Supporting Information

Synthesis and Structure of m-Terphenyl Thio-, Seleno- and Telluro-ethers

Uzma I. Zakai,[+] Anna Bloch Mechkour,[§] Neil E. Jacobsen,[+] Leif Abrell,[+] Guangxin Lin,[+] Gary S. Nichol,[+] Thomas Bally,[§] and Richard S. Glass[+]*

Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85721, and Department of Chemistry, University of Fribourg, CH-1700, Fribourg, Switzerland

CONTENTS

Yields, physical properties and spectroscopic details for **1 -3**

1a (67% yield): mp 129-130°C; ^{1}H NMR (CD_2Cl_2) δ 1.70 (s, 3H, SMe), 3.82 (d, *J* = 10.3 Hz, 6H, OMe), 7.03 (t, *J* = 8.3 Hz, 4H, ArH), 7.23-7.41 (m, 7H, ArH); ^{13}C NMR (CD_2Cl_2) δ 18.7 (CH_3), 19.0 (CH_3), 55.9 (CH_3), 56.0 (CH_3), 111.1 (CH), 120.6 (CH), 127.7 (CH), 128.0 (CH), 129.3 (CH), 130.7 (CH), 131.4 (CH), 131.6 (CH), 131.7 (Cq), 136.9 (Cq), 144.0 (Cq), 144.1 (Cq), 157.4 (Cq); IR υ_{max} (KBr)/cm^{-1} 3005 (C-H), 2948 (C-H), 2926 (C-H), 2832 (C-H), MS (DIP-EI$^+$) *m/z* (rel. intensity %) 336 (M^+, 85), 305 (100), 290 (66); HRMS (DIP-EI$^+$) Calcd for $C_{21}H_{20}O_2S$: 336.1184. Found: 336.1178.

1c recrystallized from dichloromethane/hexanes (16% yield): mp 135-136 °C; ^{1}H NMR (CD_2Cl_2) δ 1.67 (s, 3H, SMe), 3.85 (s, 6H, OMe), 6.96 (d, *J* = 8.8 Hz, 4H, ArH), 7.23 (d, *J* = 1.6 Hz, 1H, ArH), 7.26 (s, 1H, ArH), 7.33 (dd, *J* = 8.6 Hz, *J* = 6.3 Hz, 1H, ArH), 7.42 (d, *J* = 8.8, 4H, ArH); ^{13}C NMR (CD_2Cl_2) δ 19.4 (CH_3), 55.8 (CH_3), 113.7 (CH), 127.8 (CH), 130.2 (CH), 131.2 (CH), 134.5 (Cq), 135.1 (Cq), 146.7 (Cq), 159.4 (Cq); MS (EI$^+$) *m/z* (rel. intensity %) 336 (M^+, 100), 321 (39), 306 (36), 290 (24), 160 (29); IR υ_{max} (thin film) 3054 (C-H) cm^{-1}; HRMS (EI$^+$) Calcd for $C_{21}H_{20}O_2S$: 336.1184. Found: 336.1178.

1f (26% yield): mp 145-147 °C; ^{1}H NMR (CD_2Cl_2) δ 1.76 (s, 3H, SMe), 3.79 (d, *J* = 5.7 Hz, 12H, OMe), 6.85-6.95 (m, 6H, ArH), 7.25 (d, *J* = 7.2 Hz, 2H, ArH), 7.37 (t, *J* = 7.5 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 18.8 (CH_3), 19.1 (CH_3), 56.2 (CH_3), 56.5 (CH_3), 112.0 (CH), 113.5 (CH), 117.6 (CH), 127.7 (CH), 127.9 (CH), 130.7 (CH), 132.4 (Cq), 136.7 (Cq), 143.9 (Cq), 151.6 (Cq), 153.8 (Cq); IR υ_{max} (KBr) 3044, 3018, 2997, 2921, 2837 cm^{-1}; GC-MS (rel. intensity %) *m/z* 396 (M^+, 16), 365 (100), 350 (84); HRMS (TOF-EI$^+$) Calcd for $C_{23}H_{24}O_4S$: 396.1395. Found: 396.1414.

1g recrystallized from dichloromethane (59% yield): mp 144-146°C; ^{1}H NMR (CD_2Cl_2) δ 1.65 (s, 3H, SMe), 7.46 (t, *J* = 3.8 Hz, 3H, ArH), 7.53 (dd, *J* = 6.3 Hz, *J* = 3.1 Hz, 4H, ArH), 7.72 (d, *J* = 1.7 Hz, 1H, ArH), 7.74 (d, *J* = 1.6 Hz, 1H, ArH), 7.92 (d, *J* = 9.1 Hz, 6H, ArH), 7.96 (d, *J* = 1.2 Hz, 2H, ArH); ^{13}C NMR (CD_2Cl_2) δ 19.6 (CH_3), 126.6 (CH), 126.7 (CH), 127.5 (CH), 128.2 (CH), 128.2 (CH), 128.6 (CH), 128.6 (CH), 128.8 (CH), 130.9 (CH), 133.0 (Cq), 133.7 (Cq), 134.6 (Cq), 140.3 (Cq), 147.2 (Cq); IR υ_{max} (KBr)/cm^{-1} 3054, 2919; MS (EI$^+$) *m/z* (rel. intensity %) 376 (M^+, 100), 361 (100), 180 (43); HRMS (DIP-EI$^+$) Calcd for $C_{27}H_{20}S$: 376.1286. Found: 376.1288.

1h (54% yield): mp 124-125 °C; ^{1}H NMR (CD_2Cl_2) δ 3.60 (s, 3H, OMe), 3.71 (s, 3H, OMe), 6.62 (t, *J* = 3.8 Hz, 2H, ArH), 6.80-6.92 (m, 7H, ArH), 7.06 (d, *J* = 6.8 Hz, 1H, ArH), 7.26 (ddd, *J* = 15.2 Hz, *J* = 8.0 Hz, *J* = 6.3 Hz, 5H, ArH), 7.45 (t, *J* = 7.6 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 55.6 (CH_3), 55.8 (CH_3), 110.9 (CH), 120.4 (CH), 125.2 (CH), 125.4 (CH), 128.4 (CH), 128.5 (CH), 128.8 (CH), 129.0 (CH), 129.2 (CH), 131.0 (CH), 131.1 (CH), 131.2 (CH), 131.5 (CH), 134.4 (Cq), 144.7 (Cq), 157.1 (Cq), 157.2 (Cq); IR υ_{max} (KBr) 3057 (C-H), 3012 (C-H), 2962 (C-H), 2934 (C-H), 2835 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity %) 398 (M^+, 100), 367 (100), 352 (32) 199 (23); HRMS (EI$^+$) Calcd for $C_{26}H_{22}O_2S$: 398.1341. Found: 398.1360.

2a (30% yield): mp 100-102 °C; ^{1}H NMR (CD_2Cl_2) δ 1.53 (d, 3H, *J* = 4.5 Hz, SMe), 3.81 (d, *J* = 11.2 Hz, 6H, OMe), 7.01 (ddd, *J* = 13.1 Hz, *J* = 7.8 Hz, *J* = 4.1 Hz, 4H, ArH), 7.21-7.24 (m, 3H, ArH), 7.30-7.40 (m, 4H, ArH); ^{13}C NMR (CD_2Cl_2) δ 8.2 (CH_3), 8.7 (CH_3), 54.7 (CH_3), 55.9 (CH_3), 111.0 (CH), 111.1 (CH), 120.6 (CH), 120.6 (CH), 127.7 (CH), 128.1 (CH), 129.3 (CH), 130.2 (CH), 130.3 (CH), 131.4 (CH), 131.6 (CH), 132.8 (Cq), 133.2 (Cq), 133.2 (Cq), 144.3 (Cq), 144.5 (Cq), 157.3 (Cq), 157.4 (Cq); ^{77}Se NMR δ 374.7, 375.0; IR υ_{max} (KBr) 30005(C-H), 2947 (C-H), 2931 (C-H), 2832 (C-H) cm^{-1}; MS (EI^{+}) *m/z* (rel. intensity %) 384 (M+1, 98), 353 (98), 338 (52); HRMS (DIP-EI^{+}) Calcd for $C_{21}H_{20}O_2{}^{80}Se$: 384.0630. Found: 384.0622.

2b recrystallized from CH_2Cl_2 (34% yield): mp 129-131 °C; ^{1}H NMR (CD_2Cl_2) δ 1.49 (s, 3H, SeMe), 3.85 (s, 6H, OMe), 6.95 (d, *J* = 8.7 Hz, 4H, ArH), 7.22 (d, *J* = 1.2 Hz, 1H, ArH), 7.24 (s, 1H, ArH), 7.33 (dd, *J* = 8.4 Hz, *J* = 6.5 Hz, 1H, ArH) 7.41(d, *J* = 8.7 Hz, 4H, ArH); ^{13}C NMR (CD_2Cl_2) δ 9.8 (CH_3), 55.8 (CH_3), 113.7 (CH), 114.7(CH), 125.6 (CH), 127.7 (CH), 128.7 (CH), 129.7 (CH), 131.1 (CH), 136.2 (Cq), 147.0 (Cq), 159.5 (Cq); ^{77}Se NMR (CD_2Cl_2) δ 365.5; IR υ_{max} (KBr)/cm^{-1} 3036 (C-H), 3002 (C-H), 2962 (C-H), 2927 (C-H), 2831 (C-H), MS (EI^{+}) *m/z* (rel. intensity %) 384 (M+1, 95), 382 (M-1, 50); HRMS (DIP-EI^{+}) Calcd for $C_{21}H_{20}O_2{}^{80}Se$: 384.0630. Found: 384.0622.

2c recrystallized from pentanes/dichloromethane (64% yield): mp 133-135 °C; ^{1}H NMR (CD_2Cl_2) δ 1.59 (d, *J* = 6.6 Hz, 3H, SeMe), 3.79 (dd, *J* = 9.0 Hz, *J* = 5.8 Hz, 12H, OMe), 6.84 (s, 1H, ArH), 6.91 (s, 5H, ArH), 7.23 (d, *J* = 7.3 Hz, 2H, ArH), 7.38 (dd, *J* = 8.2 Hz, *J* = 6.9 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 8.3 (CH_3), 8.8 (CH_3), 56.2 (CH_3), 56.4(CH_3), 56.5 (CH_3), 111.8 (CH), 112.0 (CH), 113.5 (CH), 113.6 (CH), 117.6 (CH), 117.7 (CH), 127.7 (CH), 128.0 (CH), 130.2 (CH), 130.4 (CH), 132.9 (Cq), 132.9 (Cq), 133.5 (Cq), 144.1 (Cq), 144.3 (Cq), 151.5 (Cq), 151.6 (Cq), 157.7 (Cq); IR υ_{max} (KBr)/ cm^{-1} 2999 (C-H), 2929 (C-H), 2835 (C-H), GC-MS *m/z* (rel. intensity %) 444 (M+1, 58), 413 (100), 398 (96), 396 (55); HRMS (TOF-EI^{+}) Calcd for $C_{23}H_{24}O_4{}^{80}Se$: 444.0840. Found: 444.0847.

2d (46% yield): mp 103-104 °C; ^{1}H NMR (CD_2Cl_2) δ 6.72 (dd, *J* = 8.3 Hz, *J* = 1.3 Hz, 2H, ArH), 6.90-7.02 (m, 3H, ArH), 7.28 (s, 10H, ArH), 7.33 (d, *J*=0.9 Hz, 1H, ArH), 7.35 (s, 1H, ArH), 7.47 (dd, *J* = 8.3 Hz, *J* = 6.8 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 126.2 (CH), 127.4 (CH), 128.0 (CH), 129.0 (CH), 129.0 (CH), 129.9 (CH), 130.3 (CH), 131.3 (CH), 134.4 (Cq), 143.7 (Cq), 148.9 (Cq); ^{77}Se NMR (CD_2Cl_2) δ 557.7; IR υ_{max} (KBr) 3050 cm^{-1}; MS (EI^{+}) *m/z* (rel. intensity %) 386 (M+1, 100), 384 (M-1, 50); HRMS (EI^{+}) Calcd for $C_{24}H_{18}{}^{80}Se$: 386.0575. Found: 386.0560.

2e recrystallized from pentanes/dichloromethane (62% yield): mp 115-117 °C; ^{1}H NMR (CD_2Cl_2) 3.61 (s, 3H, OMe), 3.76 (s, 3H, OMe), 6.79 (dd, *J* = 16.0 Hz, *J* = 7.6 Hz, 3H, ArH), 6.86-7.07 (m, 7H, ArH), 7.26-7.32 (m, 5H, ArH), 7.43-7.49 (m, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 55.5 (CH_3), 55.7 (CH_3), 110.7 (CH), 110.8 (CH), 120.4 (CH), 120.4 (CH), 126.1 (CH), 126.2 (CH), 128.5 (CH), 128.6 (CH), 128.7 (CH), 129.1 (CH), 129.2 (CH), 129.2 (CH), 130.5 (CH), 130.7 (CH), 131.2 (CH), 131.6 (CH), 131.6 (CH), 132.2 (CH), 132.4 (Cq), 132.5 (Cq), 133.2 (Cq), 133.3 (Cq), 133.6 (Cq), 134.2 (Cq), 144.9 (Cq), 145.0 (Cq), 157.0 (Cq), 157.2 (Cq); ^{77}Se NMR (C_2Cl_2) δ 371.6, 374.5; IR υ_{max} (KBr) 3056 (C-H), 2931 (C-H), 2835(C-H) cm^{-1}; MS (EI^{+})

m/z (rel. intensity %) 446 (M+1, 100), 415 (85), 413 (60); HRMS (DIP-EI$^+$) Calcd for $C_{26}H_{22}O_2{}^{80}Se$: 446.0787. Found: 446.0801.

2f (45% yield): mp 107-109 °C; ^{1}H NMR (CD_2Cl_2) δ 3.85 (s, 6H, OMe), 7.00 (d, *J* = 8.8 Hz, 5H, ArH), 7.43-7.53 (m, 4H, ArH), 7.60 (d, *J* = 8.9 Hz, 5H, ArH), 7.75 (m, 2H, ArH); ^{13}C NMR (CD_2Cl_2) δ 55.9 (CH_3) 78.0 (Cq), 99.2 (CH), 114.7 (CH), 125.6 (CH), 128.7 (CH), 129.7 (CH), 134.1 (Cq), 141.8 (Cq), 159.9 (Cq); IR υ_{max} (KBr) 2956 (C-H), 2936 (C-H), 2838 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity %) 446 (M+1, 1), 290 (100); HRMS (EI$^+$) Calcd for $C_{26}H_{22}O_2{}^{80}Se$: 446.0787. Found: 446.0785.

2g recrystallized from CH_2Cl_2 (29% yield): mp 112-113 °C; ^{1}H NMR (CD_2Cl_2) δ 3.58 (s, 3H, OMe), 3.63 (s, 3H, OMe), 3.72 (s, 6H, OMe), 6.58 (t, *J* = 1.8 Hz, 1H, ArH), 6.72-6.85 (m, 7H, ArH), 6.91-7.03 (m, 3H, ArH), 7.28 (d, *J* = 7.6 Hz, 2H, ArH), 7.45 (dd, *J* = 14.8 Hz, *J* = 6.9 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 56.0 (CH_3) 56.1 (CH_3), 56.2 (CH_3), 56.3 (CH_3), 111.6 (CH), 111.8 (CH), 113.8 (CH), 113.9 (CH), 116.9 (CH), 117.5 (CH), 126.1 (CH), 126.2 (CH), 128.5 (CH), 128.6 (CH), 128.8 (CH), 129.1 (CH), 130.4 (CH), 130.6 (CH), 131.6 (CH), 132.2 (CH), 132.9 (Cq), 133.0 (Cq), 133.1 (Cq), 133.8 (Cq), 134.4 (Cq), 144.8 (Cq), 144.9 (Cq), 151.3 (Cq), 153.5 (Cq), 153.6 (Cq); IR υ_{max} (KBr) 3043 (C-H), 2988 (C-H), 2940 (C-H), 2825 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity %) 506 (M+1, 100), 475 (90); HRMS (DIP-EI$^+$) Calcd for $C_{28}H_{26}O_4{}^{80}Se$: 506.0998. Found: 506.0991.

3a viscous dark green-black oil (69% yield): ^{1}H NMR (CD_2Cl_2) δ 1.30 (d, *J* = 3.1 Hz, 3H, TeMe), 3.79 (s, 3H, OMe), 3.83 (s, 3H, OMe), 6.94-7.05 (m, 4H, ArH), 7.17-7.23 (m, 3H, ArH), 7.30-7.41 (m, 4H, ArH); ^{13}C NMR (CD_2Cl_2) δ 1.4 (CH_3) 55.8 (CH_3), 55.9 (CH_3), 111.0 (CH), 111.2 (CH), 120.7 (CH), 120.8 (CH), 128.1 (CH), 128.3 (CH), 128.7 (CH), 129.1 (CH), 129.3 (CH), 129.4 (CH), 129.4 (CH), 131.5 (CH), 131.8 (CH), 134.8 (Cq), 146.9 (Cq), 147.0 (Cq), 157.1 (Cq), 157.3 (Cq); IR υ_{max} (thin film) 3052 (C-H), 2932 (C-H), 2833 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity %) 434 (M+2, 100), 432 (M$^+$, 100), 403 (50), 290 (48); HRMS (DIP-EI$^+$) Calcd for $C_{21}H_{20}O_2{}^{130}Te$: 434.0527. Found: 434.0521.

3b purplish-red oil (37% yield): ^{1}H NMR (CD_2Cl_2) δ 1.34 (dd, *J* = 6.7 Hz, *J* = 1.0 Hz, 3H, TeMe), 3.78 (dd, *J* = 11.2 Hz, *J*=6.4 Hz, 12H, OMe), 6.81 (s, 1H, ArH), 6.89 (d, *J* = 3.6 Hz, 5H, ArH), 7.20 (dd, *J* = 7.5 Hz, *J* = 4.1 Hz, 2H, ArH), 7.36 (dt, *J* = 7.2 Hz, *J* = 7.0, *J* = 4.4, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 1.4 (CH_3) 56.3 (CH_3), 56.4 (CH_3), 111.8 (CH), 112.2 (CH), 113.8 (CH), 117.6 (CH), 117.8 (CH), 128.1 (CH), 128.2 (CH), 129.2 (CH), 129.3 (CH), 135.4 (Cq), 146.7 (Cq), 146.8 (Cq), 151.3 (Cq), 151.6 (Cq), 153.8 (Cq), 153.8 (Cq); IR υ_{max} (thin film) 3052 (C-H), 2997 (C-H), 2937 (C-H), 2832 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity %) 494 (M+2, 100), 492 (M$^+$, 90), 463 (55), 350 (30); HRMS (DIP-EI$^+$) Calcd for $C_{23}H_{24}O_4{}^{130}Te$: 494.0739. Found: 494.0752.

3c (67 % yield): mp 74-76 °C; ^{1}H NMR (CD_2Cl_2) δ 6.88 (t, *J* = 7.4 Hz, 2H, ArH), 6.96-6.99 (m, 2H, ArH), 7.03-7.13 (m, 1H, ArH), 7.22-7.31 (m, 12H, ArH), 7.40 (dd, *J* = 8.3 Hz, *J* = 6.7 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 118.4 (Cq) 120.5 (Cq), 127.1 (CH), 127.2 (CH), 127.6 (CH), 127.9 (CH), 128.2 (CH), 129.0 (CH), 129.1 (CH), 129.7 (CH), 130.5 (CH), 137.9 (CH), 146.2 (Cq), 151.1 (Cq); IR υ_{max} (KBr) 3047 (C-H), 3022 (C-H) cm^{-1}; MS (EI$^+$) *m/z* (rel. intensity

%) 436 (M+2, 100), 434 (M^+, 91), 229 (43); HRMS (DIP-EI^+) Calcd for $C_{24}H_{18}{}^{130}Te$: 436.0472. Found: 436.0483.

3d recrystallized from dichloromethane/pentanes as a orange-pink solid (21% yield): mp 121-123 °C; ^1H NMR (CD_2Cl_2) δ 3.58 (s, 3H, OMe), 3.74 (s, 3H, OMe), 6.76 (d, *J* = 8.2 Hz, 1H, ArH), 6.83-7.09 (m, 9H, ArH), 7.21-7.32 (m, 5H, ArH), 7.42 (ddd, *J* = 8.0 Hz, *J* = 7.1, *J* = 3.8 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 55.4 (CH_3), 55.7 (CH_3), 110.7 (CH), 117.1 (Cq), 117.4 (Cq), 120.6 (CH), 120.6 (CH), 127.0 (CH), 127.1 (CH), 128.8 (CH), 128.9 (CH), 128.9 (CH), 129.3 (CH), 129.3 (CH), 129.5 (CH), 131.7 (CH), 134.9 (Cq), 135.0 (Cq), 137.8 (CH), 138.3 (CH), 147.4 (Cq), 147.6 (Cq), 156.9 (Cq), 157.1 (Cq); IR υ_{max} (KBr) 3058 (C-H), 3007 (C-H), 2949 (C-H), 2929 (C-H), 2831 (C-H) cm^{-1}; MS (EI^+) *m/z* (rel. intensity %) 496 (M+2, 100), 494 (M^+, 90), 465 (30); HRMS (DIP-EI^+) Calcd for $C_{26}H_{22}O_2{}^{130}Te$: 496.0684. Found: 496.0692.

3e red solid (24% yield): mp 158-161 °C; ^1H NMR (CD_2Cl_2) δ 6.67 (t, *J* = 7.4 Hz, 2H, ArH), 6.76-6.90 (m, 3H, ArH), 7.28-7.62 (m, 13H, ArH), 7.86 (t, *J* = 11.1 Hz, *J* = 9.0 Hz, 4H, ArH); ^{13}C NMR (CD_2Cl_2) δ 116.7 (Cq), 116.8 (Cq), 123.7 (Cq), 125.5 (CH), 125.6 (CH), 126.2 (CH), 126.4 (CH), 126.5 (CH), 126.6 (CH), 126.7 (CH), 127.3 (CH), 127.4 (CH), 127.8 (CH), 128.2 (CH), 128.2 (CH), 128.3 (CH), 128.6 (CH), 128.7 (CH), 128.8 (CH), 129.0 (CH), 130.3 (CH), 132.4 (Cq), 132.7 (Cq), 134.0 (Cq), 138.0 (CH), 138.4 (CH), 143.3 (Cq), 143.4 (Cq), 149.0 (Cq); IR υ_{max} (KBr) 3041 (C-H) cm^{-1}; MS (EI^+) *m/z* (rel. intensity %) 536 (M+2, 100), 326 (55); HRMS (DIP-EI^+) Calcd for $C_{32}H_{22}{}^{130}Te$: 536.0787. Found: 536.0800.

3f red oil (41% yield): ^1H NMR (CD_2Cl_2) δ 2.37 (s, 6H, ArMe), 6.87 (t, *J* = 7.4 Hz, 2H, ArH), 6.98 (dd, *J* = 8.1 Hz, *J* = 1.5 Hz, 2H, ArH), 7.10 (dd, *J* = 14.9 Hz, *J* = 8.2 Hz, 9H, ArH), 7.25 (dd, *J* = 7.5 Hz, *J* = 0.7 Hz, 2H, ArH), 7.38 (dd, *J* = 8.2 Hz, *J* = 6.8 Hz, 1H, ArH); ^{13}C NMR (CD_2Cl_2) δ 21.5 (CH_3) 118.5 (Cq), 120.7 (Cq), 127.2 (CH), 128.8 (CH), 128.9 (CH), 129.6 (CH), 130.0 (CH), 130.0 (CH), 137.3 (Cq), 137.9 (CH), 143.4 (Cq), 151.0 (Cq); IR υ_{max} (thin film) 3050 (C-H) cm^{-1}; GC-MS (EI^+) *m/z* (rel. intensity %) 464 (M+2, 100), 462 (M^+, 88), 460 (M-2, 55), 258 (47); HRMS (DIP-EI^+) Calcd for $C_{26}H_{22}{}^{130}Te$: 464.0784. Found: 464.0759.

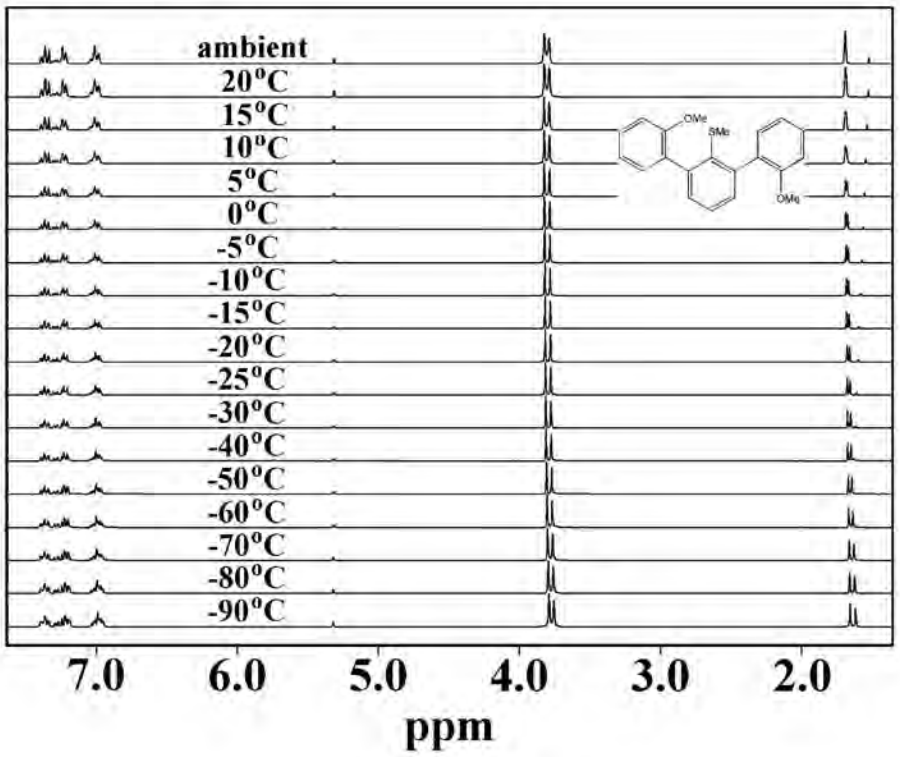


Figure S1. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **1c** in CD_2Cl_2

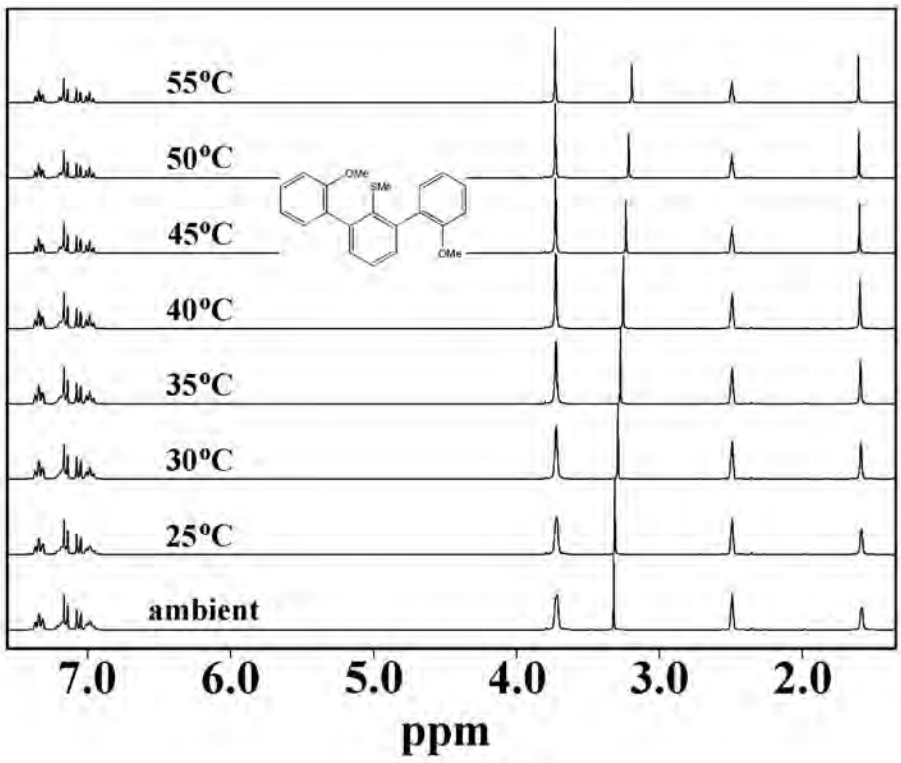


Figure S2. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **1c** in DMSO-d_6

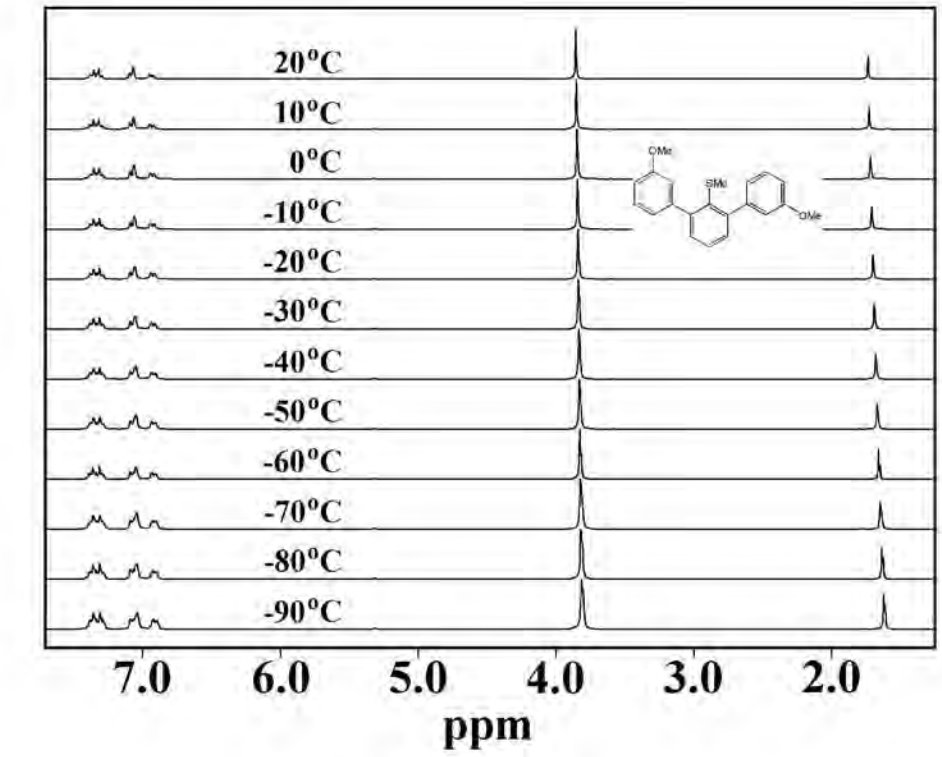


Figure S3. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **1d** in CD_2Cl_2

