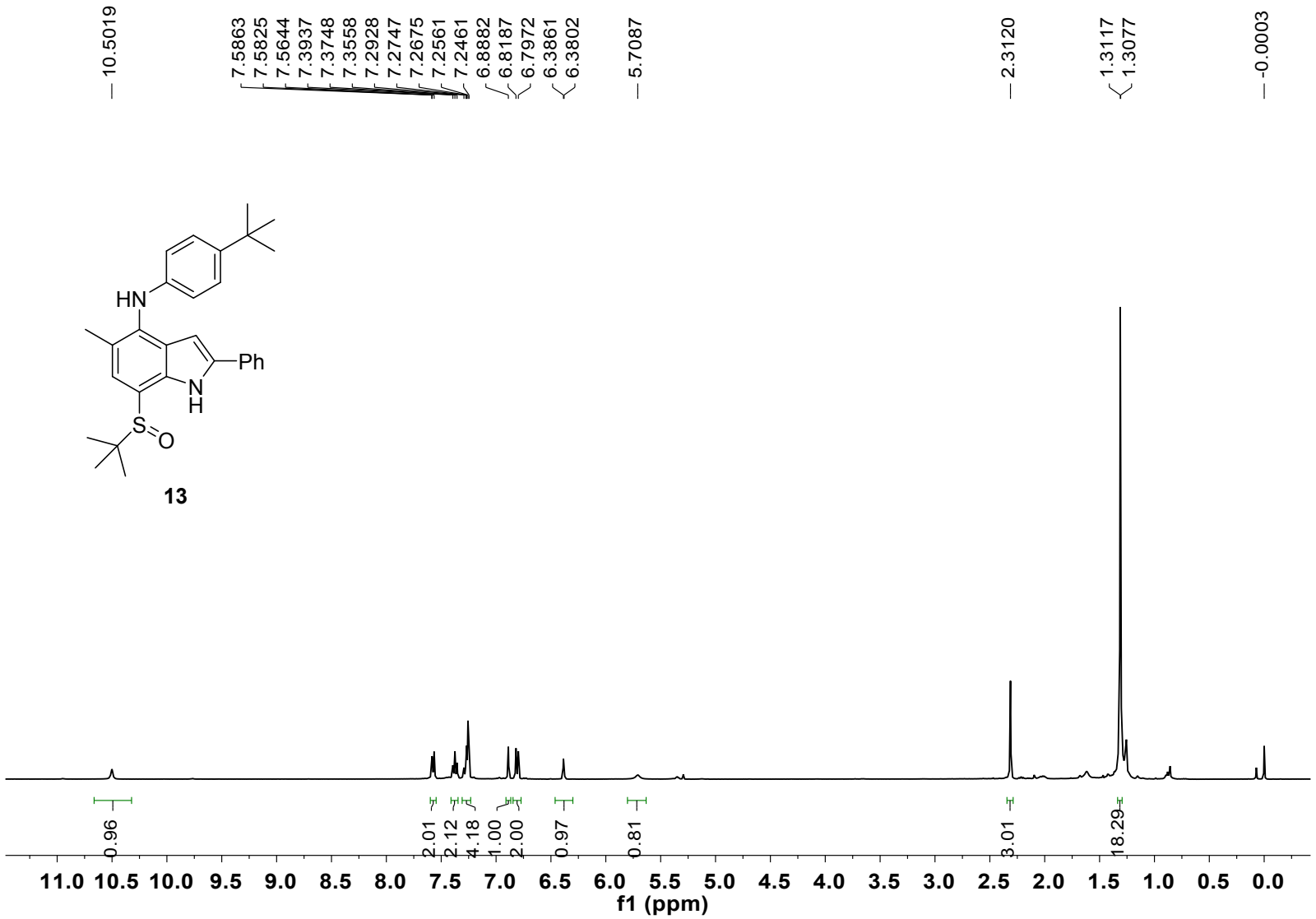
f1 (ppm)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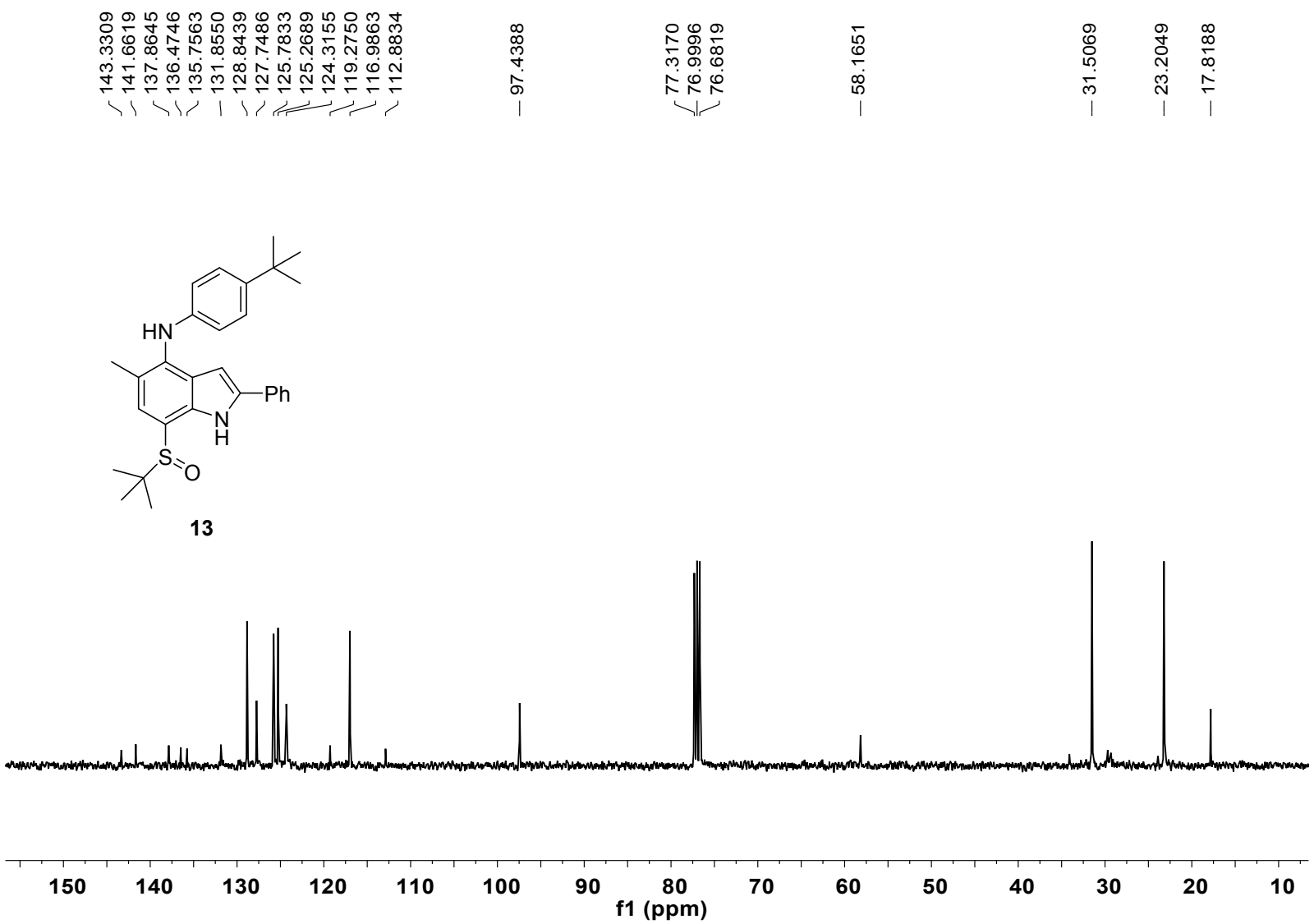
7.2461
6.8882
6.8187
6.7972
6.3861
6.3802
5.7087
2.3120
1.3117
1.3077
-0.0003
HN
Ph
N
H
S
O
13
0.96
2.01
2.12
4.18
1.00
2.00
0.97
0.81
3.01
18.29
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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116.9863
112.8834
97.4388
77.3170
76.9996
76.6819
58.1651
31.5069
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HN
Ph
N
H
S
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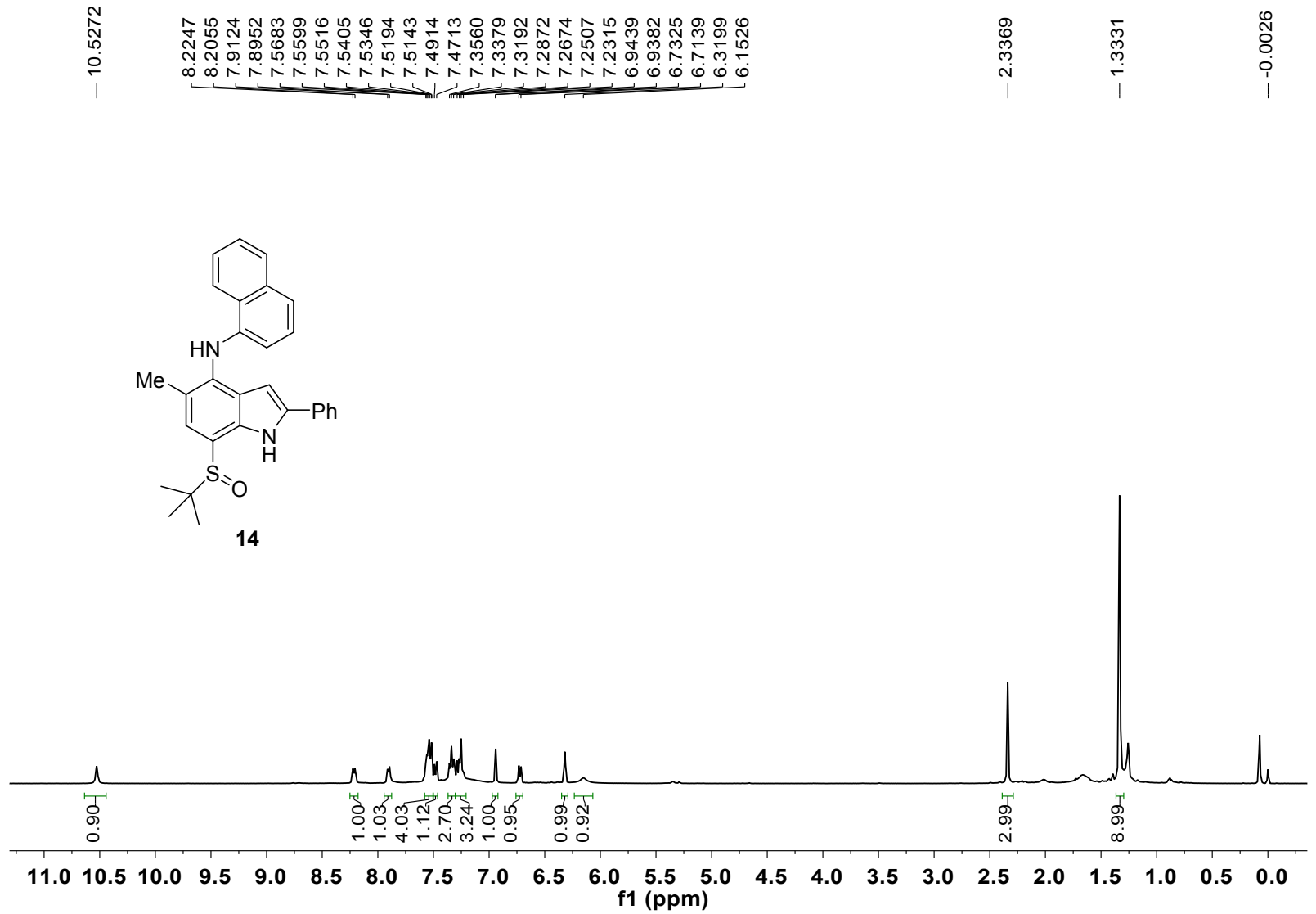
f1 (ppm)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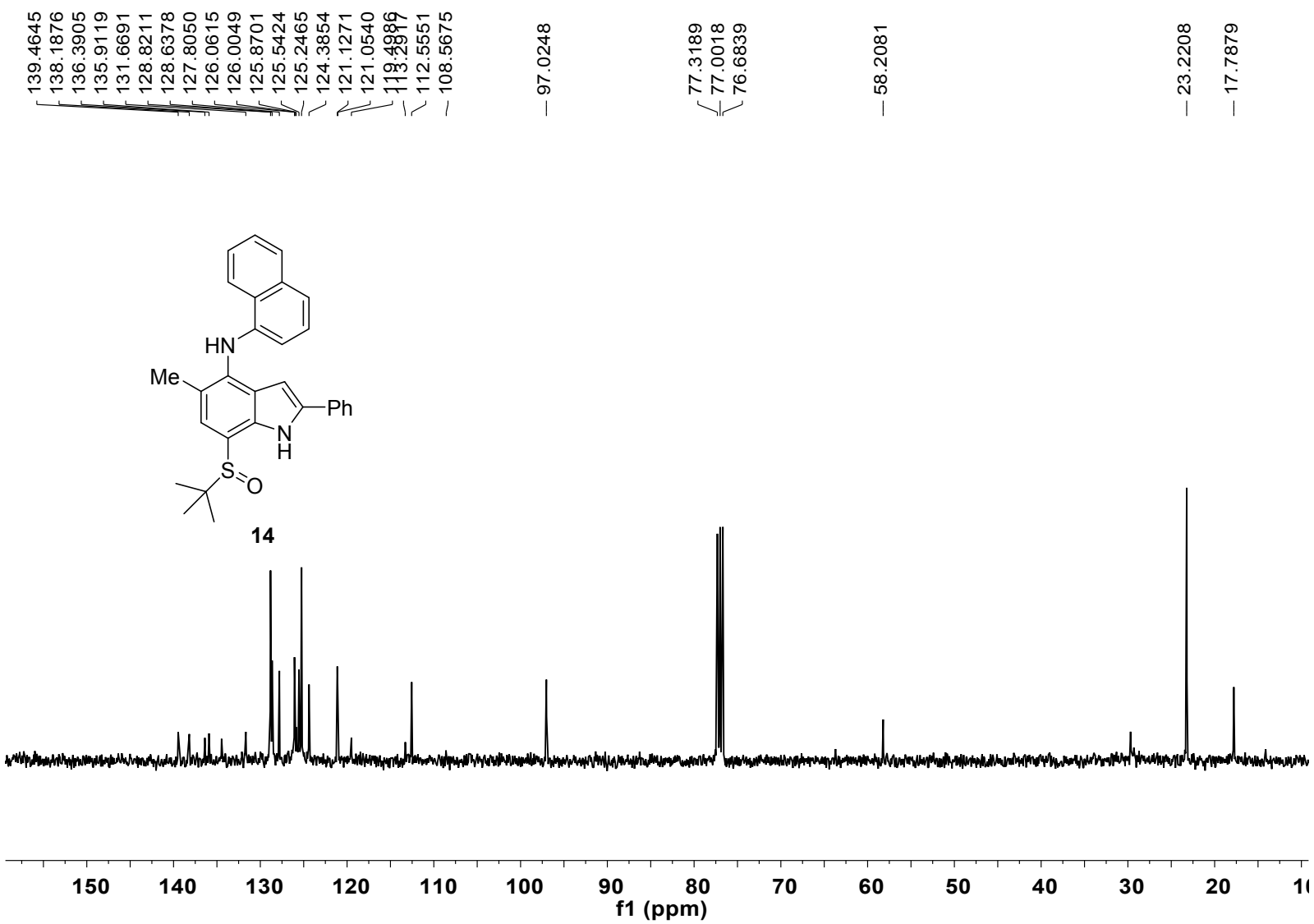
7.5346
7.5194
7.5143
7.4914
7.4713
7.3560
7.3379
7.3192
7.2872
7.2674
7.2507
7.2315
6.9439
6.9382
6.7325
6.7139
6.3199
6.1526
2.3369
1.3331
-0.0026
HN
Me
Ph
N
H
S
O
14
0.90
1.00
1.03
4.03
1.12
2.70
3.24
1.00
0.95
0.99
0.92
2.99
8.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.5424
125.2465
124.3854
121.1271
121.0540
112.5551
108.5675
97.0248
77.3189
77.0018
76.6839
58.2081
23.2208
17.7879
HN
Me
Ph
N
H
S
O
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150
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130
120
110
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70
60
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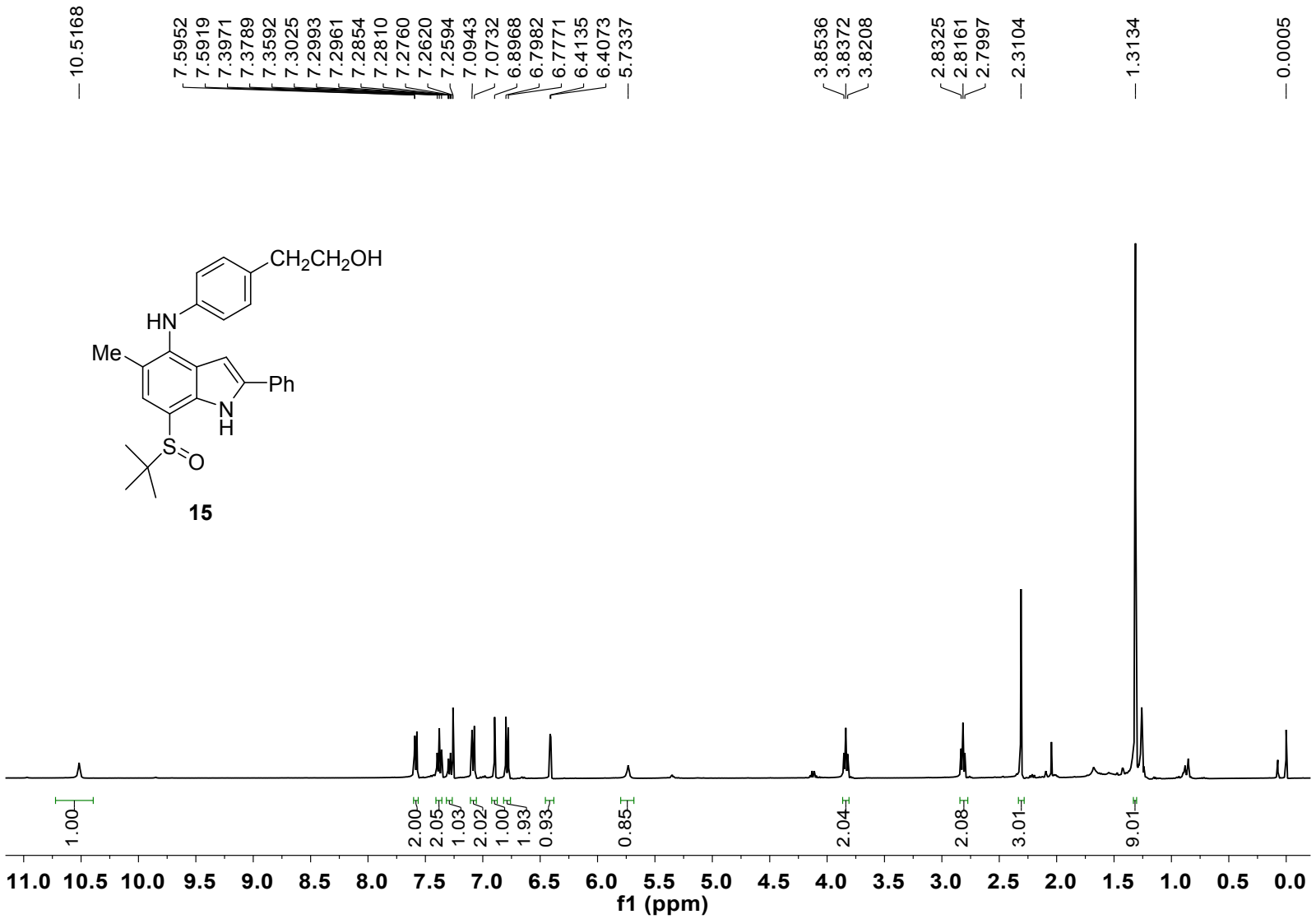
40
30
20
f1 (ppm)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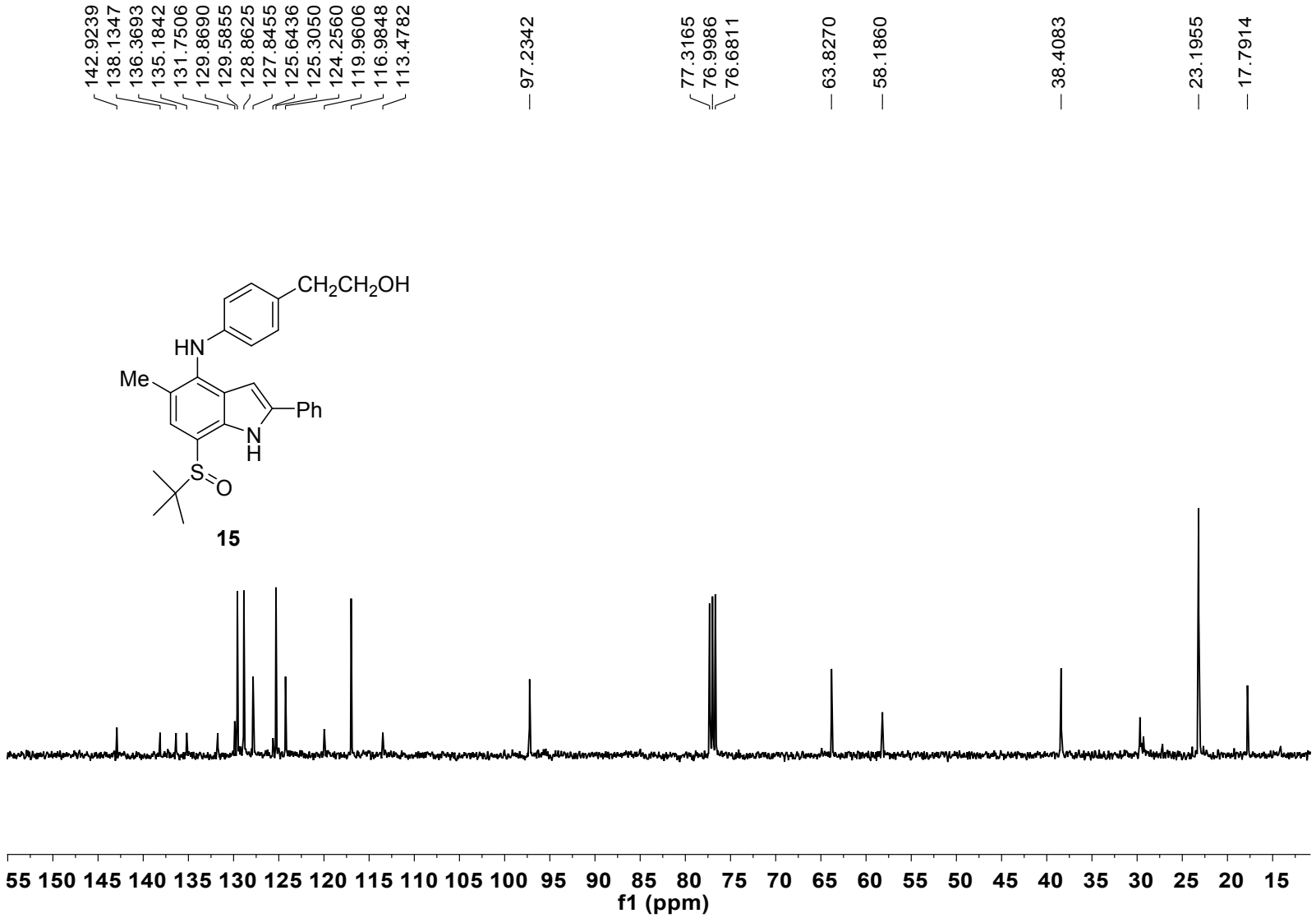
7.2810
7.2760
7.2620
7.2594
7.0943
7.0732
6.8968
6.7982
6.7771
6.4135
6.4073
5.7337
3.8536
3.8372
3.8208
2.8325
2.8161
2.7997
2.3104
1.3134
0.0005
CH2CH2OH
HN
Me
Ph
N
H
S
O
15
1.00
2.00
2.05
1.03
2.02
1.00
1.93
0.93
0.85
2.04
2.08
3.01
9.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.2560
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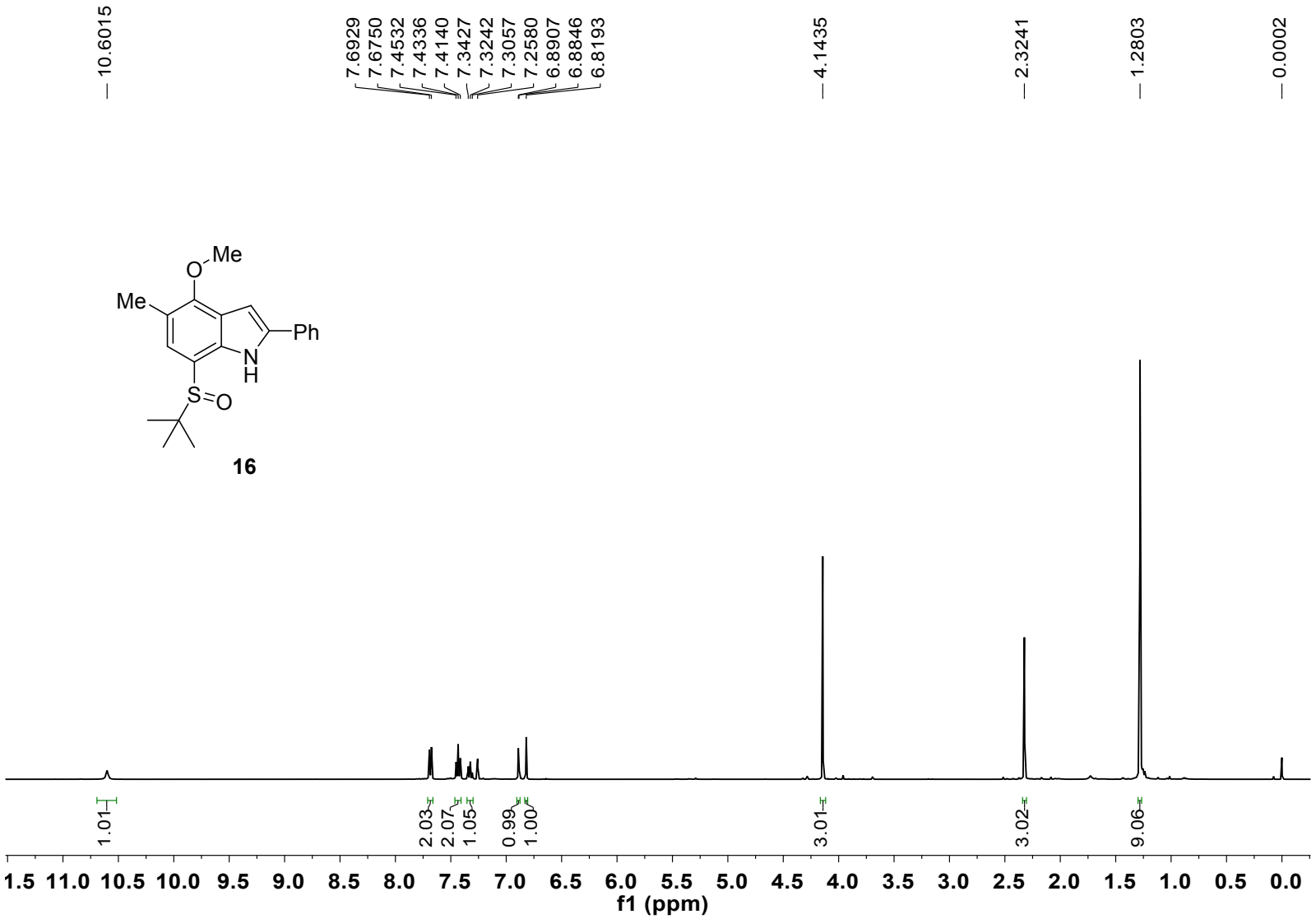
116.9848
113.4782
97.2342
77.3165
76.9986
76.6811
63.8270
58.1860
38.4083
23.1955
17.7914
CH2CH2OH
HN
Me
Ph
N
H
S
O
15
55 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)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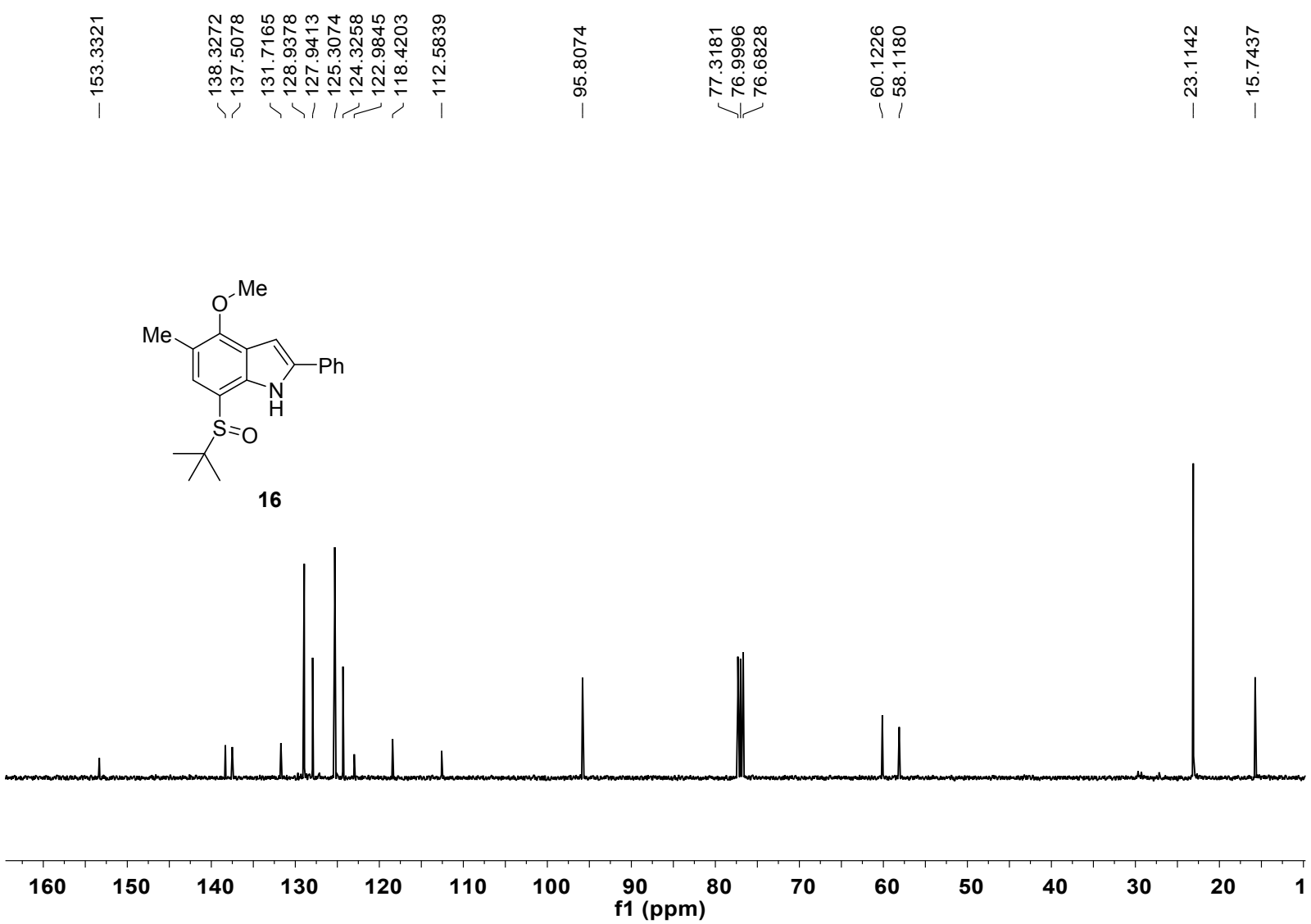
6.8846
6.8193
4.1435
2.3241
1.2803
0.0002
Me
O
Me
Ph
N
H
S
O
16
1.01
2.03
2.07
1.05
0.99
1.00
3.01
3.02
9.06
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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95.8074
77.3181
76.9996
76.6828
60.1226
58.1180
23.1142
15.7437
Me
O
Me
Ph
N
H
S
O
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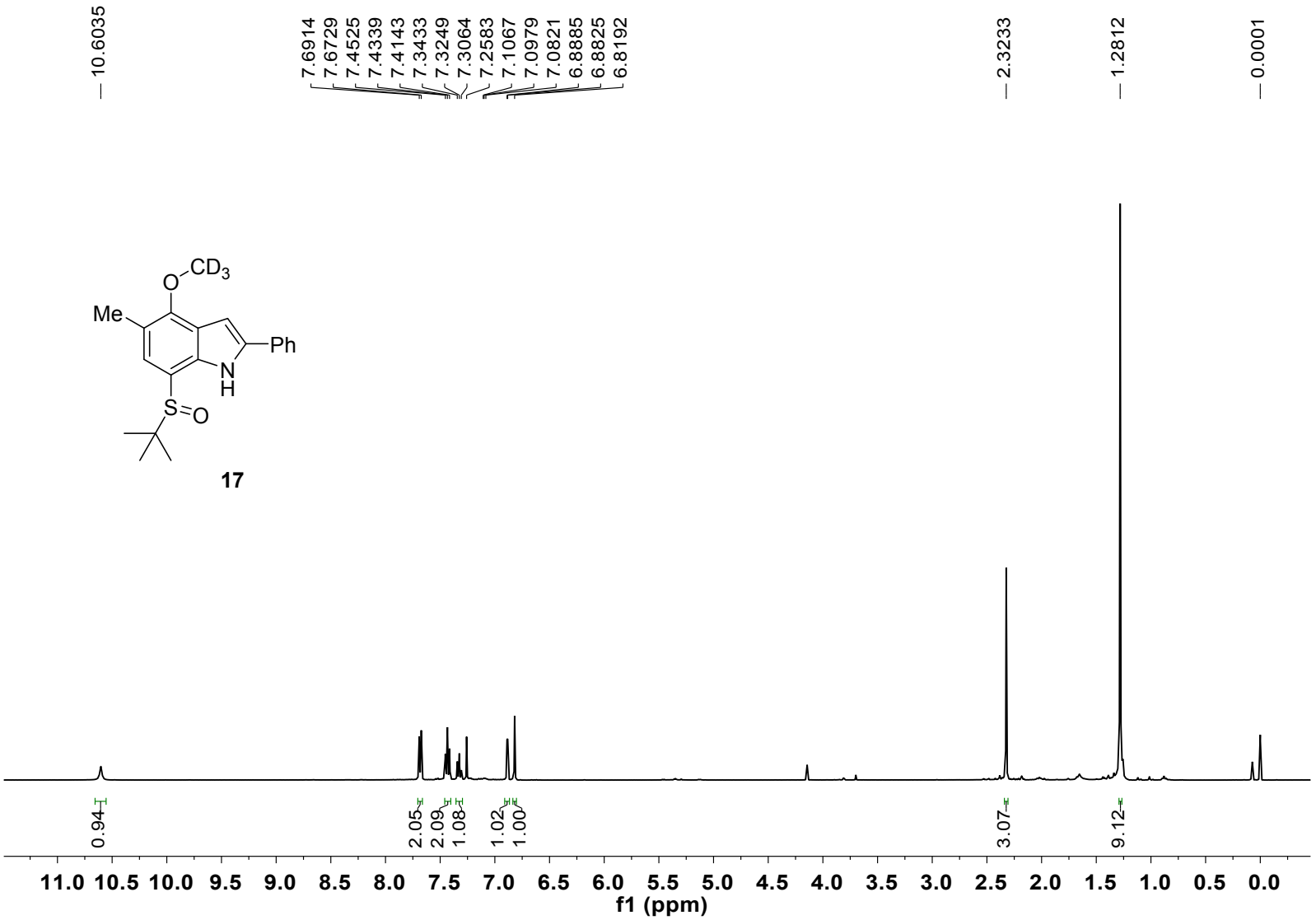
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)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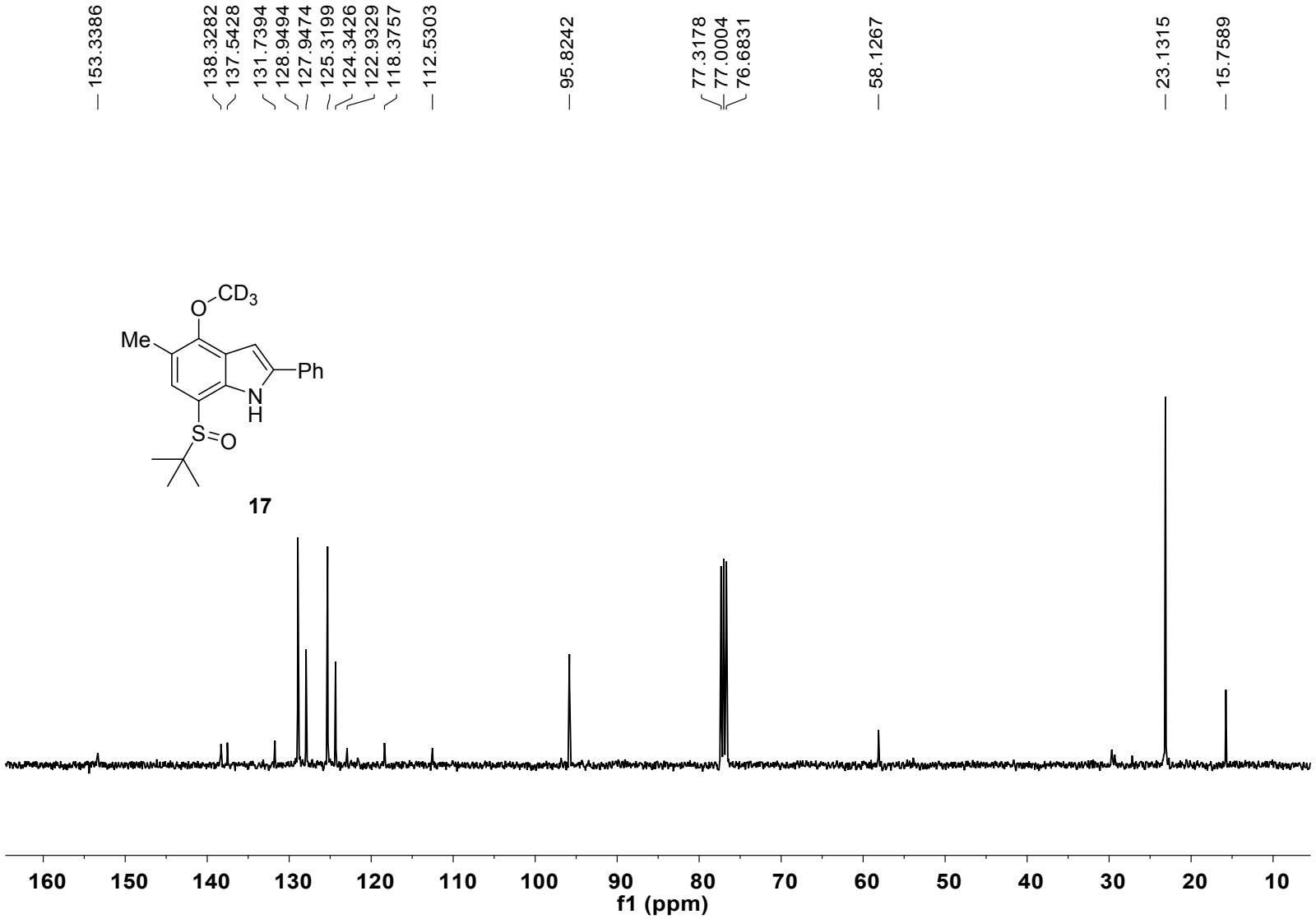