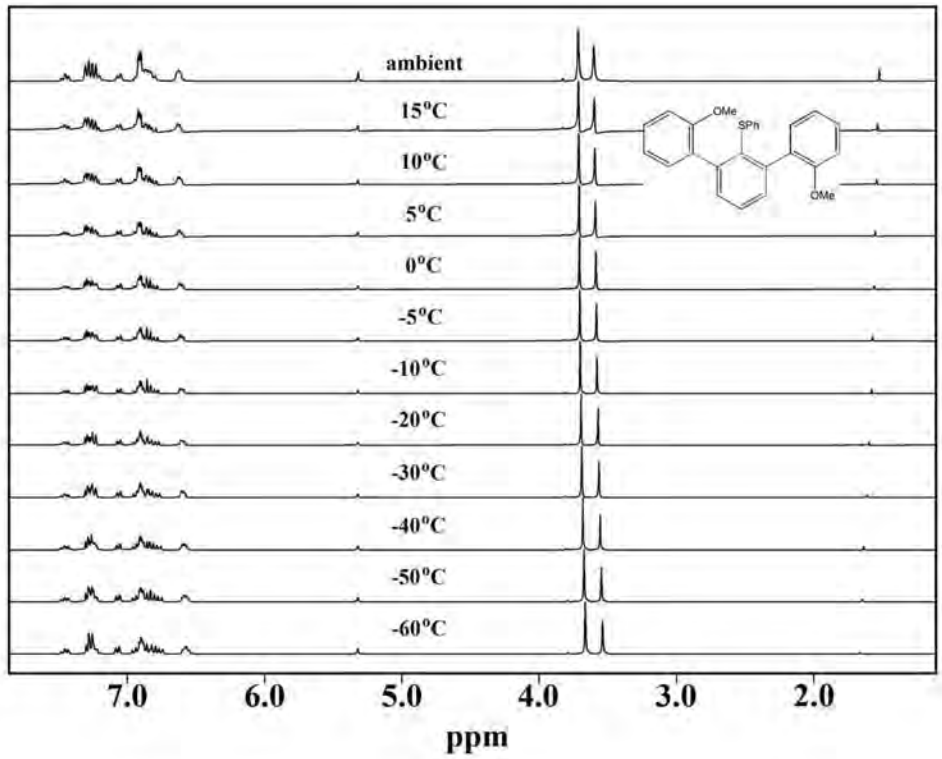


Figure S4. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **1h** in CD_2Cl_2

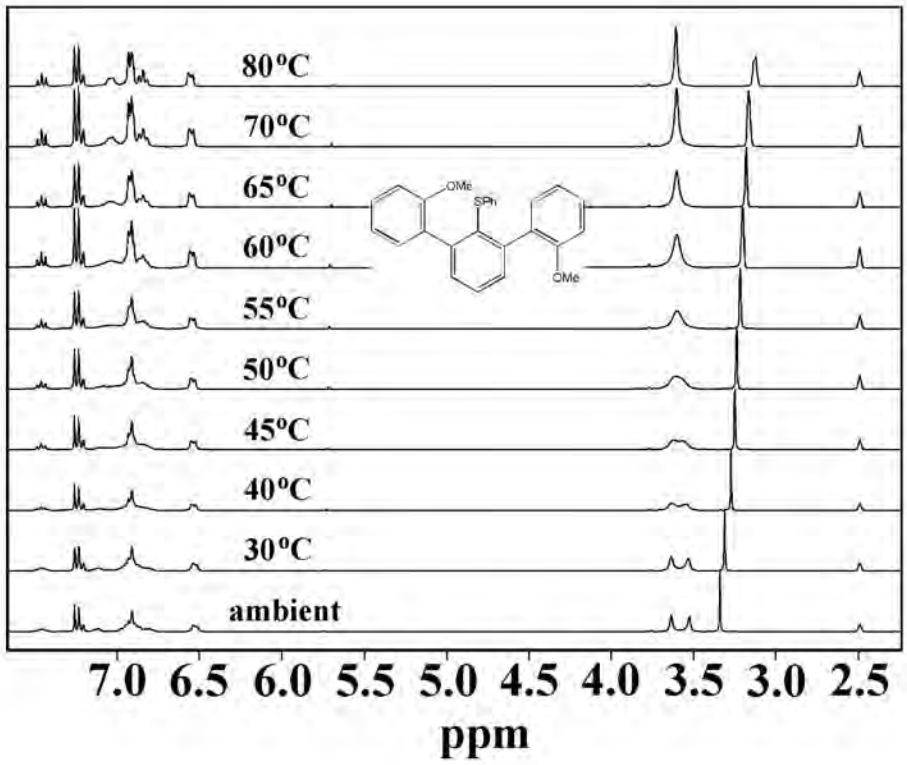


Figure S5. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **1h** in DMSO-d_6

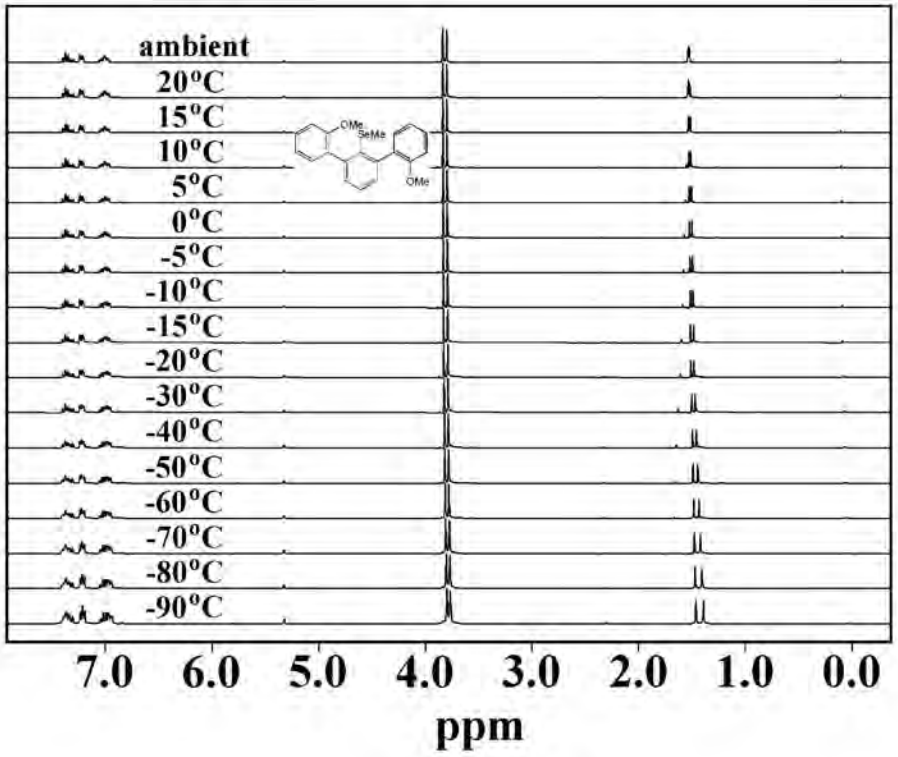


Figure S6. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **2a** in CD_2Cl_2

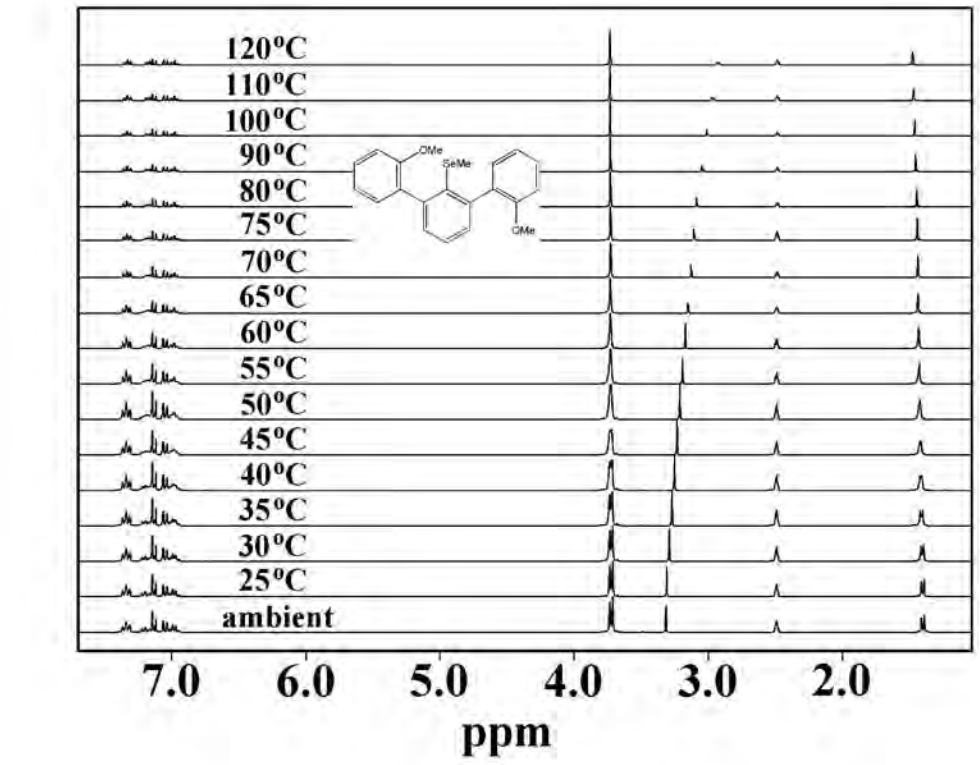


Figure S7. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **2a** in DMSO-d_6

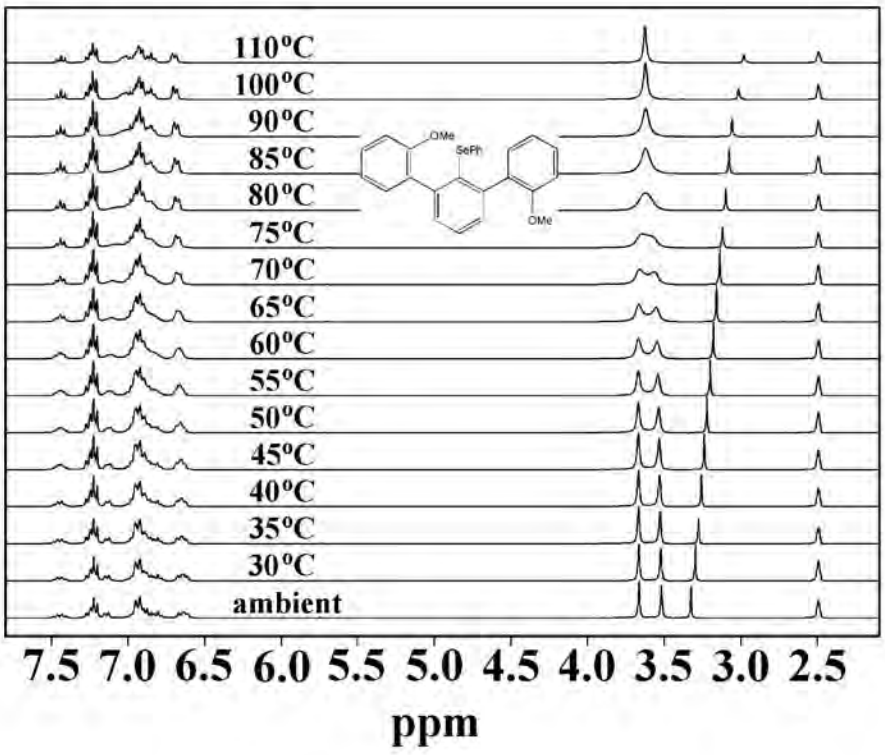


Figure S8. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **2f** in DMSO-d_6

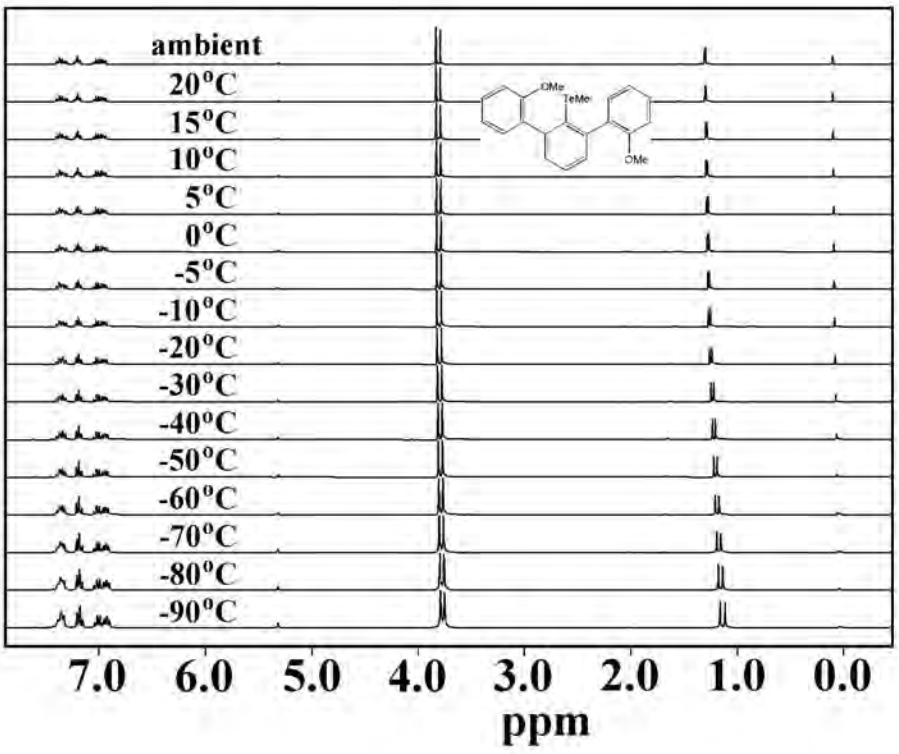


Figure S9. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **3a** in CD_2Cl_2

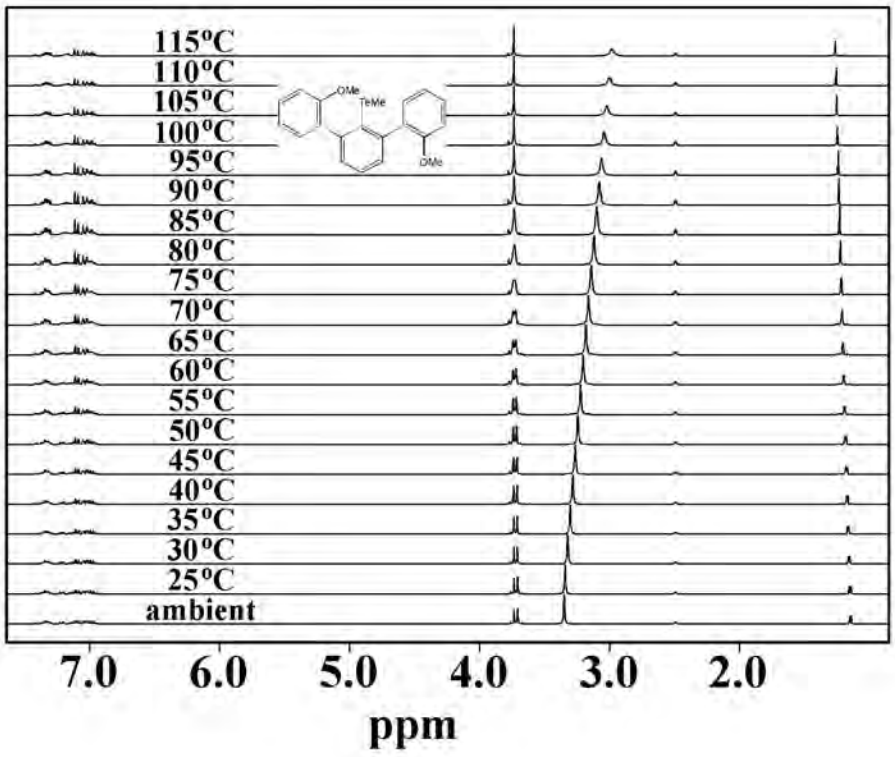


Figure S10. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **3a** in DMSO-d_6

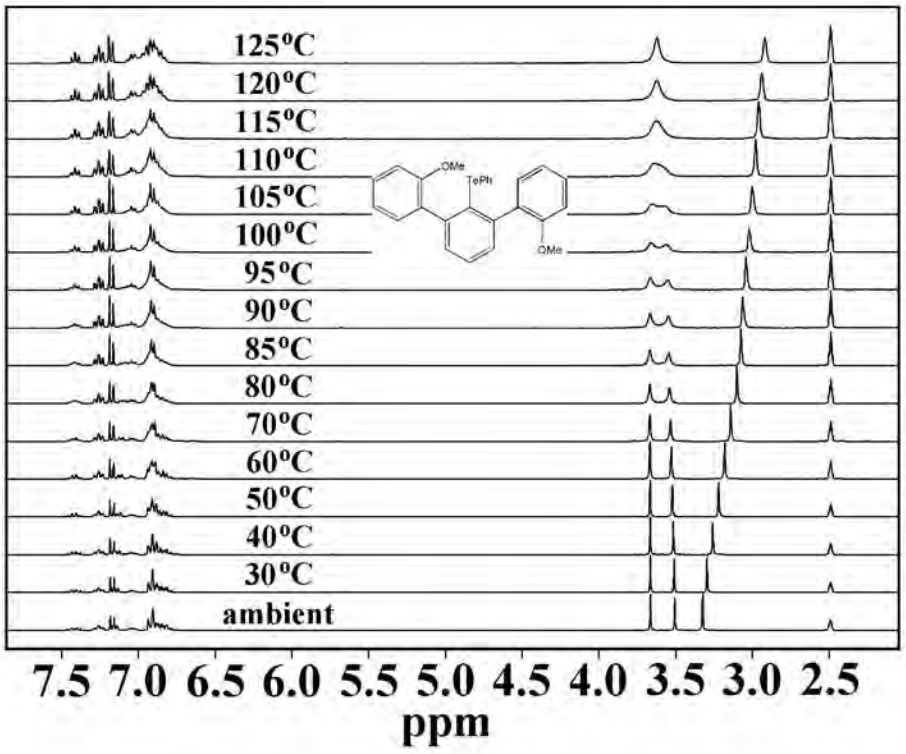
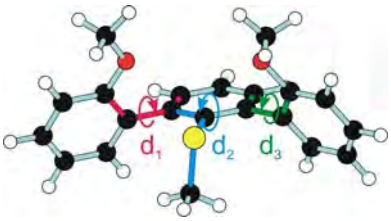
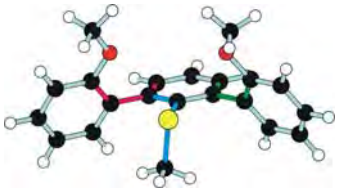
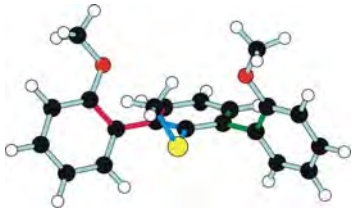
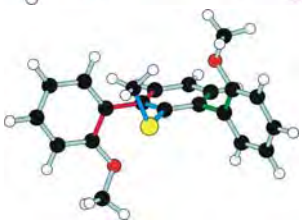
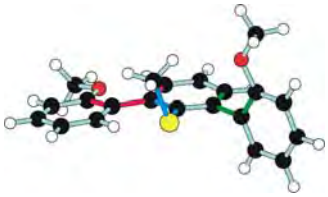
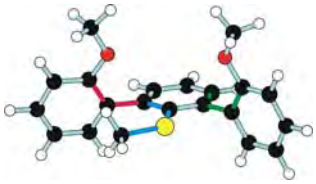
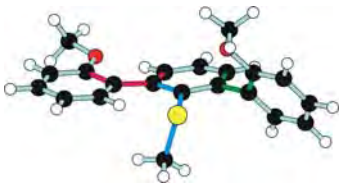
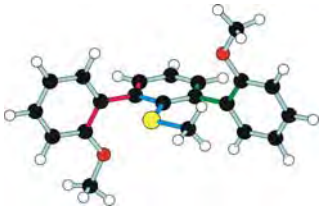


Figure S11. Variable-temperature 300 MHz ^{1}H NMR spectroscopic study of **3d** in DMSO-d_6

Table S1. Crystal data and structure refinement for 1c.

Chemical formula (moiety)	$C_{21}H_{20}O_2S$
Chemical formula (total)	$C_{21}H_{20}O_2S$
Formula weight	336.43
Temperature	150(2) K
Radiation, wavelength	MoK , 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell parameters	a = 16.805(5) Å α = 90°
	b = 7.535(2) Å β = 111.354(4)°
	c = 14.901(5) Å γ = 90°
Cell volume	1757.2(9) $Å^3$
Z	4
Calculated density	1.272 g/cm^3
Absorption coefficient	0.194 mm^{-1}
F(000) 712	
Crystal color and size	colorless, 0.49 × 0.28 × 0.14 mm^3
Reflections for cell refinement	2978 (θ range 2.6 to 25.5°)
Data collection method	Bruker SMART 1000 CCD diffractometer
	thin-slice ω scans
θ range for data collection	2.6 to 25.1°
Index ranges	h –20 to 19, k –8 to 8, l –17 to 17
Completeness to θ = 25.1°	95.6 %
Reflections collected	10573
Independent reflections	2969 (R_{int} = 0.0423)
Reflections with $F^2>2\sigma$	1972
Absorption correction	semi-empirical from equivalents
Min. and max. transmission	0.9119 and 0.9726
Structure solution	direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting parameters a, b	0.0154, 1.4642
Data / restraints / parameters	2969 / 0 / 221
Final R indices [$F^2>2\sigma$]	R1 = 0.0389, wR2 = 0.0738
R indices (all data)	R1 = 0.0781, wR2 = 0.0947
Goodness-of-fit on F^2	1.110
Extinction coefficient	0.0016(4)
Largest and mean shift/su	0.000 and 0.000
Largest diff. peak and hole	0.30 and –0.27 e $Å^{-3}$



Conformers		Dihedral angles[a]		
		d_1	d_2	d_3
syn-a		**-109.53** ***-118.90***	**81.59** ***83.28***	**112.27** ***119.66***
syn-s		**-63.25** ***-60.26***	**-67.26** ***-64.33***	**102.21** ***112.37***
anti		**107.76** ***116.02***	**-79.18** ***-68.77***	**94.81** ***109.99***
TS(*syn-s* → *anti*)		**-115.22** ***-103.63***	**107.78** ***91.65***	**5.98** ***-1.30***
TS(*syn-a* → *syn-s*)		**-98.45** ***-99.01***	**-0.02** ***-1.85***	**95.66** ***91.13***
TS(*anti* → *syn-a*)		**4.87** ***5.69***	**-71.23** ***-69.71***	**89.12** ***97.11***
TS(*anti* → *anti*)		**92.23** ***88.76***	**-178.69** ***-177.51***	**93.30** ***91.65***

[a] in bold italics for 2a

Table S2. Geometrical parameters of the species in Figure 9

Tables of coordinates for species in Figure 9

All stationary points listed in this file were located and characterized by B3LYP/6-31G*. The charge and multiplicity are indicated in the line above the cartesian coordinates.

Single point calculations by B2PLYP/cc-pVDZ for all conformers of 1a and 2a (B3LYP/6-31G* geometry) were done in gas phase phase (gas phase) and with the PCM-SCRF model, using dimethylsulfoxide as a solvent (SCRF IN DMSO).

1a syn-s

0,1

6	1.183573	-0.409201	2.408642
6	-0.055347	-0.258568	3.025822
6	-1.210822	-0.239439	2.253097
6	-1.155386	-0.379757	0.858079
6	0.107565	-0.501102	0.233283
6	1.284552	-0.519366	1.015969
1	2.093270	-0.426299	3.002257
1	-0.119990	-0.163215	4.106536
1	-2.181399	-0.133864	2.728215
6	-2.451142	-0.449694	0.114265
6	-3.352005	0.639846	0.112566
6	-2.835890	-1.624186	-0.540255
6	-4.590653	0.535833	-0.531959
6	-4.069633	-1.735525	-1.183611
1	-2.149050	-2.464427	-0.536377
6	-4.943484	-0.651647	-1.176791
1	-5.281555	1.371114	-0.536438
1	-4.342285	-2.661726	-1.680858
1	-5.908686	-0.720371	-1.671791
6	2.651413	-0.685988	0.429124
6	3.316727	-1.908359	0.543170
6	3.330097	0.392464	-0.178277
6	4.615955	-2.085379	0.058258
1	2.797027	-2.736796	1.017408
6	4.630563	0.224840	-0.663217
6	5.266660	-1.014576	-0.545028
1	5.107349	-3.049203	0.154076
1	5.155022	1.049152	-1.132591
1	6.277184	-1.130337	-0.928196
16	0.264231	-0.688405	-1.552095
6	-0.319763	0.946843	-2.136052
1	-0.184903	0.949241	-3.221686
1	-1.375901	1.101352	-1.905226

1	0.286972	1.737602	-1.690557
8	-2.927792	1.769477	0.759122
8	2.640879	1.572666	-0.241272
6	-3.792575	2.891189	0.800997
1	-3.258252	3.657857	1.365394
1	-4.014284	3.271581	-0.205283
1	-4.736529	2.657454	1.311429
6	3.296935	2.705728	-0.784582
1	3.561323	2.554951	-1.839702
1	2.584850	3.529597	-0.705967
1	4.204253	2.956571	-0.219032

SCF Done: E(RB+HF-LYP) = -1360.89177478

Thermal correction to Enthalpy= 0.380050
Thermal correction to Gibbs Free Energy= 0.303913
Sum of electronic and zero-point Energies= -1360.535008
Sum of electronic and thermal Energies= -1360.512669
Sum of electronic and thermal Enthalpies= -1360.511724
Sum of electronic and thermal Free Energies= -1360.587861

E(B2PLYPD) = -1359.8301308 (gas phase)
E(B2PLYPD) = -1359.8409341 (SCRF IN DMSO)

1a syn-a

0,1

6	1.221538	0.058345	2.409192
6	0.016068	0.304952	3.059345
6	-1.185729	0.082616	2.392726
6	-1.200367	-0.386123	1.071405
6	0.025300	-0.616914	0.409371
6	1.246676	-0.404501	1.084958
1	2.164030	0.217516	2.925562
1	0.012811	0.662902	4.085598
1	-2.132054	0.259518	2.896267
6	-2.526794	-0.572389	0.407322
6	-3.324733	0.536853	0.114069
6	-3.036974	-1.859533	0.124267
6	-4.585583	0.400667	-0.475051
6	-4.296387	-2.003027	-0.466977
6	-5.062780	-0.872895	-0.766728
1	-5.181080	1.280574	-0.700396
1	-4.689851	-2.987916	-0.690918
1	-6.039661	-1.001516	-1.225673
6	2.579341	-0.599350	0.437775
6	3.060229	-1.884557	0.101654

6	3.412604	0.499746	0.213375
6	4.328271	-2.036115	-0.467934
6	4.681549	0.356201	-0.355167
6	5.131595	-0.915055	-0.696270
1	4.699285	-3.019897	-0.731577
1	5.304626	1.228992	-0.527459
1	6.114812	-1.049018	-1.139919
16	0.034575	-1.155492	-1.311176
6	-0.194934	0.457047	-2.152673
1	-0.197667	0.248378	-3.226602
1	-1.149337	0.912650	-1.875823
1	0.629093	1.138513	-1.924414
1	-2.939198	1.526103	0.348103
1	3.047211	1.487597	0.482400
8	-2.240447	-2.906041	0.481931
8	2.224572	-2.924274	0.386637
6	-2.660834	-4.219201	0.156588
1	-2.786797	-4.345616	-0.926619
1	-1.866801	-4.880929	0.507558
1	-3.599417	-4.482263	0.663104
6	2.619732	-4.232774	0.013489
1	1.799284	-4.887589	0.312787
1	2.772566	-4.314404	-1.070513
1	3.536774	-4.542624	0.532707

SCF Done: E(UB+HF-LYP) = -1360.89273476

Thermal correction to Enthalpy= 0.379944
Thermal correction to Gibbs Free Energy= 0.303425
Sum of electronic and zero-point Energies= -1360.536126
Sum of electronic and thermal Energies= -1360.513735
Sum of electronic and thermal Enthalpies= -1360.512790
Sum of electronic and thermal Free Energies= -1360.589309

E(B2PLYPD) = -1359.8303903 (gas phase)
E(B2PLYPD) = -1359.8413224 (SCRF IN DMSO)

1a anti

0,1

6	1.163885	-0.188521	2.369639
6	-0.070452	-0.124663	3.008510
6	-1.239054	-0.293175	2.269931
6	-1.190859	-0.528443	0.889585
6	0.063497	-0.562701	0.239675
6	1.249598	-0.400988	0.985975
1	2.081341	-0.064903	2.938244

1	-0.122372	0.046723	4.080541
1	-2.206952	-0.264001	2.762670
6	-2.483710	-0.709002	0.160899
6	-3.357232	0.369799	0.000419
6	-2.886129	-1.976449	-0.317840
6	-4.590396	0.227343	-0.643589
6	-4.116359	-2.124912	-0.966816
6	-4.960650	-1.022580	-1.128962
1	-5.247096	1.084319	-0.761924
1	-4.427014	-3.093251	-1.341994
1	-5.913695	-1.154992	-1.634588
6	2.614685	-0.478516	0.375150
6	3.341899	-1.668960	0.433826
6	3.228846	0.654549	-0.198551
6	4.641260	-1.759871	-0.072746
1	2.871593	-2.539627	0.883043
6	4.529772	0.573698	-0.705013
6	5.229255	-0.634756	-0.641482
1	5.183121	-2.699636	-0.019064
1	5.004664	1.441093	-1.149081
1	6.239271	-0.684273	-1.039936
16	0.159397	-0.846712	-1.537487
6	-0.259978	0.824162	-2.168628
1	-0.140765	0.781823	-3.255364
1	-1.294428	1.085967	-1.931372
1	0.427015	1.563979	-1.753582
8	2.476766	1.799918	-0.212864
6	3.077644	2.992862	-0.689424
1	3.347493	2.916731	-1.751173
1	2.326985	3.775689	-0.564609
1	3.972678	3.252396	-0.108752
1	-3.054020	1.340692	0.384351
8	-2.019349	-3.002431	-0.085503
6	-2.322674	-4.279376	-0.620401
1	-2.410752	-4.246301	-1.714002
1	-1.485931	-4.923837	-0.344830
1	-3.248919	-4.688074	-0.194203

SCF Done: E(UB+HF-LYP) = -1360.89254528

Thermal correction to Enthalpy= 0.380091
Thermal correction to Gibbs Free Energy= 0.303491
Sum of electronic and zero-point Energies= -1360.535755
Sum of electronic and thermal Energies= -1360.513399
Sum of electronic and thermal Enthalpies= -1360.512455
Sum of electronic and thermal Free Energies= -1360.589054

E(B2PLYPD) = -1359.8303938 (gas phase)
E(B2PLYPD) = -1359.8413128 (SCRF IN DMSO)

1a TS syn-s-->anti

0,1

6	-1.031217	2.284579	0.040490
6	0.232682	2.741566	0.372057
6	1.316385	1.874261	0.344090
6	1.224881	0.506897	-0.007969
6	-0.118222	0.029256	-0.233600
6	-1.212409	0.928793	-0.244823
1	-1.888094	2.951575	0.027439
1	0.391531	3.781926	0.644437
1	2.278285	2.279086	0.596798
6	2.510763	-0.290596	-0.126763
6	2.490659	-1.670209	-0.417640
6	3.837741	0.255555	-0.006106
6	3.619051	-2.475846	-0.544188
6	4.973431	-0.558251	-0.115839
6	4.878469	-1.920767	-0.377371
1	3.496574	-3.530740	-0.772816
1	5.955338	-0.117945	0.000408
1	5.780294	-2.522158	-0.455057
6	-2.613309	0.507944	-0.581133
6	-3.078885	0.613525	-1.892919
6	-3.519822	0.102810	0.421158
6	-4.401391	0.308714	-2.228255
1	-2.384223	0.937303	-2.663542
6	-4.845115	-0.200311	0.095927
6	-5.279387	-0.098273	-1.229310
1	-4.736086	0.393269	-3.258072
1	-5.543556	-0.516962	0.862101
1	-6.312057	-0.338259	-1.468801
16	-0.643230	-1.691941	-0.475280
6	-0.409443	-2.343803	1.222346
1	-0.815227	-3.359850	1.222937
1	0.648449	-2.378559	1.499684
1	-0.968005	-1.726819	1.928447
8	-3.010613	0.028503	1.690943
6	-3.888437	-0.322788	2.747423
1	-4.298800	-1.332919	2.615649
1	-3.286786	-0.294377	3.657999
1	-4.717101	0.391990	2.838701
1	1.534368	-2.134862	-0.591321
8	4.006118	1.599558	0.205355
6	5.306261	2.164246	0.235989

1	5.848332	1.983693	-0.700748
1	5.153950	3.237922	0.363679
1	5.897650	1.782234	1.078001

SCF Done: E(RB+HF-LYP) = -1360.86917295

Thermal correction to Enthalpy= 0.379470
Thermal correction to Gibbs Free Energy= 0.306674
Sum of electronic and zero-point Energies= -1360.511896
Sum of electronic and thermal Energies= -1360.490647
Sum of electronic and thermal Enthalpies= -1360.489703
Sum of electronic and thermal Free Energies= -1360.562499

E(B2PLYPD) = -1359.8078881 (gas phase)
E(B2PLYPD) = -1359.8179930 (SCRF IN DMSO)

1a TS syn-a-->syn-s

0,1

6	-1.257166	-1.339118	2.058298
6	-0.052282	-1.587636	2.710101
6	1.135608	-1.328632	2.039537
6	1.159758	-0.827555	0.726387
6	-0.065980	-0.591411	0.063972
6	-1.281743	-0.844885	0.753021
1	-2.203199	-1.525500	2.559197
1	-0.040179	-1.973797	3.725406
1	2.087544	-1.506448	2.532522
6	2.529201	-0.618367	0.154811
6	3.289493	-1.711368	-0.269510
6	3.133669	0.657831	0.150038
6	4.604630	-1.562333	-0.719916
6	4.452276	0.815635	-0.291787
6	5.179919	-0.295014	-0.728130
1	5.169482	-2.428290	-1.052554
1	4.918588	1.794357	-0.297958
1	6.202339	-0.157928	-1.070461
6	-2.619942	-0.633947	0.112195
6	-3.242288	0.634056	0.129062
6	-3.306823	-1.705048	-0.464580
6	-4.511672	0.804014	-0.434660
6	-4.575101	-1.543389	-1.028211
6	-5.170034	-0.285394	-1.011407
1	-4.994080	1.774795	-0.425984
1	-5.086740	-2.391324	-1.474130
1	-6.155970	-0.139117	-1.445232
16	-0.342913	-0.033890	-1.622156

6	1.247492	0.224080	-2.480592
1	0.940009	0.464325	-3.503436
1	1.808021	1.065376	-2.073473
1	1.869779	-0.670435	-2.499551
1	2.830817	-2.696524	-0.247703
1	-2.826875	-2.679988	-0.474190
8	2.346881	1.687043	0.582442
8	-2.532664	1.634127	0.727191
6	2.907921	2.987093	0.652907
1	3.213674	3.353053	-0.336595
1	2.118235	3.630153	1.045297
1	3.772203	3.017983	1.329655
6	-3.069696	2.944605	0.714876
1	-2.329668	3.574238	1.212512
1	-3.225597	3.308249	-0.309473
1	-4.018961	3.000418	1.265078

SCF Done: E(UB+HF-LYP) = -1360.88502422

Thermal correction to Enthalpy= 0.379084
Thermal correction to Gibbs Free Energy= 0.304683
Sum of electronic and zero-point Energies= -1360.528358
Sum of electronic and thermal Energies= -1360.506884
Sum of electronic and thermal Enthalpies= -1360.505940
Sum of electronic and thermal Free Energies= -1360.580341

E(B2PLYPD) = -1359.8225444 (gas phase)
E(B2PLYPD) = -1359.8344437 (SCRF IN DMSO)

1a TS anti-->syn-a

0,1

6	-1.028418	2.362716	-0.626917
6	0.279128	2.804601	-0.736162
6	1.329730	1.912338	-0.577594
6	1.158246	0.532827	-0.311138
6	-0.208601	0.074648	-0.340929
6	-1.280228	0.999035	-0.444819
1	-1.863824	3.052512	-0.699792
1	0.494724	3.852494	-0.928888
1	2.326781	2.303880	-0.653216
6	2.394604	-0.297144	-0.016700
6	2.310936	-1.689982	0.186232
6	3.726176	0.229902	0.134453
6	3.392707	-2.523271	0.457977
6	4.818315	-0.610883	0.388324
6	4.667323	-1.984463	0.543928

1	3.222620	-3.586941	0.598760
1	5.809053	-0.183022	0.472061
1	5.536512	-2.607150	0.738326
6	-2.723062	0.600145	-0.412693
6	-3.541855	0.860811	-1.514859
6	-3.322390	0.059957	0.747879
6	-4.910154	0.575690	-1.501076
1	-3.086915	1.285471	-2.406043
6	-4.690650	-0.224013	0.771966
6	-5.478809	0.032359	-0.354015
1	-5.518298	0.778499	-2.377892
1	-5.150334	-0.641223	1.660576
1	-6.541135	-0.195264	-0.321220
16	-0.774857	-1.650032	-0.352334
6	-0.217654	-2.162986	-2.021061
1	-0.594878	-3.178637	-2.173131
1	-0.642078	-1.506002	-2.784107
1	0.873620	-2.170316	-2.099127
8	-2.483930	-0.150972	1.804980
6	-3.009133	-0.747797	2.978913
1	-3.424495	-1.742772	2.773068
1	-2.166960	-0.842492	3.666640
1	-3.784073	-0.119959	3.438699
1	1.334265	-2.144439	0.164189
8	3.939172	1.581413	0.047901
6	5.223412	2.123491	0.306812
1	5.962884	1.795410	-0.435012
1	5.101704	3.206266	0.235503
1	5.576786	1.863232	1.312390

SCF Done: E(UB+HF-LYP) = -1360.86960754

Thermal correction to Enthalpy= 0.379451
Thermal correction to Gibbs Free Energy= 0.306726
Sum of electronic and zero-point Energies= -1360.512323
Sum of electronic and thermal Energies= -1360.491100
Sum of electronic and thermal Enthalpies= -1360.490156
Sum of electronic and thermal Free Energies= -1360.562881

E(B2PLYPD) = -1359.8080066(gas phase)
E(B2PLYPD) = -1359.818009 (SCRF IN DMSO)

1a TS anti-->anti

0,1

6	-1.237774	0.168269	2.374439
6	-0.058562	-0.107650	3.061233

6	1.103600	-0.323492	2.332815
6	1.127384	-0.265423	0.928866
6	-0.071080	0.016884	0.236522
6	-1.262074	0.229159	0.980150
1	-2.164703	0.335863	2.916049
1	-0.046956	-0.155824	4.146433
1	2.035459	-0.541048	2.847798
6	2.460303	-0.546763	0.304074
6	2.894582	-1.863094	0.130293
6	3.354039	0.499927	-0.010021
6	4.167438	-2.156224	-0.368695
6	4.632454	0.216379	-0.503752
6	5.031263	-1.111125	-0.683566
1	4.477602	-3.188591	-0.501605
1	5.319615	1.018083	-0.749220
1	6.026165	-1.318276	-1.069057
6	-2.569032	0.541253	0.316602
6	-3.438559	-0.493474	-0.093501
6	-2.979531	1.864973	0.141913
6	-4.675558	-0.187598	-0.671653
6	-4.213885	2.178326	-0.432898
6	-5.055420	1.146772	-0.838968
1	-5.346385	-0.977469	-0.989843
1	-4.509344	3.215624	-0.560760
1	-6.019401	1.370361	-1.288880
16	-0.341371	0.149295	-1.536106
6	1.221176	-0.111488	-2.444569
1	0.910050	-0.048424	-3.492295
1	1.951074	0.673336	-2.246434
1	1.662087	-1.091529	-2.263792
1	2.212671	-2.668725	0.389621
1	-2.308936	2.658821	0.459655
8	2.874765	1.764446	0.185199
8	-2.990017	-1.764275	0.122601
6	3.735676	2.862986	-0.065641
1	4.039454	2.909539	-1.120087
1	3.157799	3.755420	0.180974
1	4.633498	2.825123	0.565578
6	-3.785437	-2.847009	-0.326860
1	-3.227027	-3.751042	-0.076565
1	-4.759940	-2.872954	0.179615
1	-3.944836	-2.807896	-1.412592

SCF Done: E(UB+HF-LYP) = -1360.88528359

Thermal correction to Enthalpy= 0.379096
Thermal correction to Gibbs Free Energy= 0.304195

Sum of electronic and zero-point Energies= -1360.528633
Sum of electronic and thermal Energies= -1360.507132
Sum of electronic and thermal Enthalpies= -1360.506188
Sum of electronic and thermal Free Energies= -1360.581089

E(B2PLYPD) = -1359.8226222 (gas phase)
E(B2PLYPD) = -1359.8342621 (SCRF IN DMSO)

2a syn-s

0,1

6	-1.132364	2.618816	-0.408005
6	0.128068	3.211210	-0.425159
6	1.266243	2.413187	-0.460547
6	1.170412	1.013346	-0.494465
6	-0.109919	0.422682	-0.454483
6	-1.269647	1.224486	-0.409123
1	-2.026524	3.234833	-0.372920
1	0.222179	4.293902	-0.413514
1	2.250318	2.870914	-0.479390
6	2.428465	0.216401	-0.624229
6	3.452198	0.302486	0.346773
6	2.642851	-0.601467	-1.739504
6	4.644407	-0.415054	0.187079
6	3.829260	-1.317292	-1.904774
1	1.854710	-0.679463	-2.480372
6	4.827697	-1.220093	-0.938859
1	5.429255	-0.352623	0.932084
1	3.970699	-1.939368	-2.783686
1	5.758041	-1.770578	-1.052358
6	-2.649116	0.649578	-0.400759
6	-3.501798	0.871164	-1.484740
6	-3.152515	-0.060528	0.713179
6	-4.815230	0.392818	-1.498293
1	-3.116918	1.422552	-2.338704
6	-4.464669	-0.541498	0.706685
6	-5.288831	-0.317002	-0.400418
1	-5.452684	0.572220	-2.359163
1	-4.854638	-1.089694	1.556503
1	-6.306237	-0.699329	-0.389936
6	0.554855	-1.975109	1.141080
1	0.274279	-3.010720	1.348922
1	1.637757	-1.898783	1.040912
1	0.184960	-1.323272	1.932151
8	3.192943	1.103868	1.425714
8	-2.296549	-0.207146	1.766819
6	4.175402	1.213018	2.440762

1	3.755216	1.886411	3.190325
1	4.388086	0.241006	2.905903
1	5.112145	1.638565	2.056325
6	-2.757888	-0.894384	2.917236
1	-3.020801	-1.935461	2.688163
1	-1.928127	-0.880223	3.626653
1	-3.625450	-0.393761	3.367428
34	-0.339550	-1.488279	-0.540359

SCF Done: E(RB+HF-LYP) = -3362.09254852

Thermal correction to Enthalpy= 0.379466
Thermal correction to Gibbs Free Energy= 0.303116
Sum of electronic and zero-point Energies= -3361.736575
Sum of electronic and thermal Energies= -3361.714027
Sum of electronic and thermal Enthalpies= -3361.713083
Sum of electronic and thermal Free Energies= -3361.789433

E(B2PLYPD) = -3362.8778709 (gas phase)
E(B2PLYPD) = -3362.888005 (SCRF IN DMSO)

2a syn-a

0,1

6	-1.220336	2.381498	-1.438751
6	-0.019181	2.946272	-1.857933
6	1.189063	2.388228	-1.448741
6	1.214473	1.261384	-0.613936
6	-0.006489	0.703796	-0.185639
6	-1.234075	1.256754	-0.599357
1	-2.166113	2.804282	-1.765859
1	-0.024482	3.814633	-2.511541
1	2.130043	2.815540	-1.783852
6	2.536387	0.730212	-0.168850
6	3.413179	1.542923	0.556257
6	2.953259	-0.579318	-0.496345
6	4.659052	1.077590	0.986602
6	4.191802	-1.055279	-0.058338
6	5.039136	-0.225892	0.682007
1	5.316085	1.726330	1.558565
1	4.507678	-2.064209	-0.299239
1	6.001178	-0.608820	1.012607
6	-2.551862	0.728388	-0.139528
6	-2.969906	-0.586843	-0.442858
6	-3.431567	1.555957	0.564365
6	-4.213829	-1.050455	-0.007280
6	-4.680899	1.102119	0.996012

6	-5.063854	-0.204831	0.711402
1	-4.531760	-2.062621	-0.230670
1	-5.339185	1.763052	1.552352
1	-6.029439	-0.578796	1.041877
6	0.203446	0.254539	2.690440
1	0.233521	-0.461065	3.515569
1	1.136426	0.819084	2.659461
1	-0.657580	0.913825	2.807640
1	3.097270	2.553758	0.801725
1	-3.114641	2.570319	0.793004
8	2.094326	-1.303538	-1.271791
8	-2.101854	-1.331957	-1.189660
6	2.230308	-2.714318	-1.283261
1	2.202859	-3.119193	-0.263869
1	1.375400	-3.091088	-1.848834
1	3.153558	-3.035328	-1.783576
6	-2.297573	-2.734354	-1.247713
1	-1.440089	-3.132188	-1.794327
1	-2.325450	-3.171169	-0.241443
1	-3.216359	-2.998215	-1.787975
34	0.003179	-0.795423	1.031431

SCF Done: E(RB+HF-LYP) = -3362.09503222

Thermal correction to Enthalpy= 0.379251
Thermal correction to Gibbs Free Energy= 0.302901
Sum of electronic and zero-point Energies= -3361.739350
Sum of electronic and thermal Energies= -3361.716725
Sum of electronic and thermal Enthalpies= -3361.715781
Sum of electronic and thermal Free Energies= -3361.792131

E(B2PLYPD) = -3362.878305 (gas phase)
E(B2PLYPD) = -3362.8882803 (SCRF IN DMSO)

2a anti

0,1

6	-1.212059	-2.080530	-1.734461
6	-0.037811	-2.452375	-2.382657
6	1.167407	-1.849161	-2.030630
6	1.215750	-0.867438	-1.031624
6	0.014176	-0.464758	-0.412538
6	-1.205633	-1.080327	-0.750462
1	-2.154537	-2.553428	-1.995823
1	-0.058790	-3.220307	-3.151441
1	2.092754	-2.155279	-2.510876
6	2.537901	-0.279373	-0.665654

6	3.284672	0.433754	-1.608443
6	3.082057	-0.455665	0.626689
6	4.522863	0.998854	-1.288771
6	4.310694	0.123523	0.958196
6	5.025181	0.848689	0.000691
1	5.078029	1.556464	-2.037504
1	4.722909	-0.001230	1.953326
1	5.981784	1.287889	0.271735
6	-2.491390	-0.753019	-0.061567
6	-3.082960	-1.697733	0.780090
6	-3.166502	0.468473	-0.277909
6	-4.303037	-1.453787	1.417208
1	-2.565124	-2.639546	0.941873
6	-4.387641	0.719046	0.354348
6	-4.947963	-0.240658	1.202878
1	-4.736209	-2.203505	2.072885
1	-4.909517	1.655594	0.195355
1	-5.896918	-0.028735	1.688670
6	0.489761	2.443123	-0.176033
1	0.389812	3.326257	0.460292
1	1.517002	2.359531	-0.531837
1	-0.214057	2.502020	-1.005685
8	-2.568126	1.338137	-1.144584
6	-3.228205	2.559498	-1.431979
1	-3.334157	3.182826	-0.534367
1	-2.597296	3.077253	-2.157185
1	-4.219431	2.389200	-1.872598
1	2.870784	0.562278	-2.605516
8	2.360422	-1.238259	1.478113
6	2.599339	-1.113727	2.870746
1	2.517104	-0.067628	3.190416
1	1.822822	-1.704689	3.360390
1	3.582261	-1.512258	3.155263
34	0.019200	0.898523	0.949873

SCF Done: E(UB+HF-LYP) = -3362.09389975

Thermal correction to Enthalpy= 0.379408
Thermal correction to Gibbs Free Energy= 0.303073
Sum of electronic and zero-point Energies= -3361.738002
Sum of electronic and thermal Energies= -3361.715436
Sum of electronic and thermal Enthalpies= -3361.714492
Sum of electronic and thermal Free Energies= -3361.790827

E(B2PLYPD) = -3362.8787498 (gas phase)
E(B2PLYPD) = -3362.8883561 (SCRF IN DMSO)

2a TS syn-s-->anti

0,1

6	-0.888430	2.526415	-0.119913
6	0.391507	2.975845	0.158386
6	1.453461	2.082164	0.182383
6	1.324206	0.693780	-0.063015
6	-0.031515	0.236946	-0.218512
6	-1.104277	1.156370	-0.286903
1	-1.729278	3.211433	-0.174601
1	0.579627	4.029791	0.346937
1	2.428216	2.481506	0.390829
6	2.590909	-0.139529	-0.151303
6	2.541459	-1.537871	-0.327832
6	3.929610	0.390480	-0.119943
6	3.653838	-2.370520	-0.417337
6	5.049386	-0.449252	-0.190381
6	4.926282	-1.826994	-0.331531
1	3.507769	-3.438313	-0.554170
1	6.040478	-0.017237	-0.139925
1	5.815963	-2.449082	-0.381838
6	-2.513893	0.731868	-0.571237
6	-3.033576	0.867691	-1.858904
6	-3.367052	0.269927	0.453431
6	-4.363046	0.544737	-2.150112
1	-2.377061	1.229233	-2.646064
6	-4.698184	-0.046542	0.173419
6	-5.189148	0.087110	-1.129990
1	-4.741781	0.653469	-3.162273
1	-5.358175	-0.404040	0.955513
1	-6.226042	-0.166901	-1.334224
6	-0.325965	-2.073692	1.561433
1	-0.771192	-3.059762	1.717401
1	0.747256	-2.121046	1.761470
1	-0.811501	-1.336538	2.199411
8	-2.806719	0.177512	1.697061
6	-3.639681	-0.195948	2.782143
1	-4.034789	-1.213198	2.659881
1	-3.007100	-0.160646	3.671306
1	-4.477593	0.502688	2.905617
1	1.576789	-2.007804	-0.437673
8	4.125612	1.744963	-0.035633
6	5.434232	2.286542	-0.099772
1	5.941176	2.011079	-1.033083
1	5.302411	3.369993	-0.066748
1	6.048642	1.972927	0.754006
34	-0.676683	-1.597658	-0.310469

SCF Done: E(UB+HF-LYP) = -3362.07202248

Thermal correction to Enthalpy= 0.379145
Thermal correction to Gibbs Free Energy= 0.305819
Sum of electronic and zero-point Energies= -3361.715302
Sum of electronic and thermal Energies= -3361.693822
Sum of electronic and thermal Enthalpies= -3361.692878
Sum of electronic and thermal Free Energies= -3361.766203

E(B2PLYPD) = -3362.8537199 (gas phase)
E(B2PLYPD) = -3362.8634989 (SCRF IN DMSO)

2a TS syn-a-->syn-s

0,1

6	-1.184723	-0.883940	2.449151
6	0.003026	-1.000510	3.161451
6	1.212072	-0.881512	2.480423
6	1.235826	-0.656580	1.103176
6	0.024435	-0.546516	0.380486
6	-1.202562	-0.652444	1.063440
1	-2.137415	-0.965596	2.965603
1	-0.013078	-1.178454	4.233047
1	2.156034	-0.963577	3.012386
6	2.555670	-0.569253	0.402469
6	3.174073	-1.719654	-0.094090
6	3.208255	0.672457	0.238211
6	4.414163	-1.664514	-0.734500
6	4.450913	0.735495	-0.402578
6	5.045366	-0.432998	-0.886016
1	4.875559	-2.572451	-1.111614
1	4.959290	1.684532	-0.528833
1	6.010376	-0.369360	-1.382372
6	-2.556313	-0.555607	0.434201
6	-3.141904	0.698615	0.155816
6	-3.314943	-1.706316	0.205716
6	-4.446661	0.775751	-0.344260
6	-4.615390	-1.639396	-0.303423
6	-5.175216	-0.394421	-0.575461
1	-4.900669	1.736996	-0.556726
1	-5.180915	-2.549924	-0.478839
1	-6.186548	-0.320869	-0.966821
6	-1.380525	-0.150413	-2.436923
1	-1.085112	-0.109666	-3.489180
1	-2.010110	-1.021035	-2.266257
1	-1.892910	0.769372	-2.164526

1	2.662981	-2.671227	0.024903
1	-2.868953	-2.671045	0.433078
8	2.556873	1.756179	0.748414
8	-2.352703	1.786259	0.398335
6	3.122114	3.039625	0.548205
1	3.233157	3.269200	-0.519799
1	2.423016	3.746449	0.999118
1	4.099447	3.134972	1.040718
6	-2.899701	3.078979	0.201117
1	-2.112102	3.780420	0.481835
1	-3.176758	3.248570	-0.848154
1	-3.779745	3.246400	0.836340
34	0.348720	-0.301901	-1.506653

SCF Done: E(UB+HF-LYP) = -3362.08132985

Thermal correction to Enthalpy= 0.378444
Thermal correction to Gibbs Free Energy= 0.302917
Sum of electronic and zero-point Energies= -3361.725694
Sum of electronic and thermal Energies= -3361.703830
Sum of electronic and thermal Enthalpies= -3361.702886
Sum of electronic and thermal Free Energies= -3361.778413

E(B2PLYPD) = -3362.8717671 (gas phase)
E(B2PLYPD) = -3362.883512 (SCRF IN DMSO)

2a TS anti-->syn-a

0,1

6	-0.878095	2.537987	-0.230954
6	0.421750	2.994110	-0.099238
6	1.470273	2.091236	0.006630
6	1.311231	0.684597	-0.007569
6	-0.053406	0.237014	-0.100391
6	-1.119286	1.161294	-0.221871
1	-1.711869	3.227271	-0.324594
1	0.635261	4.059940	-0.081334
1	2.459103	2.497515	0.099789
6	2.566402	-0.174775	0.047221
6	2.489051	-1.582198	0.044717
6	3.916580	0.327262	0.086349
6	3.581462	-2.444049	0.082762
6	5.016882	-0.540186	0.125910
6	4.864815	-1.922013	0.125337
1	3.411443	-3.517103	0.080779
1	6.016880	-0.127652	0.157369
1	5.740942	-2.564342	0.156908

6	-2.552592	0.747406	-0.388746
6	-3.194999	0.935772	-1.613985
6	-3.323141	0.304361	0.710099
6	-4.555626	0.653628	-1.780649
1	-2.611046	1.306383	-2.452850
6	-4.682243	0.024560	0.553927
6	-5.292425	0.197548	-0.693582
1	-5.027624	0.797117	-2.748359
1	-5.273762	-0.324121	1.392826
1	-6.351281	-0.023155	-0.800979
6	-0.638980	-1.951973	-1.960833
1	-0.981468	-2.979281	-2.108888
1	-1.305335	-1.265961	-2.486903
1	0.386419	-1.853016	-2.323418
8	-2.644450	0.173175	1.887386
6	-3.331010	-0.360257	3.006942
1	-3.711171	-1.369363	2.801188
1	-2.596079	-0.407438	3.812636
1	-4.164782	0.284331	3.315957
1	1.513174	-2.039004	0.027358
8	4.147500	1.679199	0.080730
6	5.471721	2.184458	0.108365
1	6.048312	1.862512	-0.768095
1	5.368424	3.271345	0.091082
1	6.001953	1.886863	1.021936
34	-0.729475	-1.591591	-0.035205

SCF Done: E(UB+HF-LYP) = -3362.07204260

Thermal correction to Enthalpy= 0.378959
Thermal correction to Gibbs Free Energy= 0.305079
Sum of electronic and zero-point Energies= -3361.715619
Sum of electronic and thermal Energies= -3361.694028
Sum of electronic and thermal Enthalpies= -3361.693084
Sum of electronic and thermal Free Energies= -3361.766964

E(B2PLYPD) = -3362.8523799 (gas phase)
E(B2PLYPD) = -3362.8618811 (SCRF IN DMSO)

2a TS anti-->anti

0,1

6	-1.137370	-0.866573	2.472574
6	-0.529436	-2.015338	1.980187
6	0.675404	-1.898623	1.291176
6	1.270014	-0.650577	1.099818
6	0.652161	0.515266	1.610215

6	-0.570088	0.406725	2.300443
1	-2.080252	-0.938351	3.008222
1	-0.989916	-2.988204	2.127711
1	1.169197	-2.779440	0.889761
6	2.571303	-0.568195	0.365394
6	3.783964	-0.638226	1.055981
6	2.600948	-0.429573	-1.039652
6	5.009080	-0.585991	0.387622
6	3.825015	-0.375164	-1.716172
6	5.021116	-0.453421	-0.998292
1	5.939140	-0.644482	0.945355
1	3.855881	-0.272108	-2.794819
1	5.964749	-0.410123	-1.536215
6	-1.357647	1.556692	2.846155
6	-1.145393	2.027556	4.159726
6	-2.386993	2.127330	2.094145
6	-1.947446	3.047839	4.683664
6	-3.187667	3.152891	2.606184
6	-2.962068	3.607726	3.902336
1	-1.788976	3.412623	5.692090
1	-3.978778	3.583510	1.999235
1	-3.576359	4.400909	4.320541
6	0.787710	3.655664	2.019545
1	1.431364	4.487336	1.719057
1	-0.215333	3.804265	1.626278
1	0.780342	3.574103	3.104142
1	3.754999	-0.731243	2.138217
1	-2.557088	1.754279	1.087603
8	1.385209	-0.369108	-1.654959
8	-0.123090	1.432994	4.843329
6	1.345960	-0.152454	-3.054770
1	1.816457	-0.977210	-3.607119
1	0.287880	-0.101902	-3.318510
1	1.834242	0.791426	-3.330917
6	0.119957	1.831875	6.182128
1	0.956552	1.221425	6.526675
1	0.396322	2.892880	6.246711
1	-0.752402	1.648313	6.823456
34	1.679253	2.100072	1.204318

SCF Done: E(UB+HF-LYP) = -3362.08160397

Thermal correction to Enthalpy= 0.378431
Thermal correction to Gibbs Free Energy= 0.302748
Sum of electronic and zero-point Energies= -3361.725984
Sum of electronic and thermal Energies= -3361.704117
Sum of electronic and thermal Enthalpies= -3361.703173

Sum of electronic and thermal Free Energies= -3361.778856

E(B2PLYPD) = -3362.8719118 (gas phase)
E(B2PLYPD) = -3362.883353 (SCRF IN DMSO)

1H NMR Spectroscopic Chemical Shifts for Me Groups in
1a and 2a were done by GIAO/WP04/cc-pVDZ with
the PCM-SCRF model, using dimethylsulfoxide as a solvent (SCRF IN DMSO).
Obtained data were scaled following the protocol outlined
in reference 21.