7.0979
7.0821
6.8885
6.8825
6.8192
2.3233
1.2812
0.0001
CD3
O
Me
Ph
N
H
S
O
17
0.94
2.05
2.09
1.08
1.02
1.00
3.07
9.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.0004
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O
CD3
Me
Ph
N
H
S
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140
130
120
110
100
90
80
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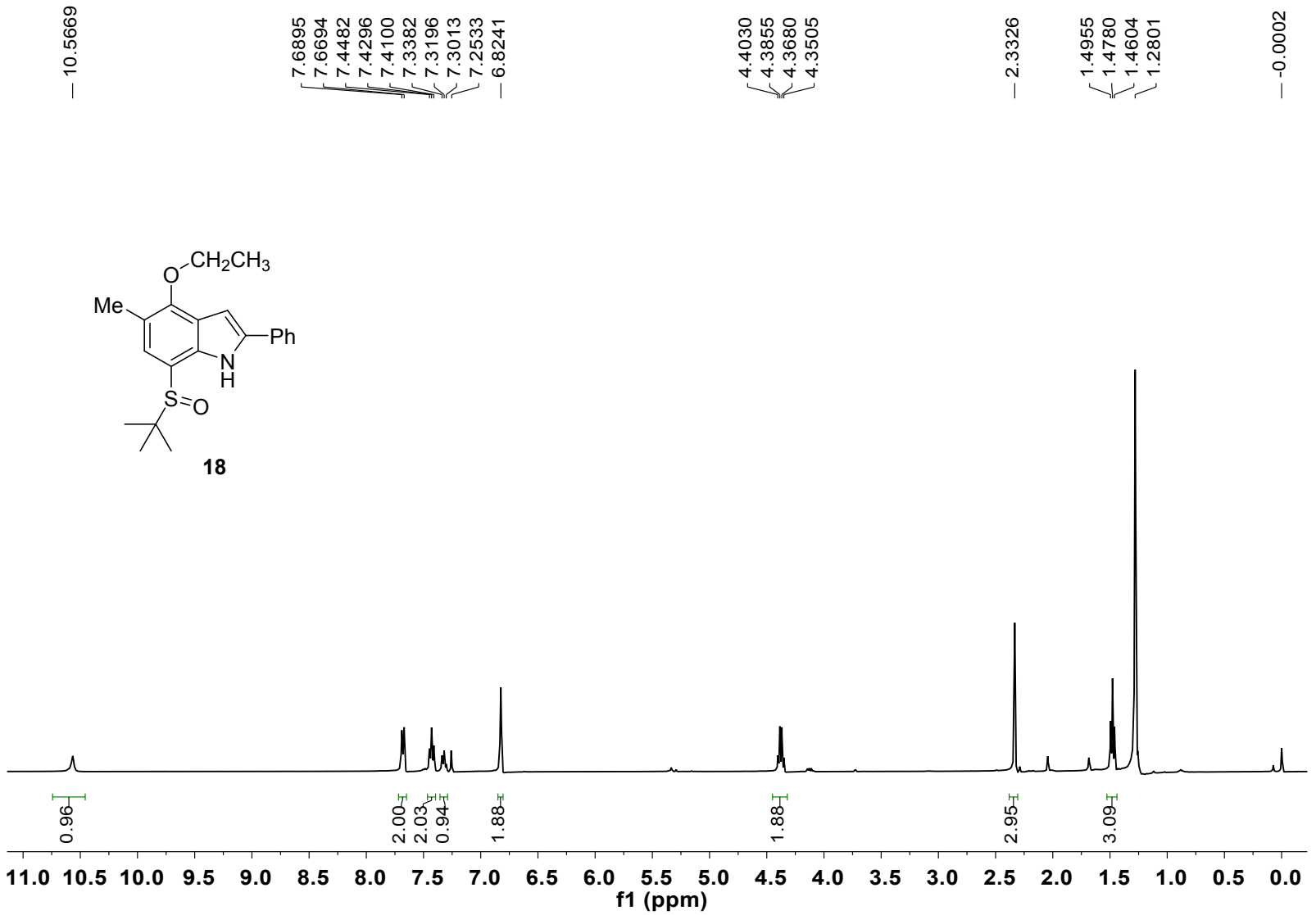
60
50
40
30
20
10
f1 (ppm)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4.3680
4.3505
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1.4780
1.4604
1.2801
-0.0002
O
CH2CH3
Me
Ph
N
H
S
O
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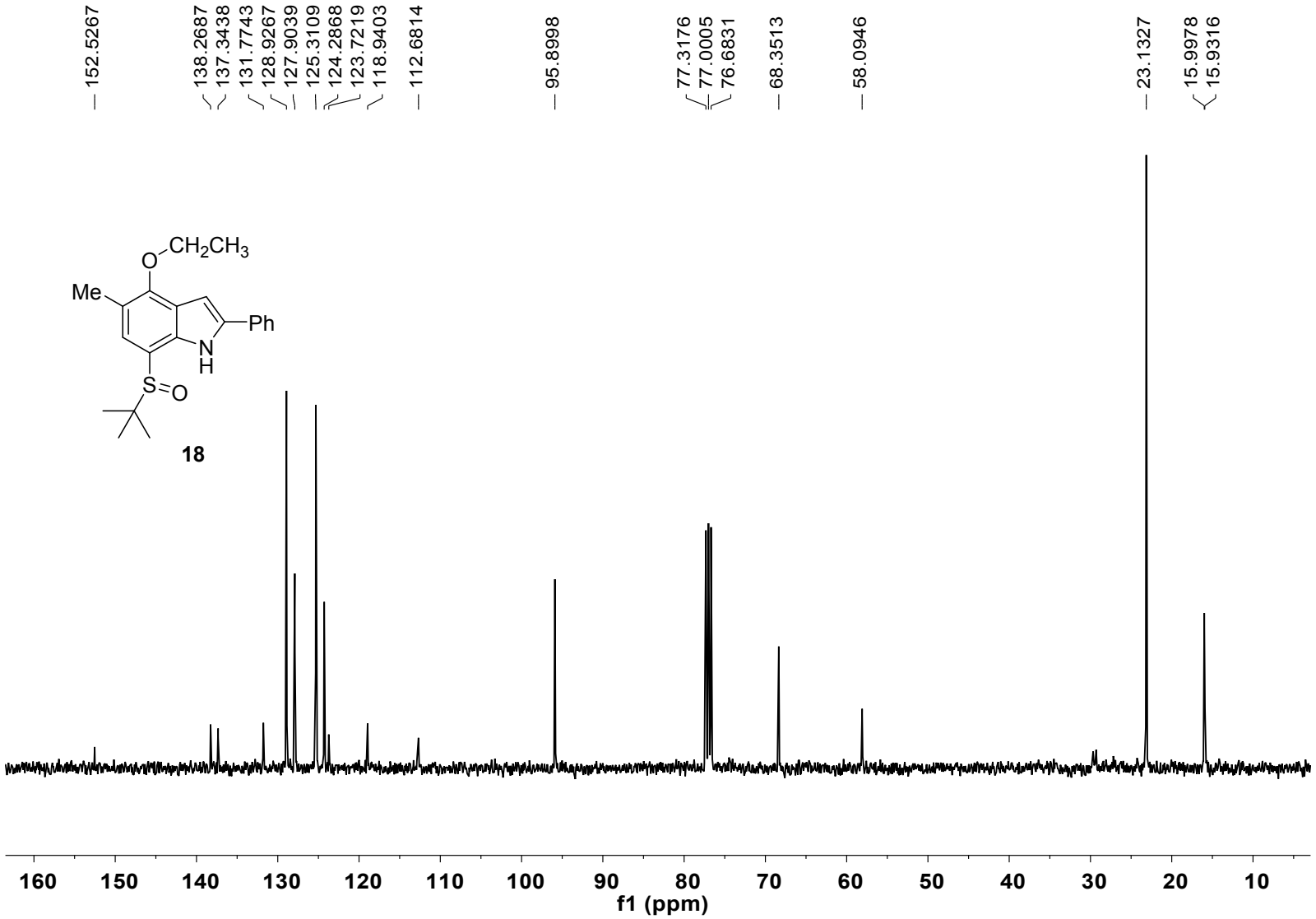
2.00
2.03
0.94
1.88
1.88
2.95
3.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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68.3513
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O
CH2CH3
Me
Ph
N
H
S
O
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140
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120
110
100
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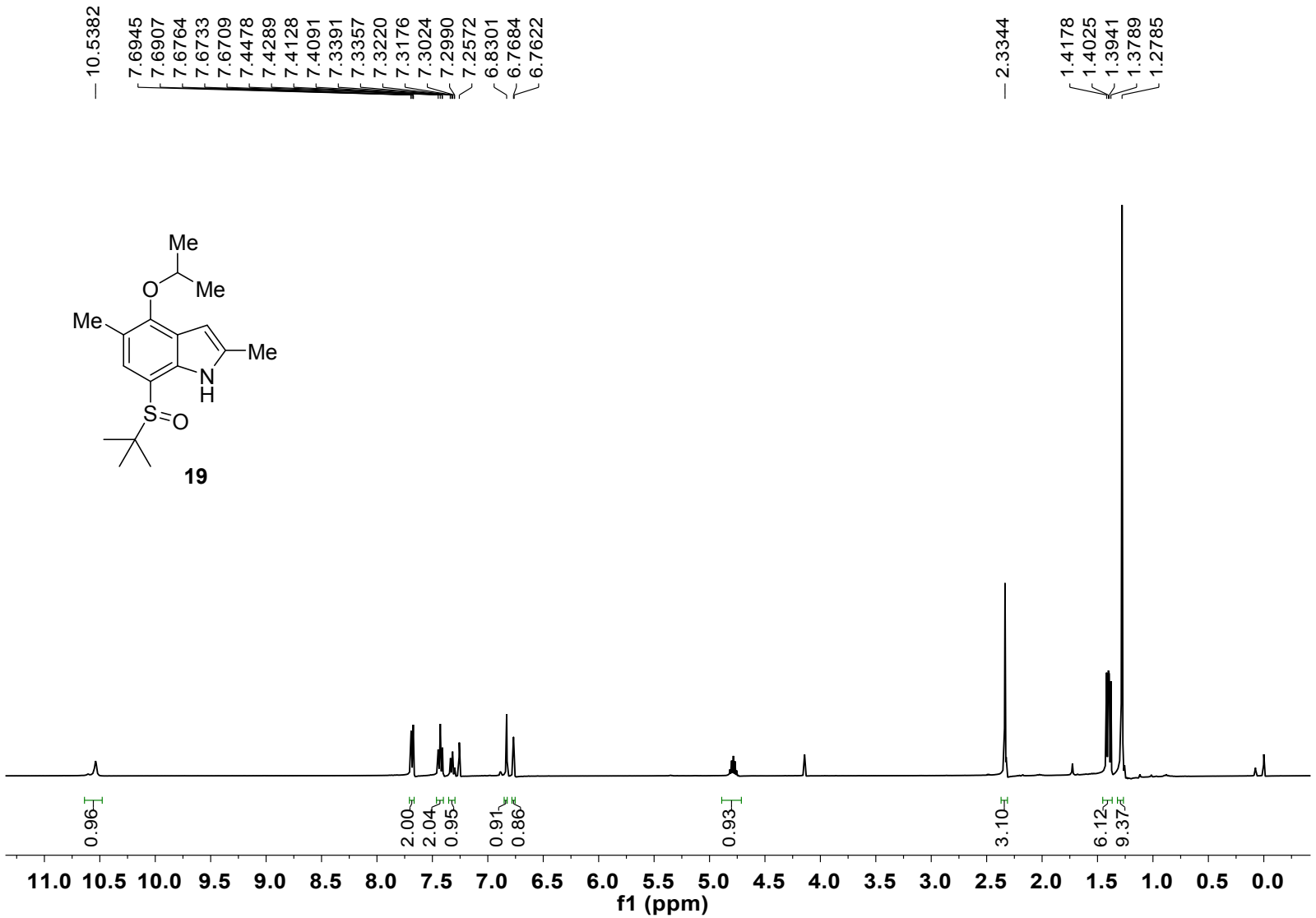
80
70
60
50
40
30
20
10
f1 (ppm)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7.2990
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6.8301
6.7684
6.7622
2.3344
1.4178
1.4025
1.3941
1.3789
1.2785
Me
O
Me
Me
Me
N
H
S
O
19
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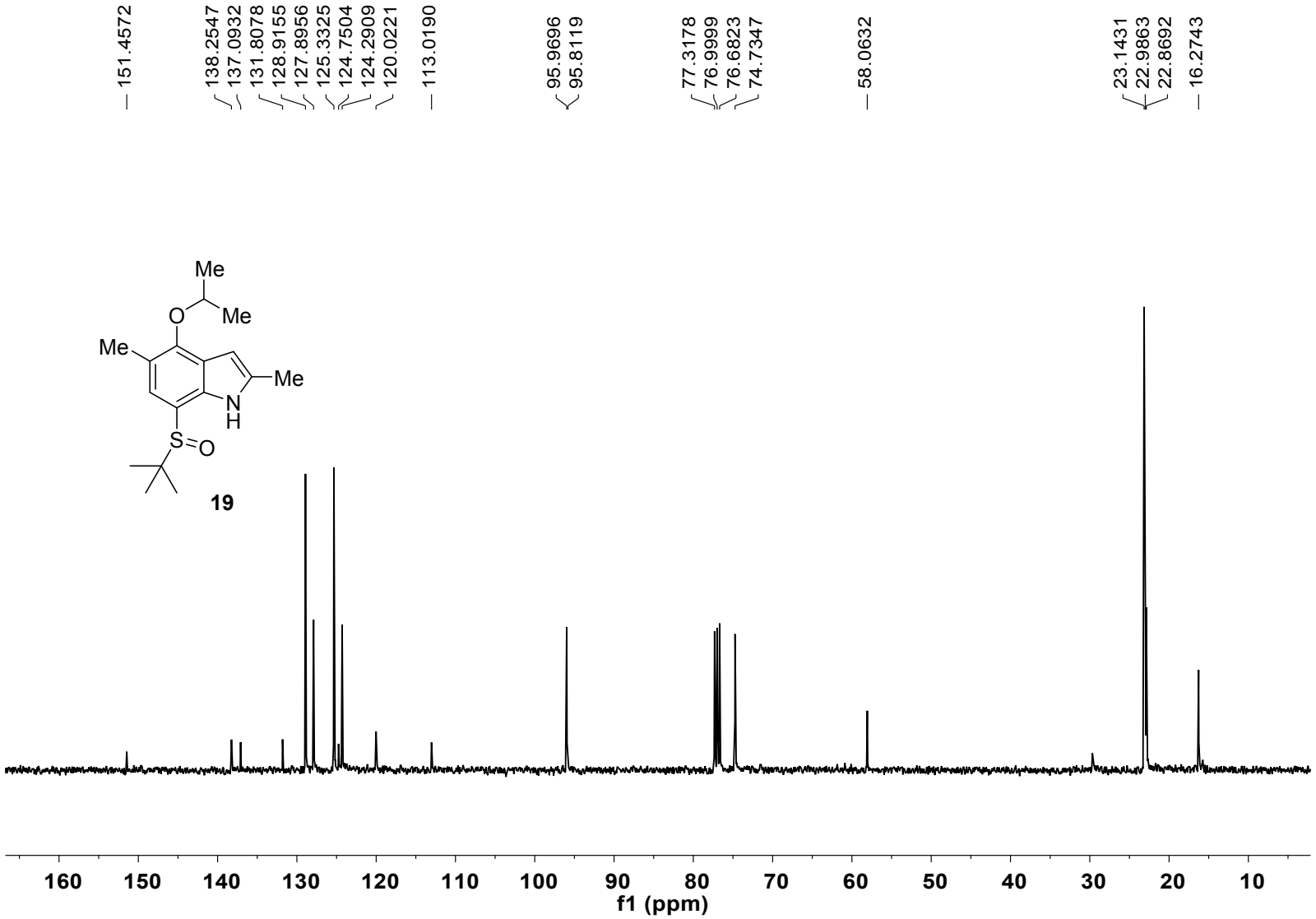
2.00
2.04
0.95
0.91
0.86
0.93
3.10
6.12
9.37
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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95.9696
95.8119
77.3178
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76.6823
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58.0632
23.1431
22.9863
22.8692
16.2743
Me
O
Me
Me
Me
N
H
S
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140
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120
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100
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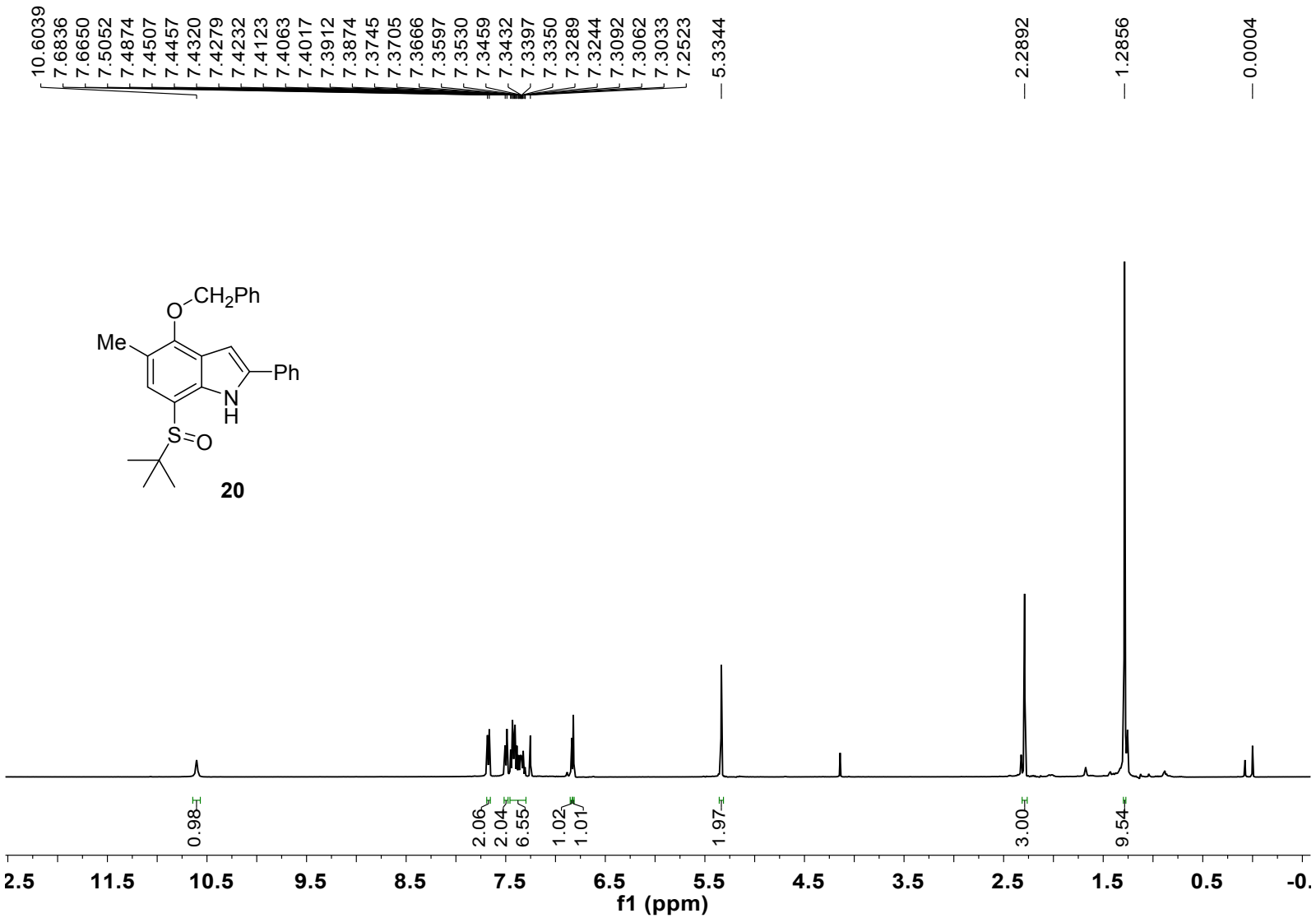
80
70
60
50
40
30
20
10
f1 (ppm)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7.3745
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7.3597
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7.3432
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7.3350
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O
Me
Ph
N
H
S
O
20
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2.04
6.55
1.02
1.01
1.97
3.00
9.54
2.5
11.5
10.5
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6.5
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4.5
3.5
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1.5
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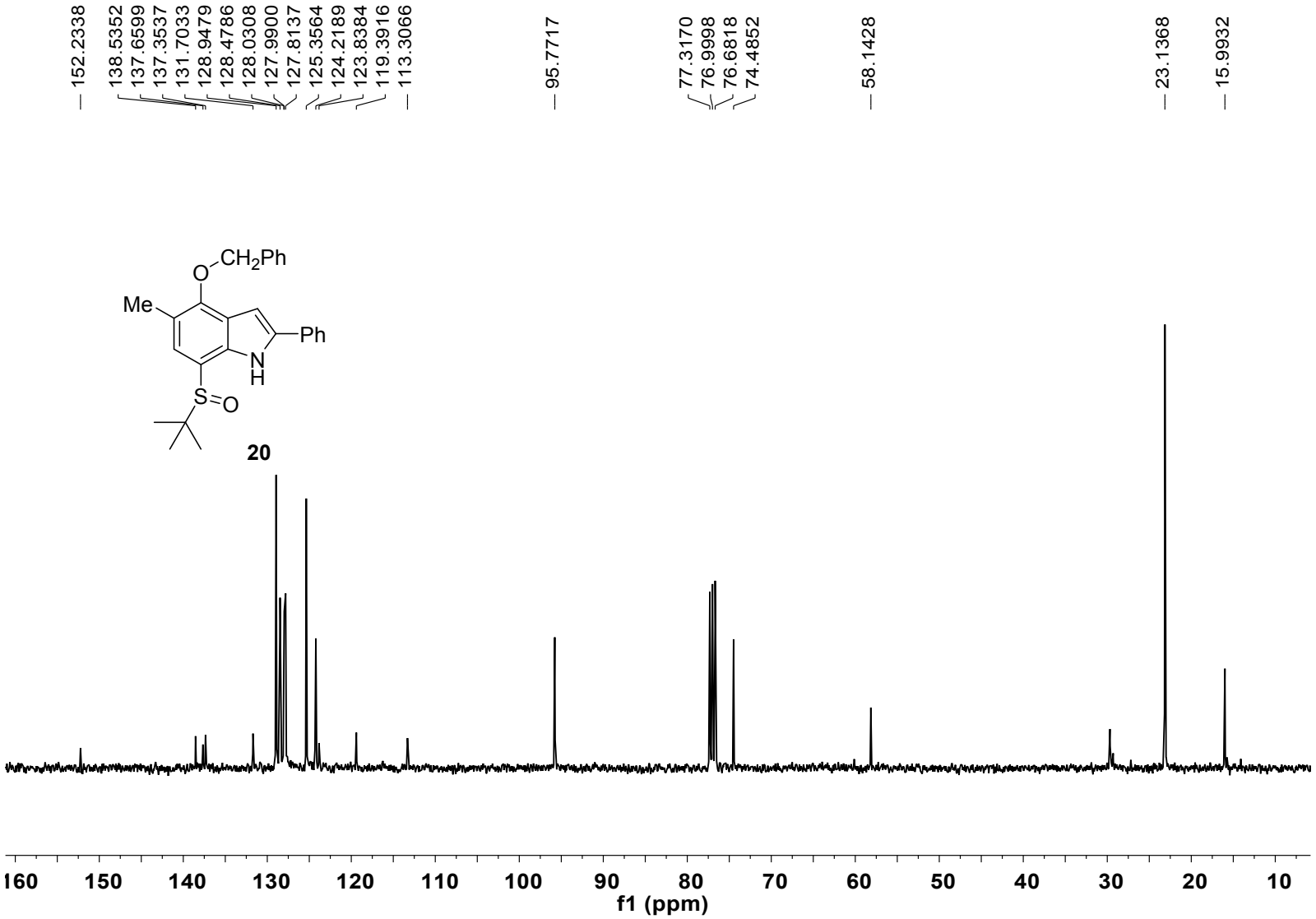
f1 (ppm)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77.3170
76.9998
76.6818
74.4852
58.1428
23.1368
15.9932
O
CH2Ph
Me
Ph
N
H
S
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120
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100
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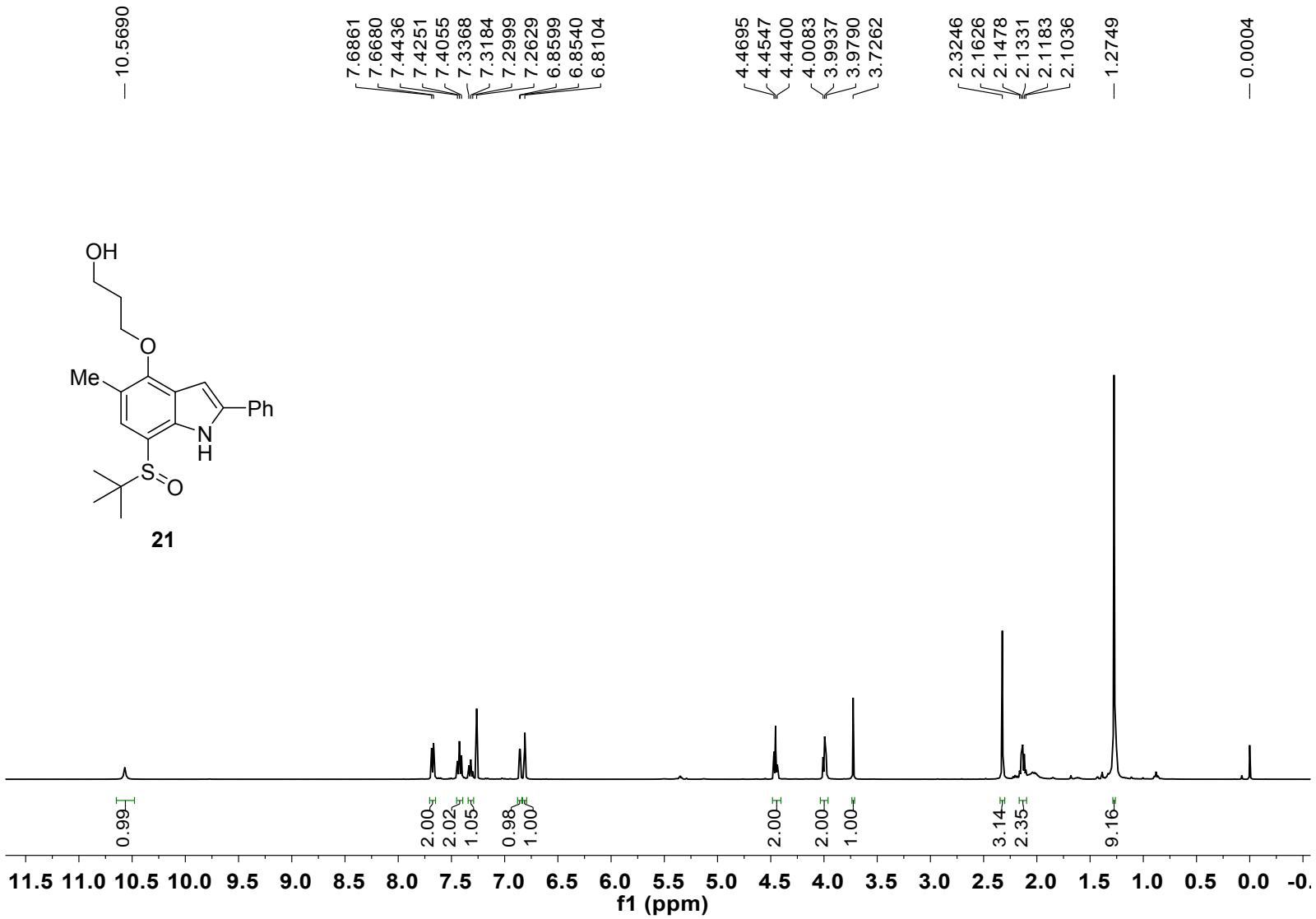
60
50
40
30
20
10
f1 (ppm)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6.8104
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3.9937
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2.3246
2.1626
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2.1331
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OH
O
Me
Ph
N
H
S
O
21
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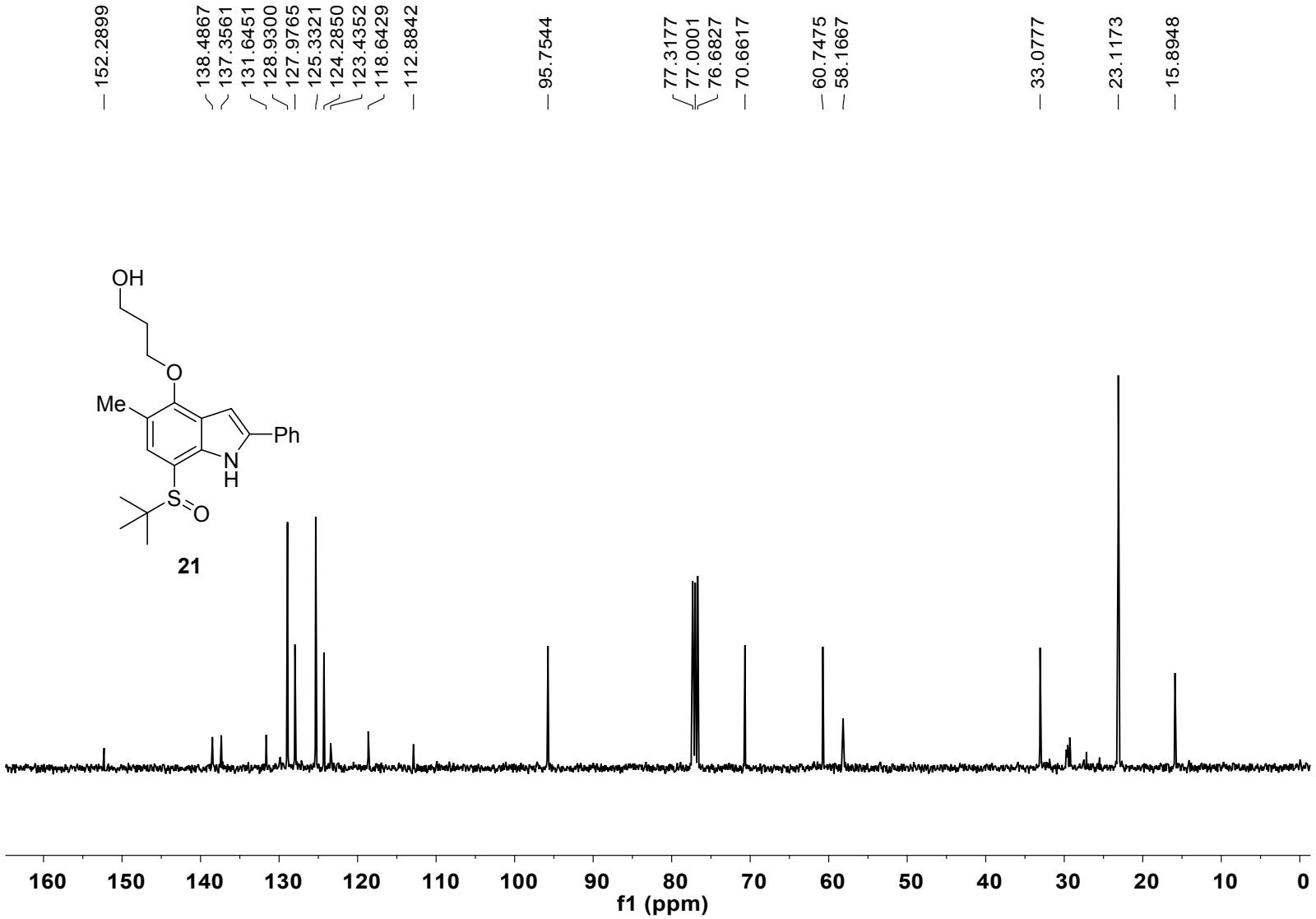
2.00
2.02
1.05
0.98
1.00
2.00
2.00
1.00
3.14
2.35
9.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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77.3177
77.0001
76.6827
70.6617
60.7475
58.1667
33.0777
23.1173
15.8948
OH
O
Me
Ph
N
H
S
O
21
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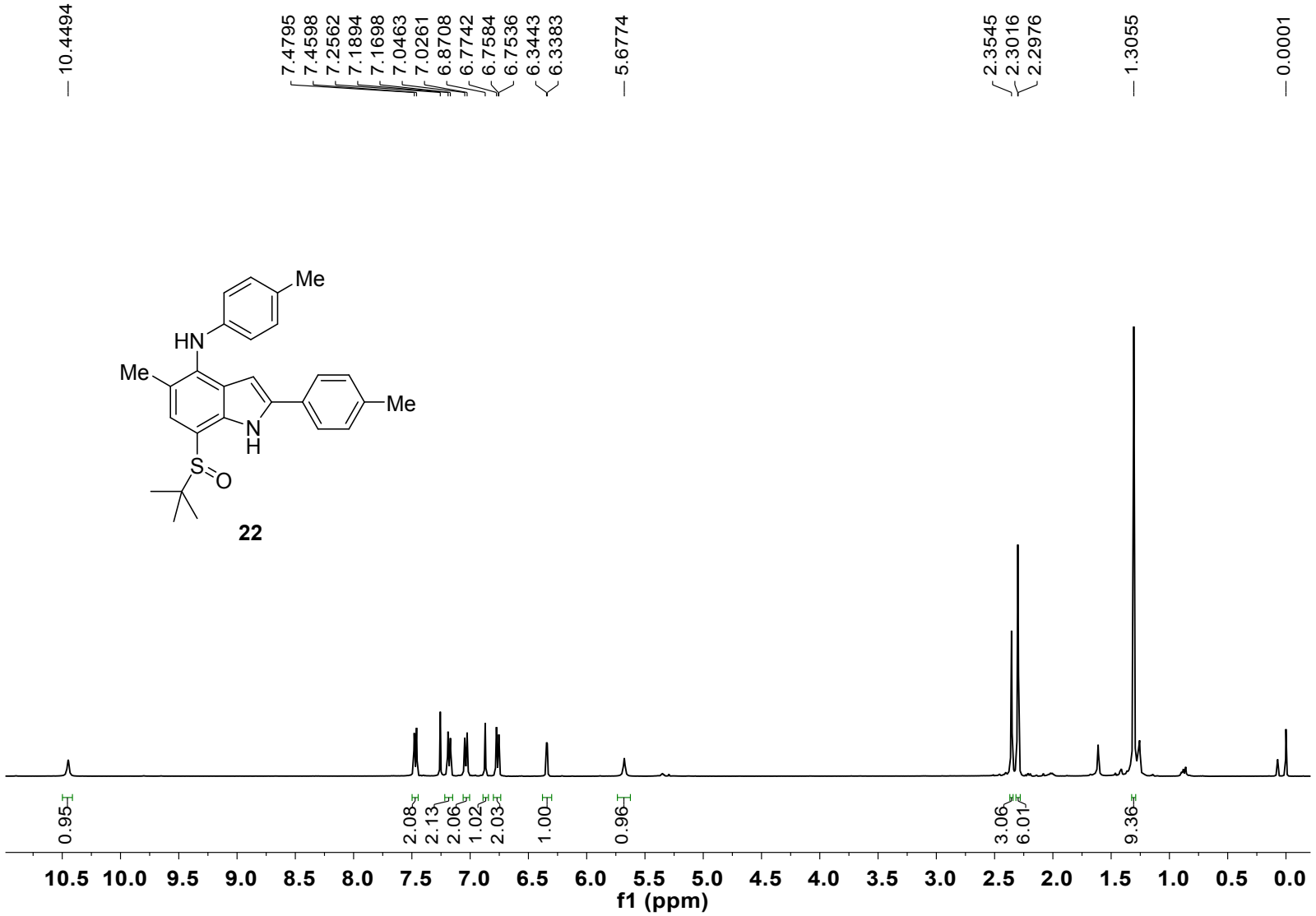
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Me
Me
N
H
S
O
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2.13
2.06
1.02
2.03
1.00
0.96
3.06
6.01
9.36
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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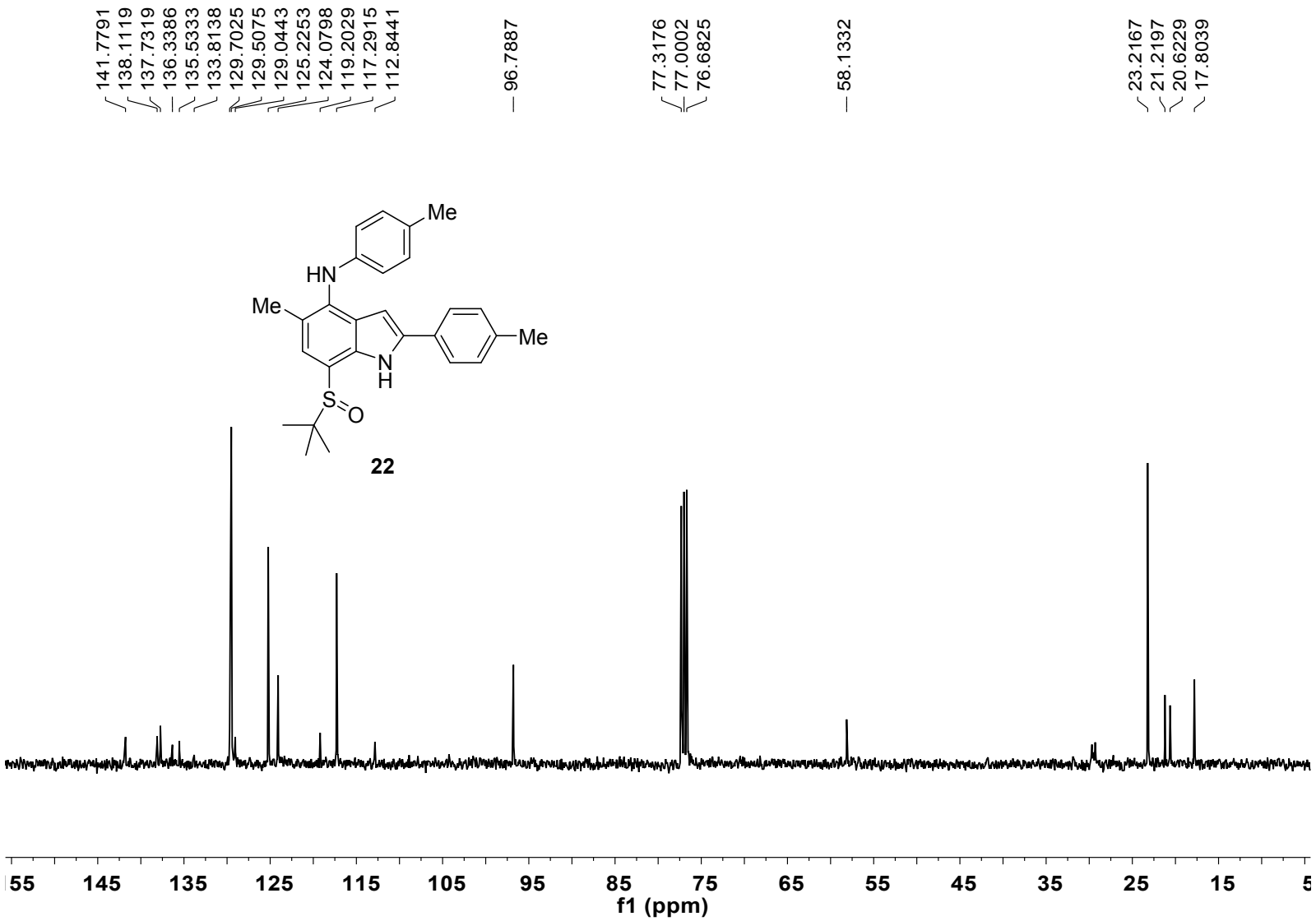
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119.2029
117.2915
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76.6825
58.1332
23.2167
21.2197
20.6229
17.8039
Me
HN
Me
Me
N
H
S
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85
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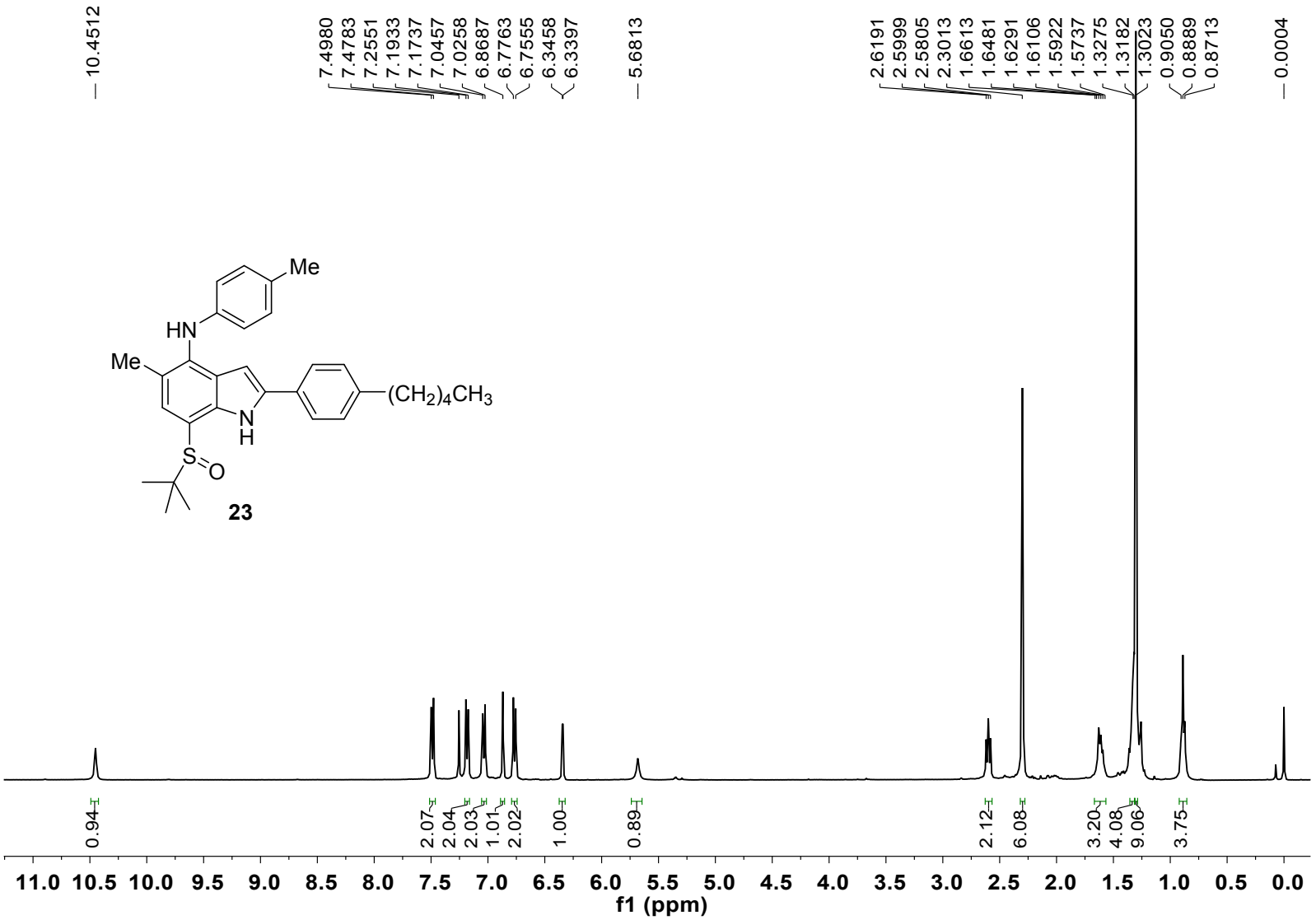
f1 (ppm)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6.7555
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2.3013
1.6613
1.6481
1.6291
1.6106
1.5922
1.5737
1.3275
1.3182
1.3023
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0.8713
0.0004
Me
HN
Me
(CH2)4CH3
N
H
S
O
23
0.94
2.07
2.04
2.03
1.01
2.02
1.00
0.89
2.12
6.08
3.20
4.08
9.06
3.75
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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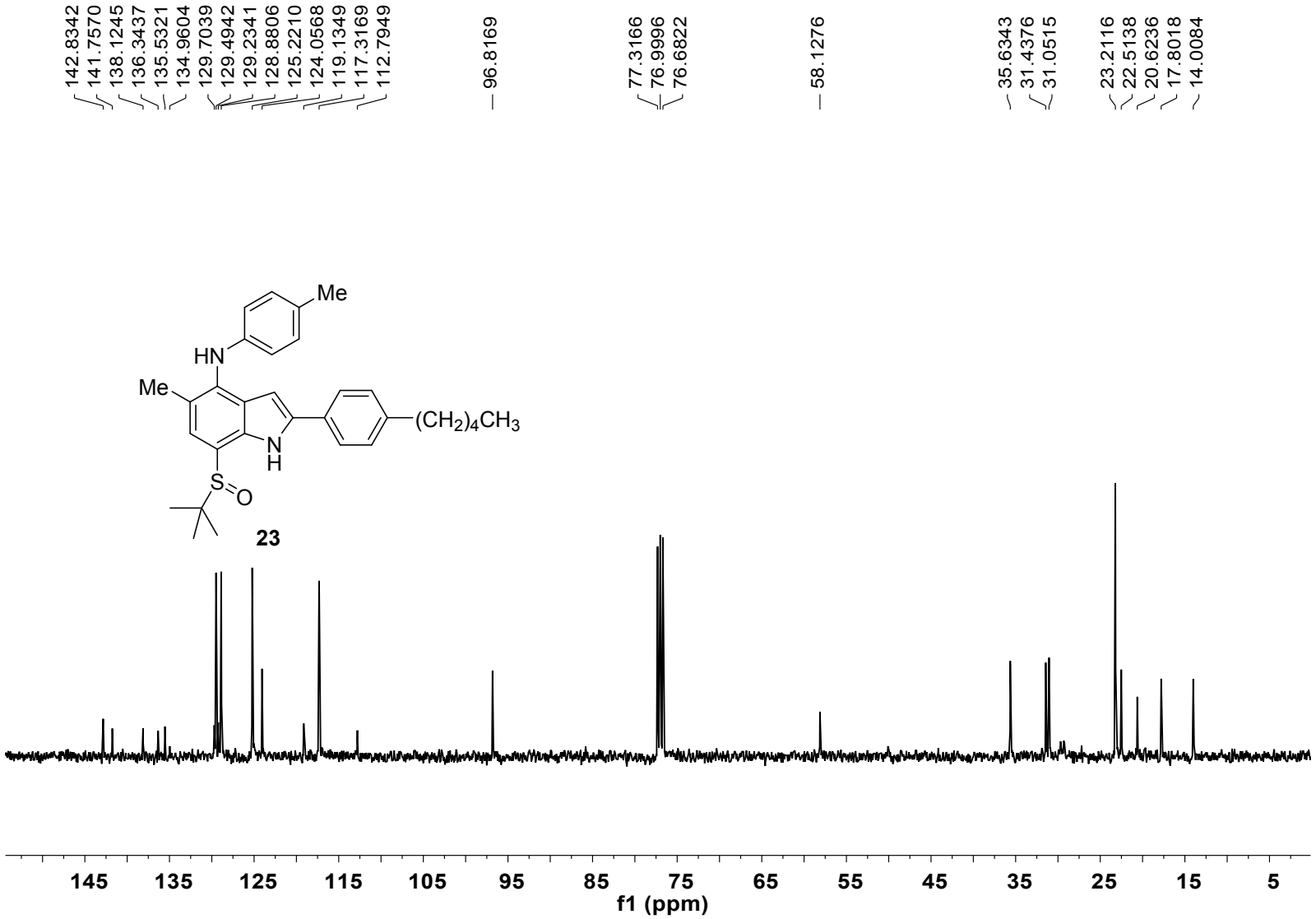
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Me
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H
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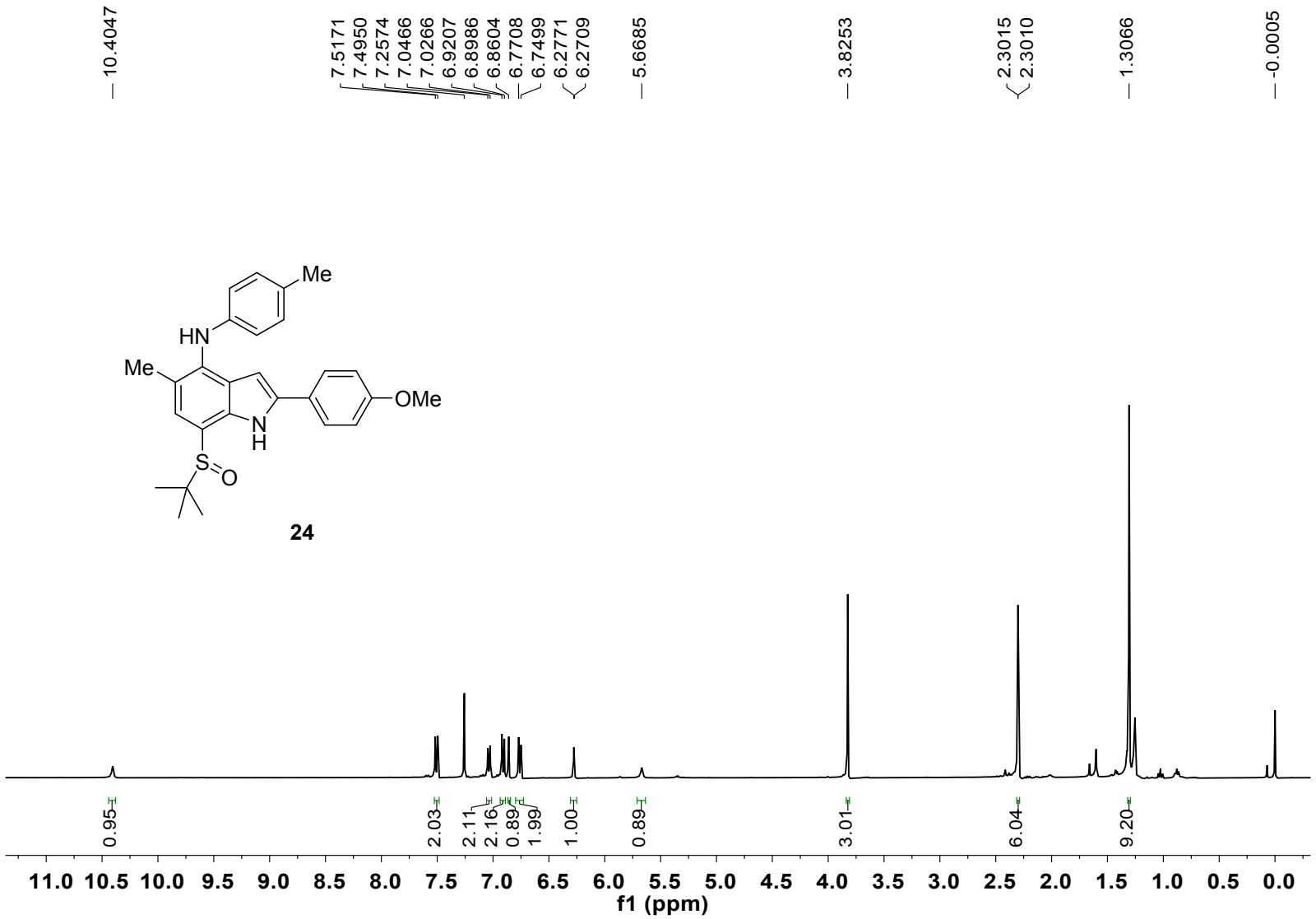
f1 (ppm)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6.2771
6.2709
5.6685
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HN