1a syn-s

Me-S
32 H Isotropic = 30.4680 Anisotropy = 11.7146
XX= 27.7898 YX= -0.3688 ZX= 0.5471
XY= 0.1319 YY= 26.9958 ZY= -4.2425
XZ= 0.0370 YZ= -4.3823 ZZ= 36.6186
Eigenvalues: 25.3460 27.7803 38.2778
33 H Isotropic = 29.8518 Anisotropy = 9.9493
XX= 35.6636 YX= -0.9557 ZX= -2.0166
XY= -2.4497 YY= 27.0522 ZY= -3.8086
XZ= -3.4765 YZ= -4.2989 ZZ= 26.8395
Eigenvalues: 22.1508 30.9199 36.4846
34 H Isotropic = 29.5131 Anisotropy = 8.4089
XX= 29.9019 YX= 1.5744 ZX= 1.9968
XY= 3.6063 YY= 33.7678 ZY= -1.8033
XZ= 1.7813 YZ= -1.6514 ZZ= 24.8697
Eigenvalues: 23.6118 29.8085 35.1191
Me-O
38 H Isotropic = 27.9659 Anisotropy = 8.8448
XX= 26.6698 YX= -2.4794 ZX= 0.0891
XY= -1.5756 YY= 32.3355 ZY= 3.4708
XZ= 0.8874 YZ= 2.6484 ZZ= 24.8923
Eigenvalues: 23.3611 26.6740 33.8624
39 H Isotropic = 28.1387 Anisotropy = 8.9684
XX= 27.4265 YX= -2.3933 ZX= 2.3895
XY= -4.0147 YY= 30.6259 ZY= -3.1904
XZ= 1.3558 YZ= -2.5401 ZZ= 26.3636
Eigenvalues: 24.8433 25.4551 34.1176
40 H Isotropic = 28.1125 Anisotropy = 9.2852
XX= 31.3136 YX= -2.1760 ZX= -2.7542
XY= -4.2393 YY= 26.4665 ZY= 1.6804
XZ= -2.5884 YZ= 2.2900 ZZ= 26.5574
Eigenvalues: 24.4559 25.5790 34.3026
Me-O
42 H Isotropic = 28.0737 Anisotropy = 8.7450

XX= 26.9180 YX= 0.6795 ZX= -1.9219
XY= 2.5460 YY= 27.5538 ZY= -4.7207
XZ= -2.0570 YZ= -3.6229 ZZ= 29.7493
Eigenvalues: 24.3356 25.9818 33.9037
43 H Isotropic = 28.0226 Anisotropy = 8.6449
XX= 26.9833 YX= 0.2582 ZX= -0.8458
XY= -0.9766 YY= 33.3251 ZY= -1.9432
XZ= -0.5549 YZ= -2.3249 ZZ= 23.7594
Eigenvalues: 23.1540 27.1279 33.7858
44 H Isotropic = 28.2274 Anisotropy = 9.7102
XX= 28.8483 YX= 3.5264 ZX= 0.8837
XY= 5.2752 YY= 31.2842 ZY= 0.5328
XZ= -0.3622 YZ= 1.1639 ZZ= 24.5498
Eigenvalues: 24.3971 25.5844 34.7009

1a syn-a

Me-S
30 H Isotropic = 30.6375 Anisotropy = 12.4211
XX= 27.3609 YX= -0.0922 ZX= -0.4992
XY= -0.2784 YY= 25.6579 ZY= 0.6579
XZ= -0.4206 YZ= -0.1007 ZZ= 38.8938
Eigenvalues: 25.6340 27.3603 38.9183
31 H Isotropic = 30.0108 Anisotropy = 8.2827
XX= 33.0194 YX= -2.8820 ZX= 1.0814
XY= -5.4734 YY= 27.4745 ZY= 4.3002
XZ= 0.9401 YZ= 4.0488 ZZ= 29.5385
Eigenvalues: 22.6796 31.8202 35.5326
32 H Isotropic = 30.1003 Anisotropy = 8.9667
XX= 30.7902 YX= 2.7191 ZX= -0.3435
XY= 4.3774 YY= 30.2103 ZY= 5.2857
XZ= -0.0429 YZ= 4.6911 ZZ= 29.3002
Eigenvalues: 23.7535 30.4693 36.0780
Me-O
38 H Isotropic = 28.1379 Anisotropy = 8.5761
XX= 26.4983 YX= 0.6034 ZX= -0.8297
XY= 1.9513 YY= 32.1302 ZY= -4.0162
XZ= 0.0224 YZ= -2.8004 ZZ= 25.7852
Eigenvalues: 24.2917 26.2667 33.8553
39 H Isotropic = 27.9634 Anisotropy = 8.5785
XX= 27.2567 YX= 0.0483 ZX= -1.0805
XY= -1.3745 YY= 32.6780 ZY= 2.9592
XZ= -1.2839 YZ= 2.7634 ZZ= 23.9555
Eigenvalues: 22.8927 27.3152 33.6824
40 H Isotropic = 28.1052 Anisotropy = 9.7329
XX= 28.5322 YX= 2.7898 ZX= 1.9926
XY= 4.7120 YY= 29.8187 ZY= 2.8764

XZ= 1.8077 YZ= 3.6524 ZZ= 25.9648
Eigenvalues: 24.0805 25.6414 34.5938
Me-O
42 H Isotropic = 27.9727 Anisotropy = 8.5362
XX= 27.4303 YX= 0.0093 ZX= 1.1163
XY= 1.5437 YY= 32.8772 ZY= 2.5195
XZ= 1.3076 YZ= 2.3820 ZZ= 23.6105
Eigenvalues: 22.7868 27.4678 33.6635
43 H Isotropic = 28.1417 Anisotropy = 8.5537
XX= 26.5538 YX= -0.5946 ZX= 0.8867
XY= -1.9637 YY= 31.8166 ZY= -4.2812
XZ= 0.1174 YZ= -3.0215 ZZ= 26.0548
Eigenvalues: 24.2792 26.3017 33.8442
44 H Isotropic = 28.1312 Anisotropy = 9.7467
XX= 28.4449 YX= -2.8295 ZX= -1.8484
XY= -4.7101 YY= 30.2105 ZY= 2.7893
XZ= -1.5703 YZ= 3.5767 ZZ= 25.7384
Eigenvalues: 24.0622 25.7025 34.6290

1a anti

Me-S
31 H Isotropic = 30.4963 Anisotropy = 11.8233
XX= 27.6682 YX= -0.1619 ZX= 0.5759
XY= 0.3222 YY= 28.1875 ZY= 5.3588
XZ= 0.8573 YZ= 5.1161 ZZ= 35.6332
Eigenvalues: 25.4541 27.6563 38.3785
32 H Isotropic = 29.8504 Anisotropy = 8.3275
XX= 32.8003 YX= -2.2626 ZX= 2.8297
XY= -4.2049 YY= 31.1644 ZY= 3.1536
XZ= 3.9783 YZ= 3.1440 ZZ= 25.5865
Eigenvalues: 22.2633 31.8859 35.4020
33 H Isotropic = 29.3767 Anisotropy = 9.6822
XX= 32.5635 YX= 2.6938 ZX= -2.3374
XY= 4.9810 YY= 31.2997 ZY= 2.4834
XZ= -2.6021 YZ= 2.3154 ZZ= 24.2668
Eigenvalues: 22.2357 30.0628 35.8315
Me-O
36 H Isotropic = 28.0712 Anisotropy = 8.8961
XX= 27.4792 YX= 1.1487 ZX= 2.9210
XY= 3.0330 YY= 28.1099 ZY= 4.4338
XZ= 2.4993 YZ= 3.2522 ZZ= 28.6244
Eigenvalues: 24.4472 25.7644 34.0019
37 H Isotropic = 28.0692 Anisotropy = 8.9651
XX= 26.8590 YX= 2.1199 ZX= 1.0648
XY= 0.9537 YY= 33.6944 ZY= -0.0196
XZ= 1.1386 YZ= 0.5166 ZZ= 23.6543

Eigenvalues: 23.3072 26.8545 34.0460
38 H Isotropic = 28.2522 Anisotropy = 9.7104
XX= 31.1655 YX= 3.4111 ZX= -1.4464
XY= 5.3600 YY= 28.5625 ZY= -0.8743
XZ= -0.6767 YZ= -1.8547 ZZ= 25.0286
Eigenvalues: 24.4872 25.5436 34.7258
Me-O
42 H Isotropic = 28.2379 Anisotropy = 8.7285
XX= 26.7560 YX= 0.4455 ZX= -1.8869
XY= 2.2294 YY= 27.7931 ZY= -4.8326
XZ= -1.6417 YZ= -3.6556 ZZ= 30.1646
Eigenvalues: 24.5722 26.0847 34.0569
43 H Isotropic = 28.0806 Anisotropy = 9.0154
XX= 26.6830 YX= 0.6168 ZX= -1.3583
XY= -0.6261 YY= 33.7638 ZY= -1.6364
XZ= -1.0616 YZ= -1.9998 ZZ= 23.7951
Eigenvalues: 23.0790 27.0720 34.0909
44 H Isotropic = 28.1479 Anisotropy = 9.8309
XX= 29.9517 YX= 3.6980 ZX= 0.4215
XY= 5.4294 YY= 30.3117 ZY= -0.1185
XZ= -0.6009 YZ= 0.7826 ZZ= 24.1805
Eigenvalues: 24.1175 25.6245 34.7019

2a syn-s

Me-Se
31 H Isotropic = 30.5382 Anisotropy = 12.7953
XX= 27.8294 YX= -0.1008 ZX= 0.2943
XY= 0.2617 YY= 35.3587 ZY= -6.7942
XZ= -0.2669 YZ= -5.7714 ZZ= 28.4266
Eigenvalues: 24.7163 27.8300 39.0685
32 H Isotropic = 30.1636 Anisotropy = 10.4602
XX= 36.8836 YX= 0.8641 ZX= 0.4823
XY= 2.4389 YY= 26.2073 ZY= -4.5506
XZ= 1.1899 YZ= -4.1772 ZZ= 27.3999
Eigenvalues: 22.1799 31.1738 37.1371
33 H Isotropic = 29.8681 Anisotropy = 8.0857
XX= 29.4857 YX= -1.5444 ZX= -0.1663
XY= -1.1889 YY= 25.0893 ZY= 0.6435
XZ= -1.9896 YZ= -0.1042 ZZ= 35.0293
Eigenvalues: 24.6990 29.6468 35.2586
Me-O
37 H Isotropic = 27.9714 Anisotropy = 8.9366
XX= 26.7479 YX= 0.3802 ZX= 2.8207
XY= -0.5496 YY= 25.8972 ZY= 3.3903
XZ= 2.0758 YZ= 4.3249 ZZ= 31.2691

Eigenvalues: 23.3806 26.6045 33.9291
38 H Isotropic = 28.1743 Anisotropy = 8.9482
XX= 27.5179 YX= -2.0962 ZX= 2.7614
XY= -0.8347 YY= 25.9002 ZY= -1.9925
XZ= 4.2127 YZ= -2.6247 ZZ= 31.1048
Eigenvalues: 24.9878 25.3953 34.1398
39 H Isotropic = 28.0958 Anisotropy = 9.4165
XX= 31.8106 YX= 2.8750 ZX= 1.7607
XY= 3.0010 YY= 26.7541 ZY= 2.0421
XZ= 3.7818 YZ= 1.4101 ZZ= 25.7228
Eigenvalues: 24.3657 25.5482 34.3735
Me-O
41 H Isotropic = 28.1162 Anisotropy = 8.6335
XX= 27.1235 YX= 1.5617 ZX= -0.8944
XY= 1.8043 YY= 30.2801 ZY= -3.6075
XZ= -2.6190 YZ= -4.5765 ZZ= 26.9451
Eigenvalues: 24.0822 26.3946 33.8719
42 H Isotropic = 28.0406 Anisotropy = 8.5208
XX= 27.3268 YX= 0.5227 ZX= -0.1604
XY= 0.0801 YY= 23.8481 ZY= -2.8524
XZ= 1.0840 YZ= -2.5963 ZZ= 32.9470
Eigenvalues: 23.0546 27.3461 33.7212
43 H Isotropic = 28.1828 Anisotropy = 10.0418
XX= 28.4556 YX= -0.6252 ZX= -3.5386
XY= 0.7372 YY= 24.1210 ZY= 0.4022
XZ= -5.0996 YZ= -0.1734 ZZ= 31.9718
Eigenvalues: 24.1121 25.5590 34.8773

2a syn-a

Me-Se
29 H Isotropic = 30.9630 Anisotropy = 13.8267
XX= 27.0364 YX= -0.0839 ZX= 0.6035
XY= -0.0241 YY= 26.5425 ZY= -3.2682
XZ= 0.6513 YZ= -3.4992 ZZ= 39.3100
Eigenvalues: 25.6937 27.0144 40.1808
30 H Isotropic = 30.3714 Anisotropy = 9.3015
XX= 32.5581 YX= 3.6838 ZX= 0.4060
XY= 5.9064 YY= 26.5181 ZY= 3.9708
XZ= 0.8770 YZ= 3.2546 ZZ= 32.0381
Eigenvalues: 22.9327 31.6091 36.5724
31 H Isotropic = 30.3387 Anisotropy = 10.1337
XX= 30.8701 YX= -3.2032 ZX= -0.8055
XY= -4.8049 YY= 27.7210 ZY= 5.3391
XZ= -1.3036 YZ= 4.3545 ZZ= 32.4251
Eigenvalues: 23.4752 30.4464 37.0945

Me-O
37 H Isotropic = 28.1756 Anisotropy = 7.4511
XX= 27.1040 YX= -0.3676 ZX= -0.7811
XY= -1.1653 YY= 32.4624 ZY= -2.8341
XZ= -1.6963 YZ= -1.7813 ZZ= 24.9603
Eigenvalues: 23.7240 27.6598 33.1430
38 H Isotropic = 27.9767 Anisotropy = 8.3631
XX= 27.9899 YX= 0.4233 ZX= 1.1517
XY= 1.8221 YY= 31.2364 ZY= 4.1833
XZ= 1.3555 YZ= 3.7710 ZZ= 24.7037
Eigenvalues: 22.7385 27.6395 33.5521
39 H Isotropic = 27.7810 Anisotropy = 9.8640
XX= 27.9722 YX= -2.3626 ZX= -1.5314
XY= -4.2774 YY= 30.2480 ZY= 3.6684
XZ= -1.4193 YZ= 4.0039 ZZ= 25.1229
Eigenvalues: 23.0522 25.9338 34.3571
Me-O
41 H Isotropic = 27.9658 Anisotropy = 8.3134
XX= 28.0096 YX= -0.1648 ZX= -1.0765
XY= -1.6632 YY= 31.2821 ZY= 4.1680
XZ= -1.4035 YZ= 3.8775 ZZ= 24.6057
Eigenvalues: 22.6133 27.7761 33.5081
42 H Isotropic = 28.1867 Anisotropy = 7.7658
XX= 27.0602 YX= 0.5194 ZX= 0.3553
XY= 1.4600 YY= 32.5927 ZY= -2.9672
XZ= 1.2694 YZ= -1.8236 ZZ= 24.9073
Eigenvalues: 23.8680 27.3283 33.3639
43 H Isotropic = 27.8671 Anisotropy = 9.9437
XX= 28.1018 YX= 2.4565 ZX= 1.7821
XY= 4.2968 YY= 29.8824 ZY= 3.7051
XZ= 1.6928 YZ= 4.2167 ZZ= 25.6170
Eigenvalues: 23.2336 25.8714 34.4962

2a anti

Me-Se
30 H Isotropic = 30.6415 Anisotropy = 12.7968
XX= 27.6475 YX= 0.4334 ZX= -0.3797
XY= -0.1415 YY= 38.6731 ZY= 2.2622
XZ= -0.1552 YZ= 2.9406 ZZ= 25.6038
Eigenvalues: 25.0723 27.6794 39.1727
31 H Isotropic = 30.1447 Anisotropy = 10.1748
XX= 35.0362 YX= -0.8333 ZX= -3.8553
XY= -1.2970 YY= 31.2461 ZY= -2.5023
XZ= -5.9704 YZ= -2.4327 ZZ= 24.1518
Eigenvalues: 21.5208 31.9854 36.9279

32 H Isotropic = 29.7859 Anisotropy = 9.7366
XX= 31.0484 YX= -0.1664 ZX= 2.6728
XY= -1.7030 YY= 29.6942 ZY= -4.8558
XZ= 4.1358 YZ= -5.7482 ZZ= 28.6151
Eigenvalues: 23.3061 29.7746 36.2770
Me-O
35 H Isotropic = 28.0980 Anisotropy = 8.6679
XX= 27.3258 YX= -2.0178 ZX= -1.1413
XY= -3.1873 YY= 32.5043 ZY= 2.2009
XZ= 0.1028 YZ= 0.9477 ZZ= 24.4638
Eigenvalues: 24.1662 26.2511 33.8765
36 H Isotropic = 28.0661 Anisotropy = 8.7917
XX= 26.9756 YX= -1.8217 ZX= 0.1130
XY= -0.8199 YY= 30.5178 ZY= -5.0484
XZ= -0.5054 YZ= -4.5747 ZZ= 26.7049
Eigenvalues: 23.2130 27.0581 33.9272
37 H Isotropic = 28.1949 Anisotropy = 10.0938
XX= 30.4534 YX= -2.5294 ZX= 3.0179
XY= -4.4591 YY= 26.8767 ZY= -2.2873
XZ= 3.4240 YZ= -3.3430 ZZ= 27.2545
Eigenvalues: 24.1907 25.4699 34.9240
Me-O
41 H Isotropic = 28.3575 Anisotropy = 7.6203
XX= 27.1410 YX= -0.4393 ZX= 0.6708
XY= -1.5252 YY= 25.7424 ZY= 2.3812
XZ= 1.8333 YZ= 3.5012 ZZ= 32.1890
Eigenvalues: 23.9936 27.6412 33.4377
42 H Isotropic = 28.1931 Anisotropy = 8.9439
XX= 26.9588 YX= 1.2903 ZX= 0.0505
XY= 1.4194 YY= 25.0182 ZY= -3.2835
XZ= -0.9487 YZ= -3.9092 ZZ= 32.6023
Eigenvalues: 23.2550 27.1686 34.1557
43 H Isotropic = 27.9162 Anisotropy = 10.0380
XX= 28.5772 YX= -1.2375 ZX= 2.9904
XY= -1.0076 YY= 24.7220 ZY= -3.2693
XZ= 5.0696 YZ= -2.7635 ZZ= 30.4494
Eigenvalues: 23.3290 25.8114 34.6082

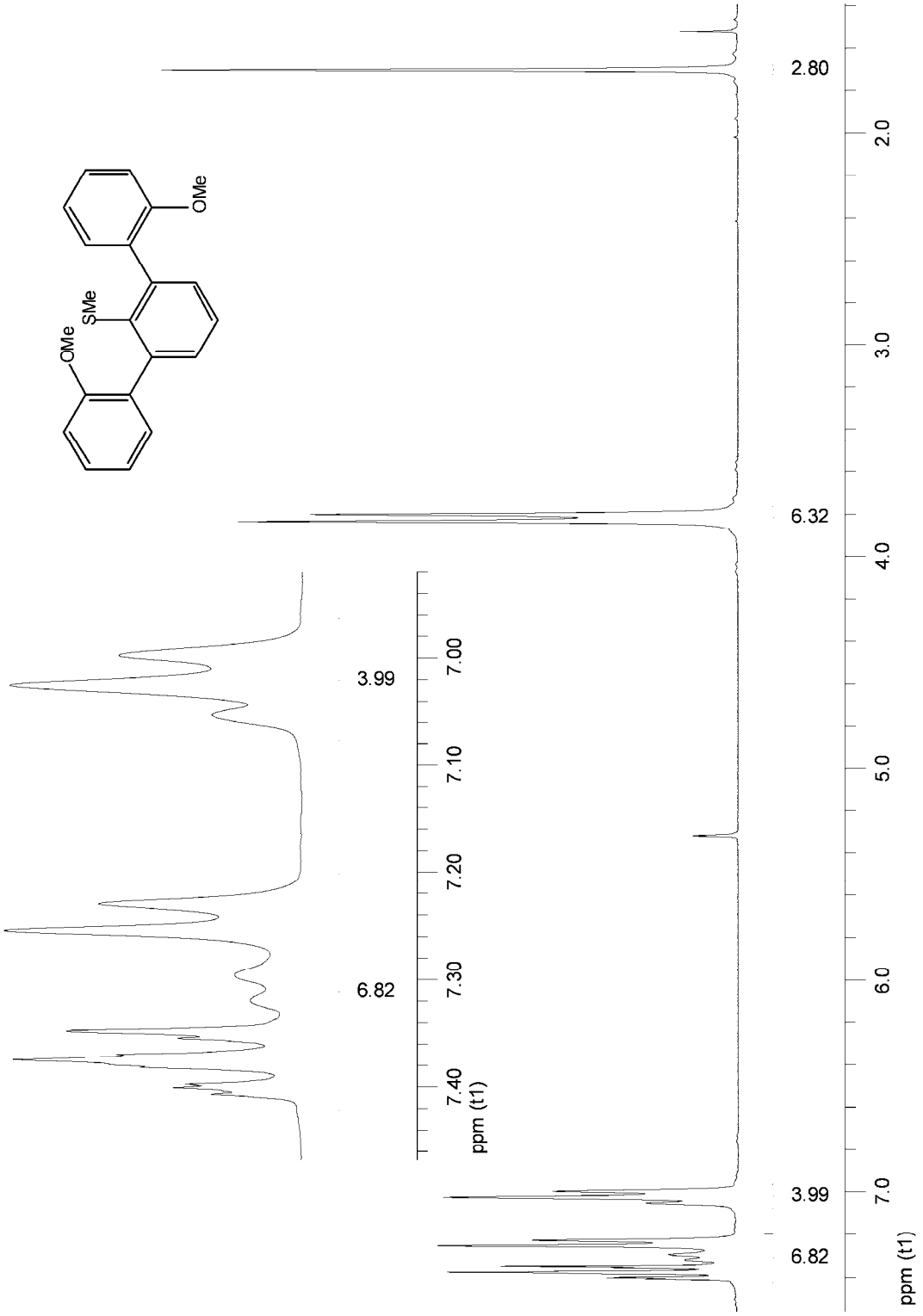


Figure S12. ^{1}H NMR spectrum of **1a**.

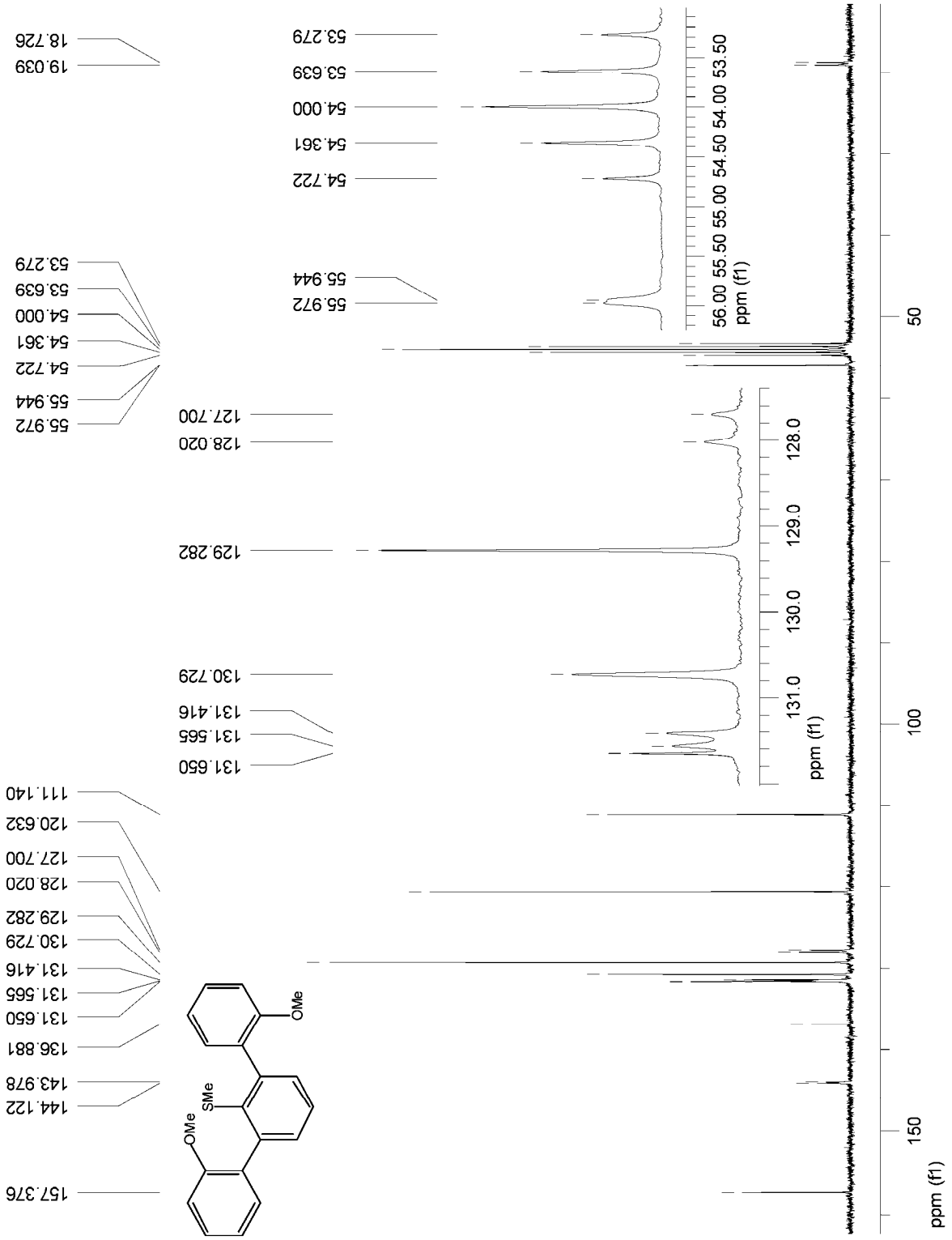


Figure S13. ^{13}C NMR spectrum of **1a**.

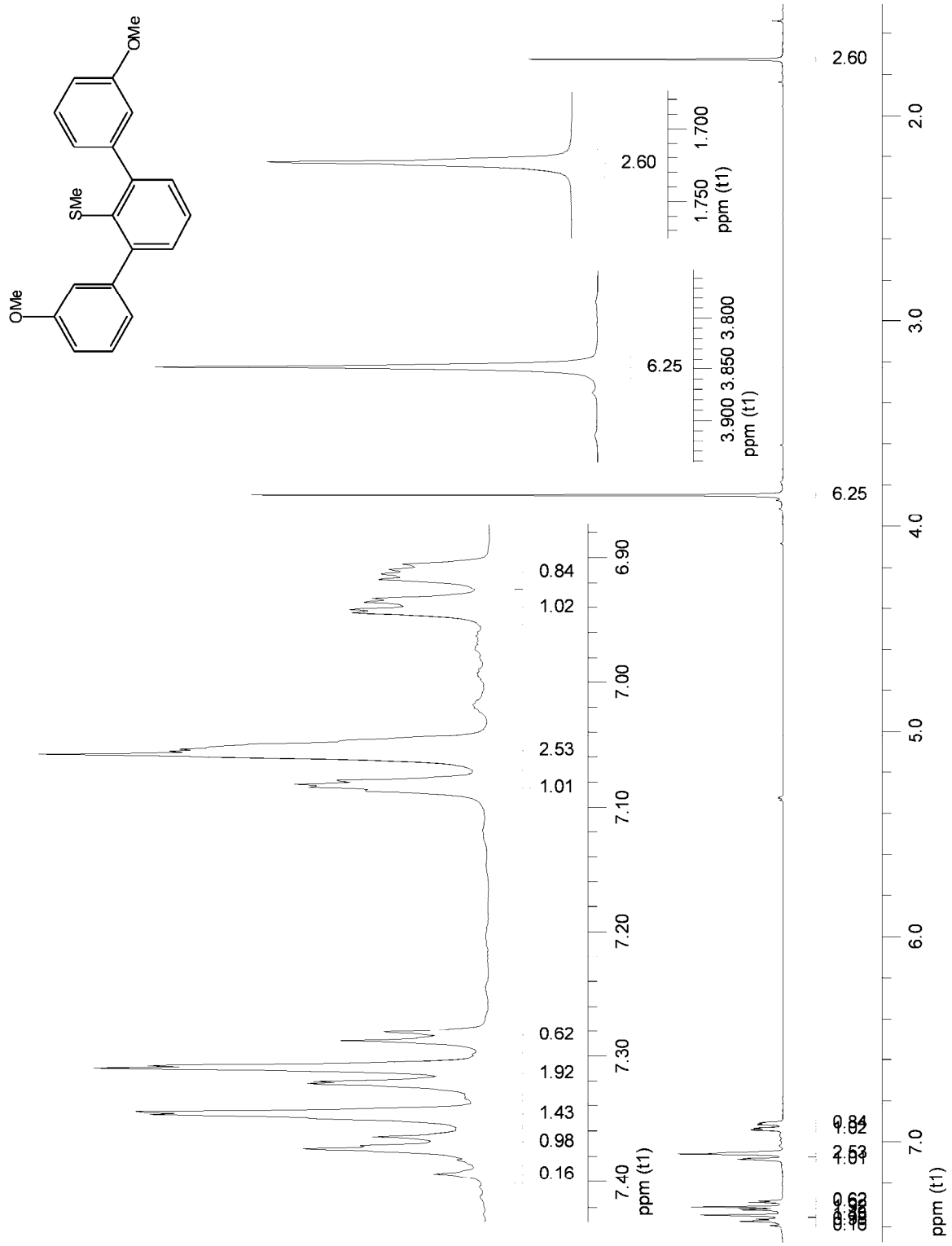


Figure S14. ^{1}H NMR spectrum of **1b**.

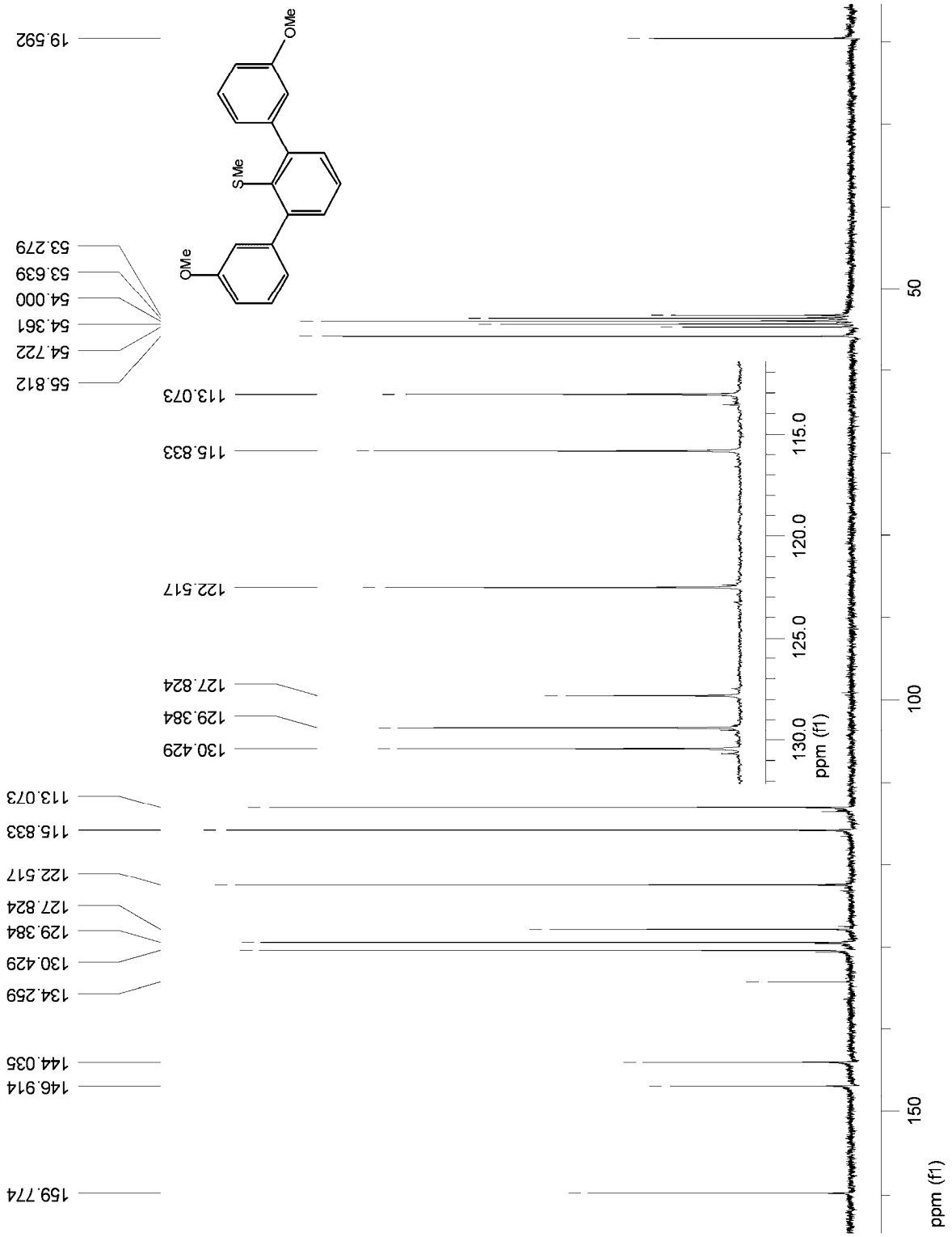


Figure S15. ^{13}C NMR spectrum of **1b**.

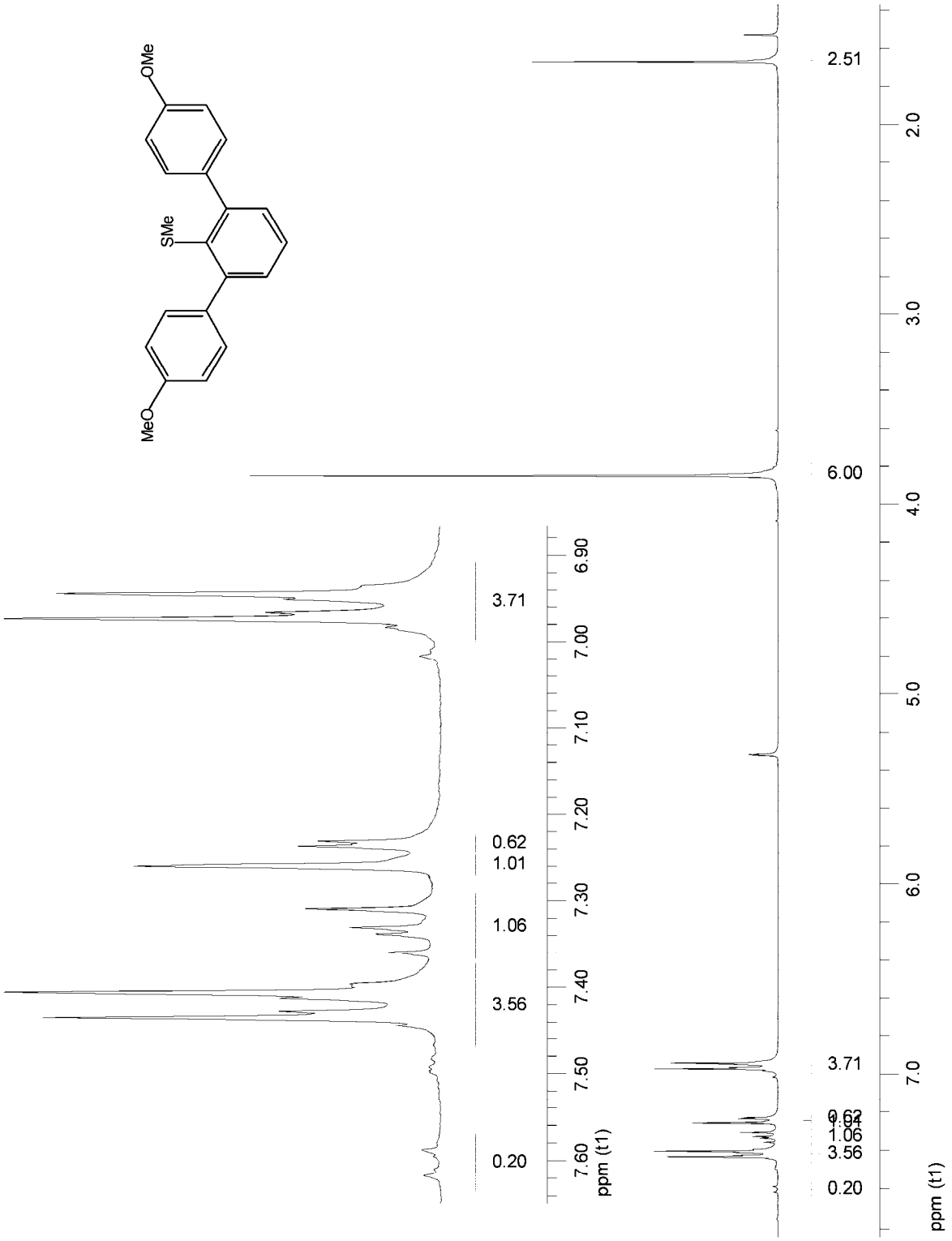


Figure S16. ^{1}H NMR spectrum of **1c**.