Me
OMe
N
H
S
O
24
0.95
2.03
2.11
2.16
0.89
1.99
1.00
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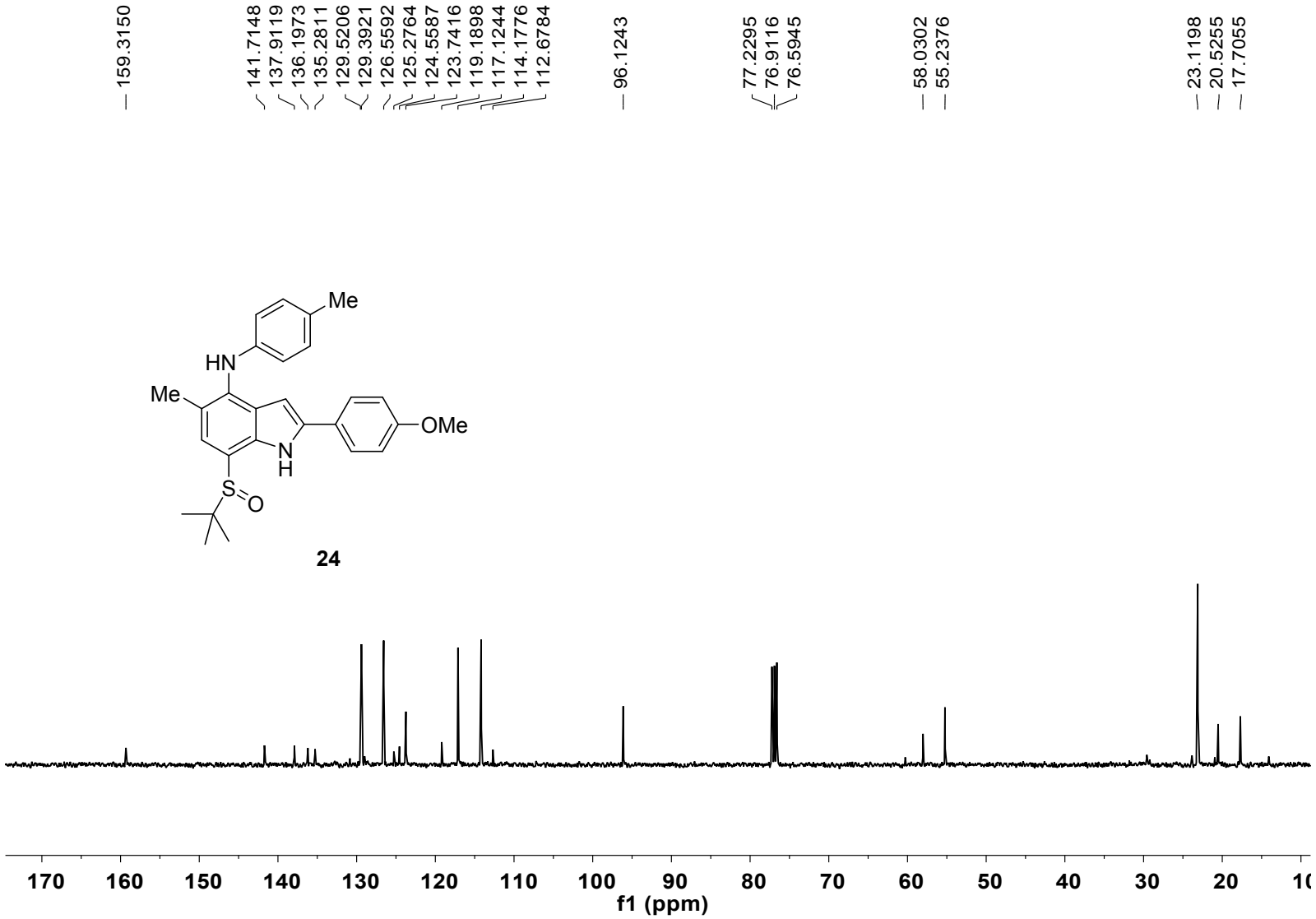
3.01
6.04
9.20
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.2295
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76.5945
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55.2376
23.1198
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Me
HN
Me
OMe
N
H
S
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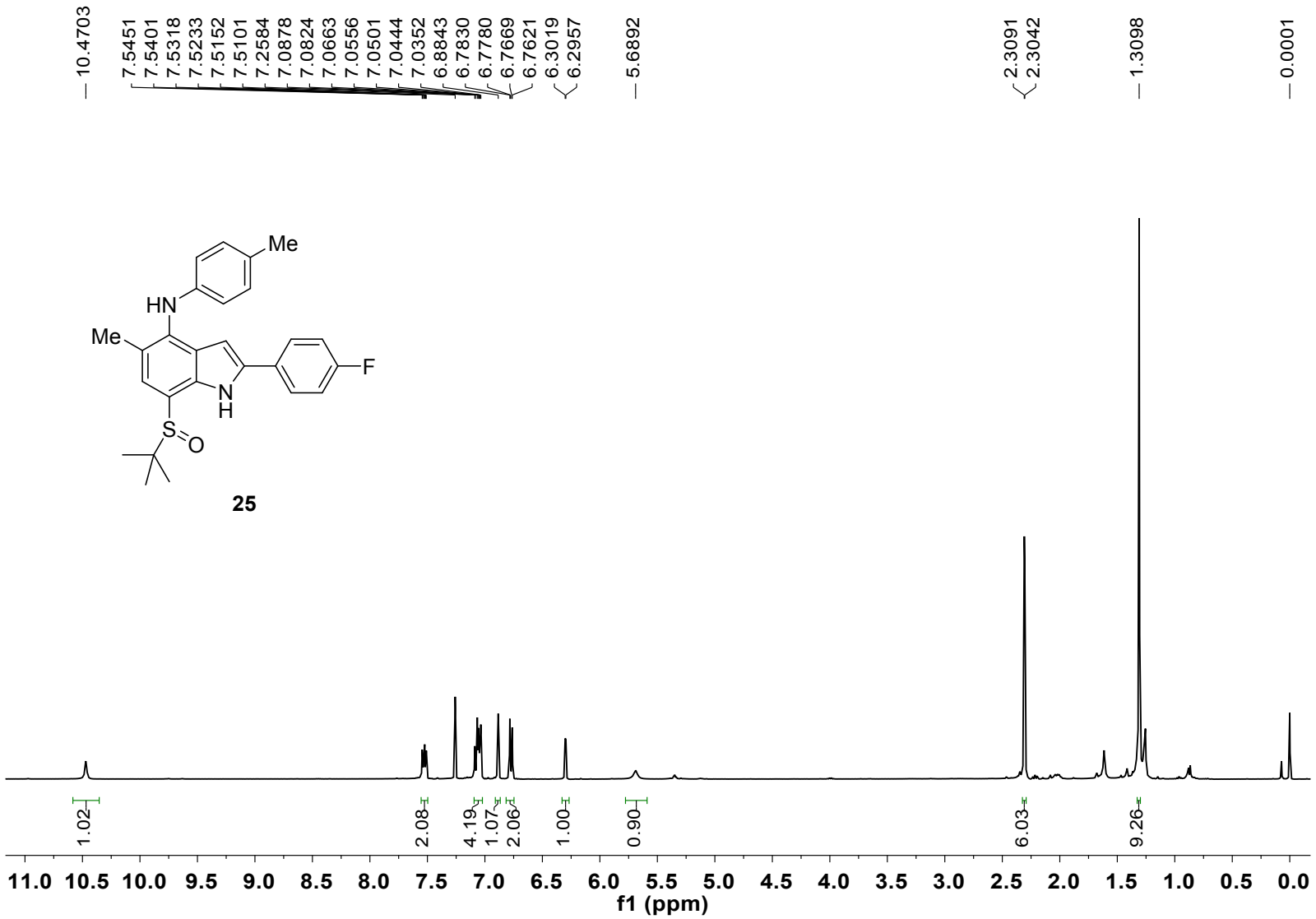
f1 (ppm)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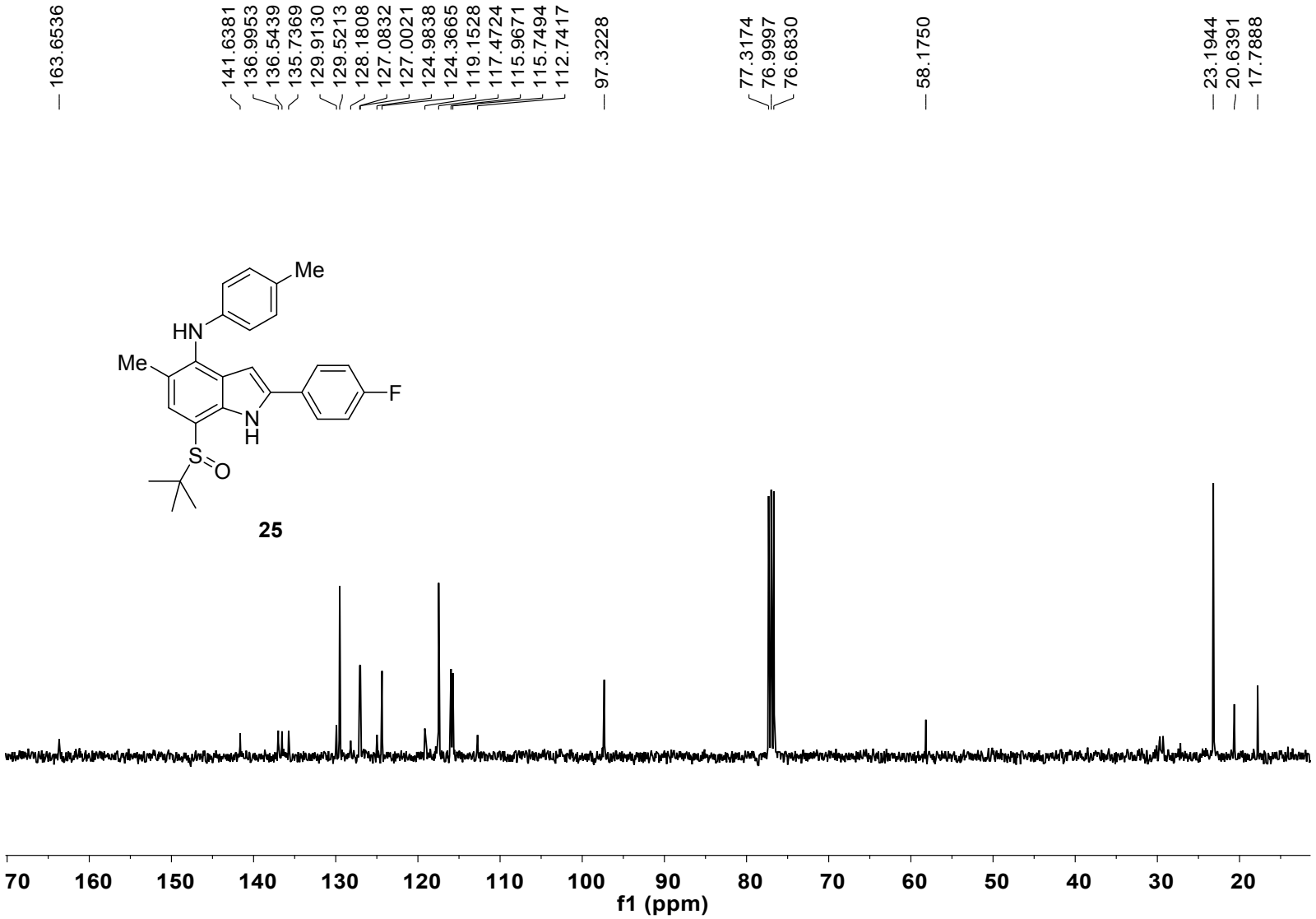
7.0556
7.0501
7.0444
7.0352
6.8843
6.7830
6.7780
6.7669
6.7621
6.3019
6.2957
5.6892
2.3091
2.3042
1.3098
0.0001
Me
HN
Me
F
N
H
S
O
25
1.02
2.08
4.19
1.07
2.06
1.00
0.90
6.03
9.26
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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115.9671
115.7494
112.7417
97.3228
77.3174
76.9997
76.6830
58.1750
23.1944
20.6391
17.7888
Me
HN
Me
F
N
H
S
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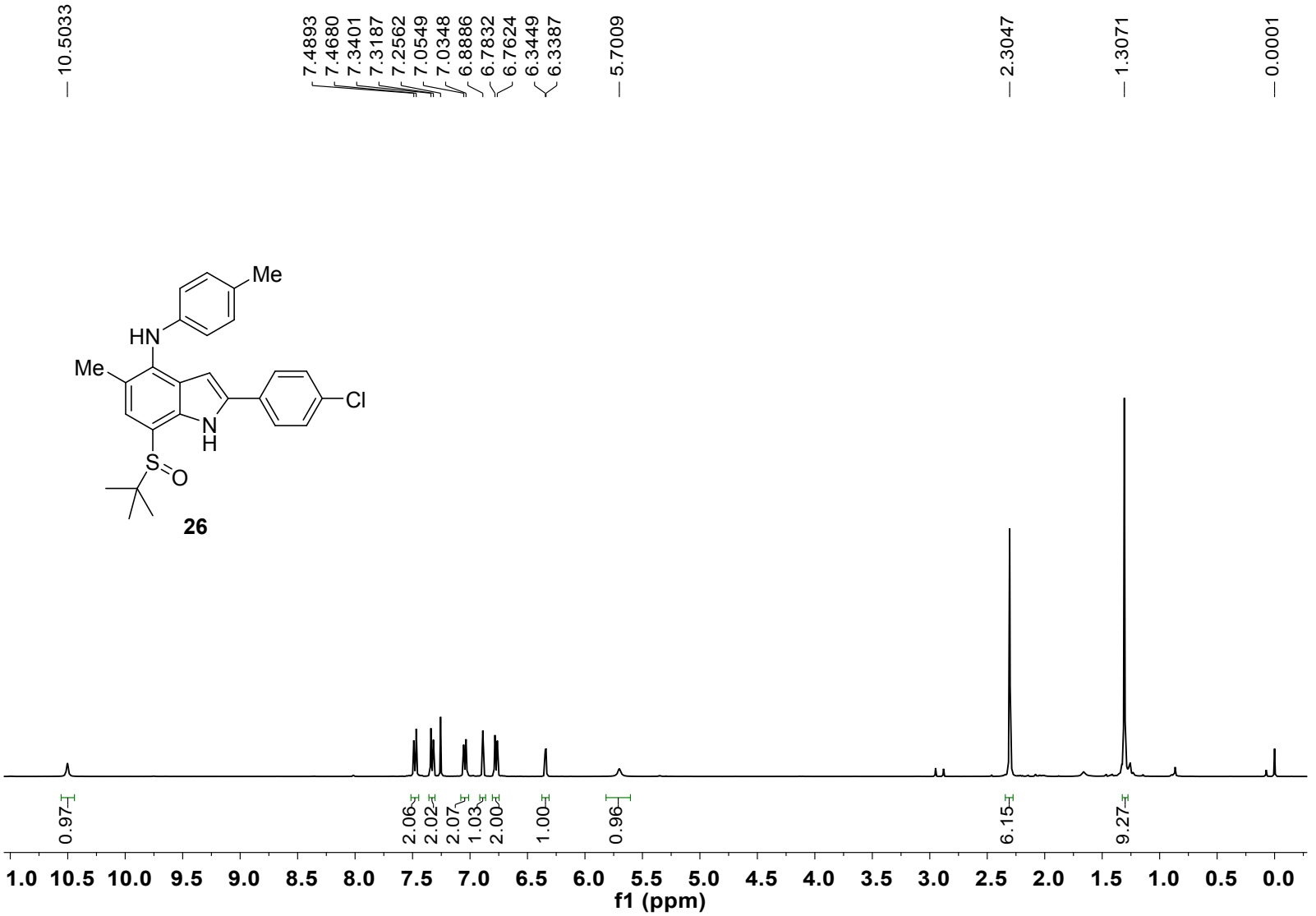
30
20
f1 (ppm)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6.3449
6.3387
5.7009
2.3047
1.3071
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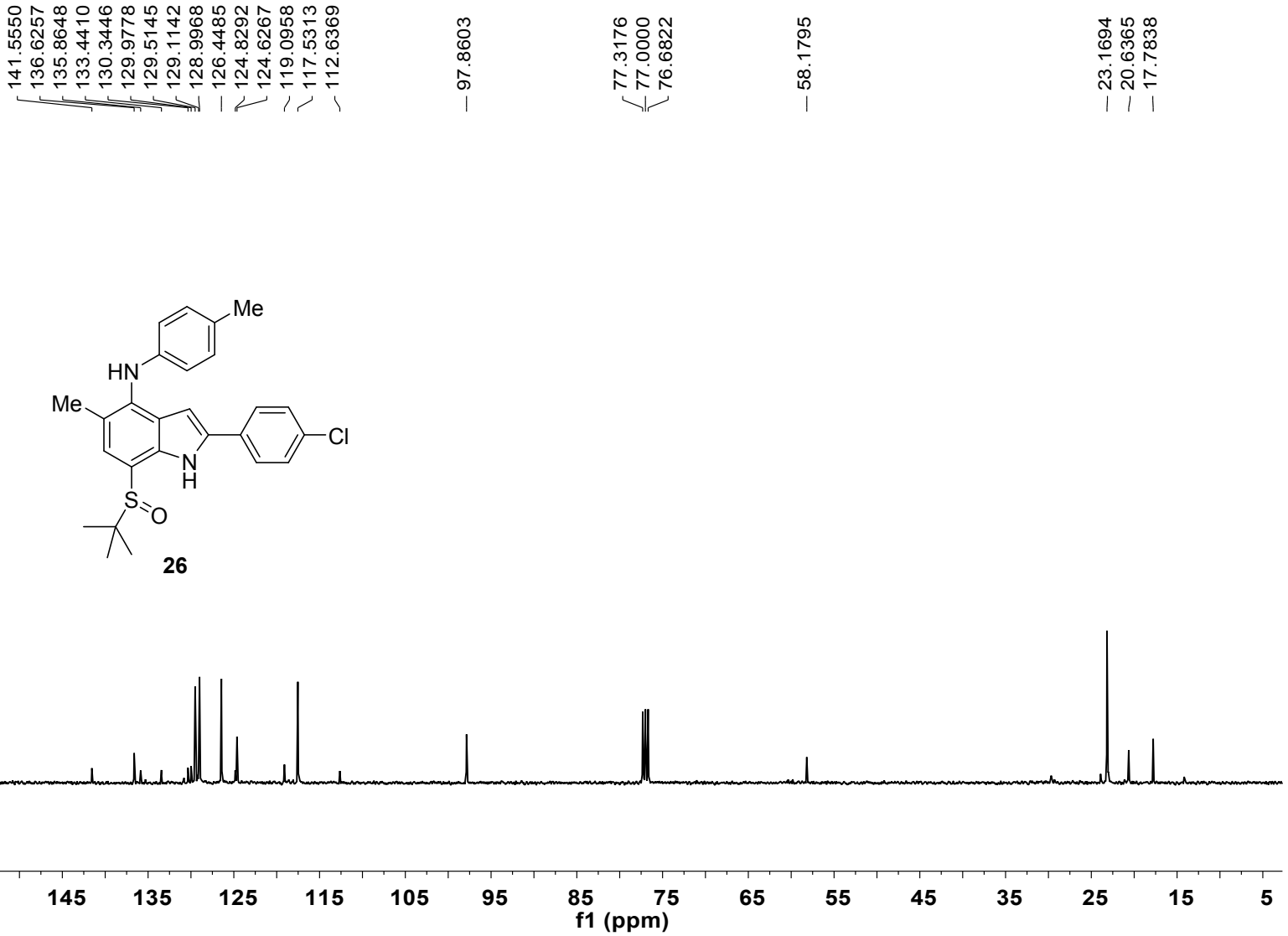
Me
HN
Me
Cl
N
H
S
O
26
0.97
2.06
2.02
2.07
1.03
2.00
1.00
0.96
6.15
9.27
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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58.1795
23.1694
20.6365
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Me
HN
Me
Cl
N
H
S
O
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115
105
95
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75
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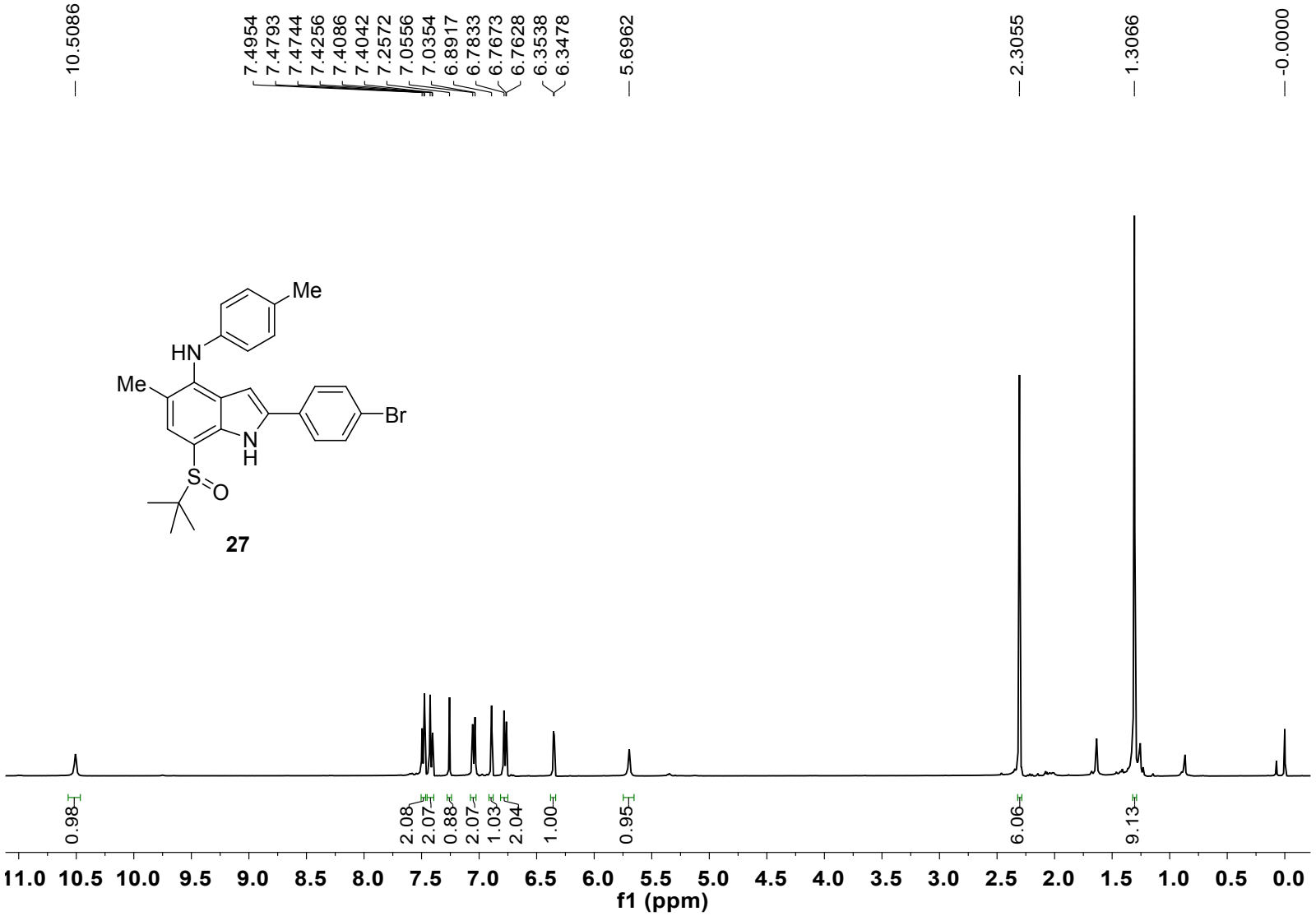
55
45
35
25
15
5
f1 (ppm)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6.7673
6.7628
6.3538
6.3478
5.6962
2.3055
1.3066
-0.0000
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HN
Me
Br
N
H
S
O
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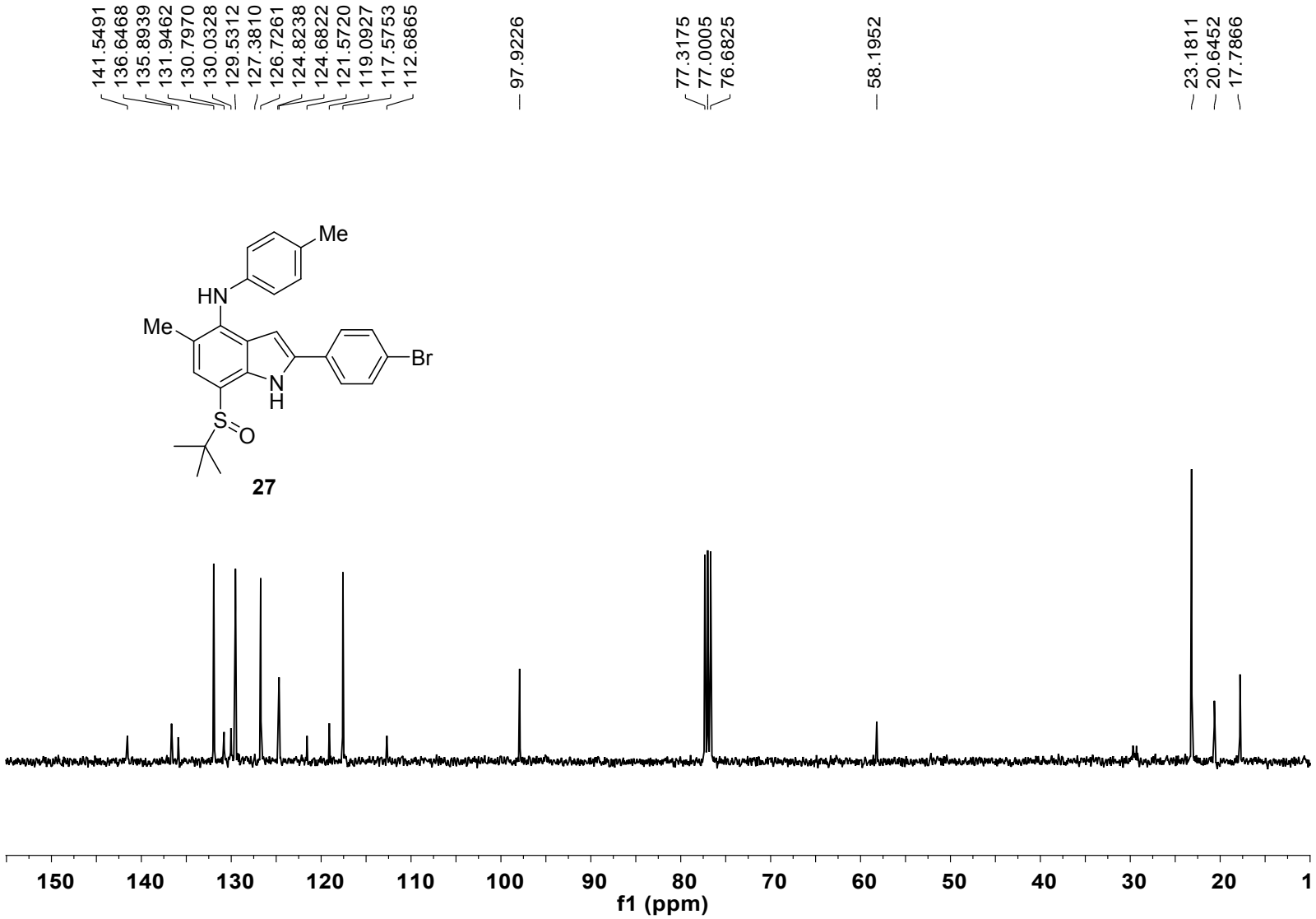
0.98
2.08
2.07
0.88
2.07
1.03
2.04
1.00
0.95
6.06
9.13
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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Me
HN
Me
Br
N
H
S
O
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140
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120
110
100
90
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70
60
50
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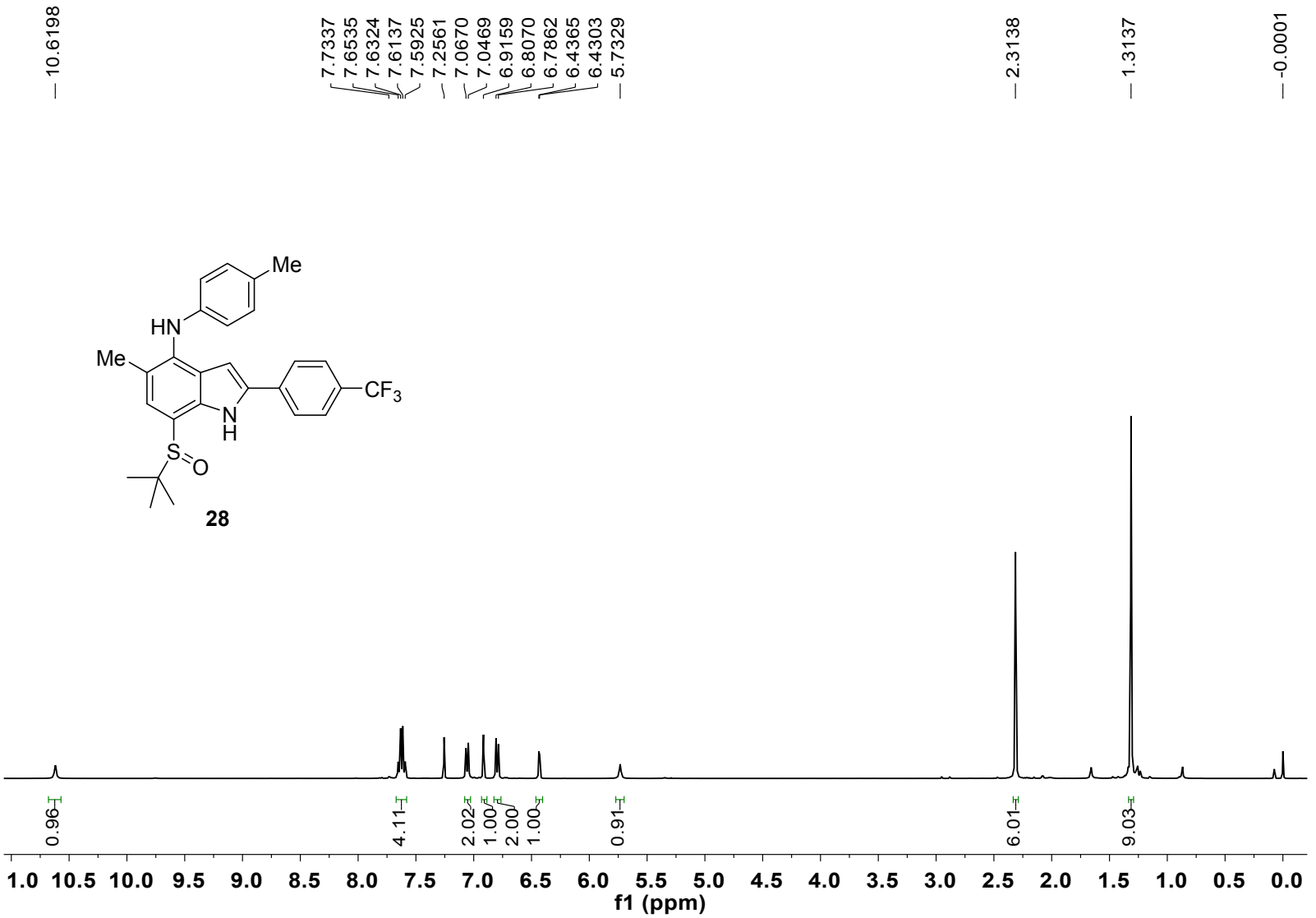
30
20
1
f1 (ppm)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6.4365
6.4303
5.7329
2.3138