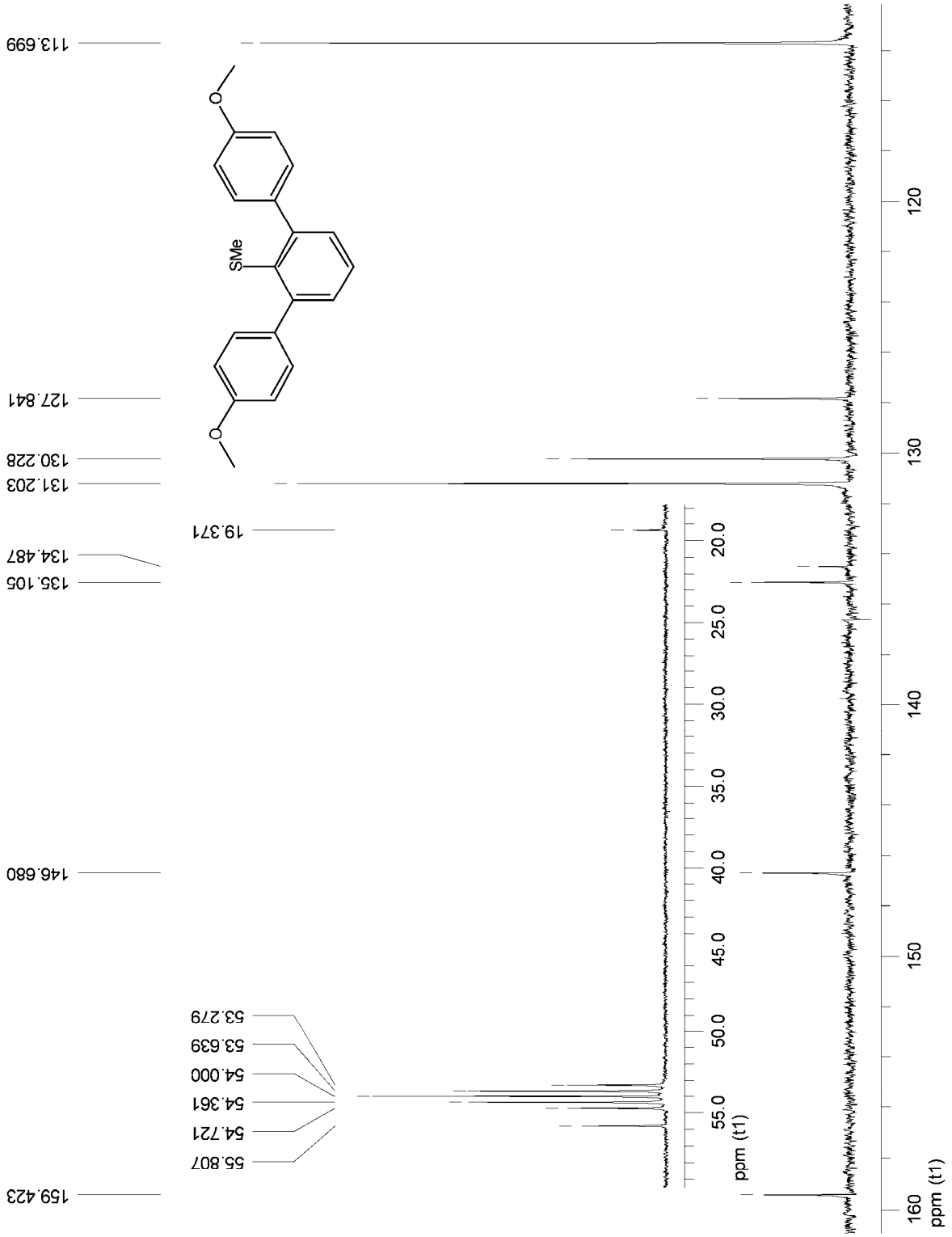


Figure S17. ^{13}C NMR spectrum of **1c**.

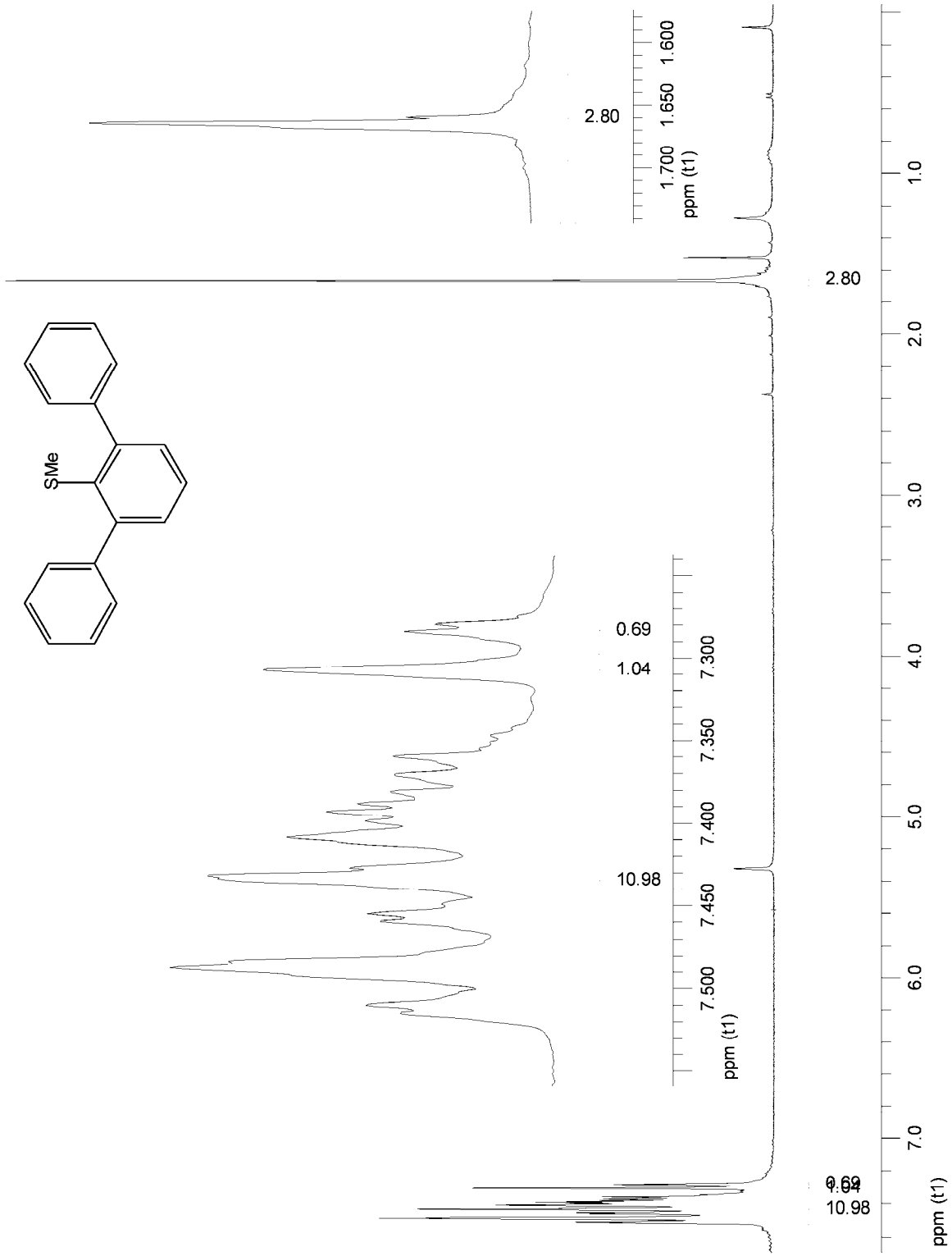


Figure S18. ^{1}H NMR spectrum of **1d**.

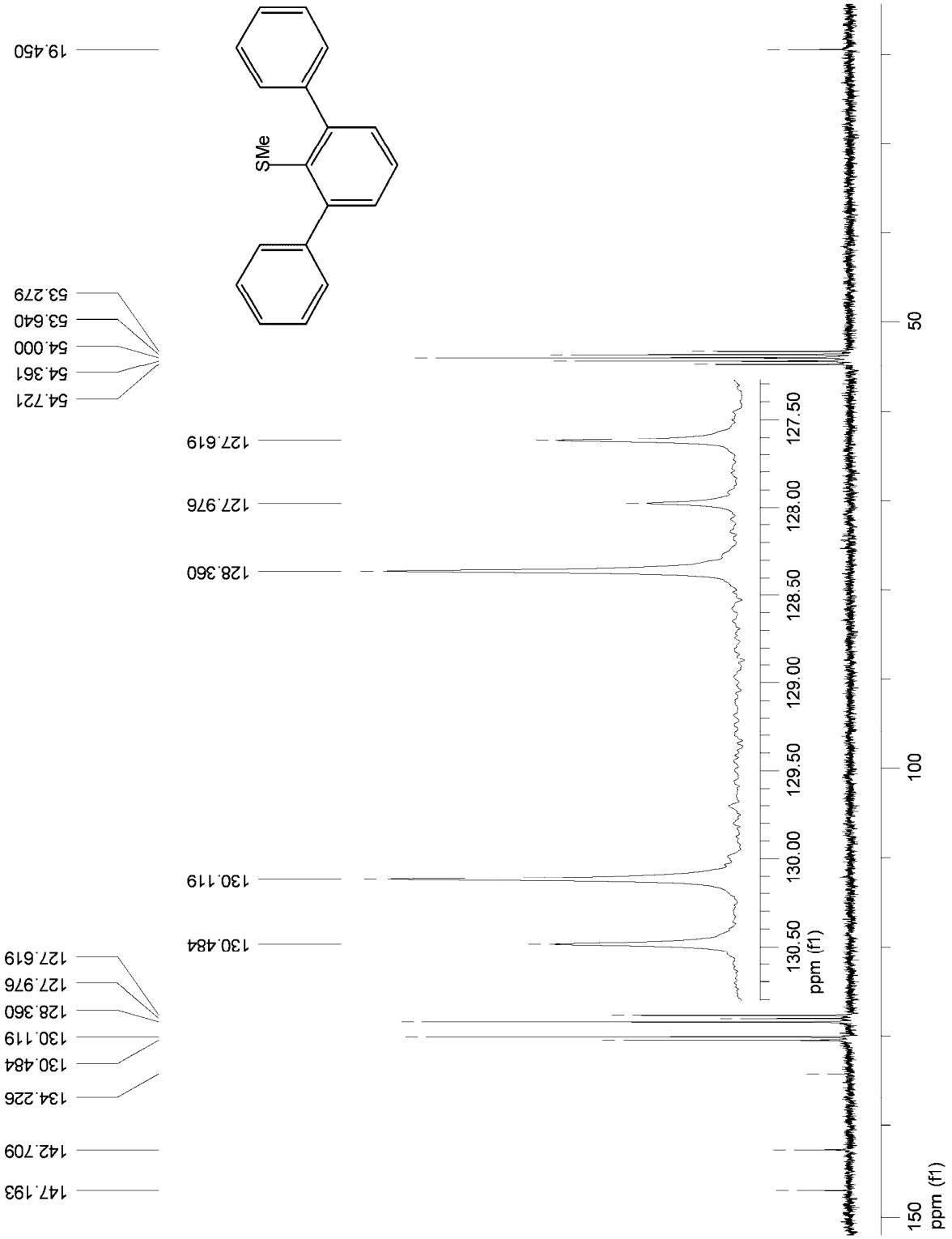


Figure S19. ^{13}C NMR spectrum of **1d**.

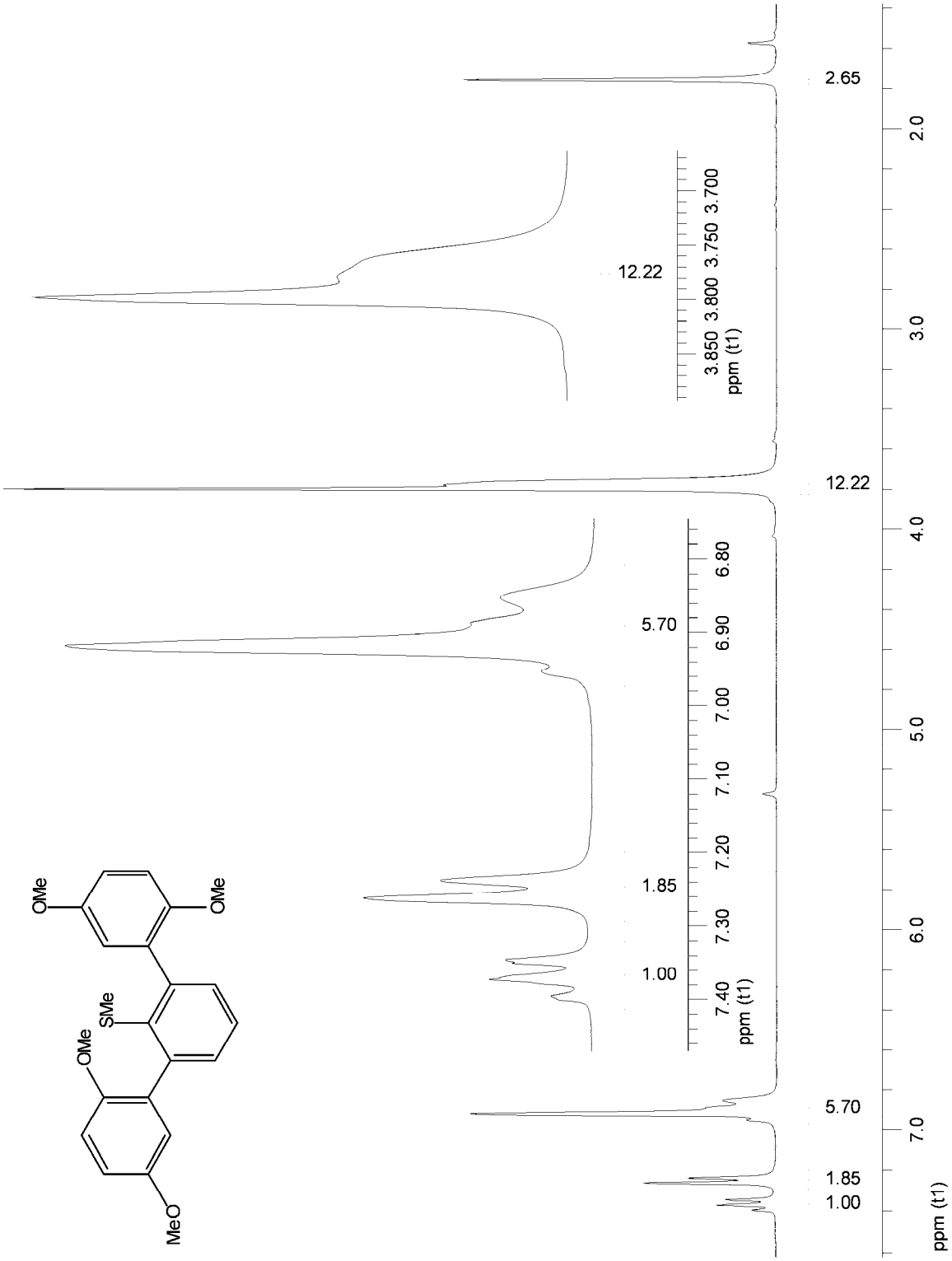


Figure S20. ^{1}H NMR spectrum of **1f**.

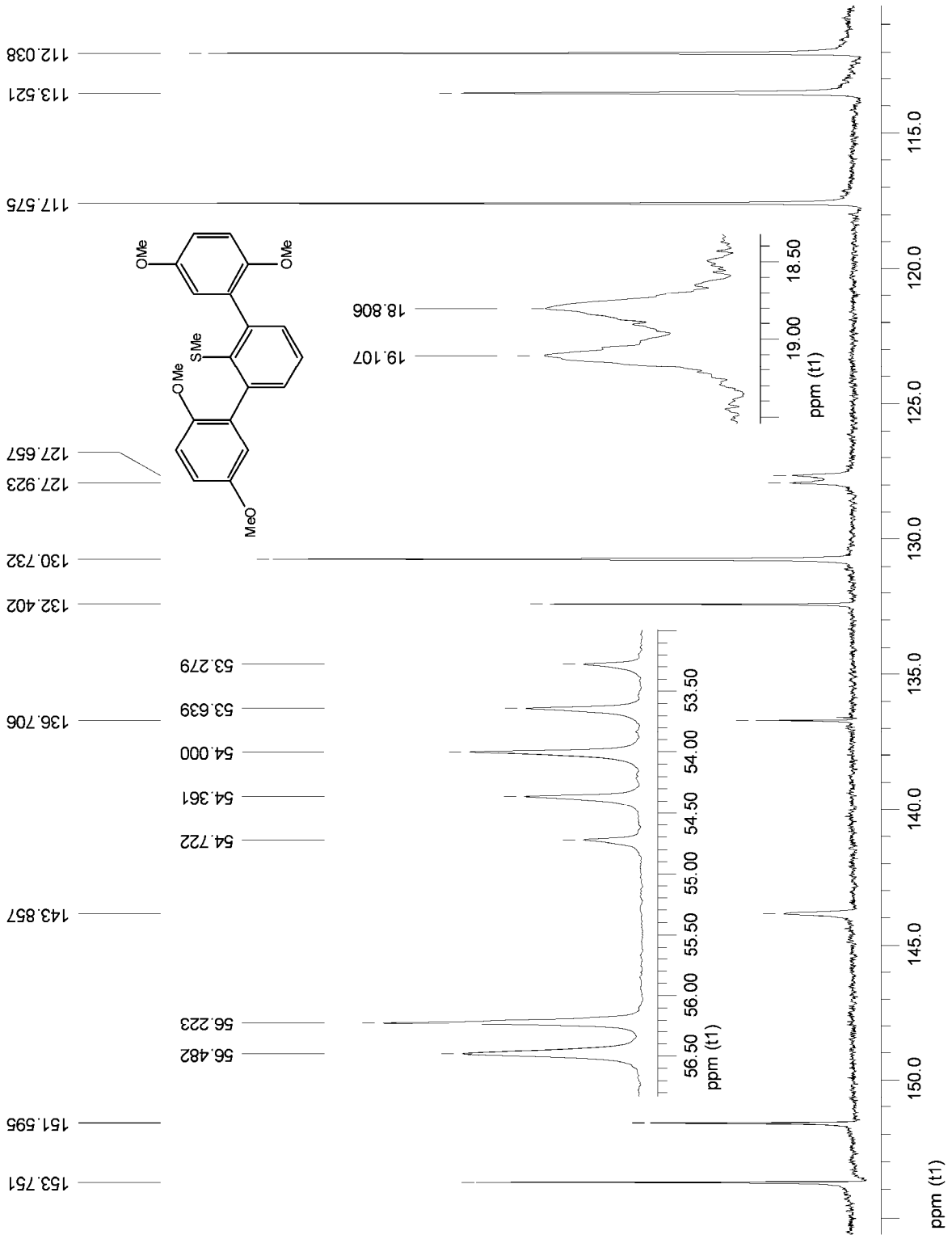


Figure S21. ^{13}C NMR spectrum of **1f**.

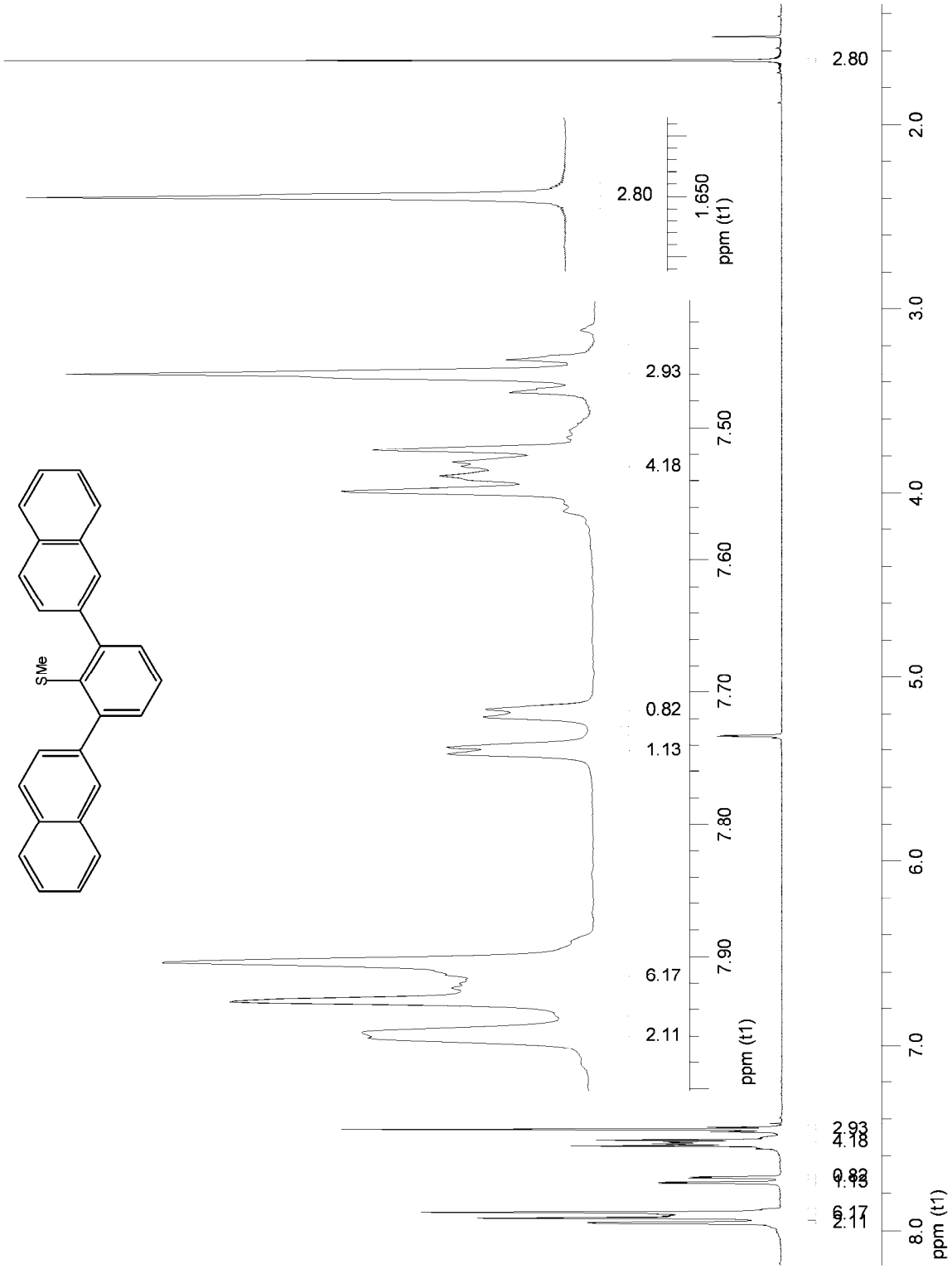


Figure S22. ^{1}H NMR spectrum of **1g**.

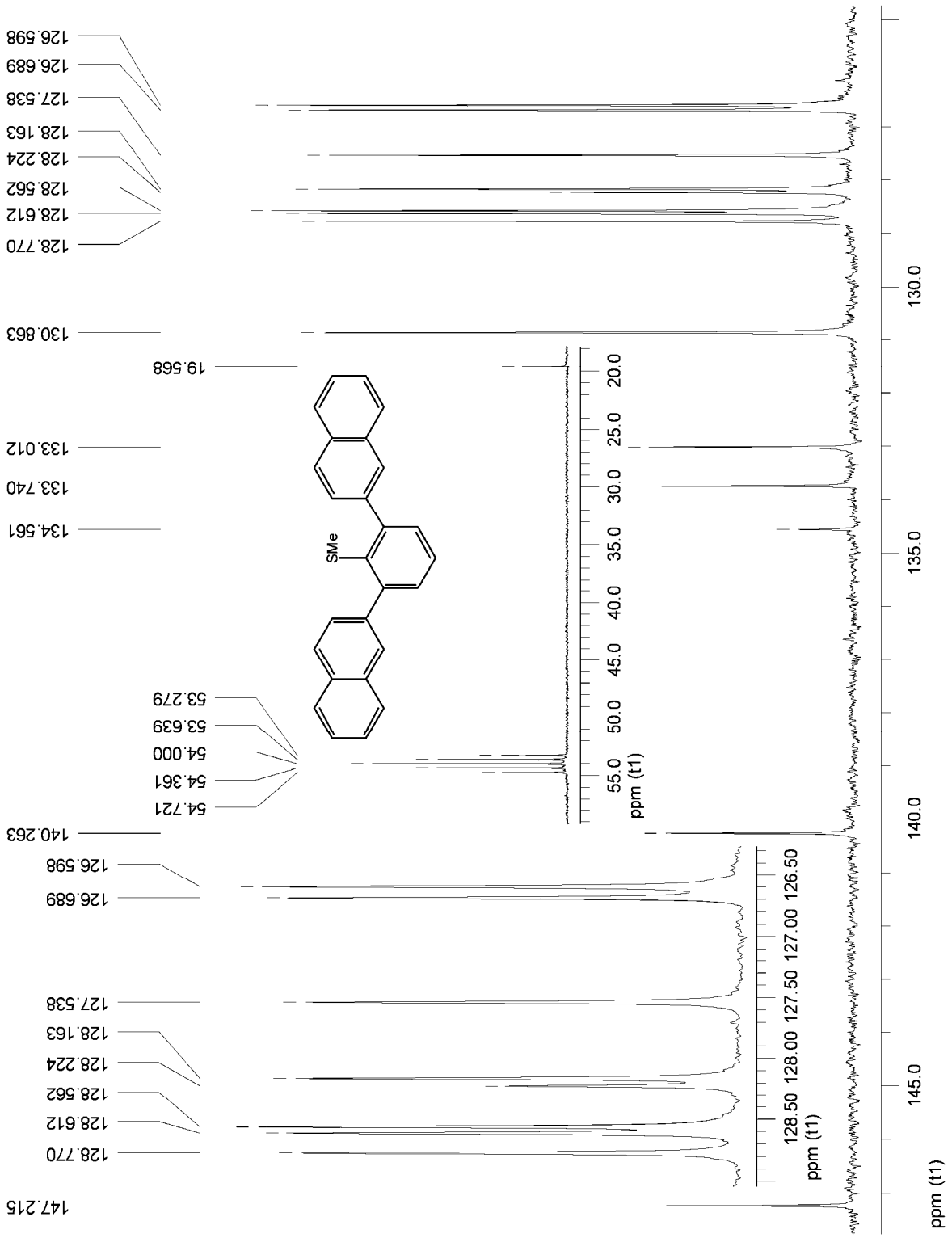


Figure S23. ^{13}C NMR spectrum of **1g**.

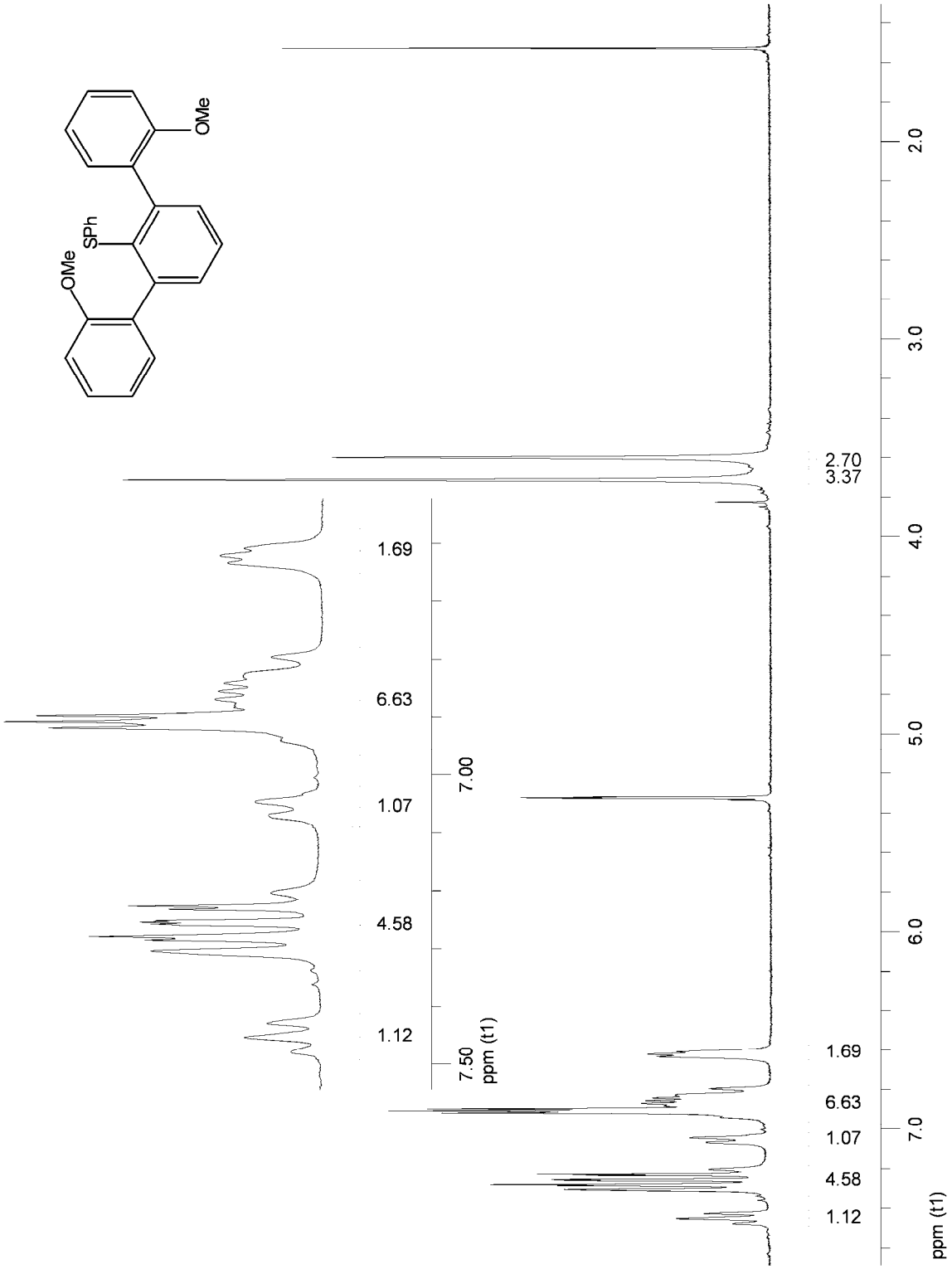


Figure S24. ^{1}H NMR spectrum of **1h**.

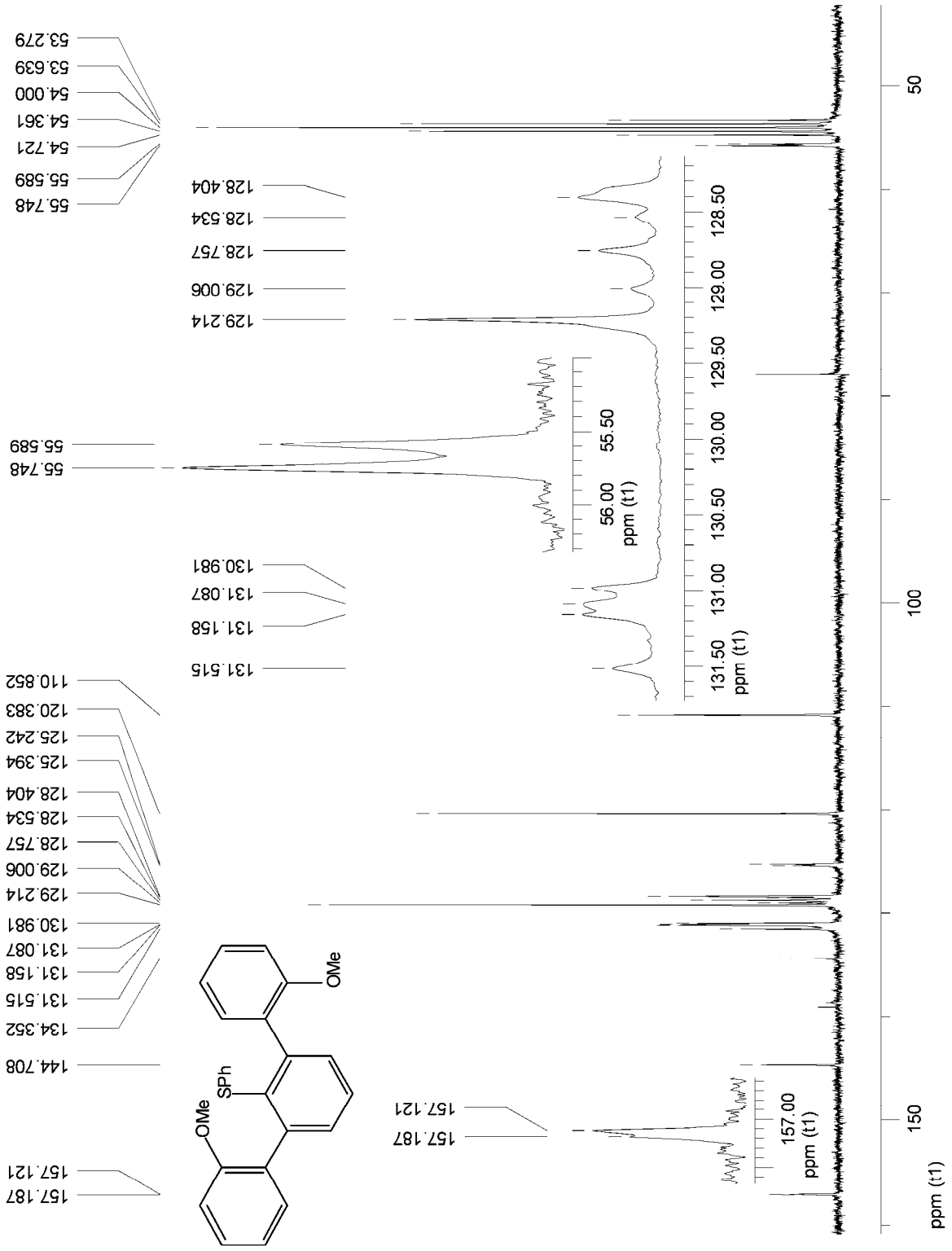


Figure S25. ^{13}C NMR spectrum of **1h**.

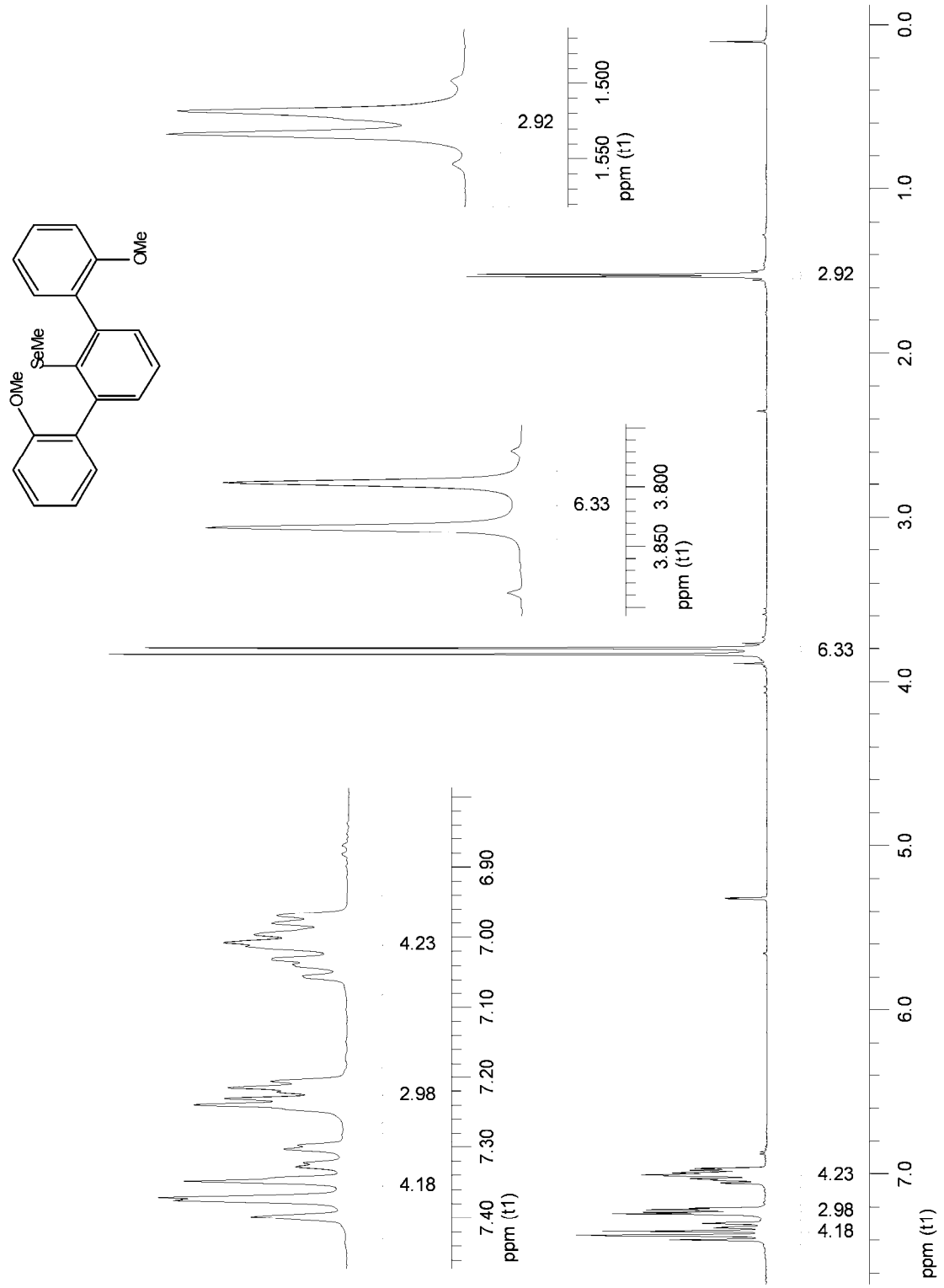


Figure S26. ^{1}H NMR spectrum of **2a**.

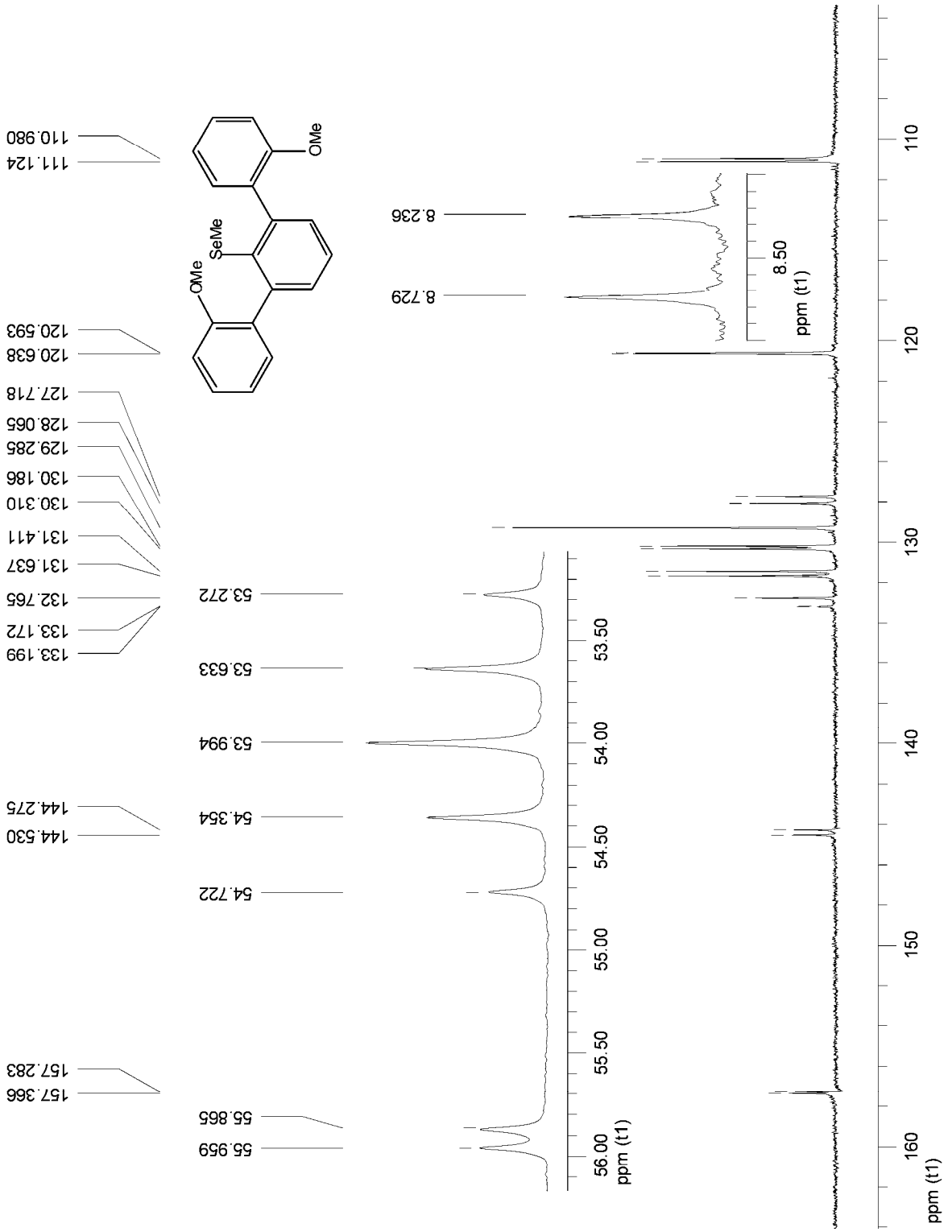


Figure S27. ^{13}C NMR spectrum of **2a**.

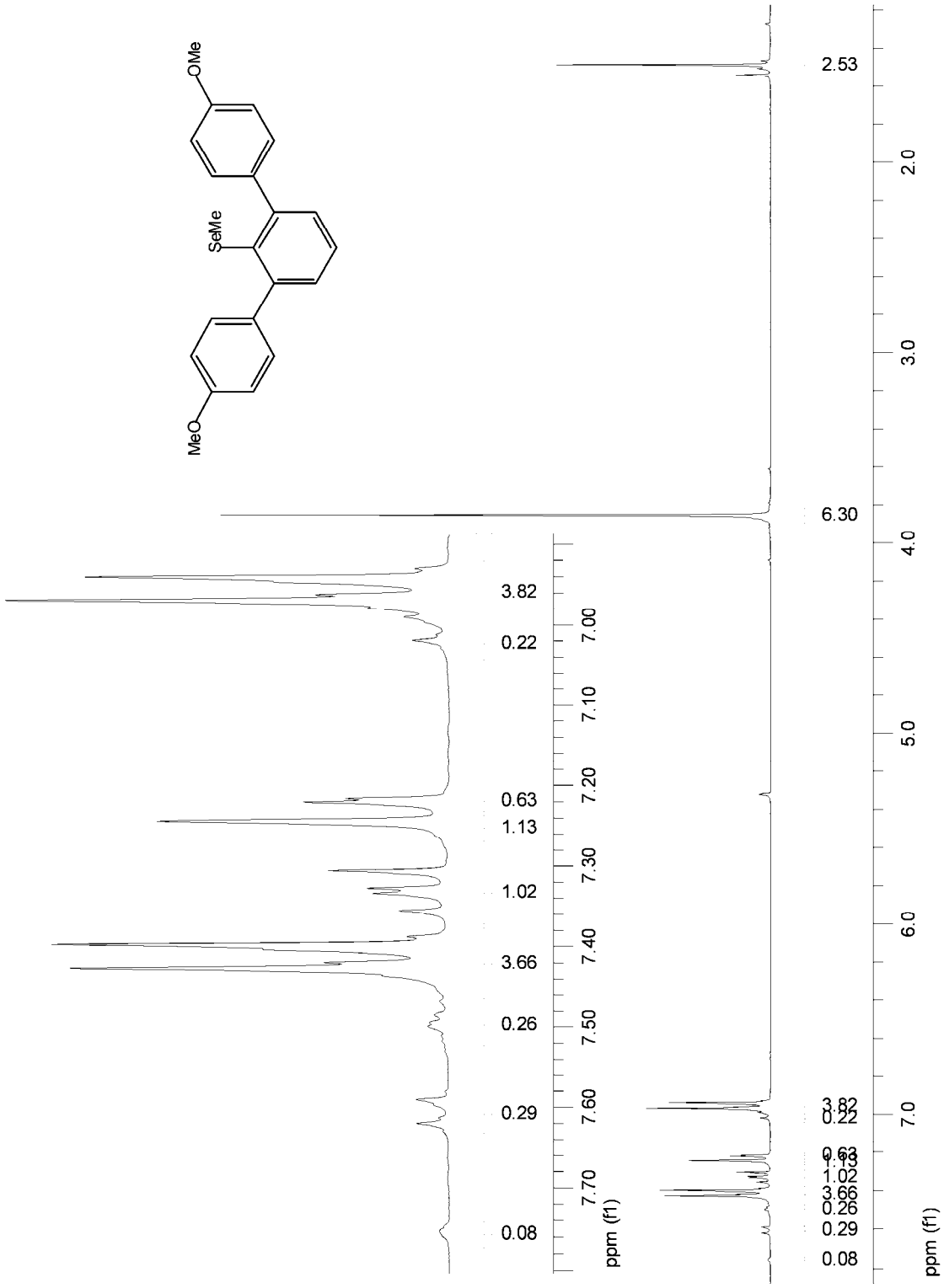


Figure S28. ^{1}H NMR spectrum of **2b**.

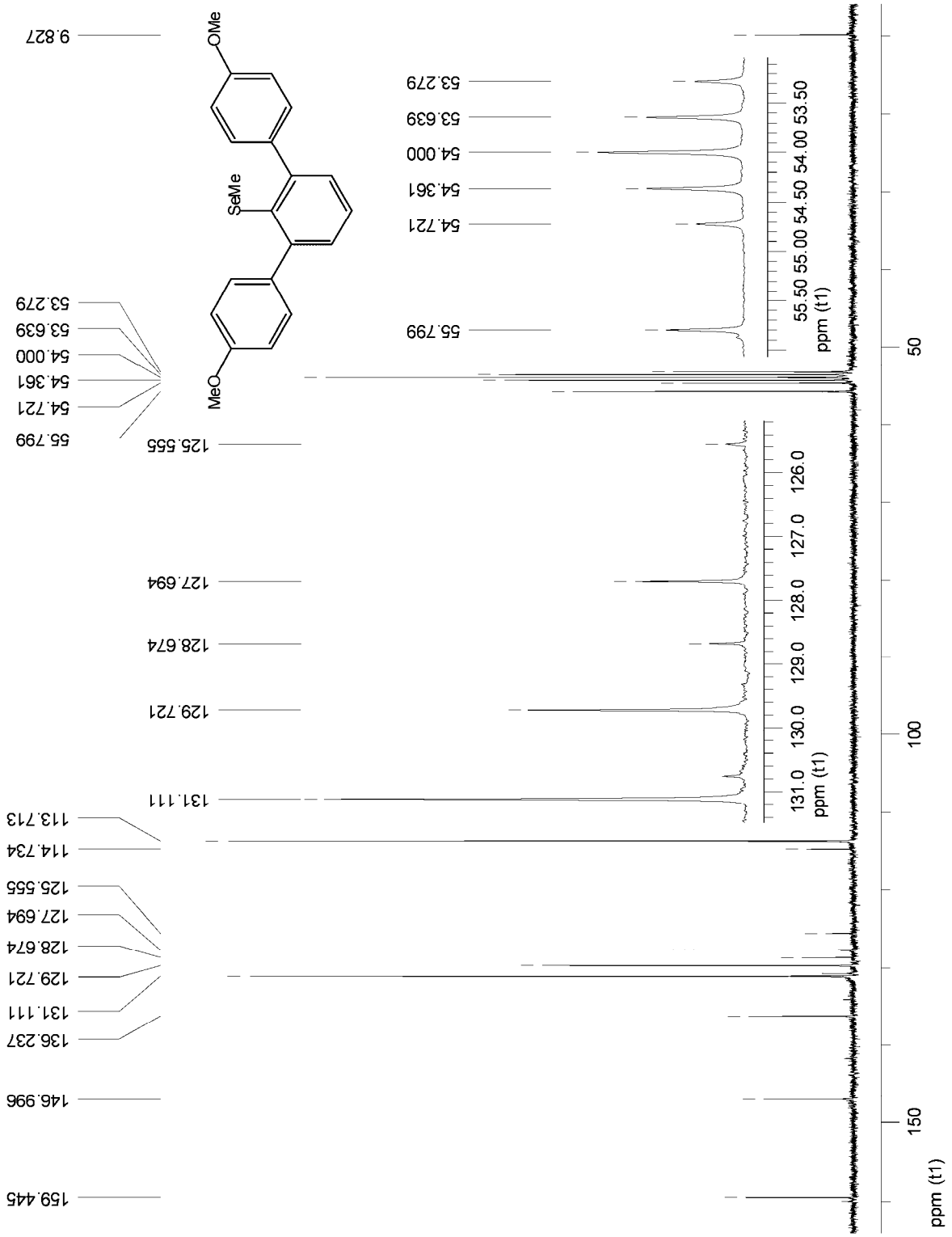


Figure S29. ^{13}C NMR spectrum of **2b**.

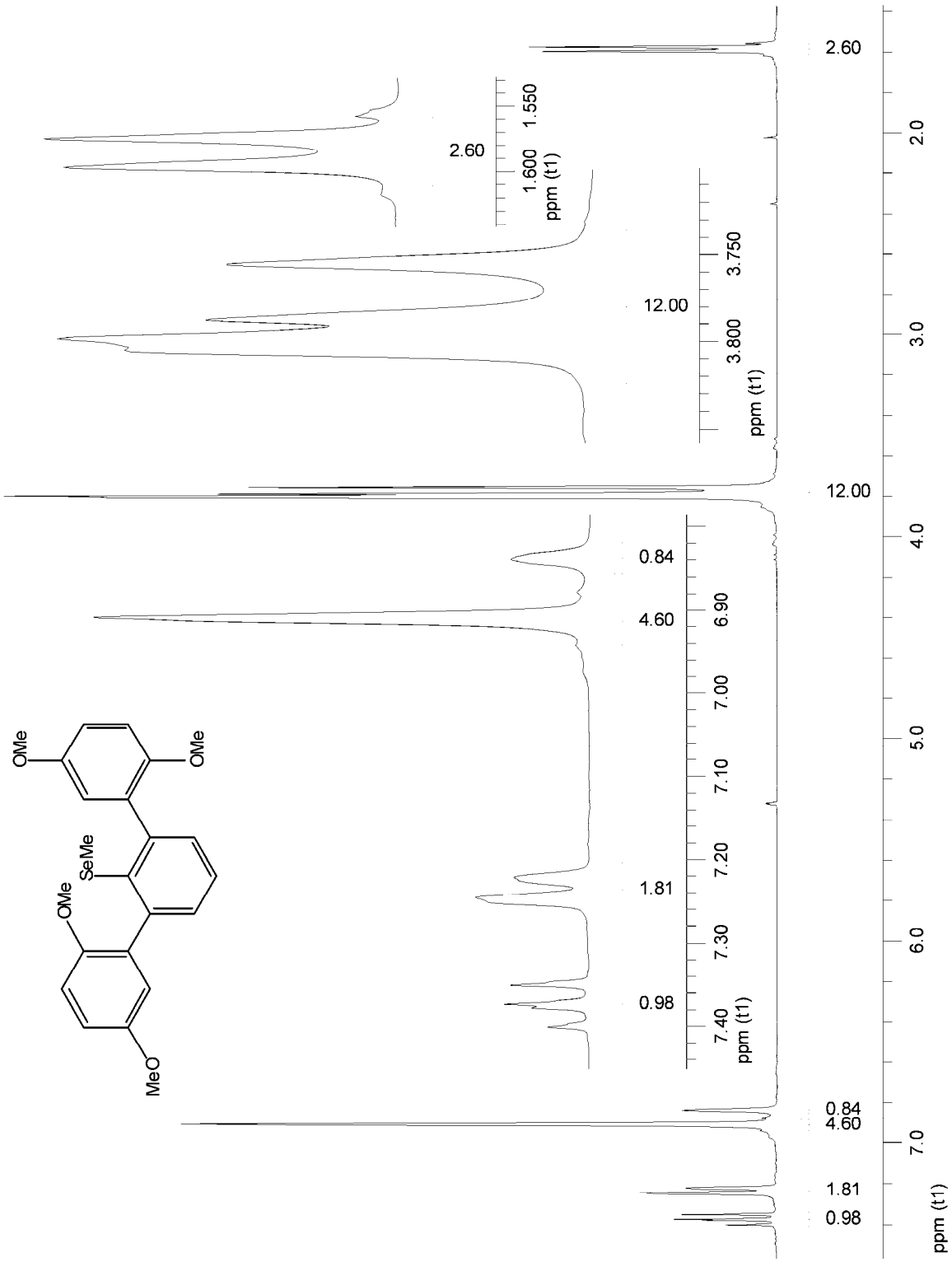


Figure S30. ^{1}H NMR spectrum of **2c**.

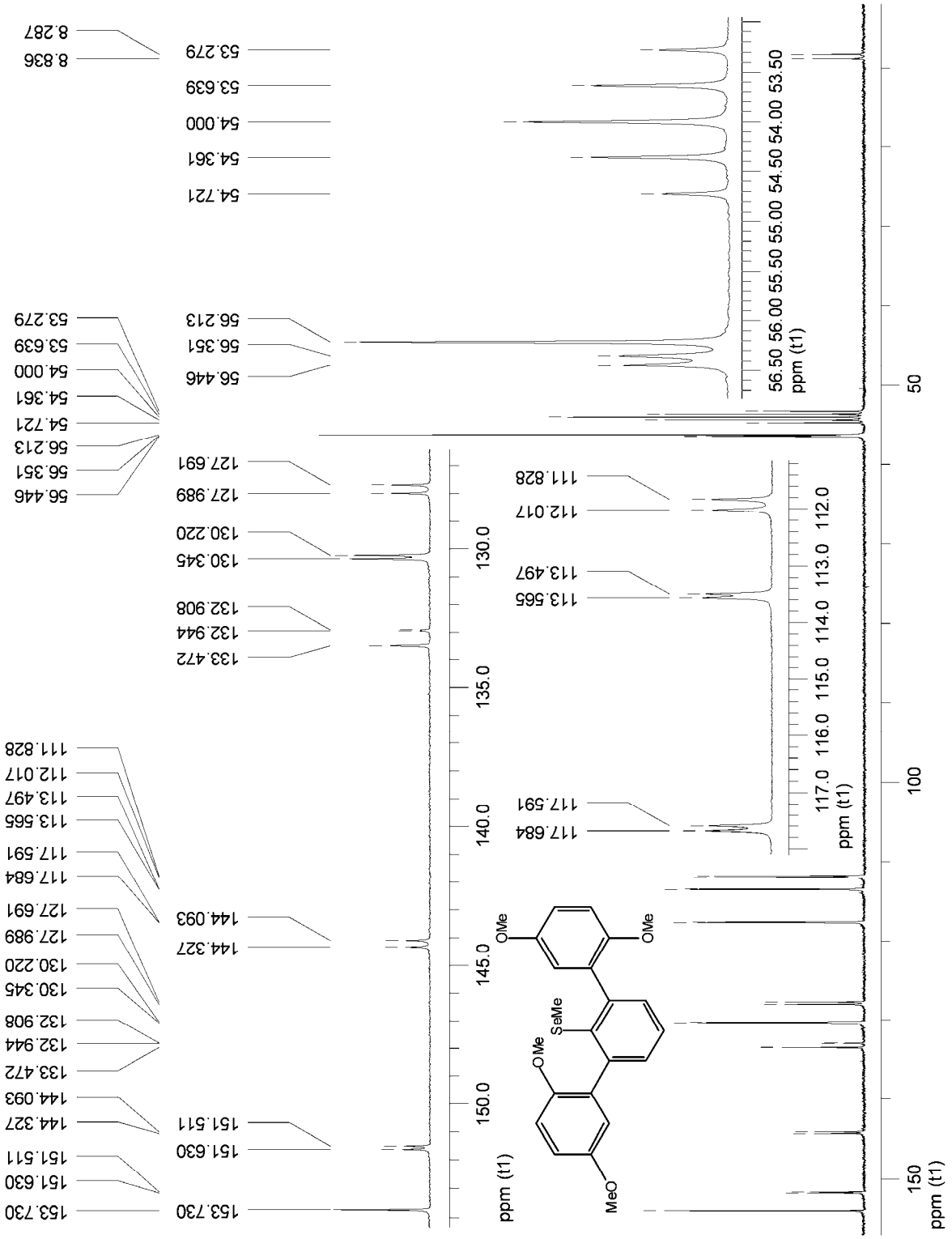


Figure S31. ^{13}C NMR spectrum of **2c**.

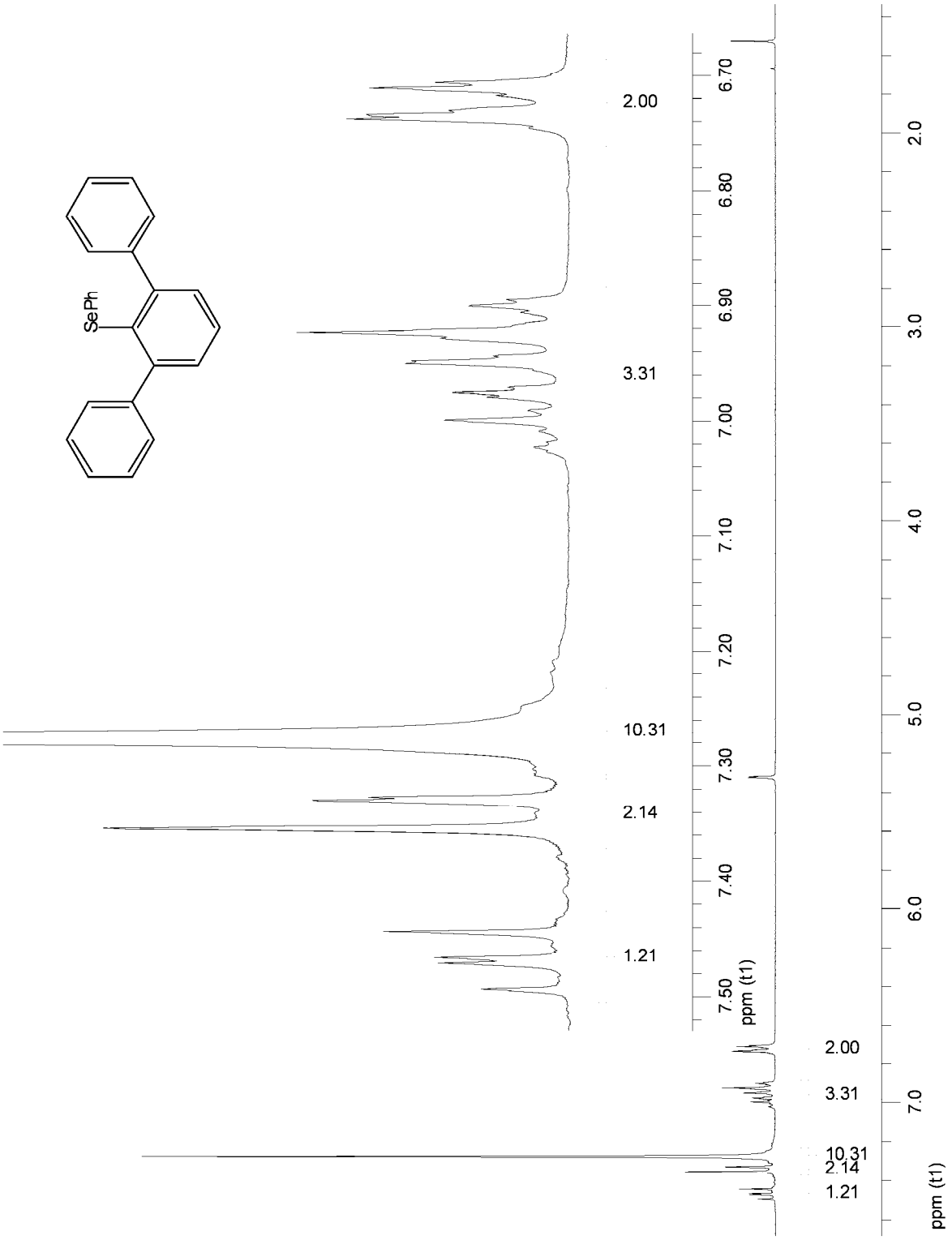


Figure S32. ^{1}H NMR spectrum of **2d**.