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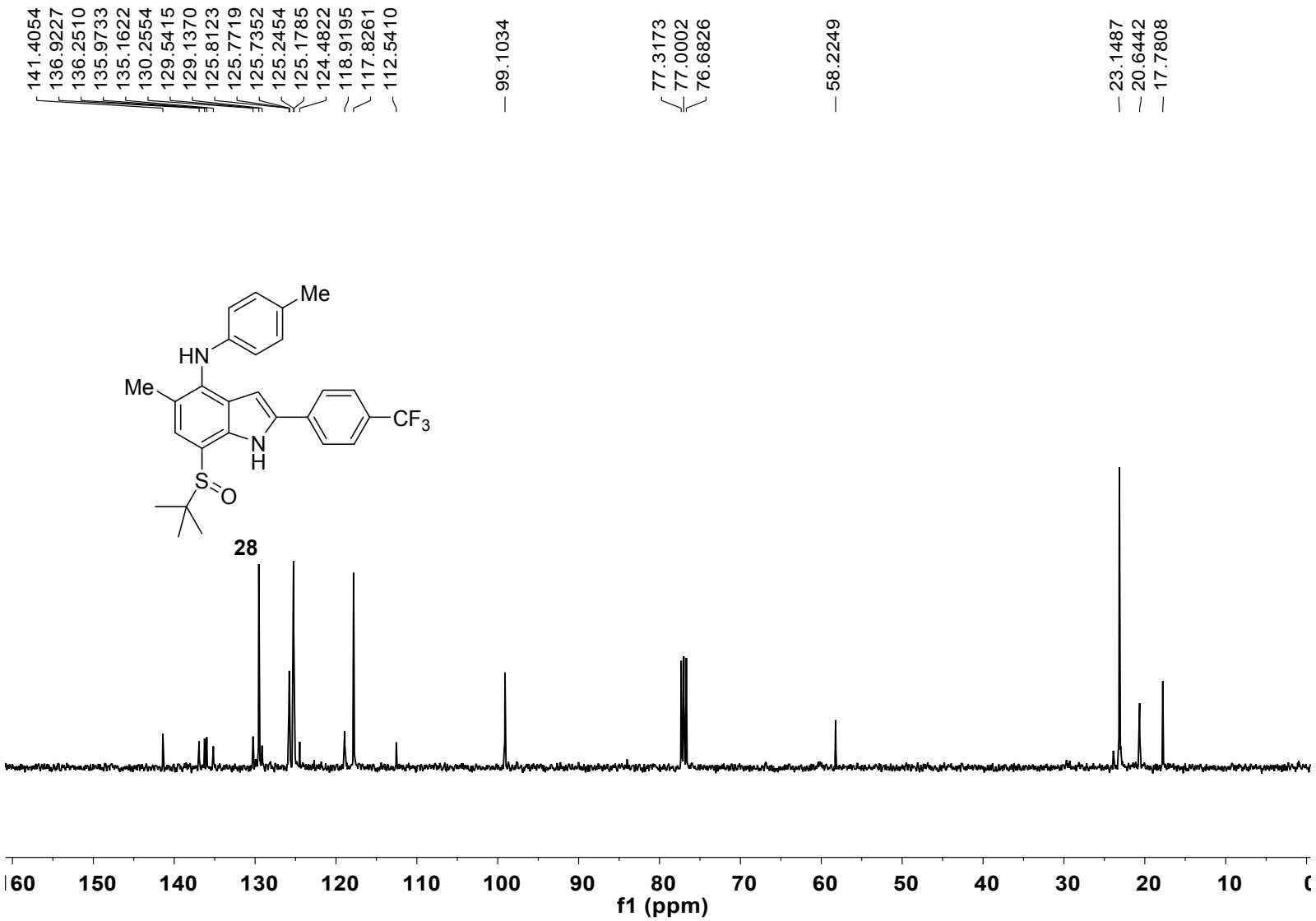
-0.0001
Me
HN
Me
CF3
N
H
S
O
28
0.96
4.11
2.02
1.00
2.00
1.00
0.91
6.01
9.03
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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CF3
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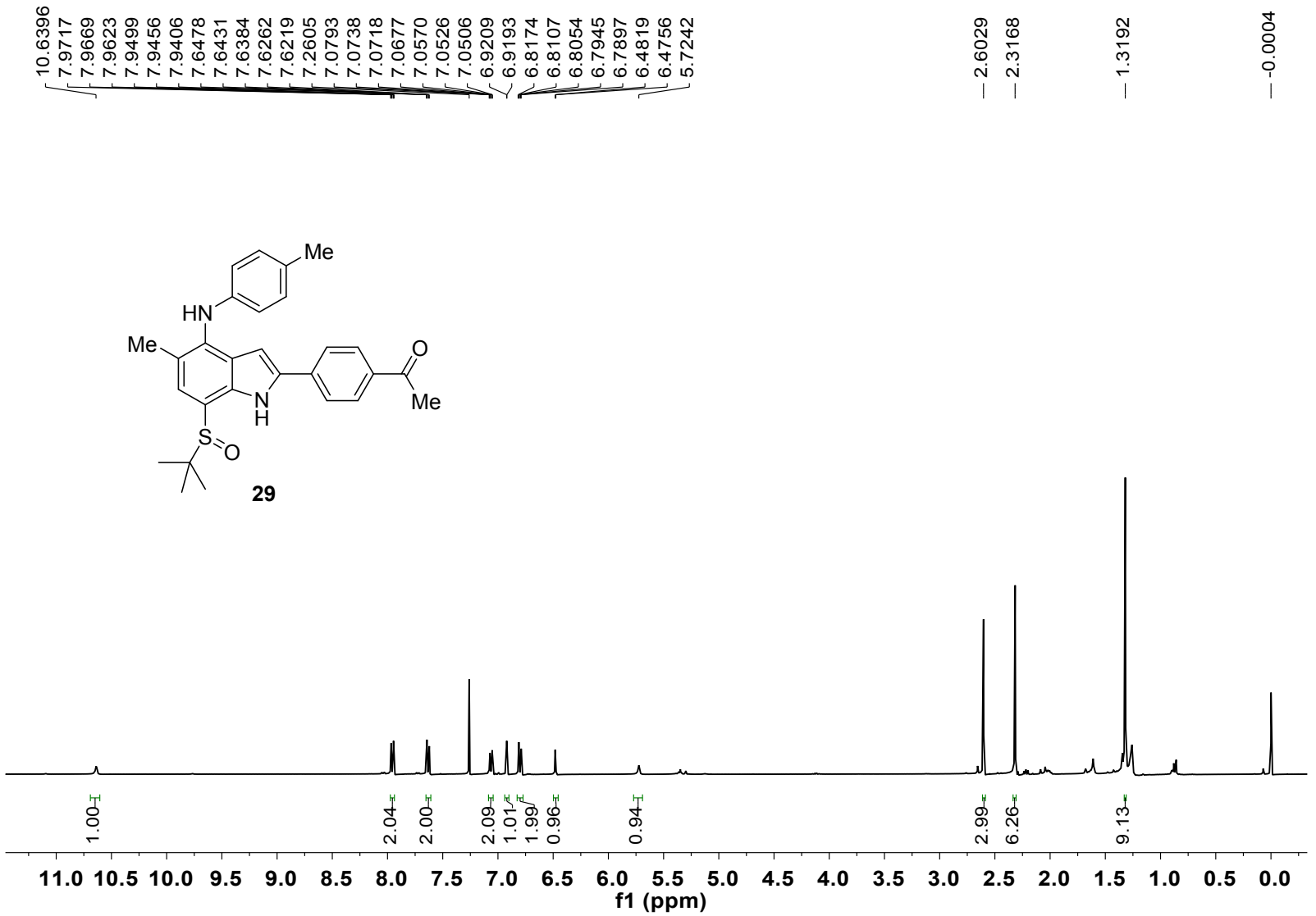
S
O
28
f1 (ppm)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Me
O
Me
N
H
S
O
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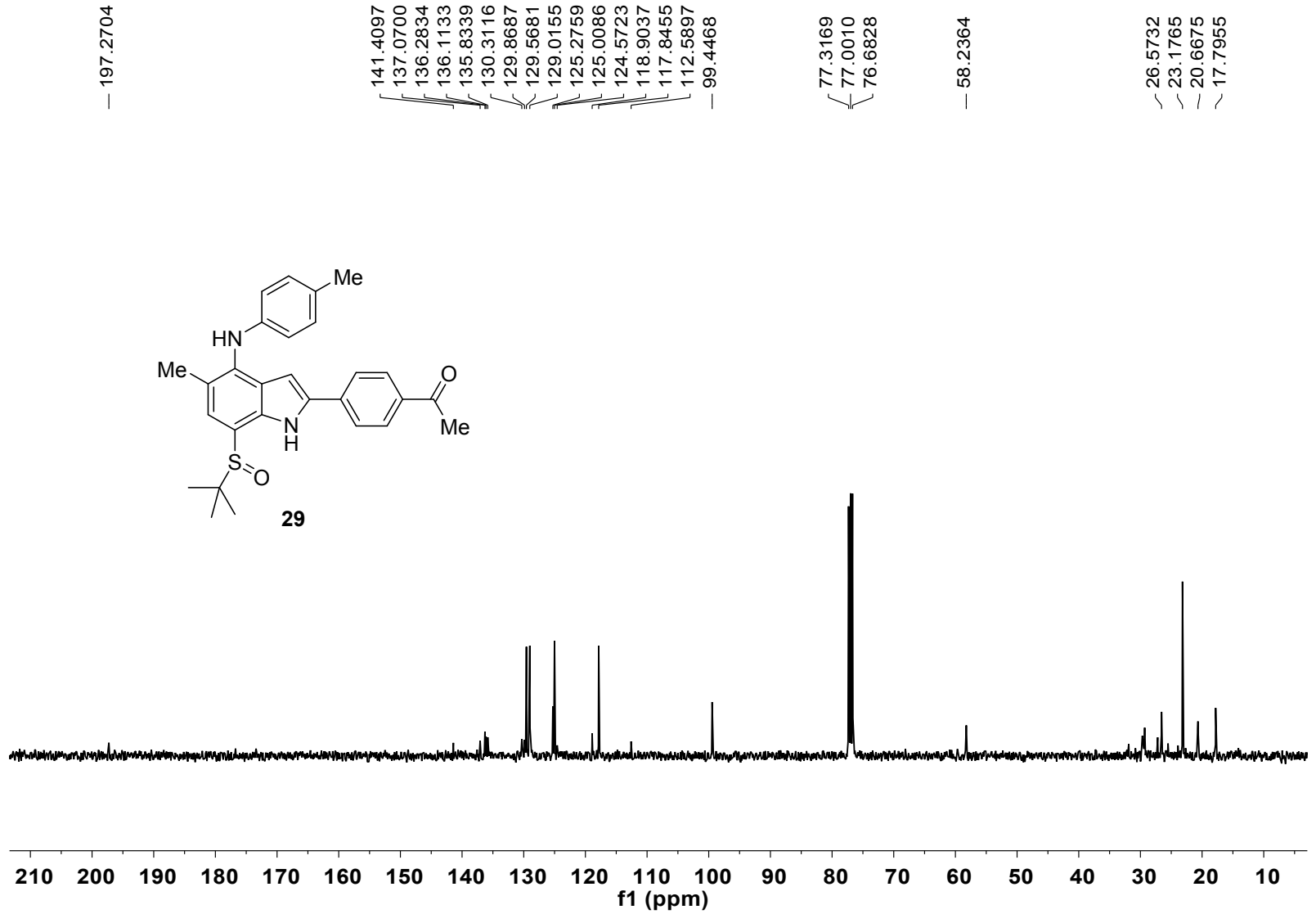
2.04
2.00
2.09
1.01
1.99
0.96
0.94
2.99
6.26
9.13
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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58.2364
26.5732
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20.6675
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Me
N
H
S
O
29
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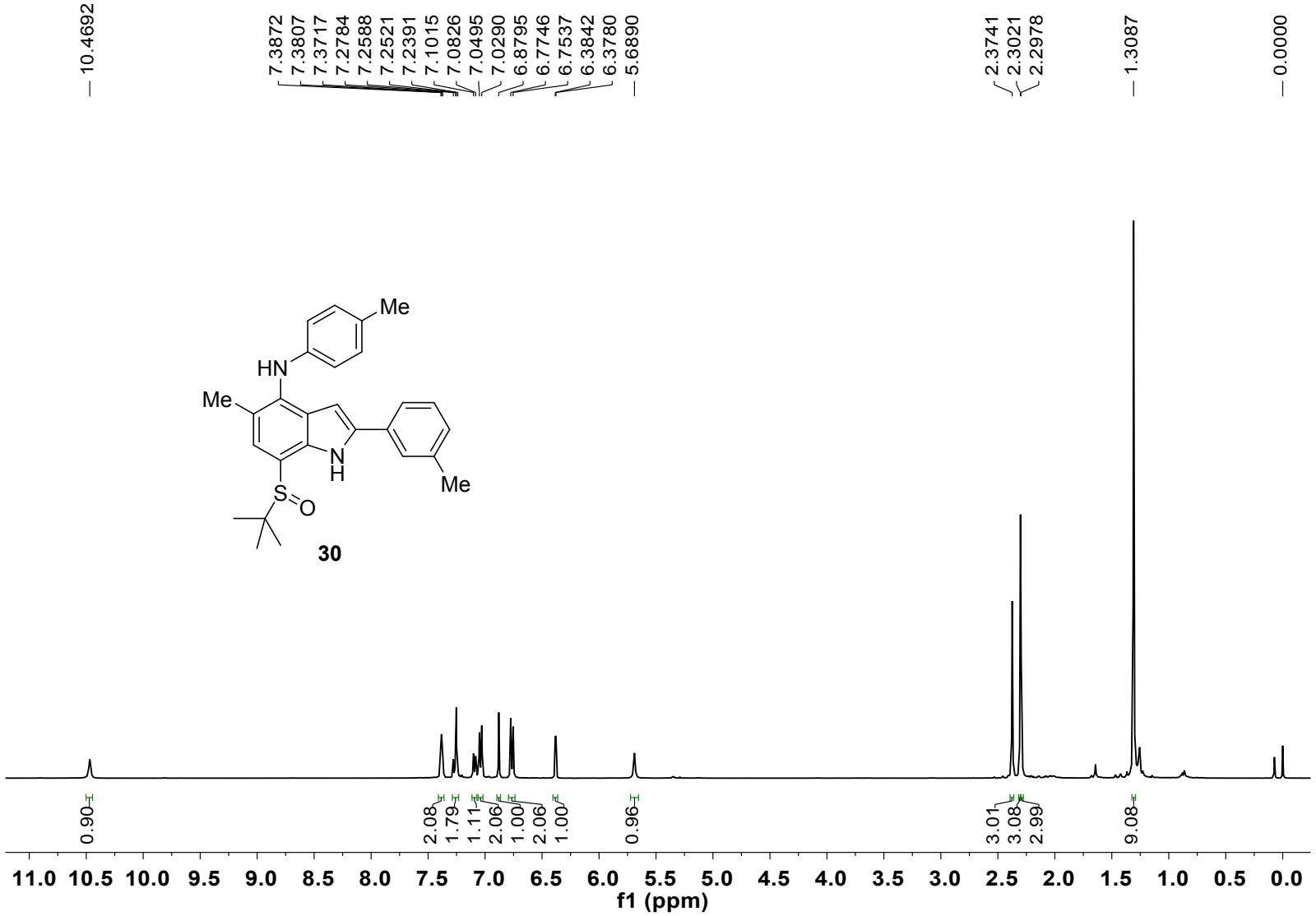
f1 (ppm)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Me
N
H
Me
S
O
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1.79
1.11
2.06
1.00
2.06
1.00
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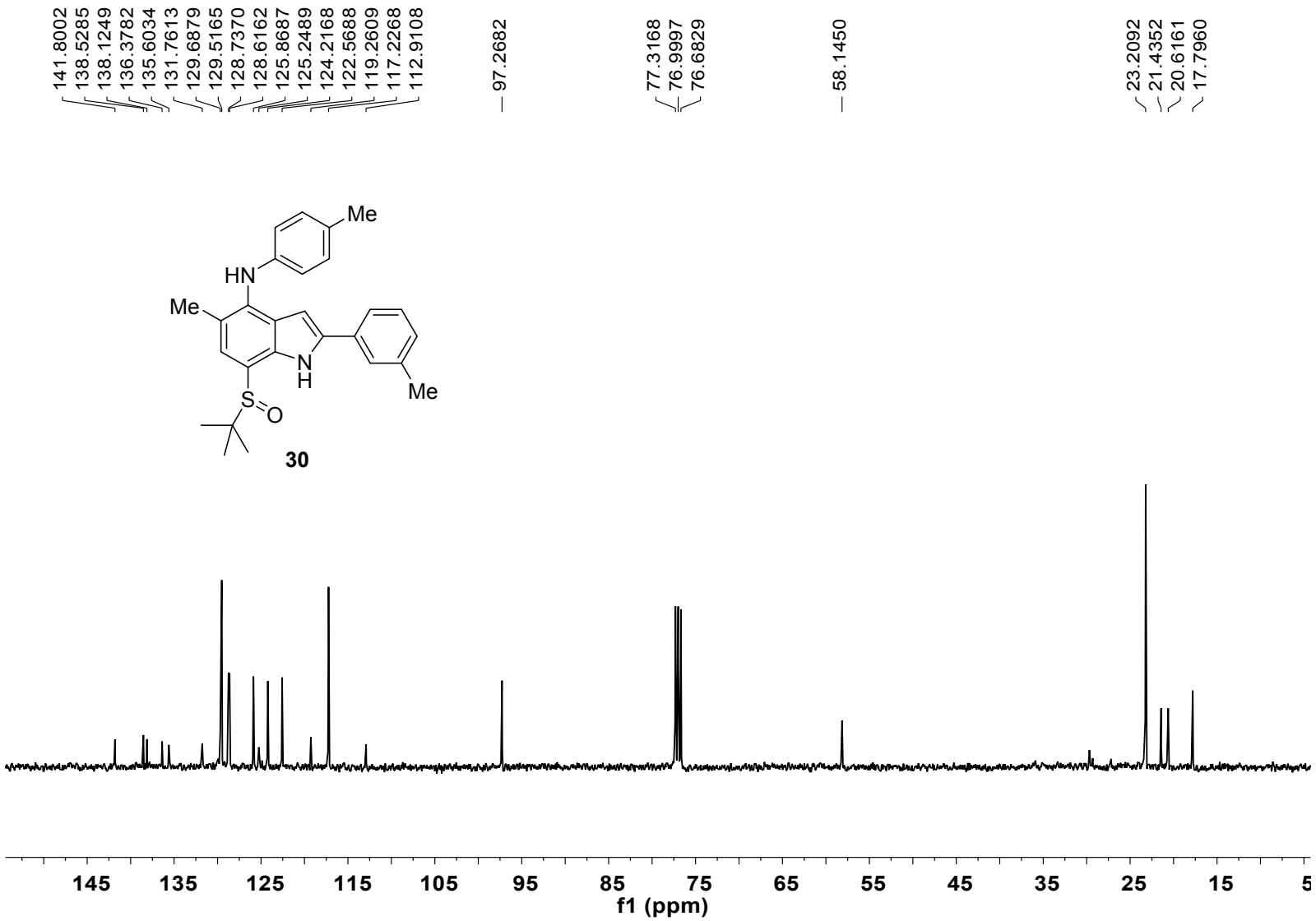
3.01
3.08
2.99
9.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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Me
HN
Me
N
H
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S
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125
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105
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65
55
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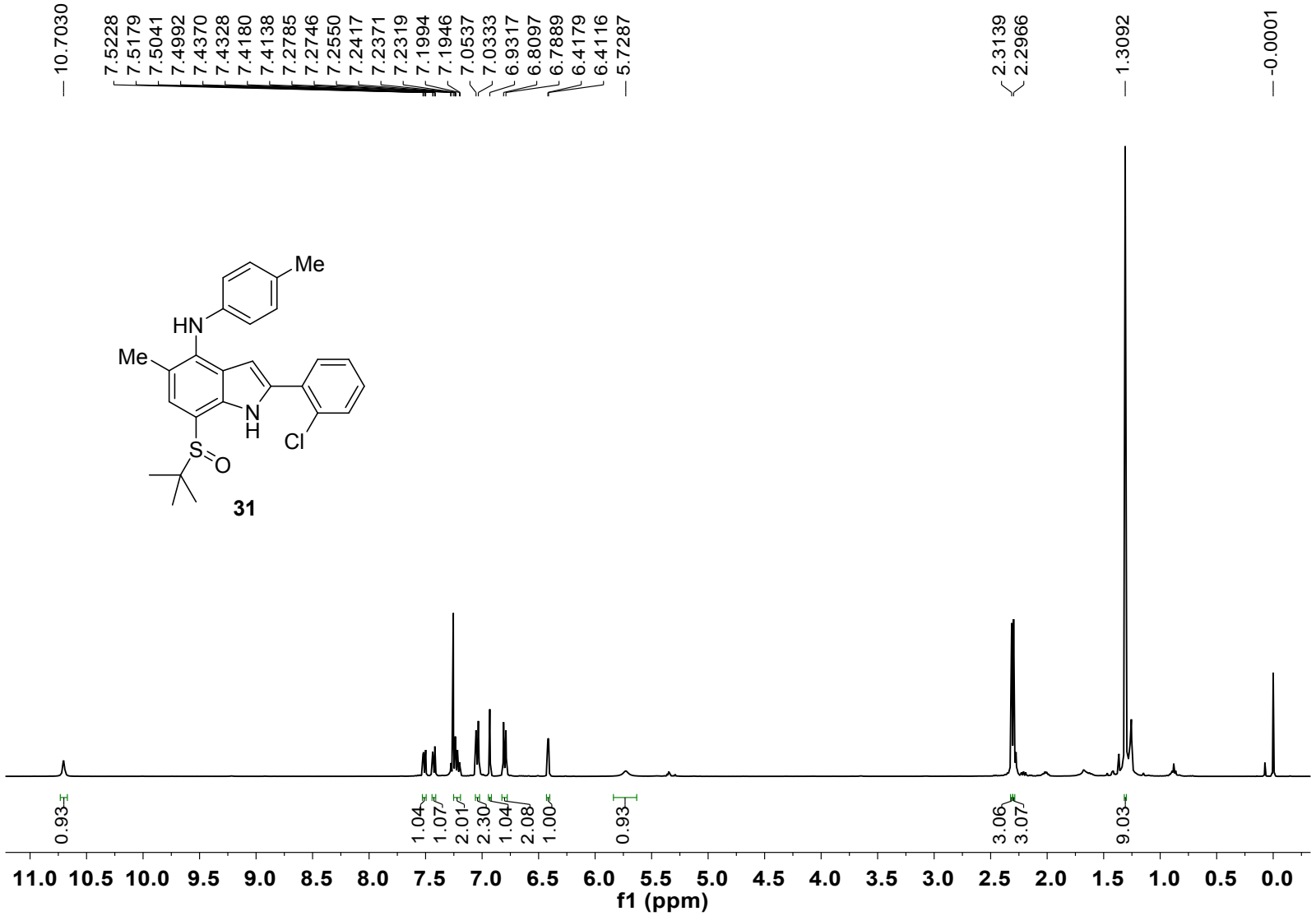
25
15
f1 (ppm)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7.1994
7.1946
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6.4179
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-0.0001
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Me
N
H
Cl
S
O
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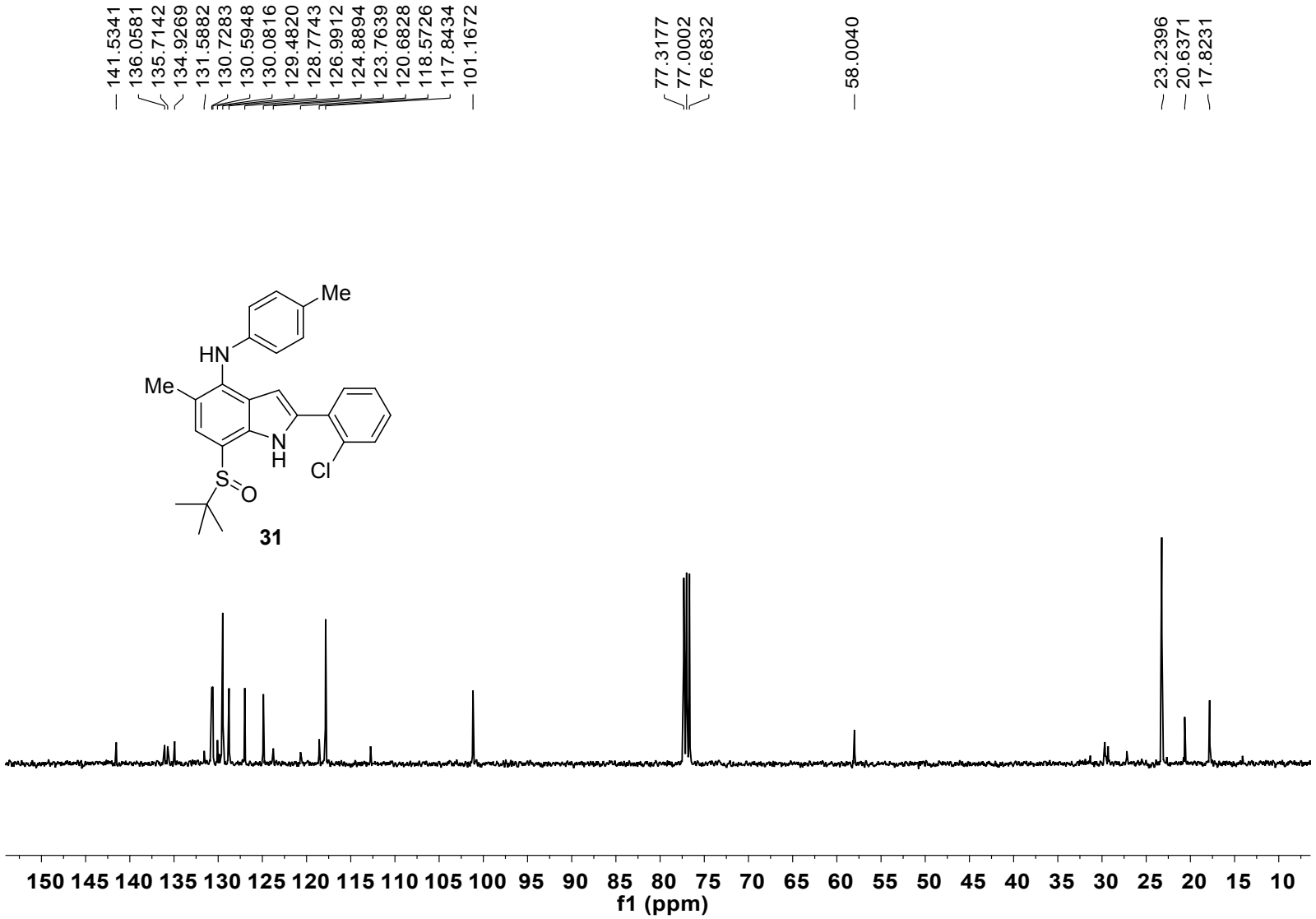
1.07
2.01
2.30
1.04
2.08
1.00
0.93
3.06
3.07
9.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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101.1672
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76.6832
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23.2396
20.6371
17.8231
Me
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Cl
S
O
31
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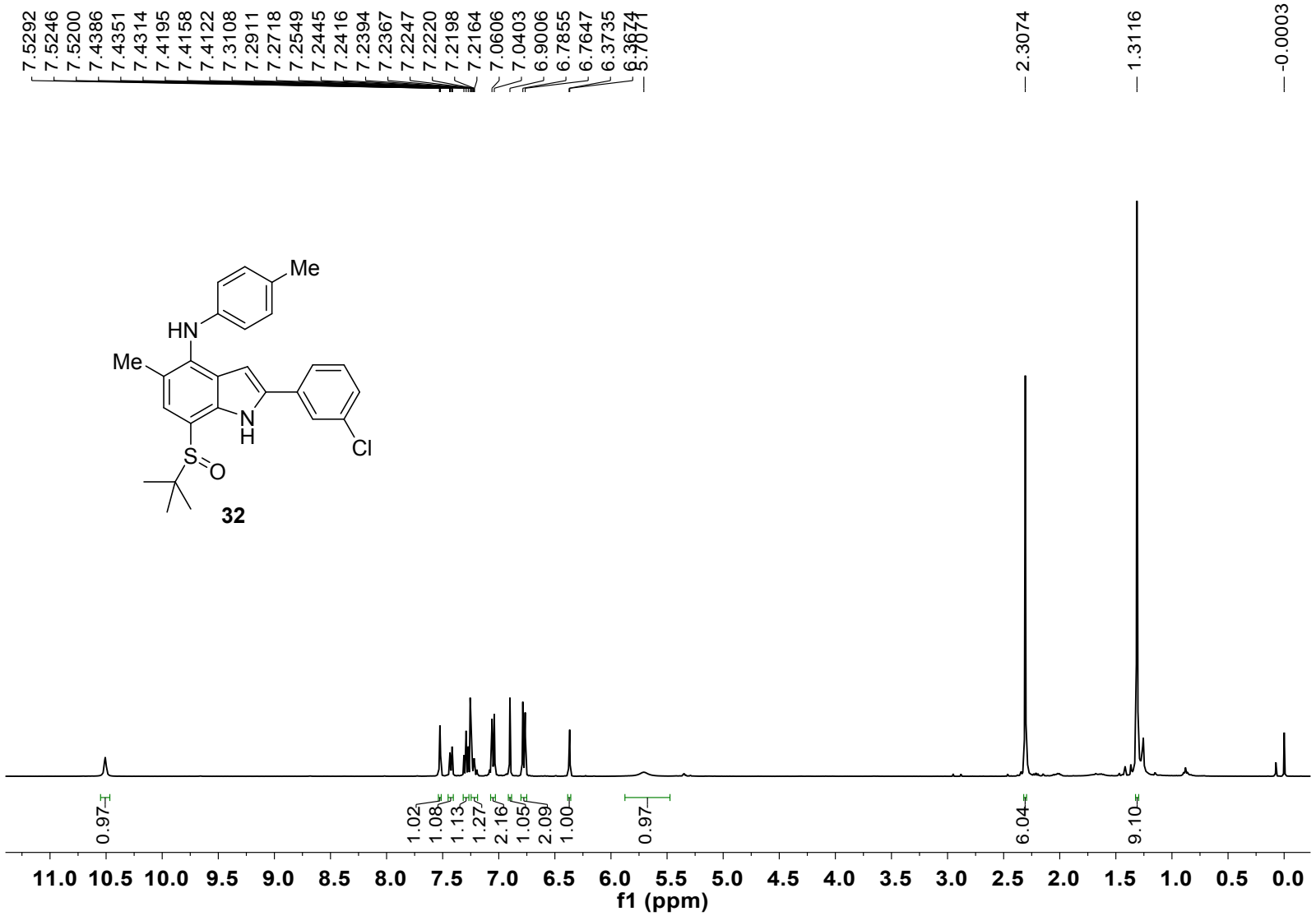
f1 (ppm)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7.2445
7.2416
7.2394
7.2367
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7.2220
7.2198
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6.7647
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HN
Me