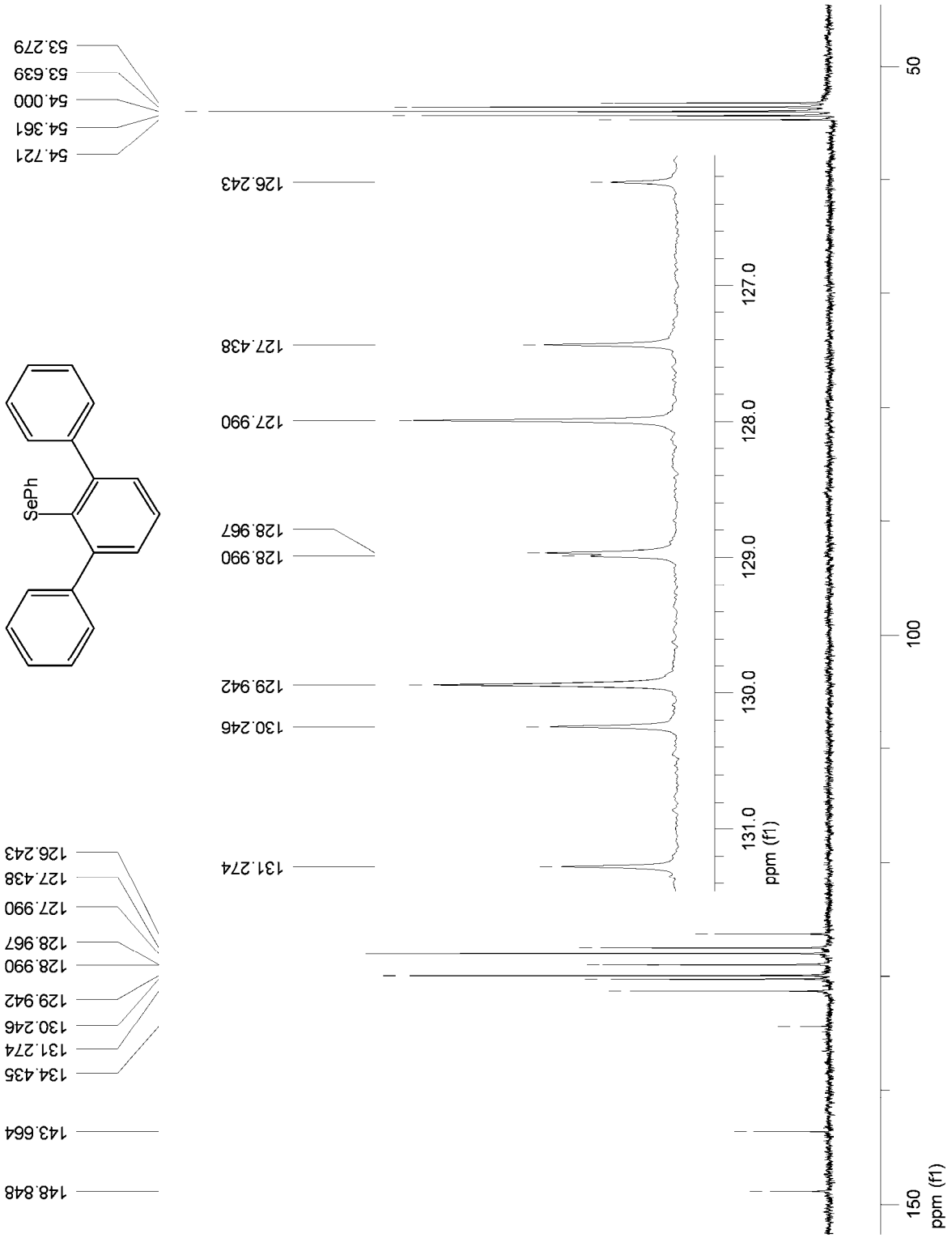


Figure S33. ^{13}C NMR spectrum of **2d**.

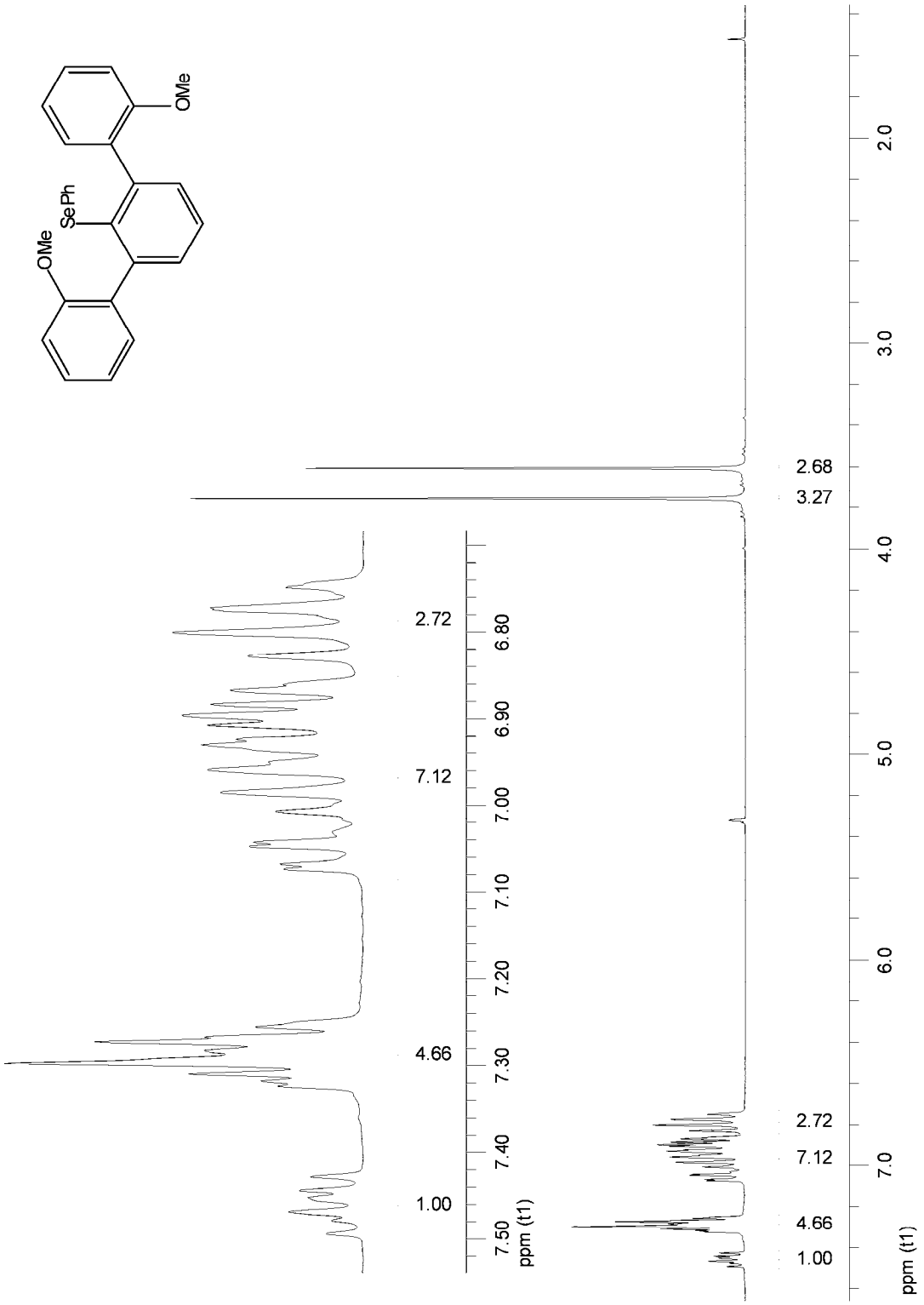


Figure S34. ^{1}H NMR spectrum of **2e**.

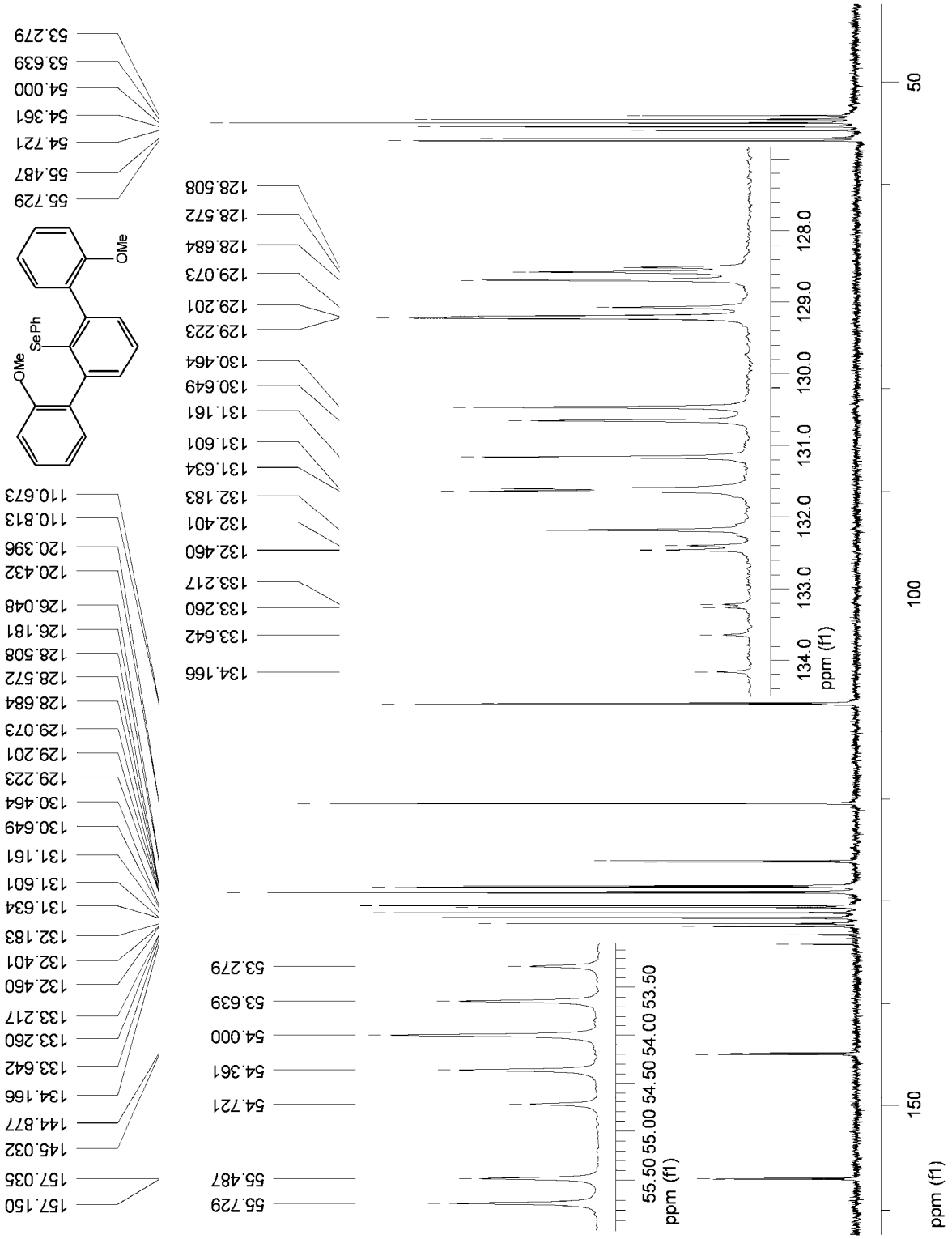


Figure S35. ^{13}C NMR spectrum of **2e**.

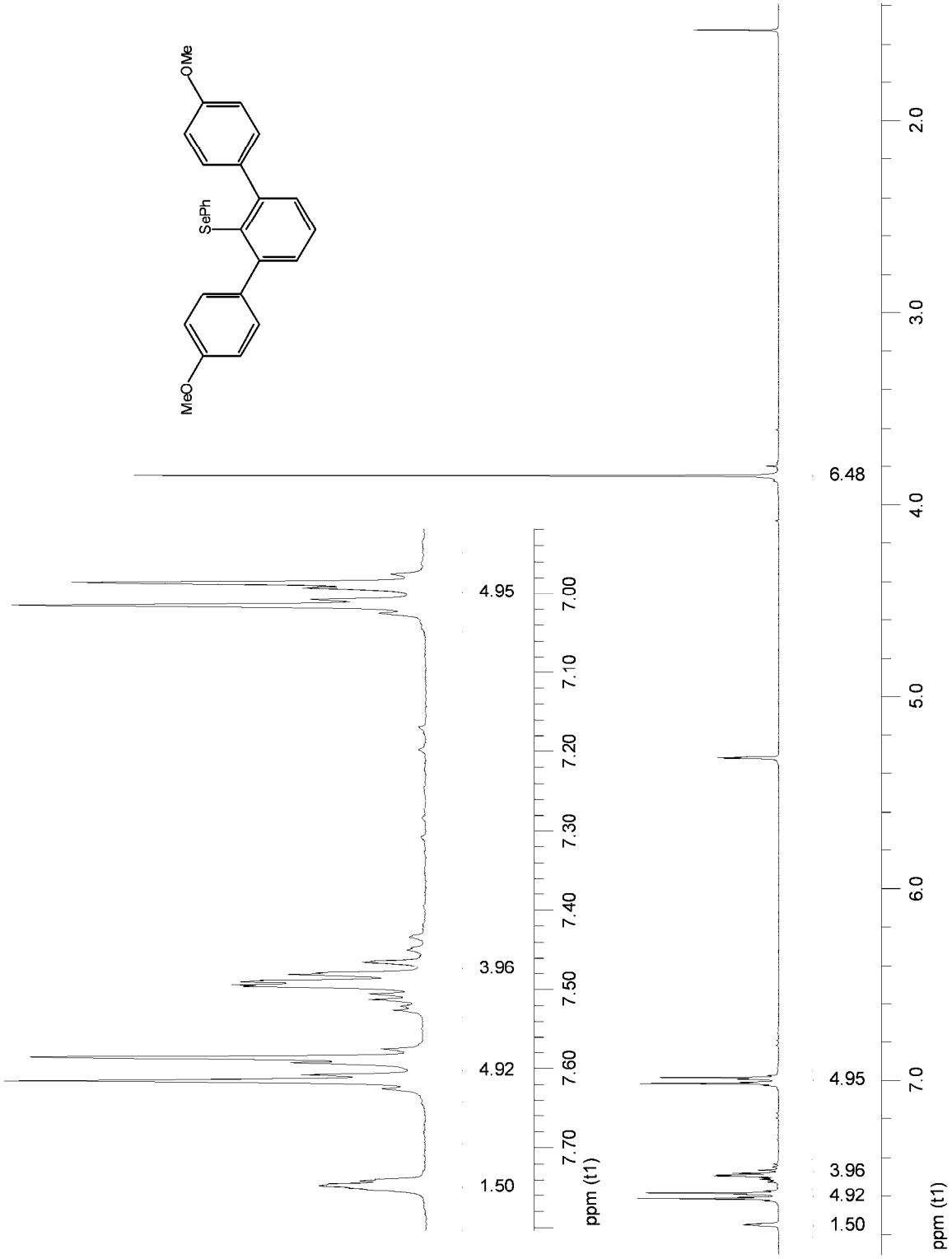


Figure S36. ^{1}H NMR spectrum of **2f**.

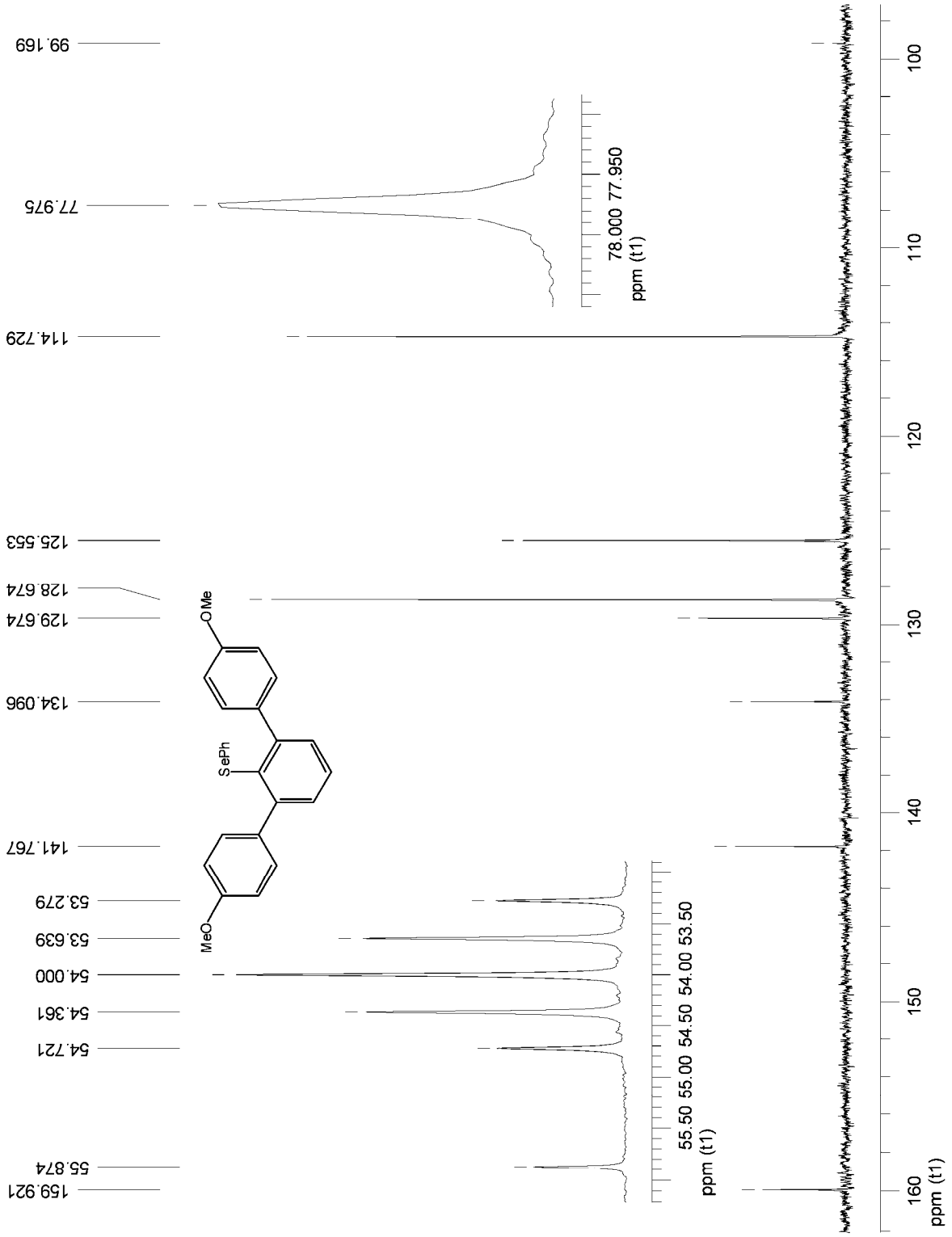


Figure S37. ^{13}C NMR spectrum of **2f**.

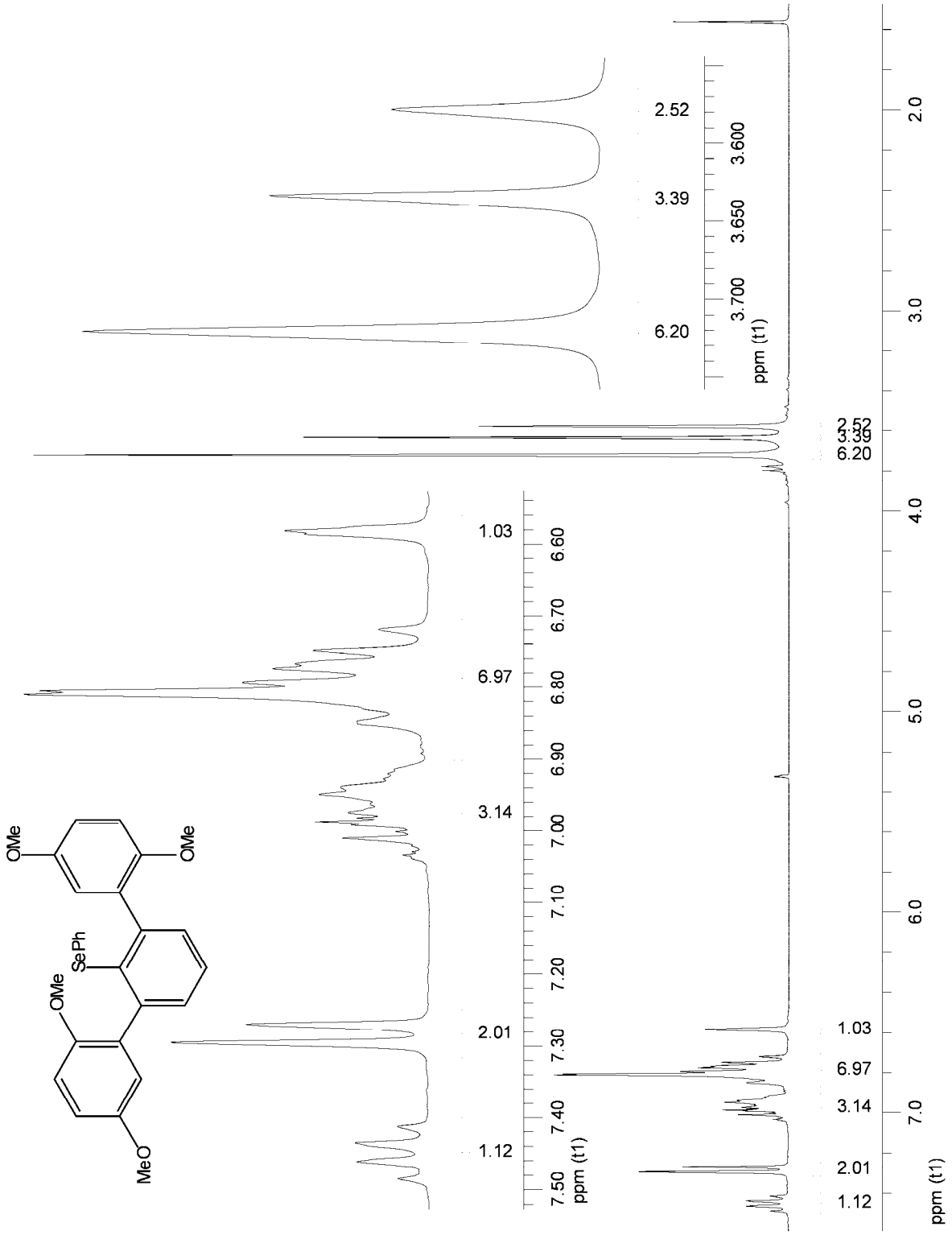


Figure S38. ^{1}H NMR spectrum of **2g**.

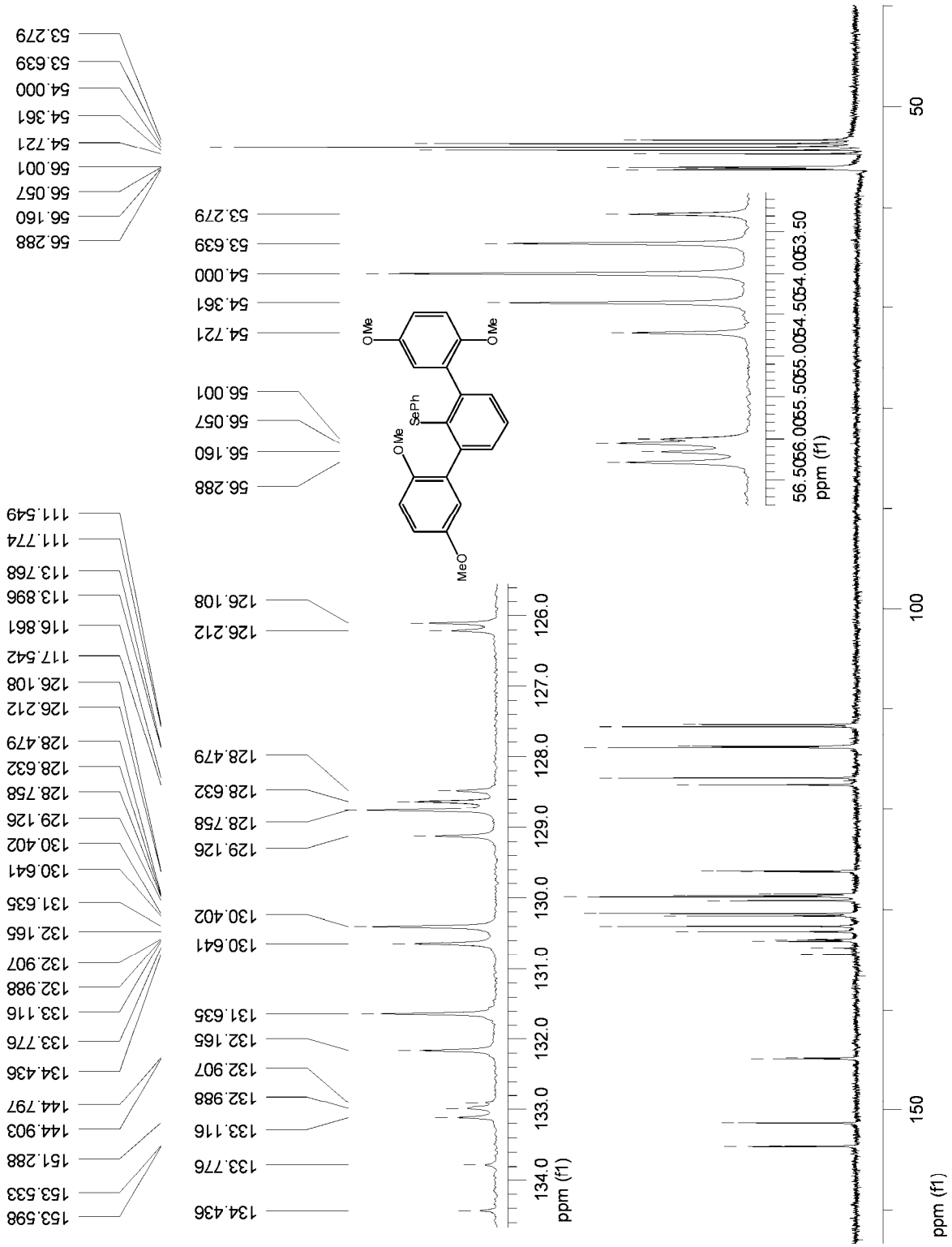


Figure S39. ^{13}C NMR spectrum of **2g**.

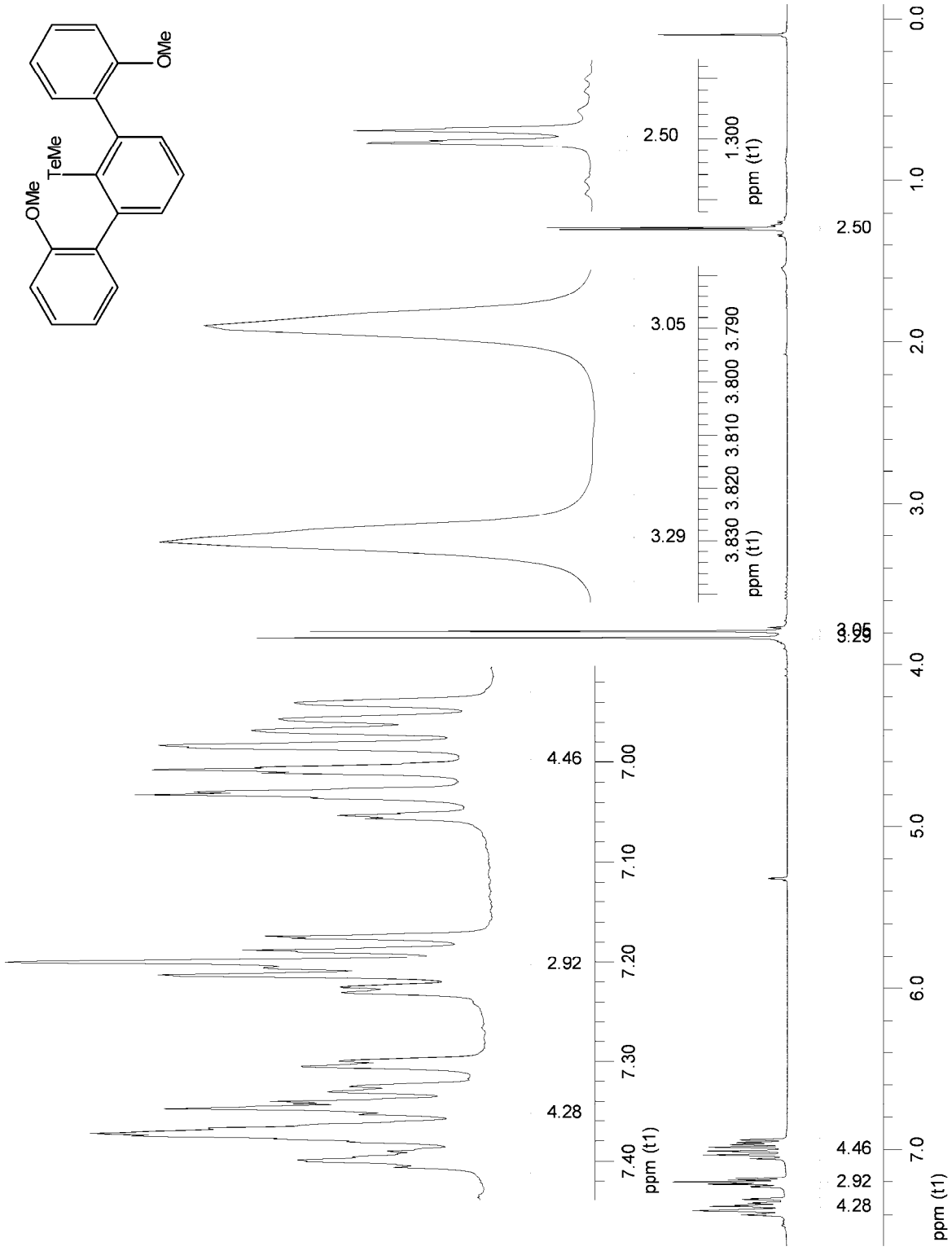


Figure S40. ^{1}H NMR spectrum of **3a**.

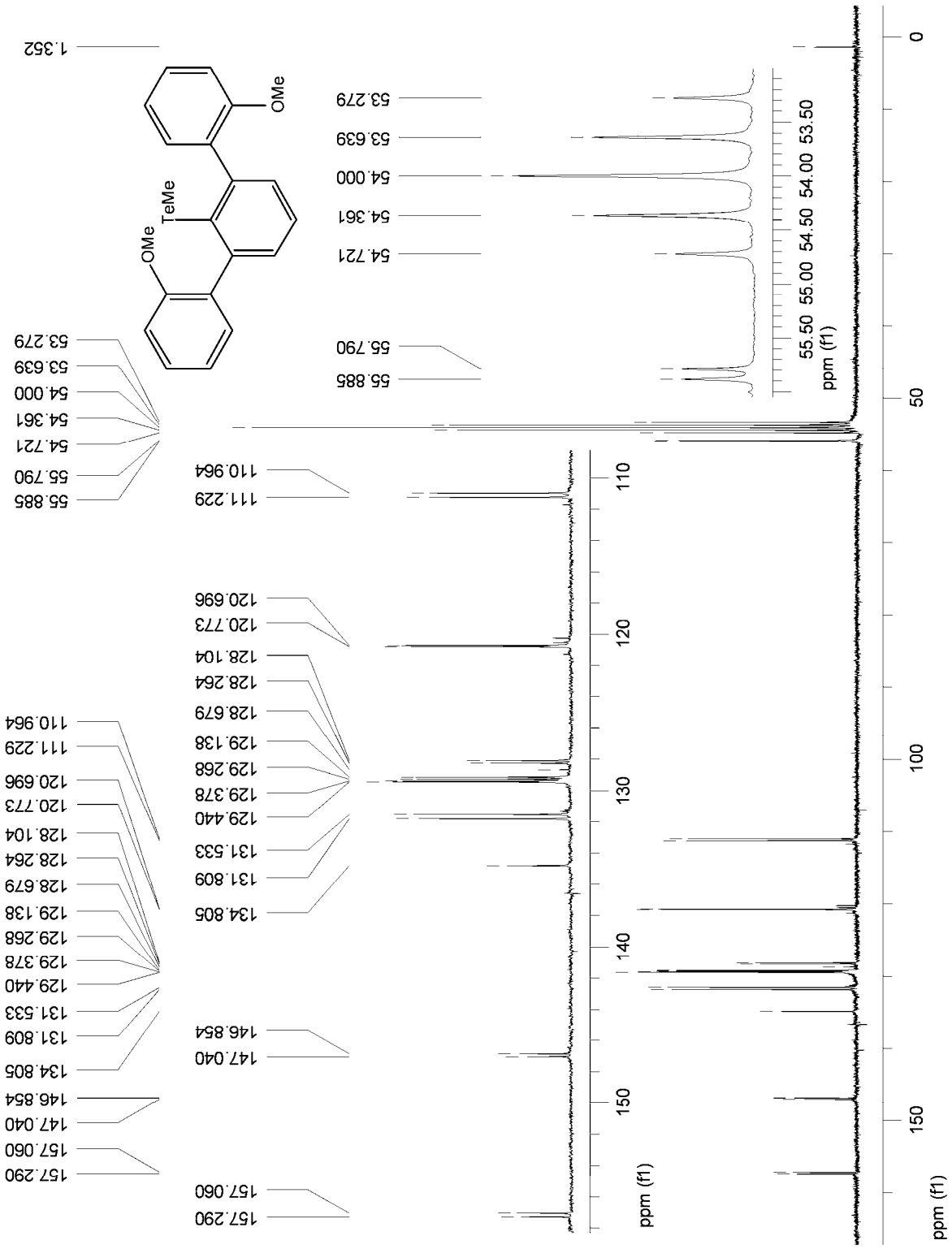


Figure S41. ^{13}C NMR spectrum of **3a**.