N
H
Cl
S
O
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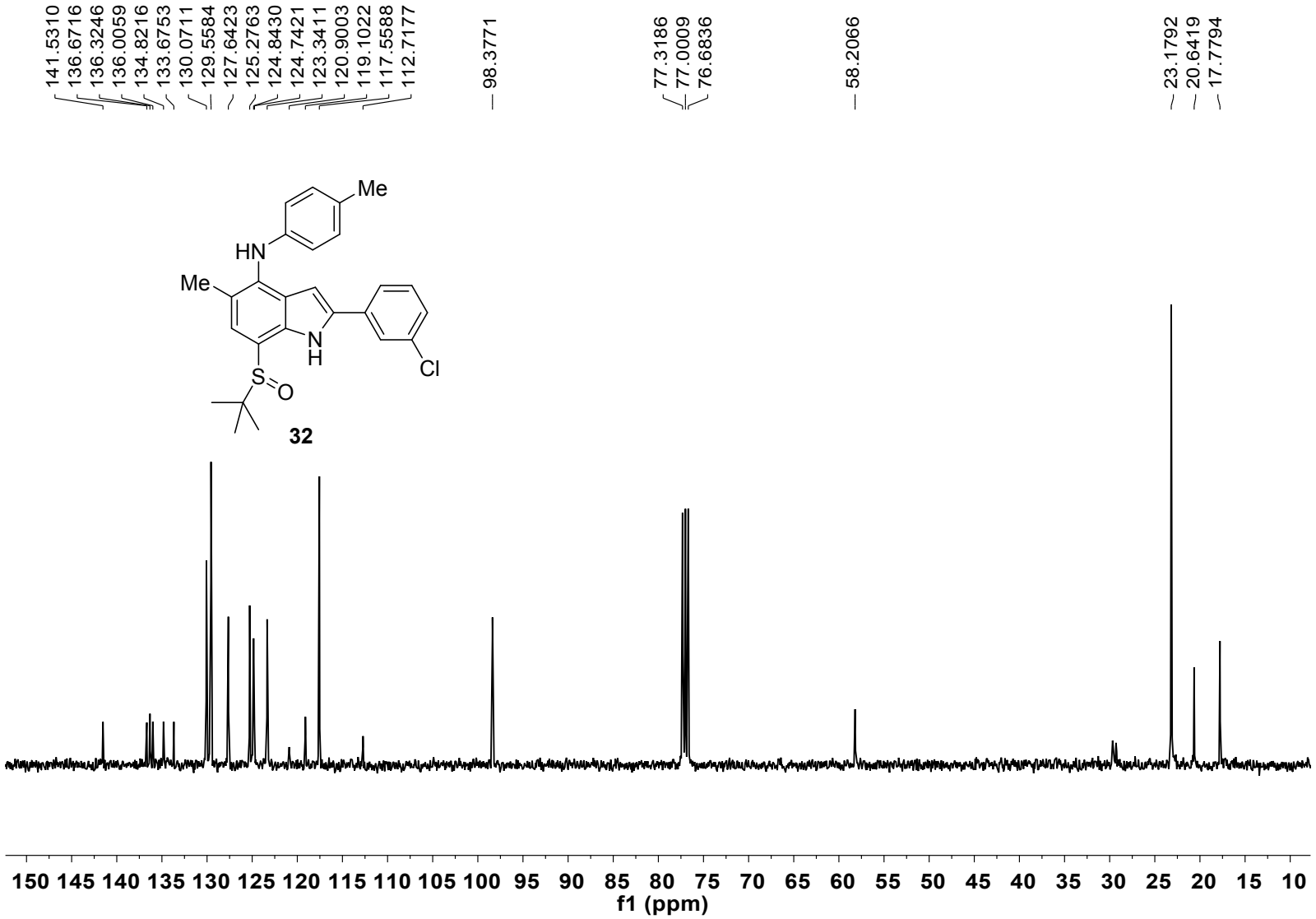
1.02
1.08
1.13
1.27
2.16
1.05
2.09
1.00
0.97
6.04
9.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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120.9003
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112.7177
98.3771
77.3186
77.0009
76.6836
58.2066
23.1792
20.6419
17.7794
Me
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Me
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S
O
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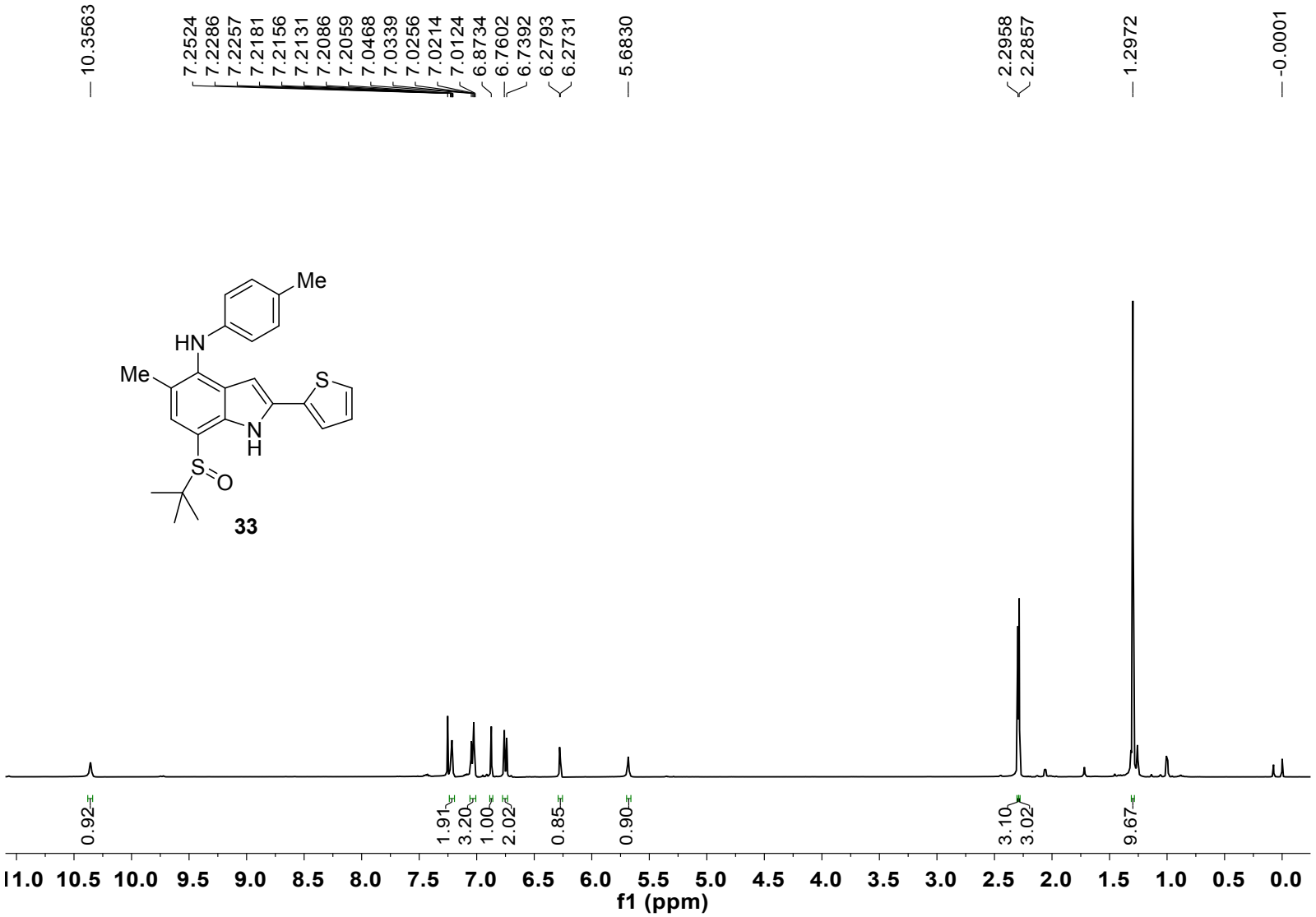
f1 (ppm)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7.0256
7.0214
7.0124
6.8734
6.7602
6.7392
6.2793
6.2731
5.6830
2.2958
2.2857
1.2972
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HN
Me
S
N
H
S
O
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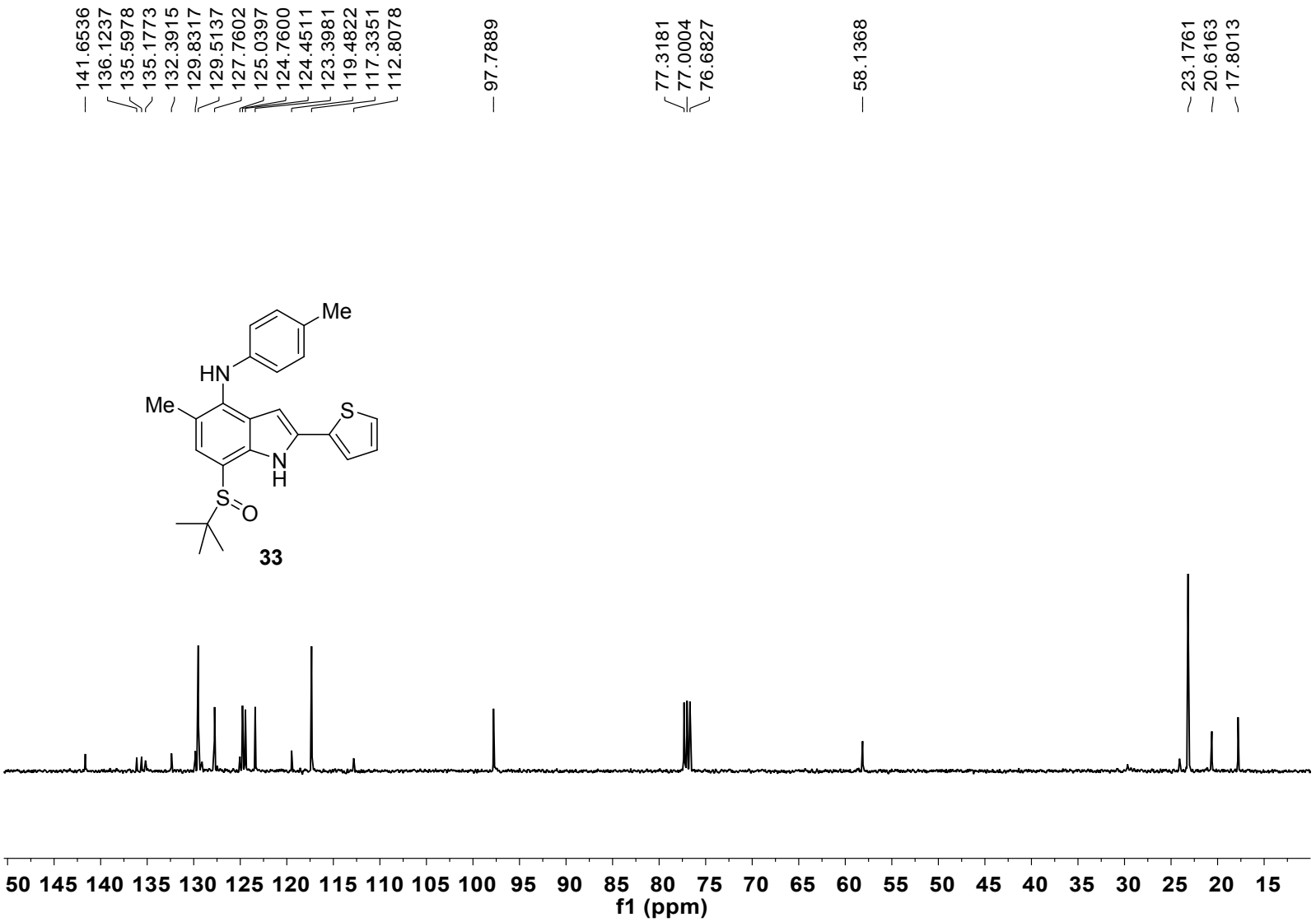
0.92
1.91
3.20
1.00
2.02
0.85
0.90
3.10
3.02
9.67
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.3981
119.4822
117.3351
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97.7889
77.3181
77.0004
76.6827
58.1368
23.1761
20.6163
17.8013
Me
HN
Me
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N
H
S
O
33
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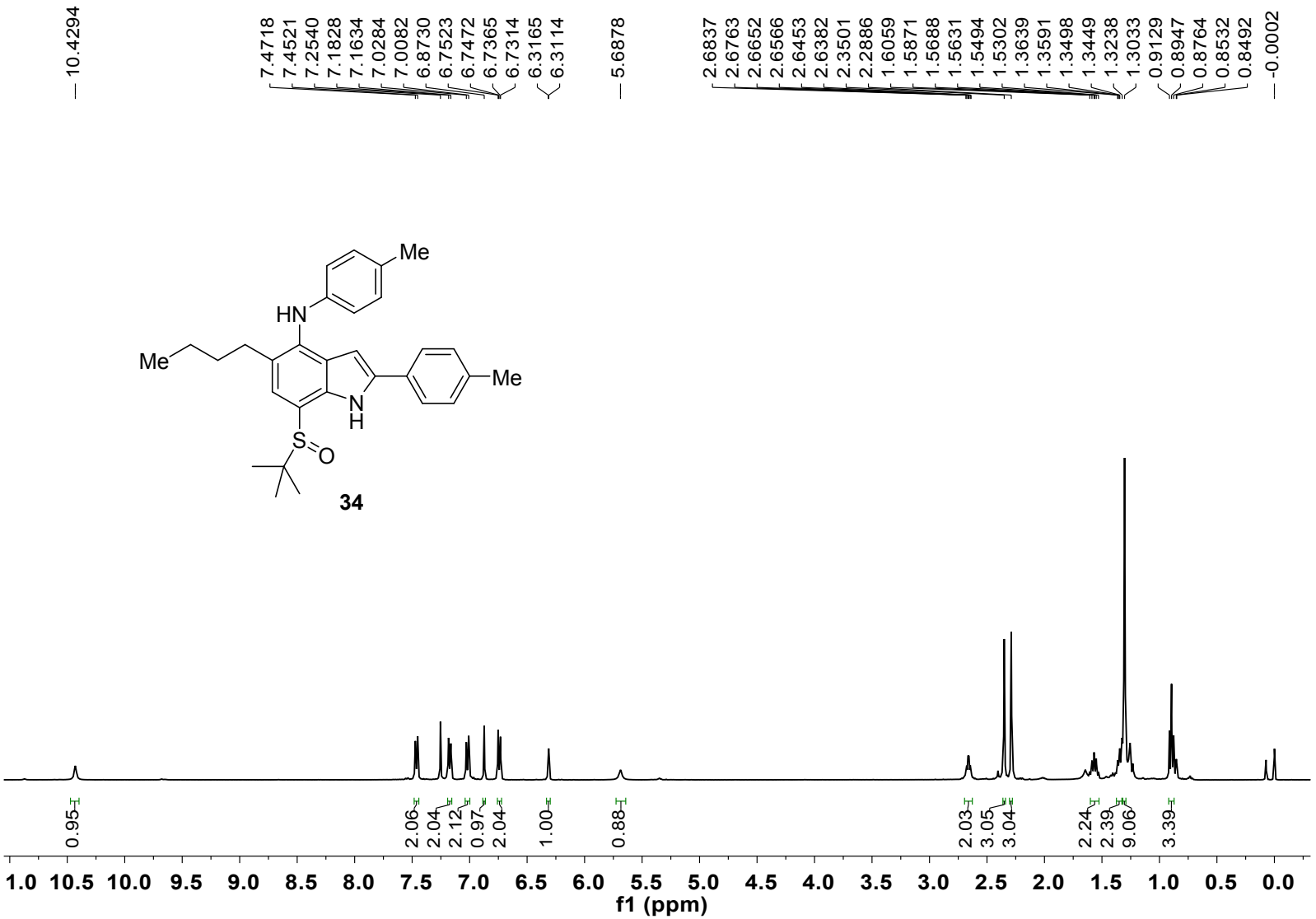
f1 (ppm)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6.3165
6.3114
5.6878
2.6837
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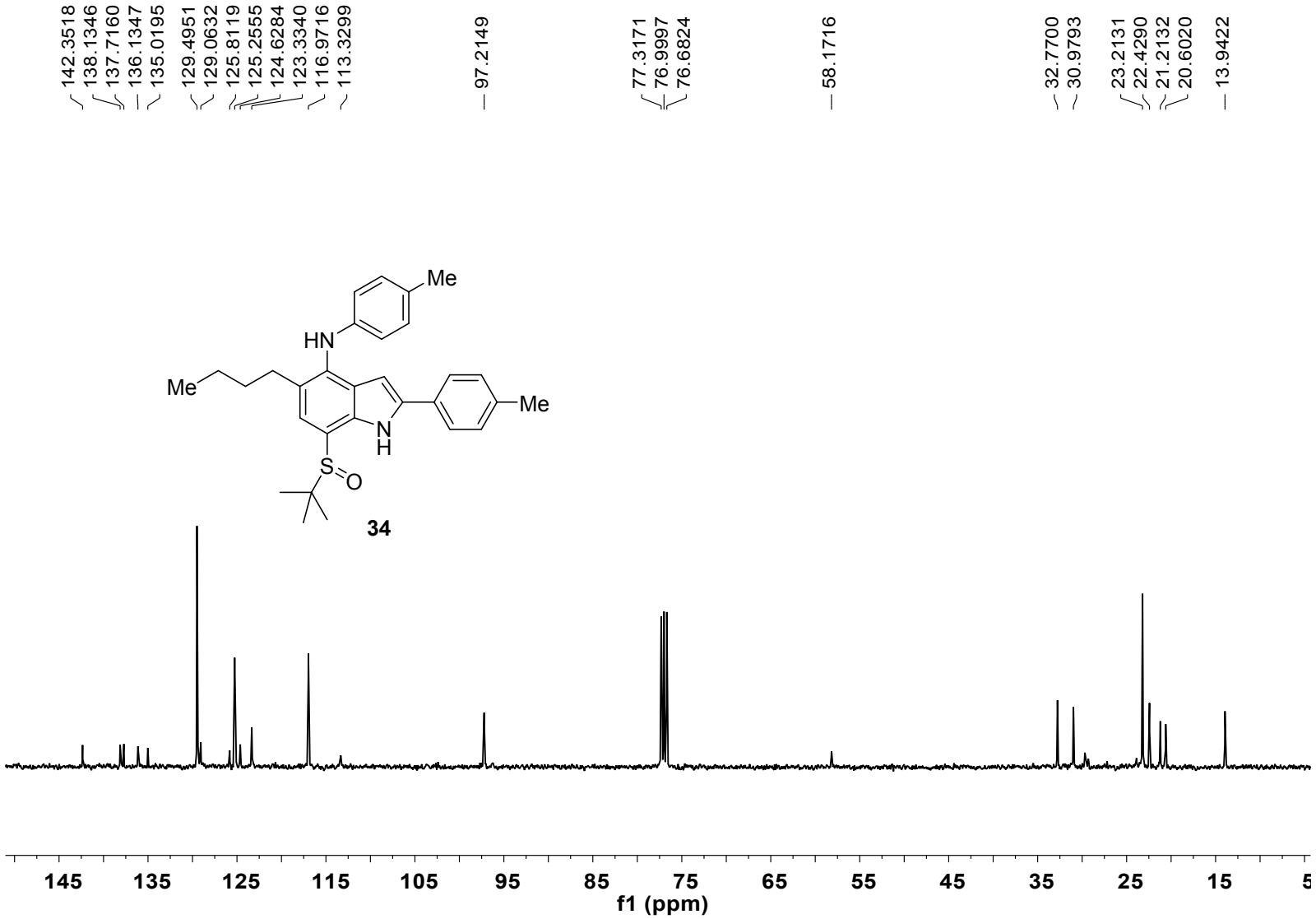
2.6566
2.6453
2.6382
2.3501
2.2886
1.6059
1.5871
1.5688
1.5631
1.5494
1.5302
1.3639
1.3591
1.3498
1.3449
1.3238
1.3033
0.9129
0.8947
0.8764
0.8532
0.8492
-0.0002
Me
HN
Me
Me
N
H
S
O
34
0.95
2.06
2.04
2.12
0.97
2.04
1.00
0.88
2.03
3.05
3.04
2.24
2.39
9.06
3.39
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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113.3299
97.2149
77.3171
76.9997
76.6824
58.1716
32.7700
30.9793
23.2131
22.4290
21.2132
20.6020
13.9422
Me
HN
Me
Me
N
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105
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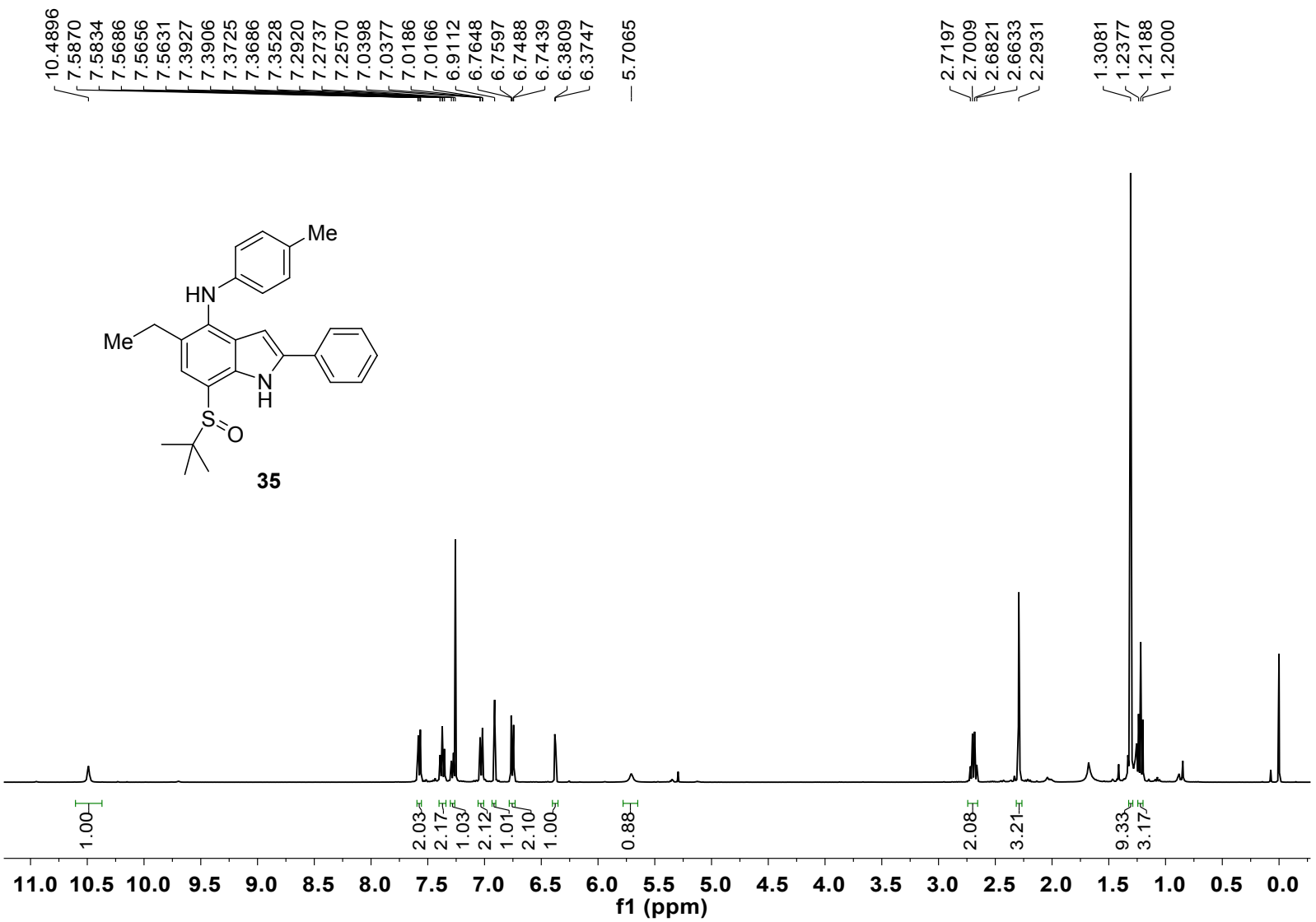
f1 (ppm)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7.2920
7.2737
7.2570
7.0398
7.0377
7.0186
7.0166
6.9112
6.7648
6.7597
6.7488
6.7439
6.3809
6.3747
5.7065
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2.7009
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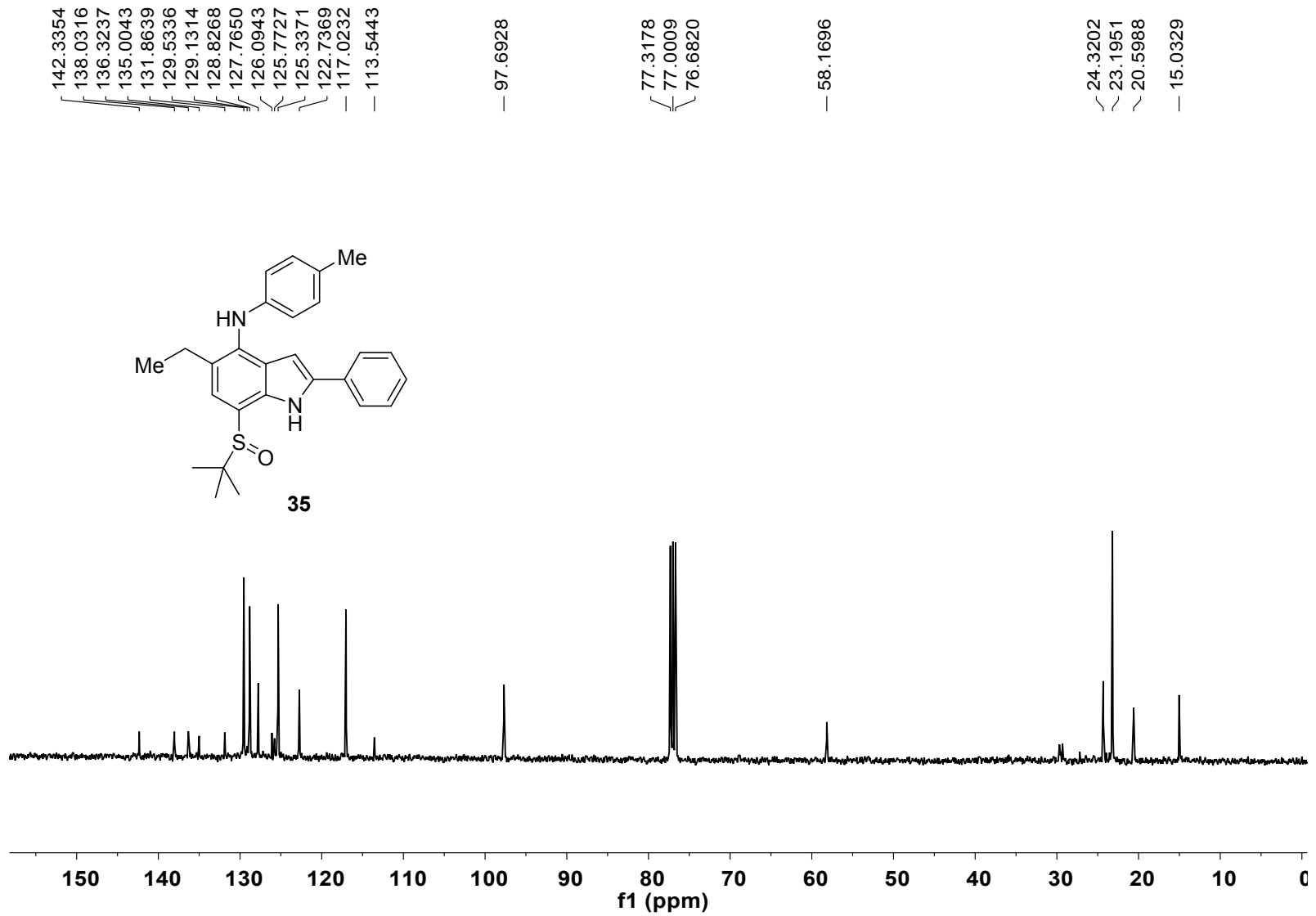
2.6633
2.2931
1.3081
1.2377
1.2188
1.2000
Me
HN
Me
N
H
S
O
35
1.00
2.03
2.17
1.03
2.12
1.01
2.10
1.00
0.88
2.08
3.21
9.33
3.17
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.3371
122.7369
117.0232
113.5443
97.6928
77.3178
77.0009
76.6820
58.1696
24.3202
23.1951
20.5988
15.0329
Me
HN
Me
N
H
S
O
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130
120
110
100
90
80
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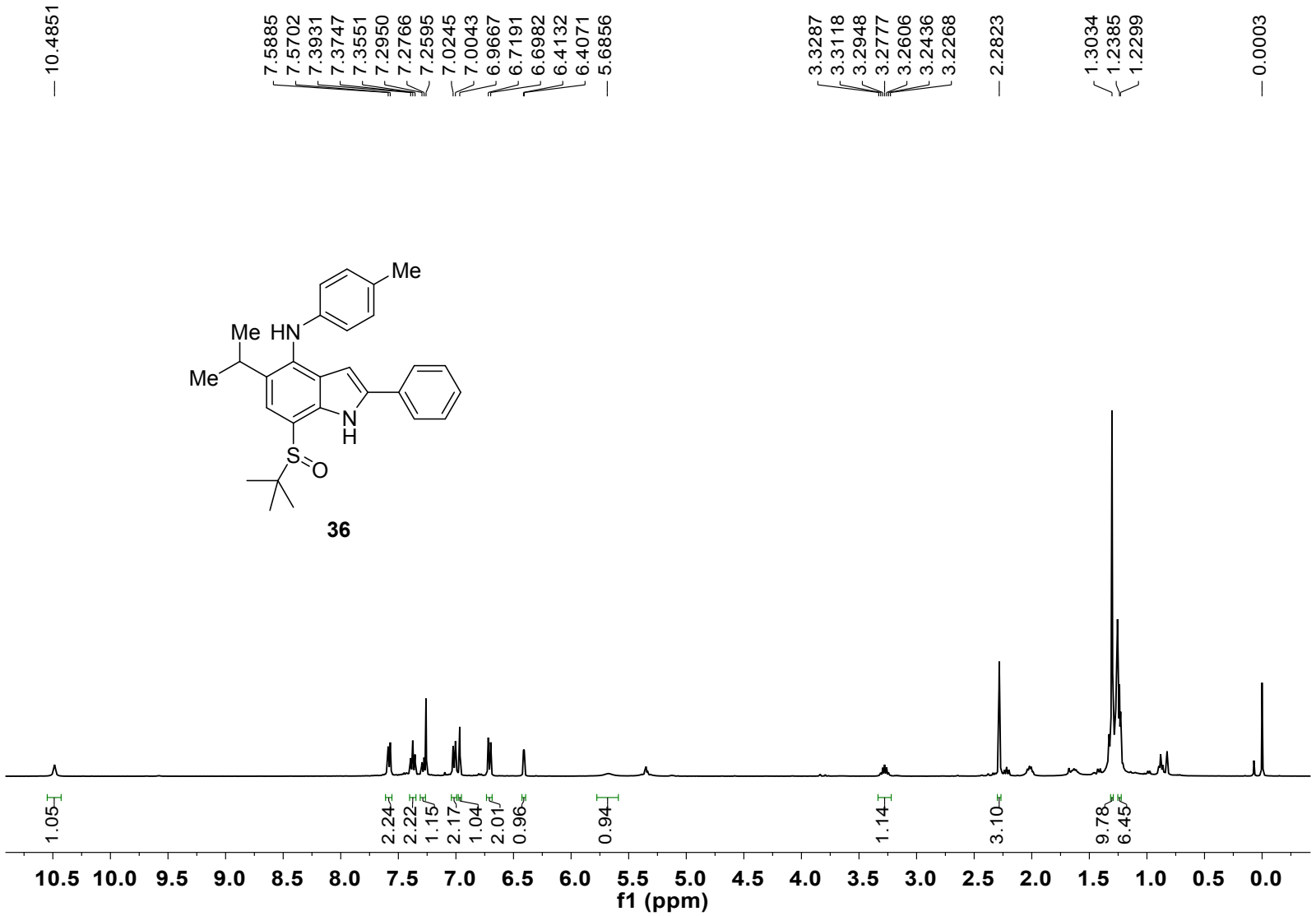
50
40
30
20
10
0
f1 (ppm)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6.7191
6.6982
6.4132
6.4071
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3.3118
3.2948
3.2777
3.2606
3.2436
3.2268
2.2823
1.3034
1.2385
1.2299
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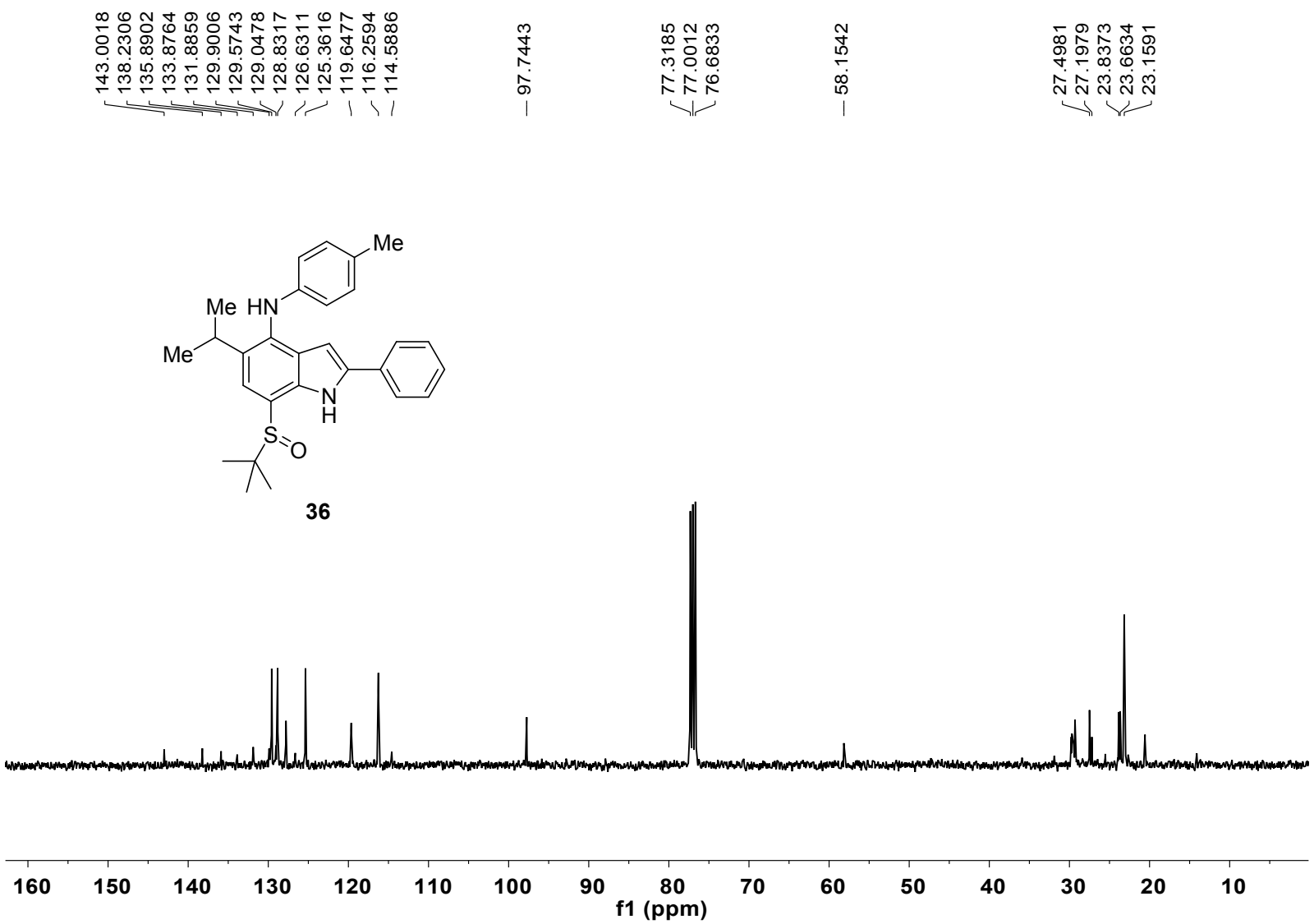
Me HN
Me
N
H
S
O
1.05
2.24
2.22
1.15
2.17
1.04
2.01
0.96
0.94
1.14
3.10
9.78
6.45
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

36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23.1591
Me
Me HN
Me
N
H
S
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120
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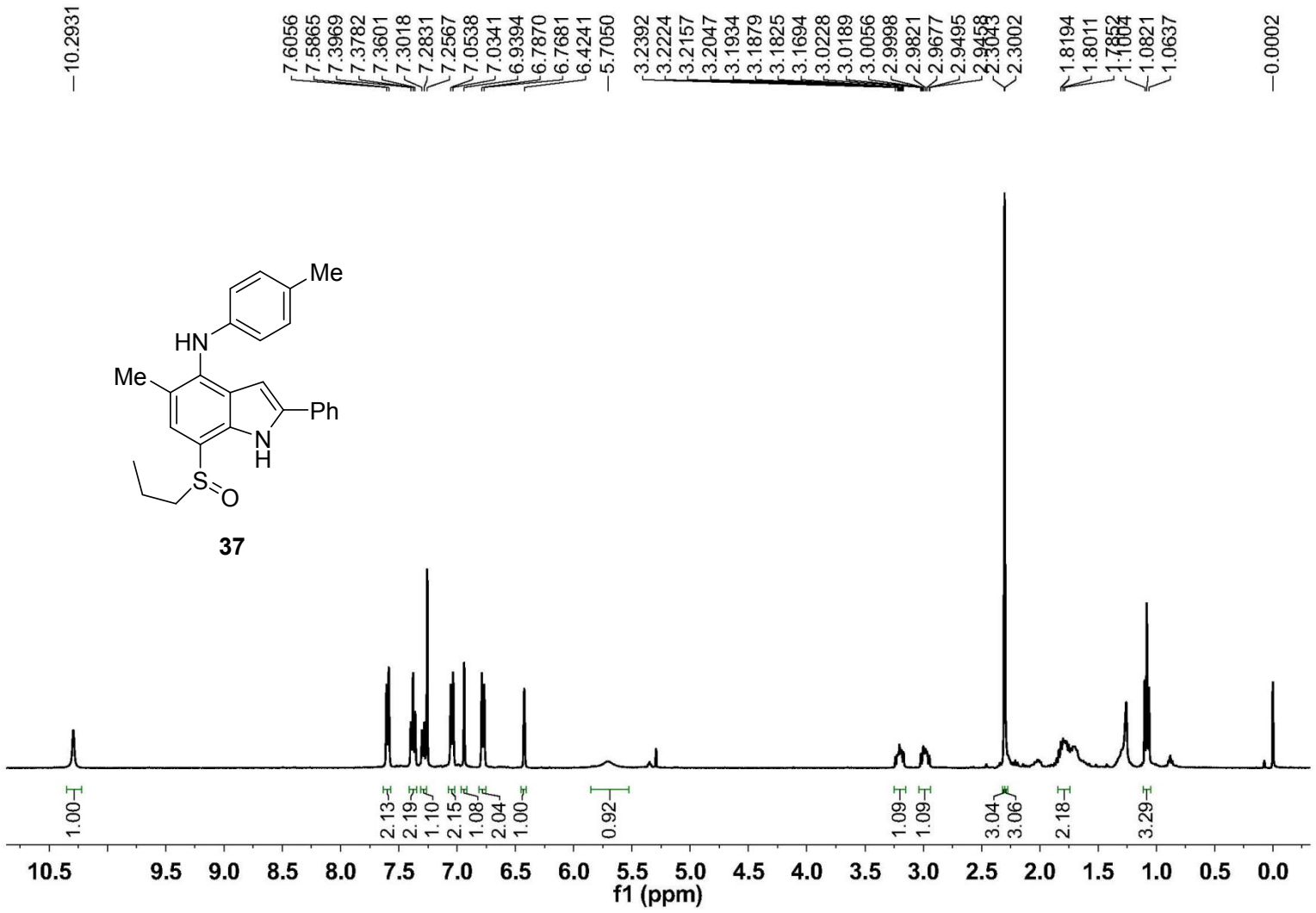
10
f1 (ppm)

36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6.7870
6.7681
6.4241
5.7050
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3.2224
3.2157
3.2047
3.1934
3.1879
3.1825
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3.0228
3.0189
3.0056
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2.9821
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1.8194
1.8011
1.0821
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HN
Me
Ph
N
H
S
O
37
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2.13
2.19
1.10
2.15
1.08
2.04
1.00
0.92
1.09
1.09
3.04
3.06
2.18
3.29
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
1.0
0.5
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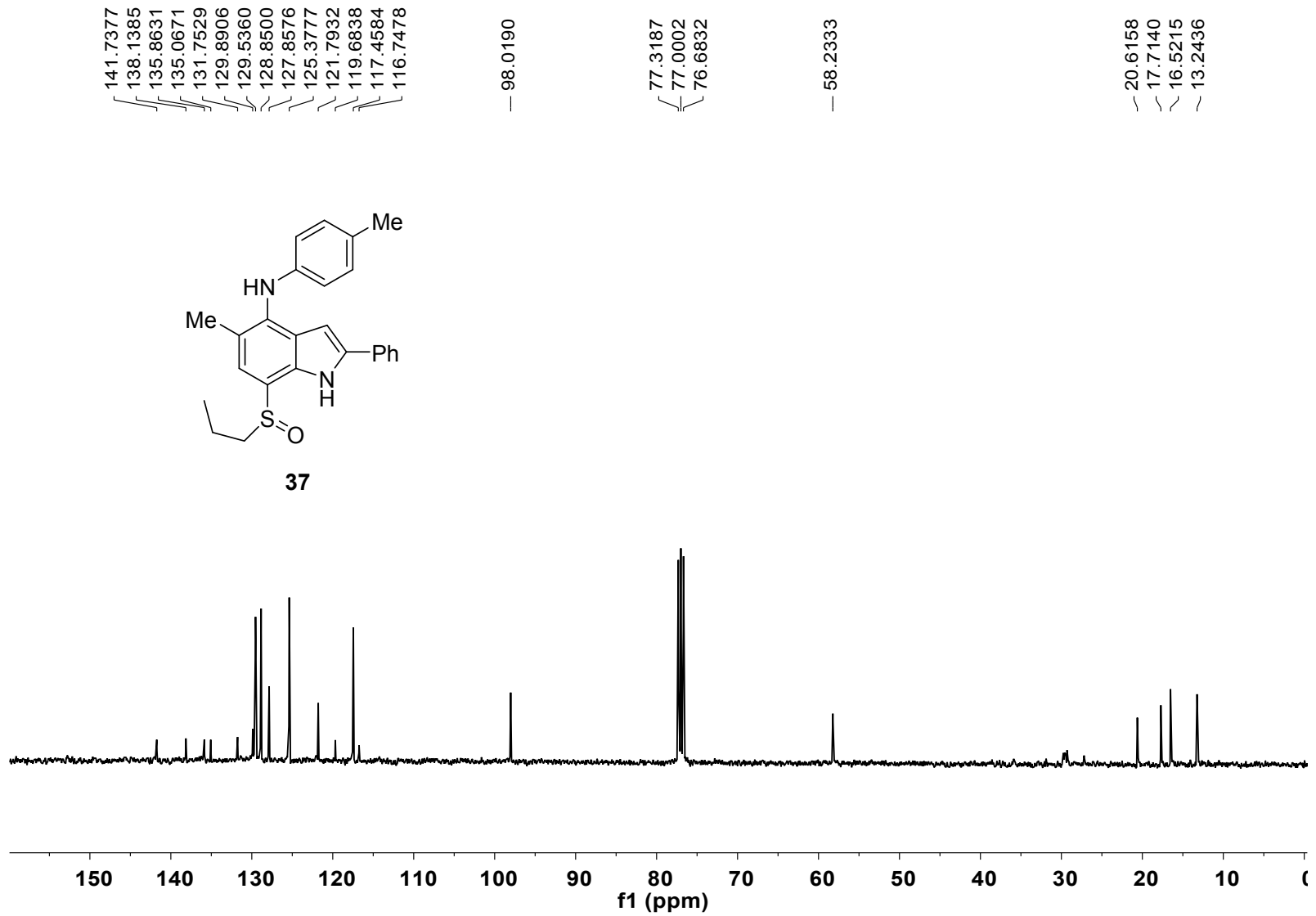
f1 (ppm)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20.6158
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16.5215
13.2436
Me
HN
Me
Ph
N
H
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120
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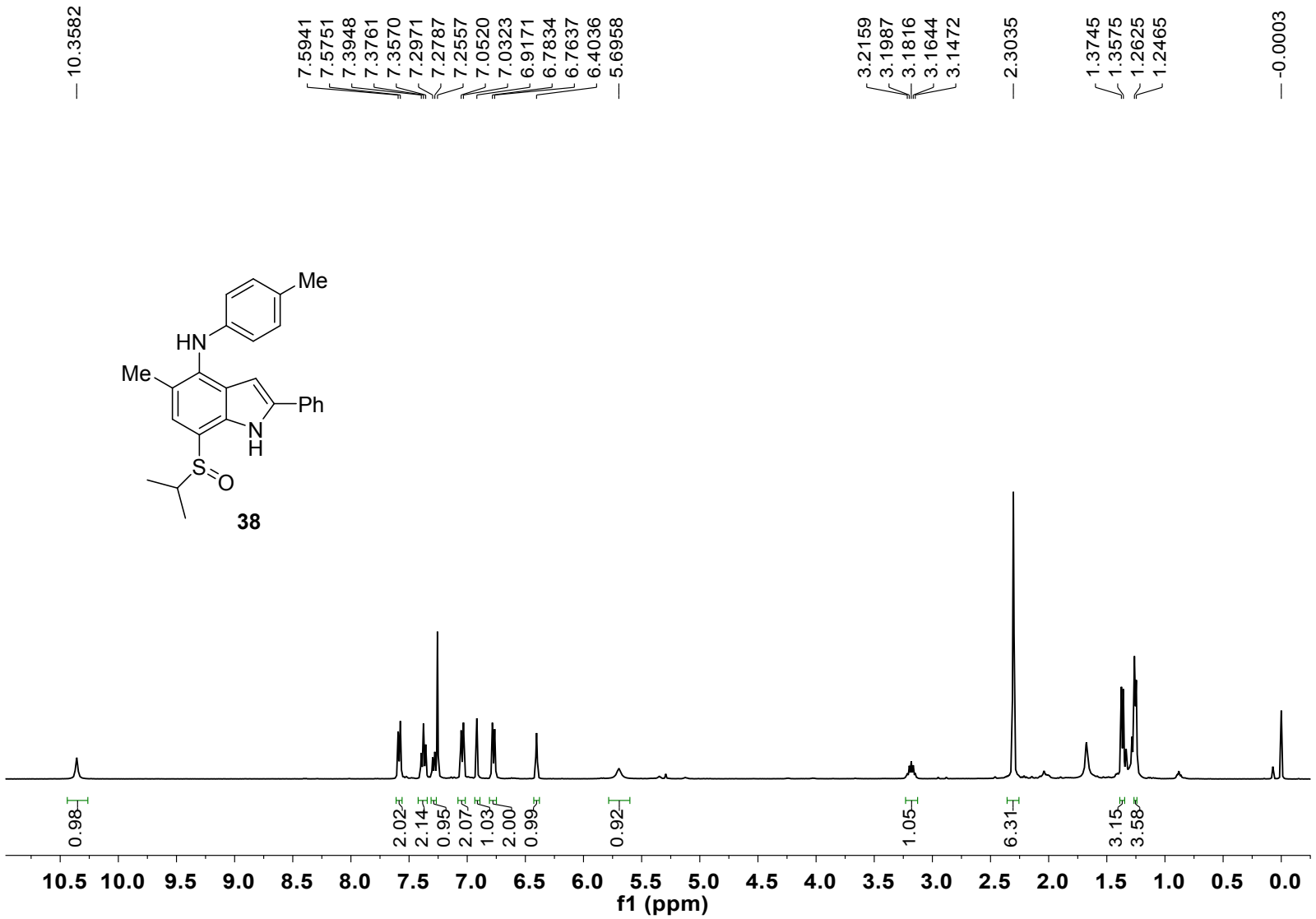
10
f1 (ppm)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6.7637
6.4036
5.6958
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3.1987
3.1816
3.1644
3.1472
2.3035
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1.3575
1.2625
1.2465
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Me
Ph
N
H
S
O
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1.05
6.31
3.15
3.58
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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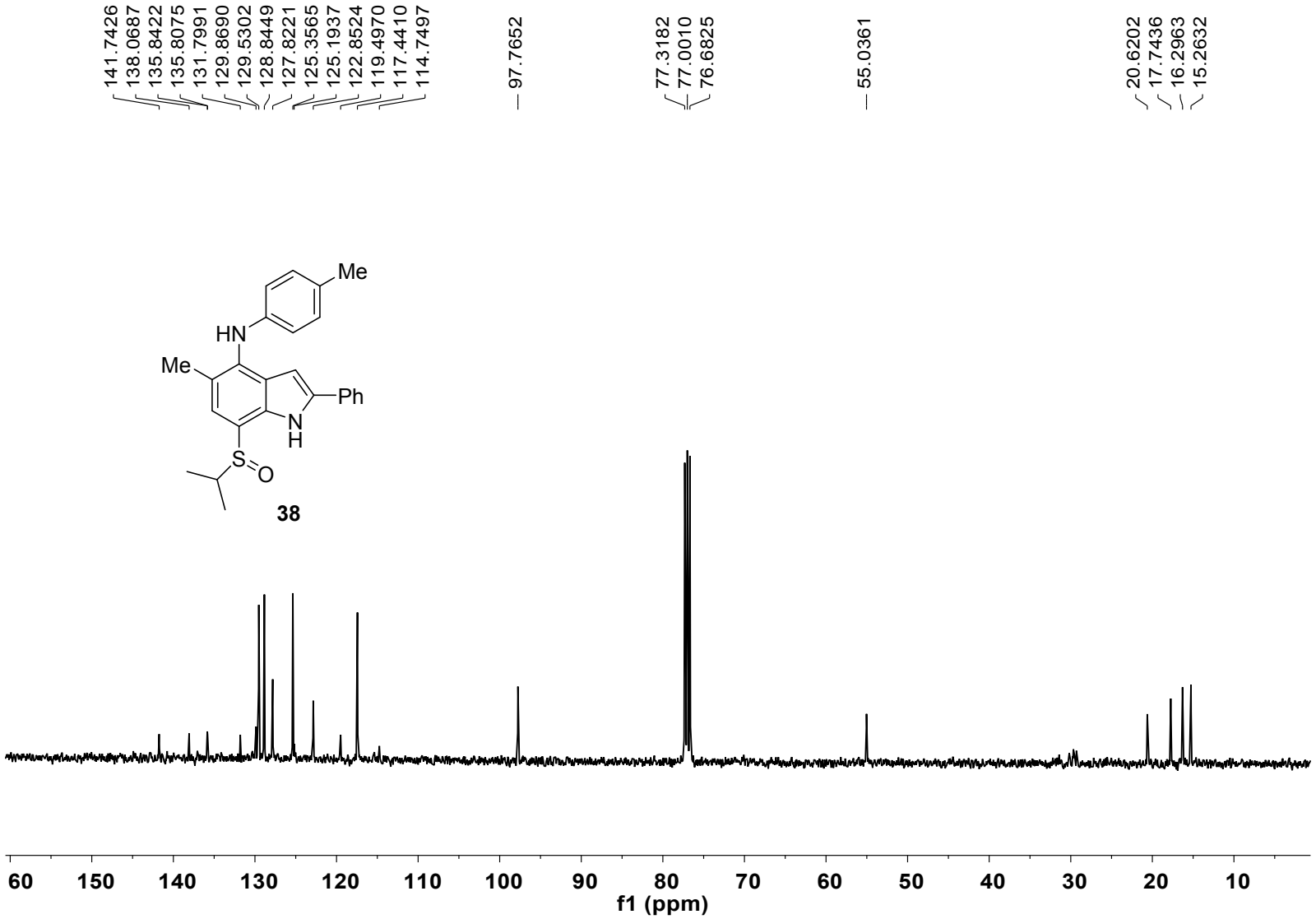
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77.0010
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55.0361
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16.2963
15.2632
Me
HN
Me
Ph
N
H
S
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120
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100
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80
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60
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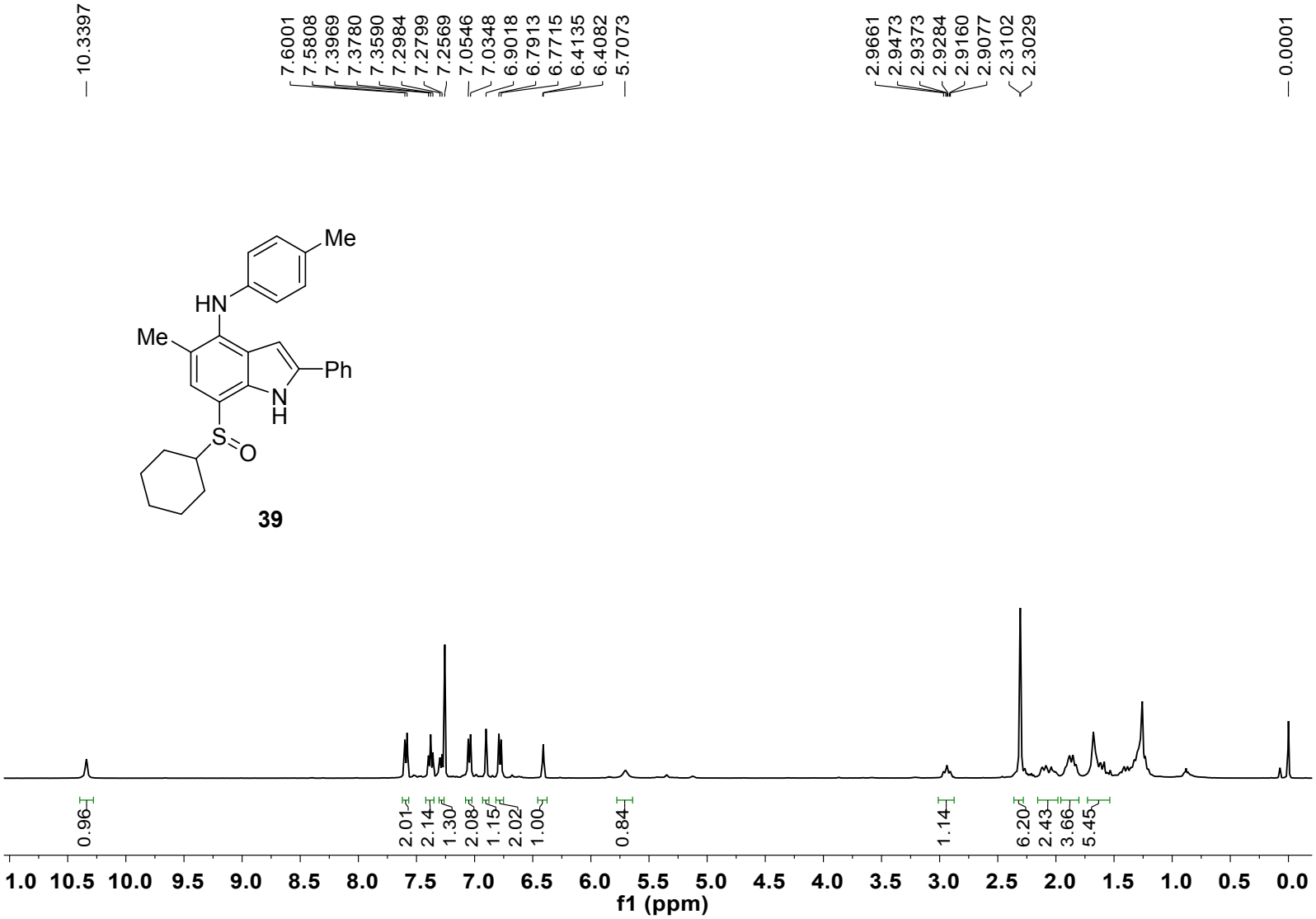
20
10
f1 (ppm)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7.0348
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6.7913
6.7715
6.4135
6.4082
5.7073
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2.9473
2.9373
2.9284
2.9160
2.9077
2.3102
2.3029
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Me
HN
Me
Ph
N
H
S
O
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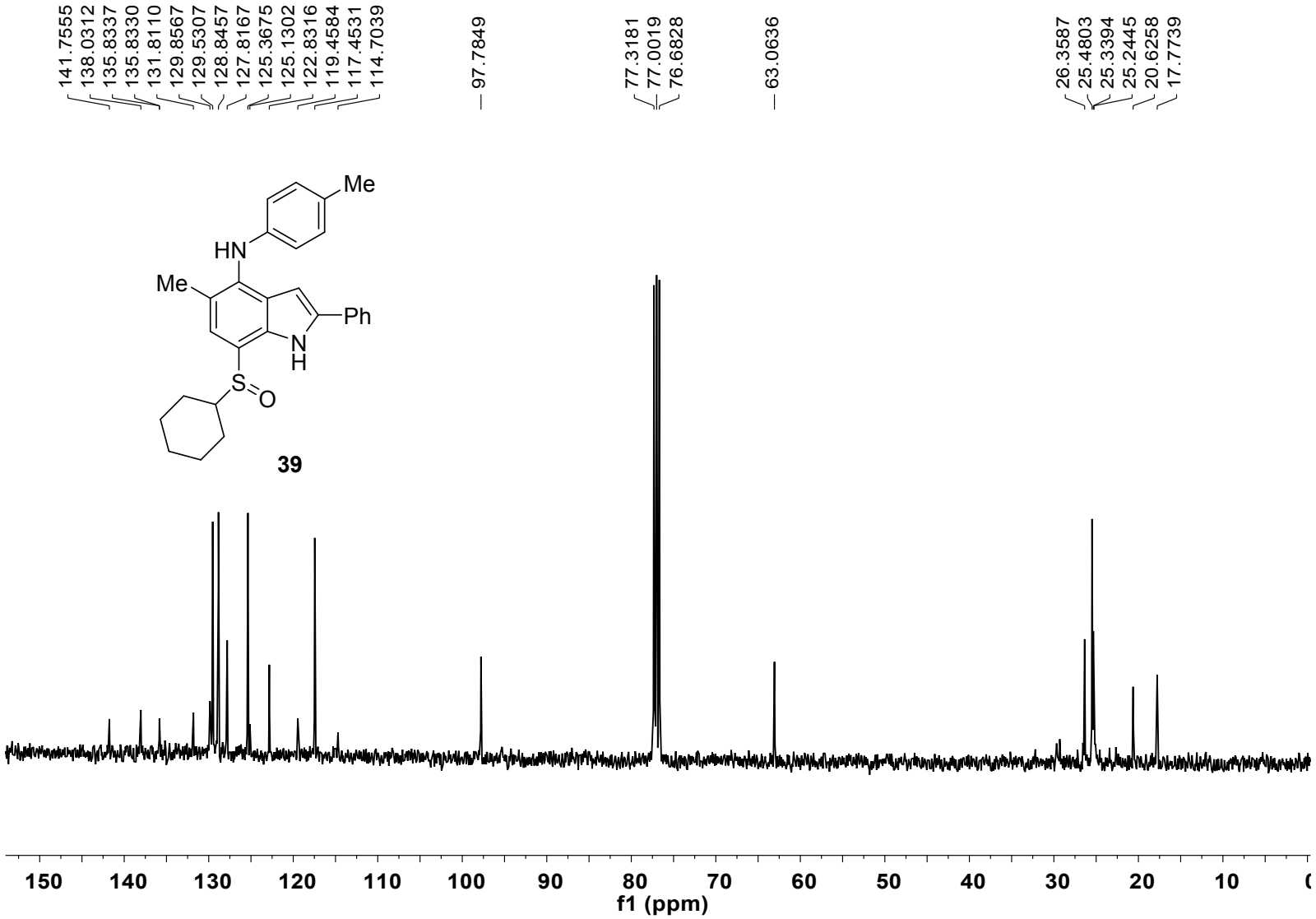
2.14
1.30
2.08
1.15
2.02
1.00
0.84
1.14
6.20
2.43
3.66
5.45
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.8316
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117.4531
114.7039
97.7849
77.3181
77.0019
76.6828
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26.3587
25.4803
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Me
HN
Me
Ph
N
H
S
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140
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100
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80
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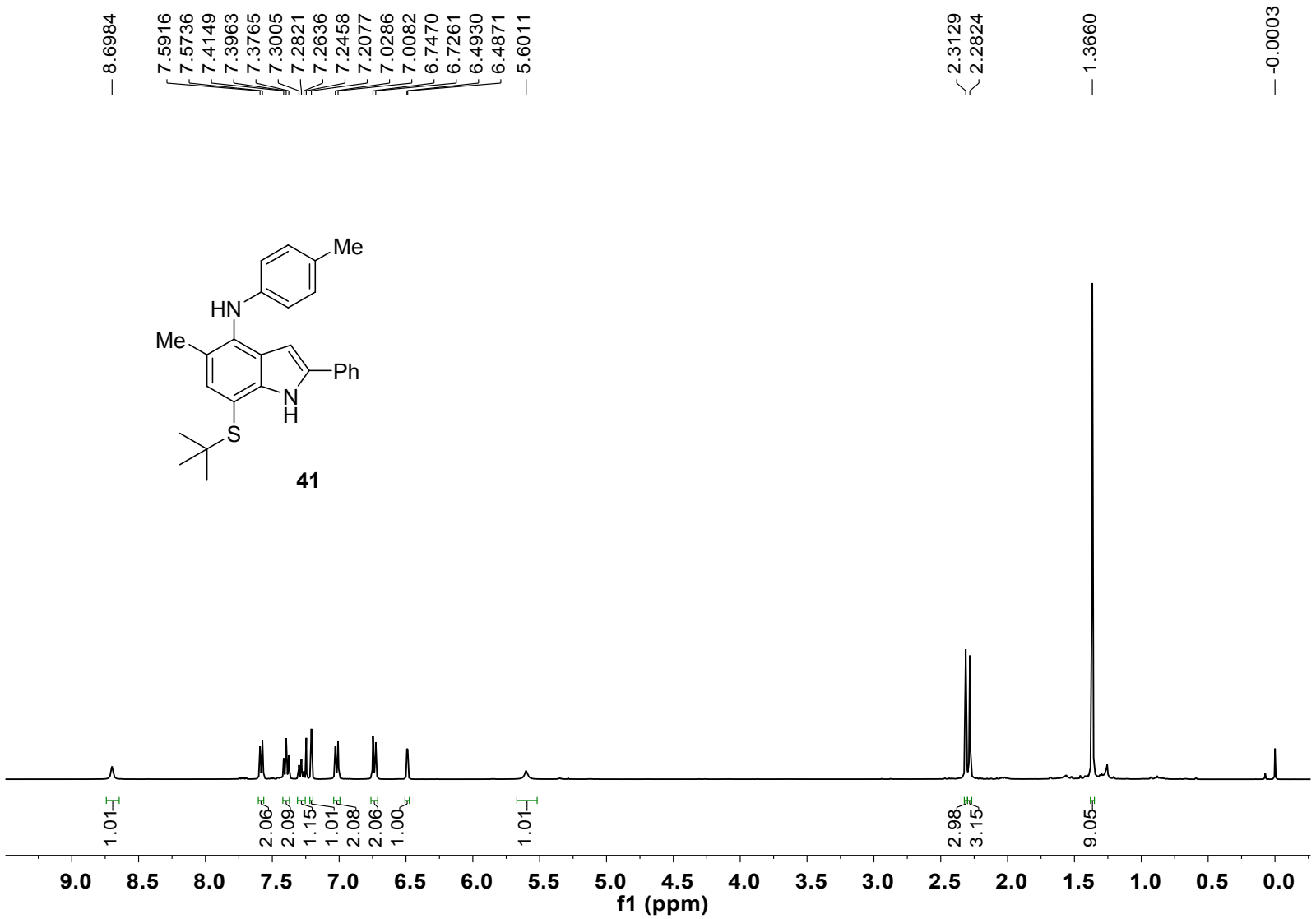
60
50
40
30
20
10
f1 (ppm)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7.0082
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2.3129
2.2824
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HN
Me
Ph
N
H
S
41
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2.06
2.09
1.15
1.01
2.08
2.06
1.00
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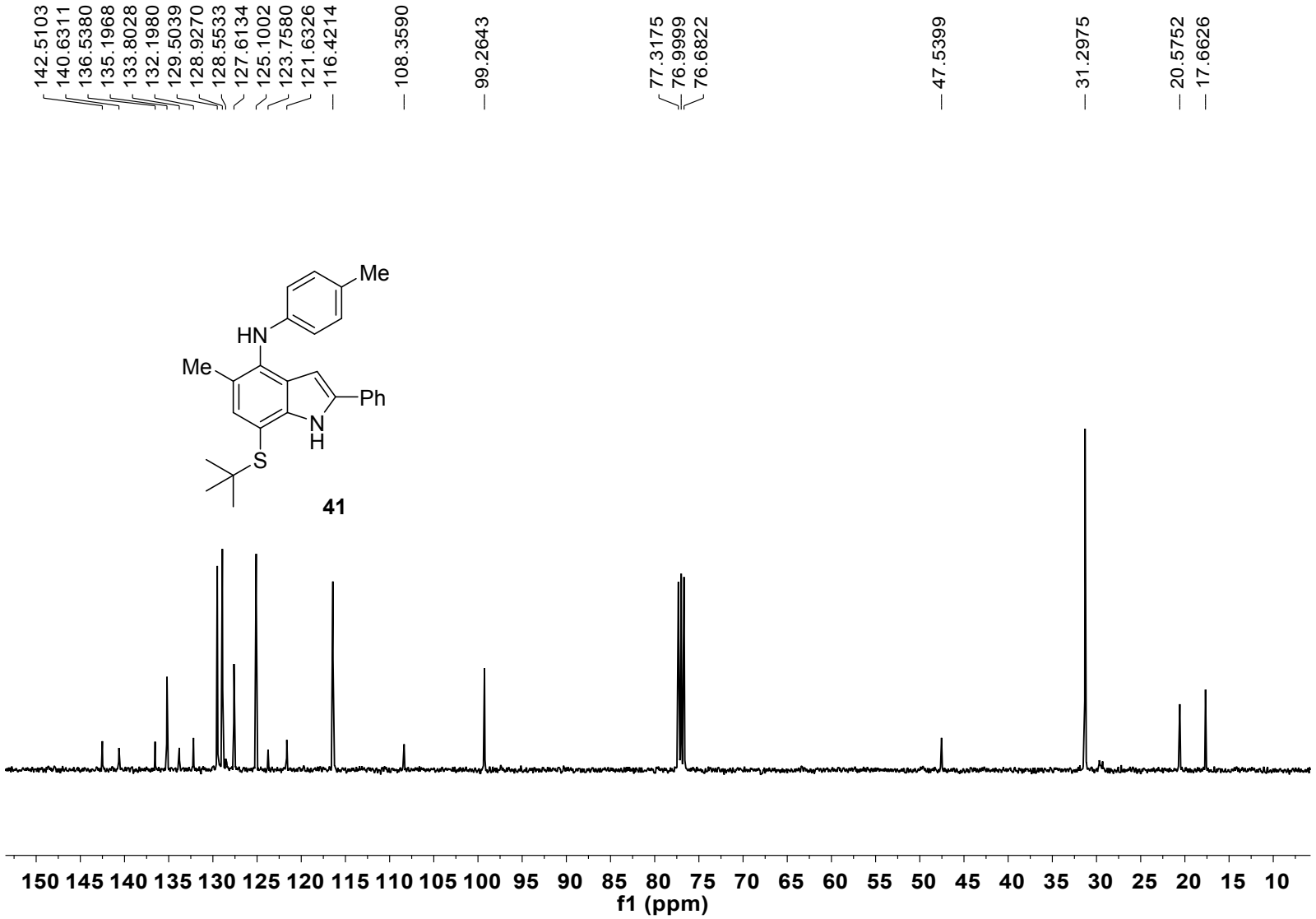
3.15
9.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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108.3590
99.2643
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76.9999
76.6822
47.5399
31.2975
20.5752
17.6626
Me
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N
H
S
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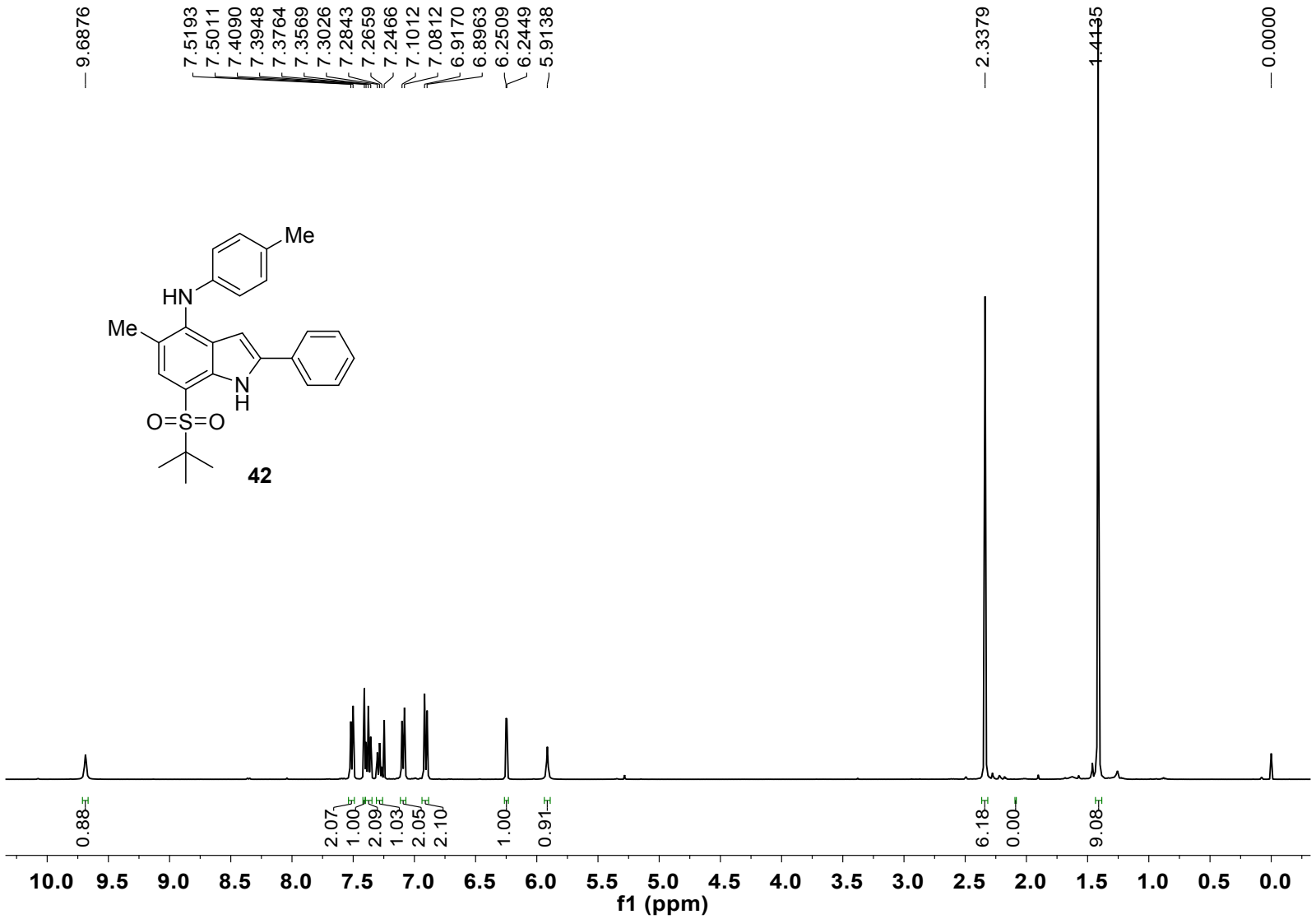
f1 (ppm)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HN
Me
N
H
O=S=O
42
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1.00
2.09
1.03
2.05
2.10
1.00
0.91
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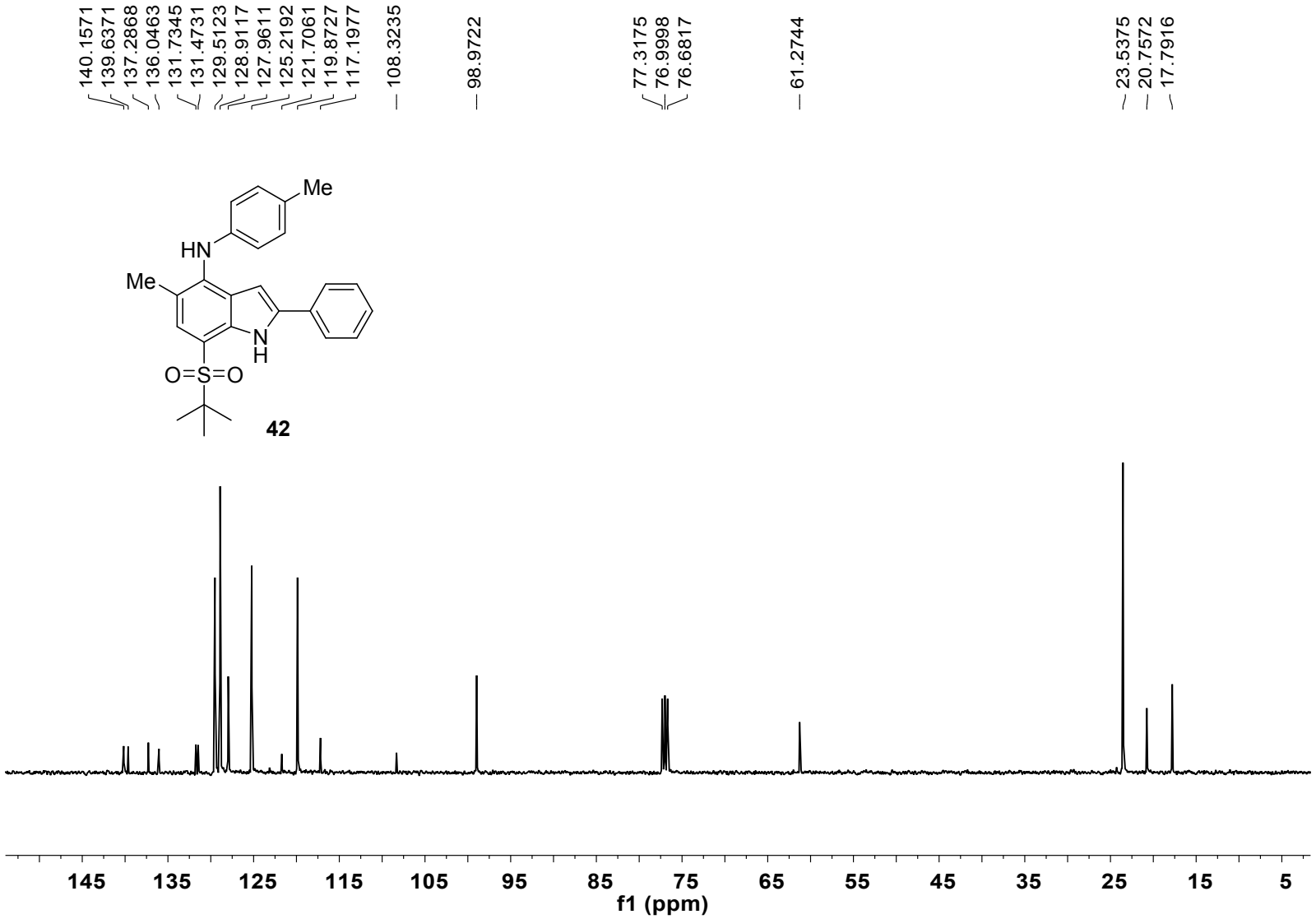
0.00
9.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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117.1977
108.3235
98.9722
77.3175
76.9998
76.6817
61.2744
23.5375
20.7572
17.7916
Me
HN
Me
N
H
O=S=O
42
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
f1 (ppm)