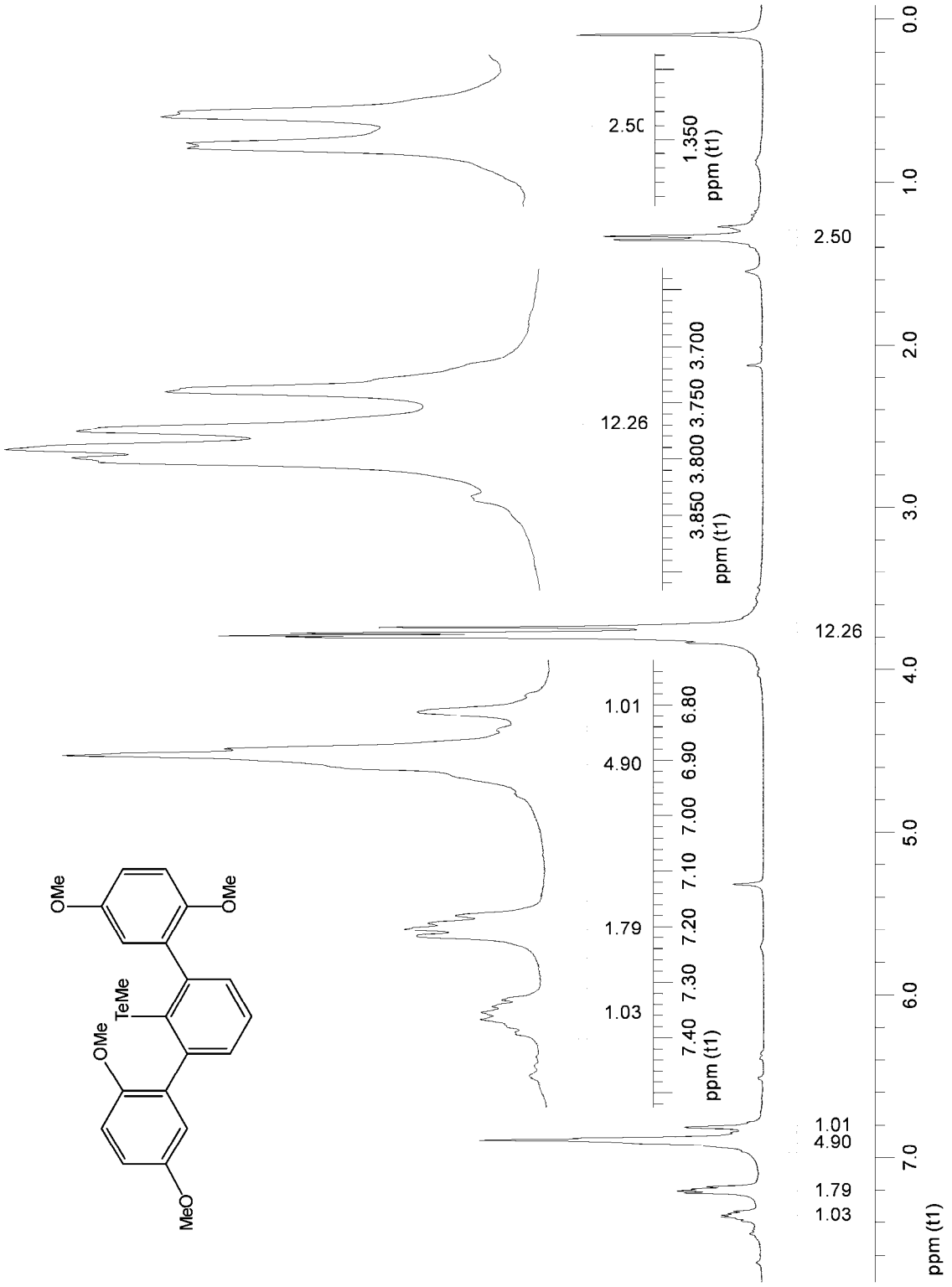


Figure S42. ^{1}H NMR spectrum of **3b**.

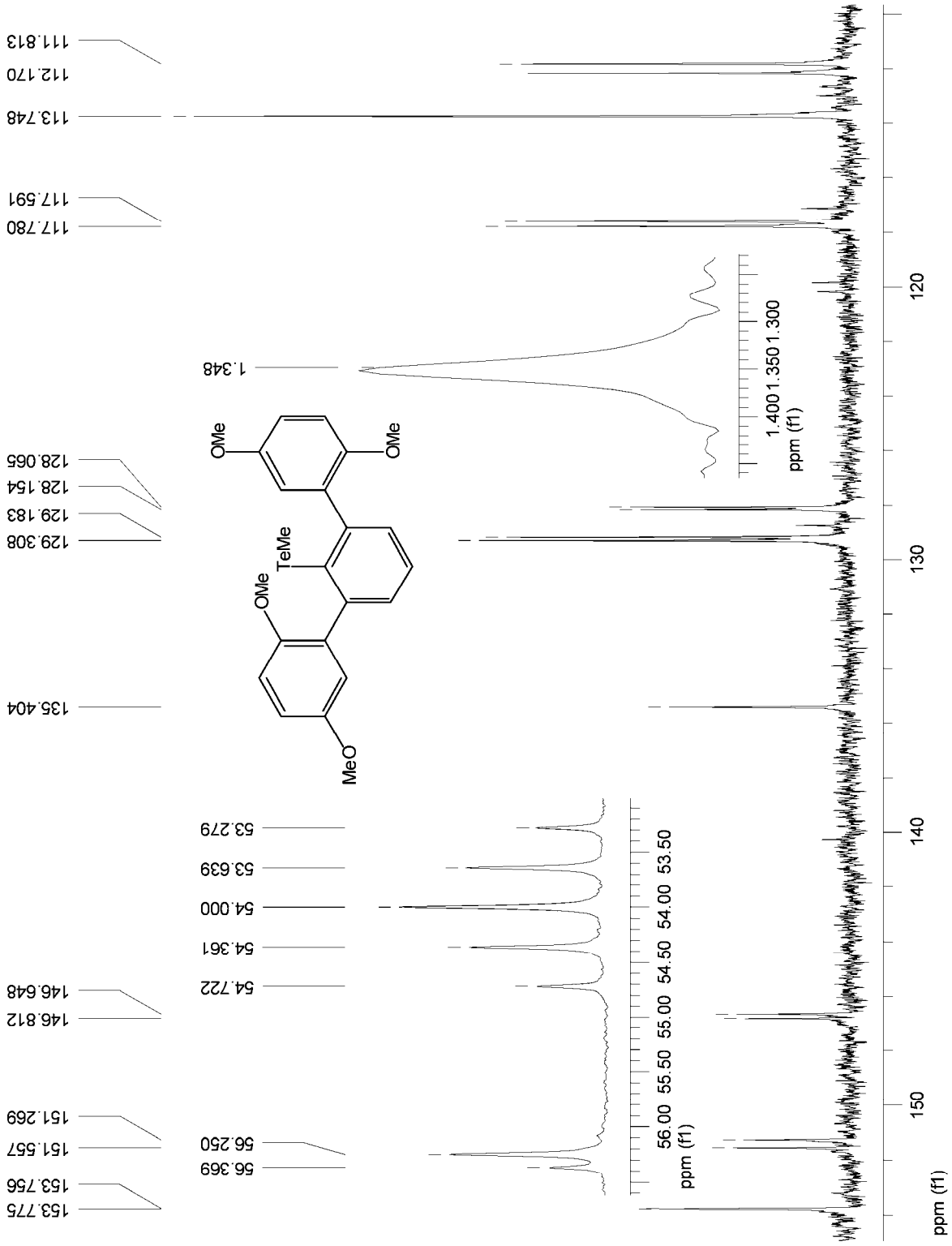


Figure S43. ^{13}C NMR spectrum of **3b**.

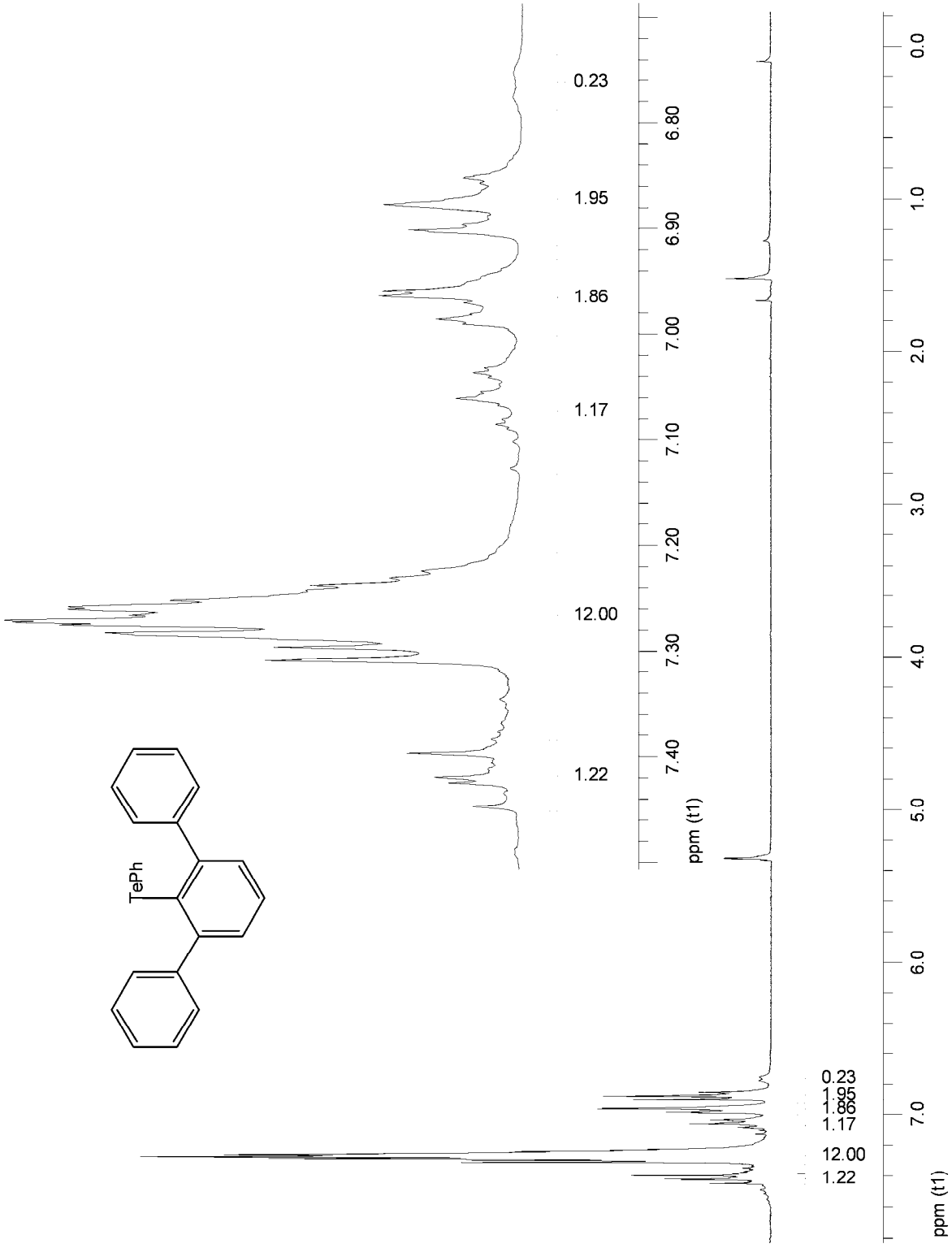


Figure S44. ^{1}H NMR spectrum of **3c**.

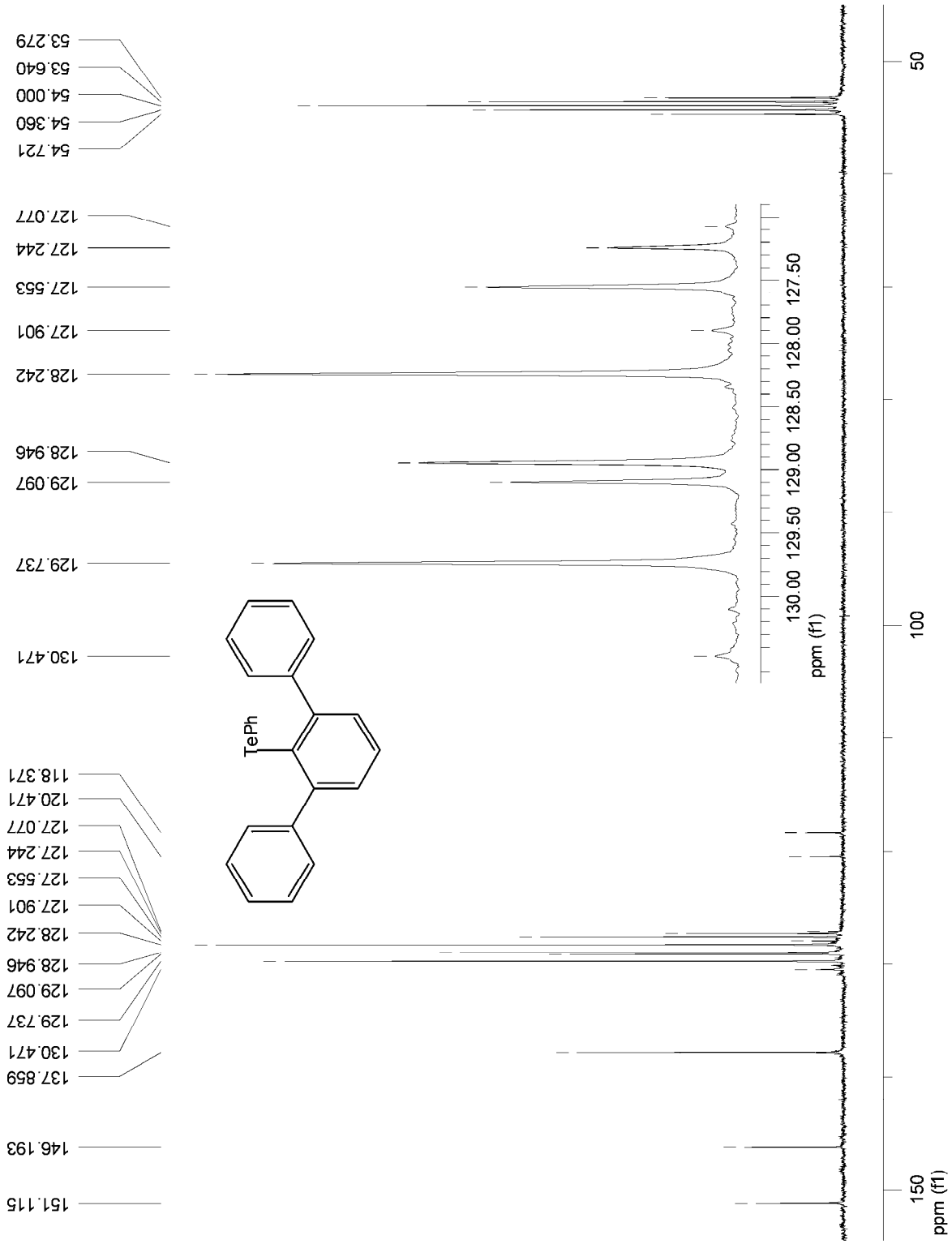


Figure S45. ^{13}C NMR spectrum of **3c**.

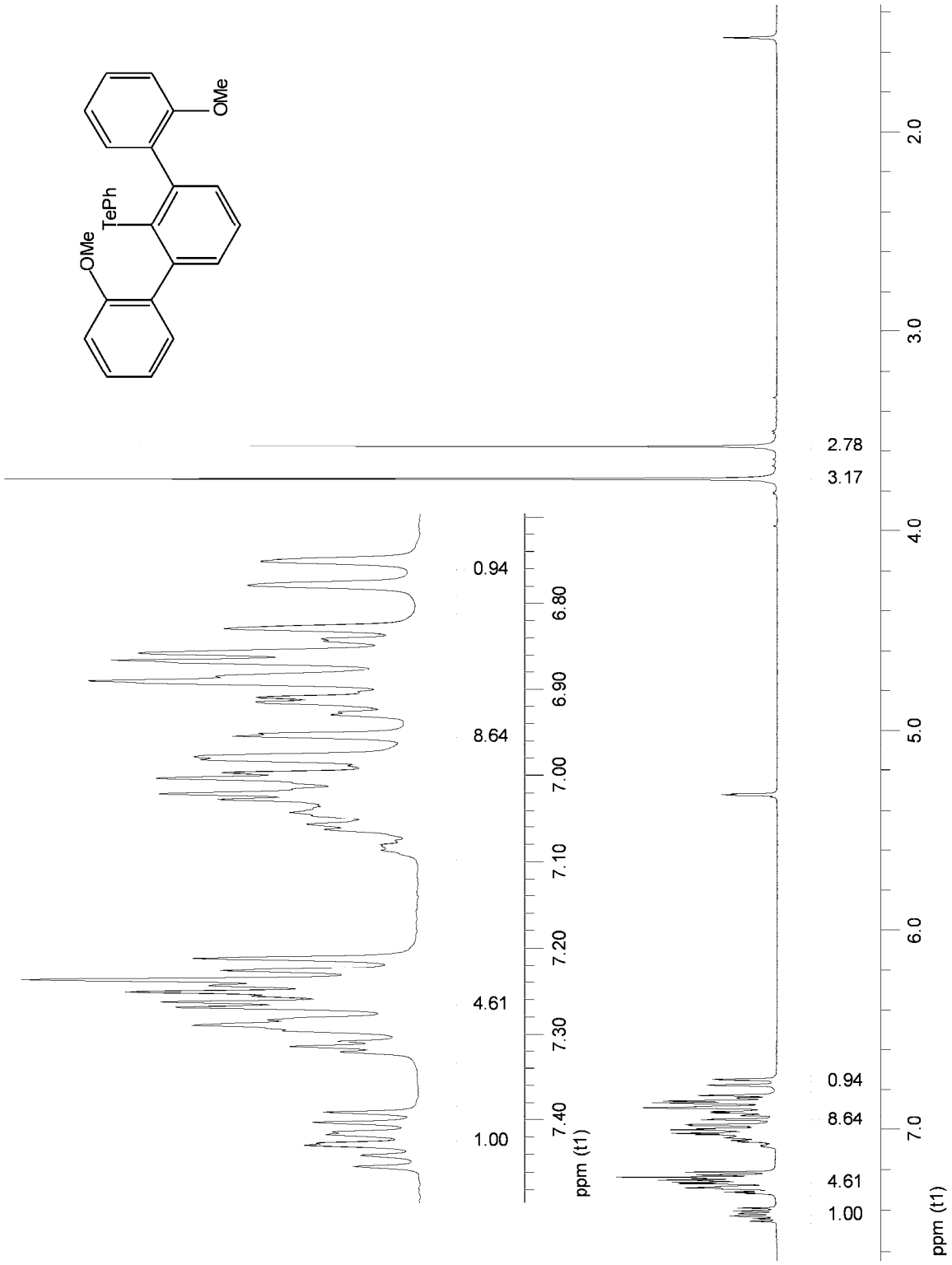


Figure S46. ^{1}H NMR spectrum of **3d**.

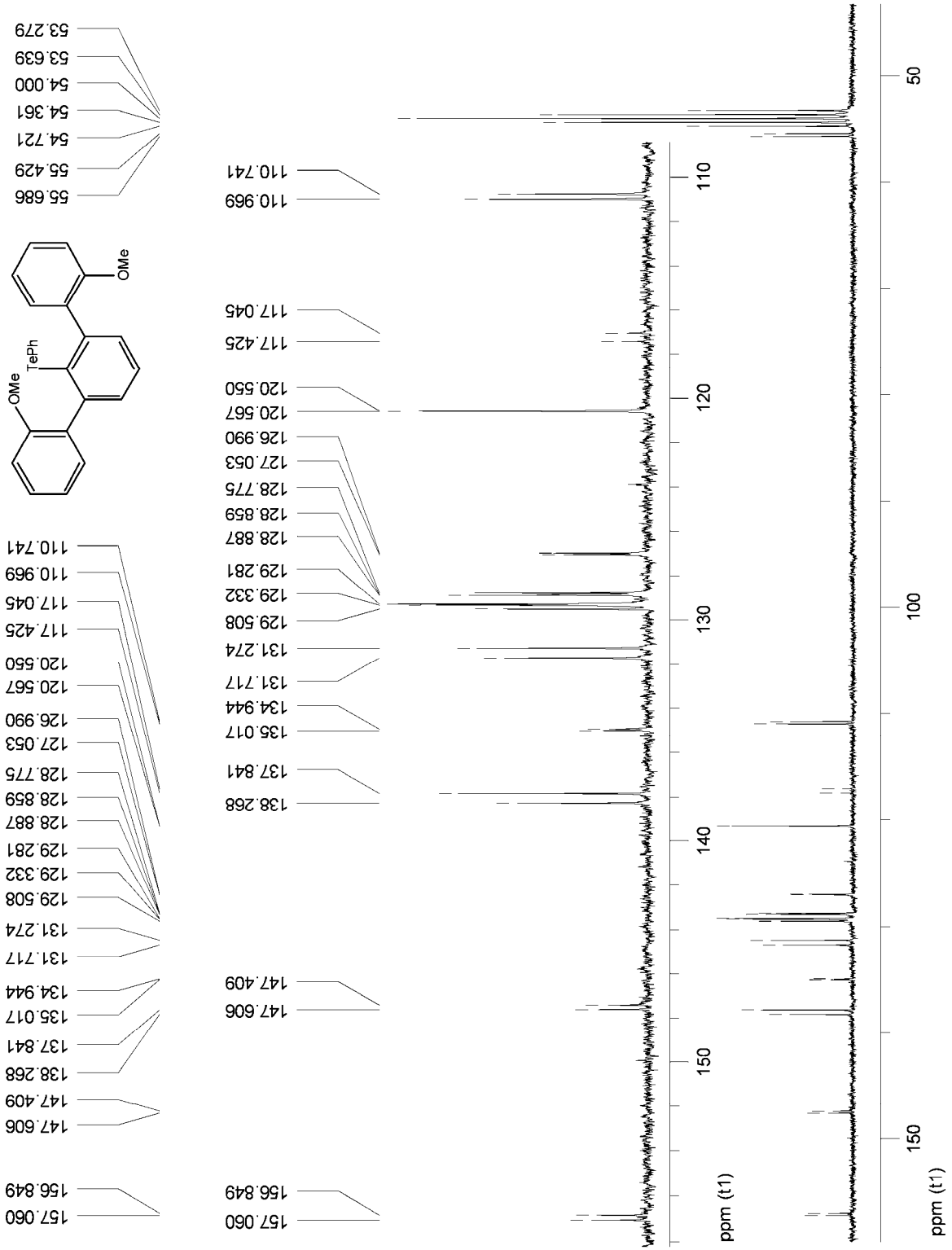


Figure S47. ^{13}C NMR spectrum of **3d**.

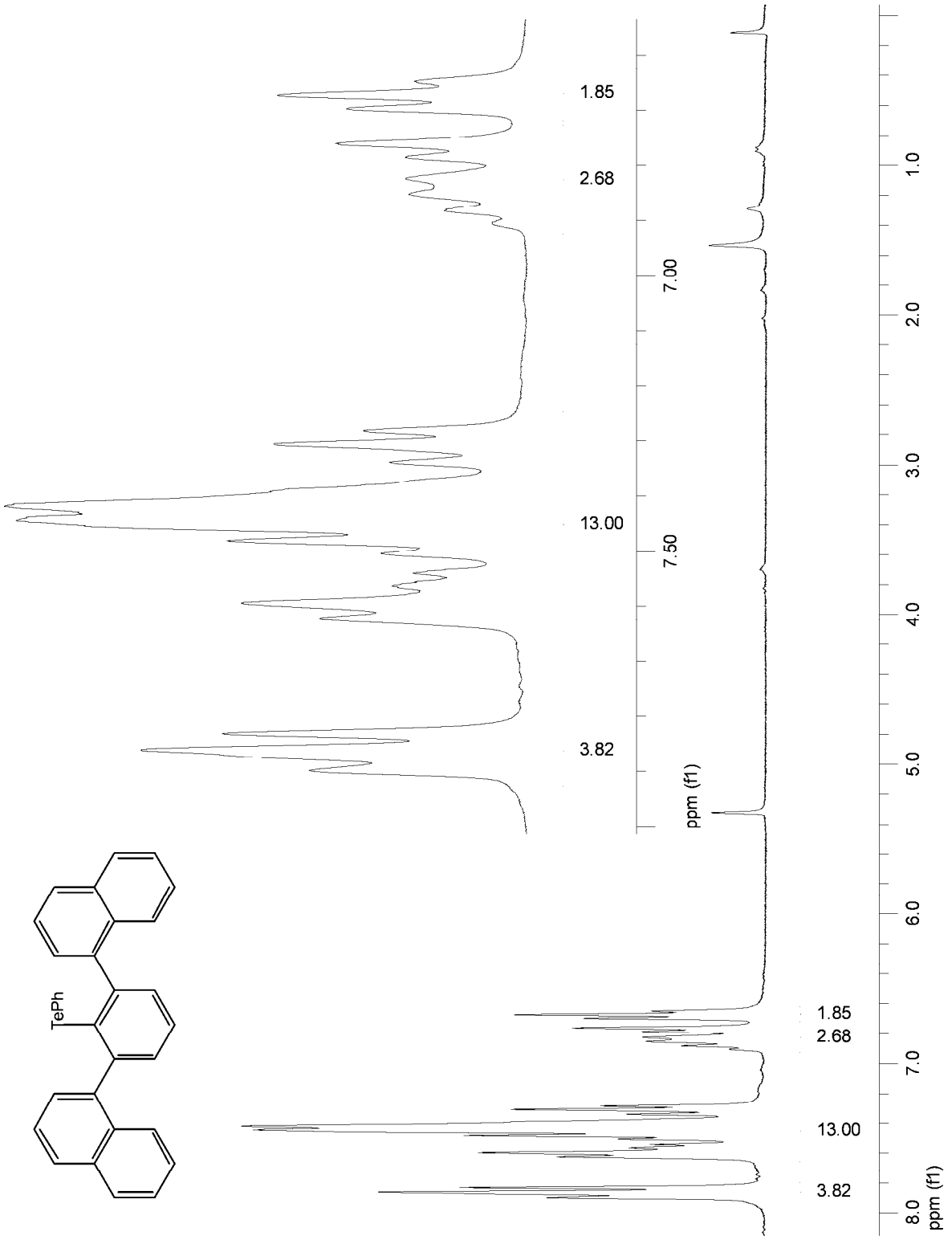


Figure S48. ^{1}H NMR spectrum of **3e**.

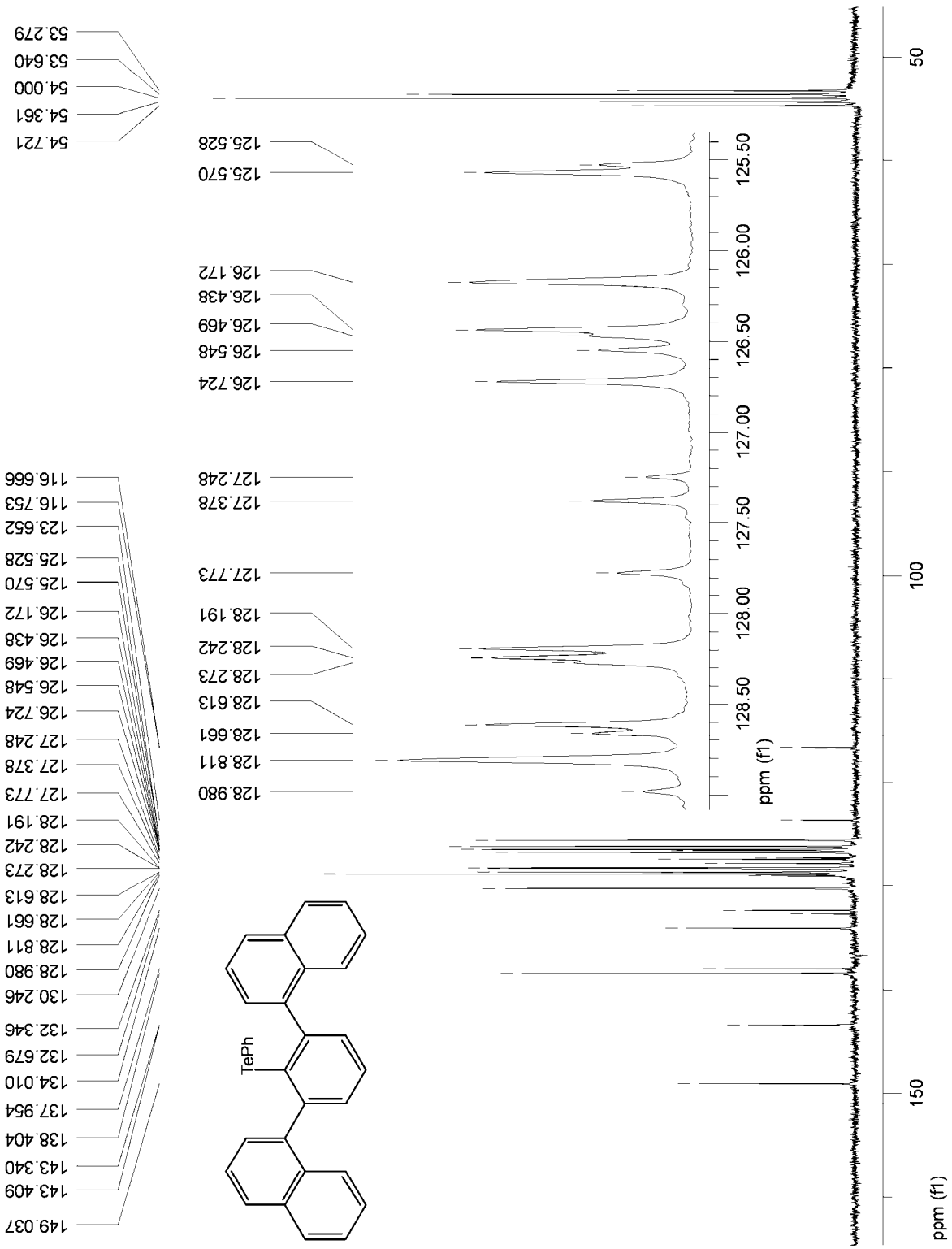


Figure S49. ^{13}C NMR spectrum of **3e**.

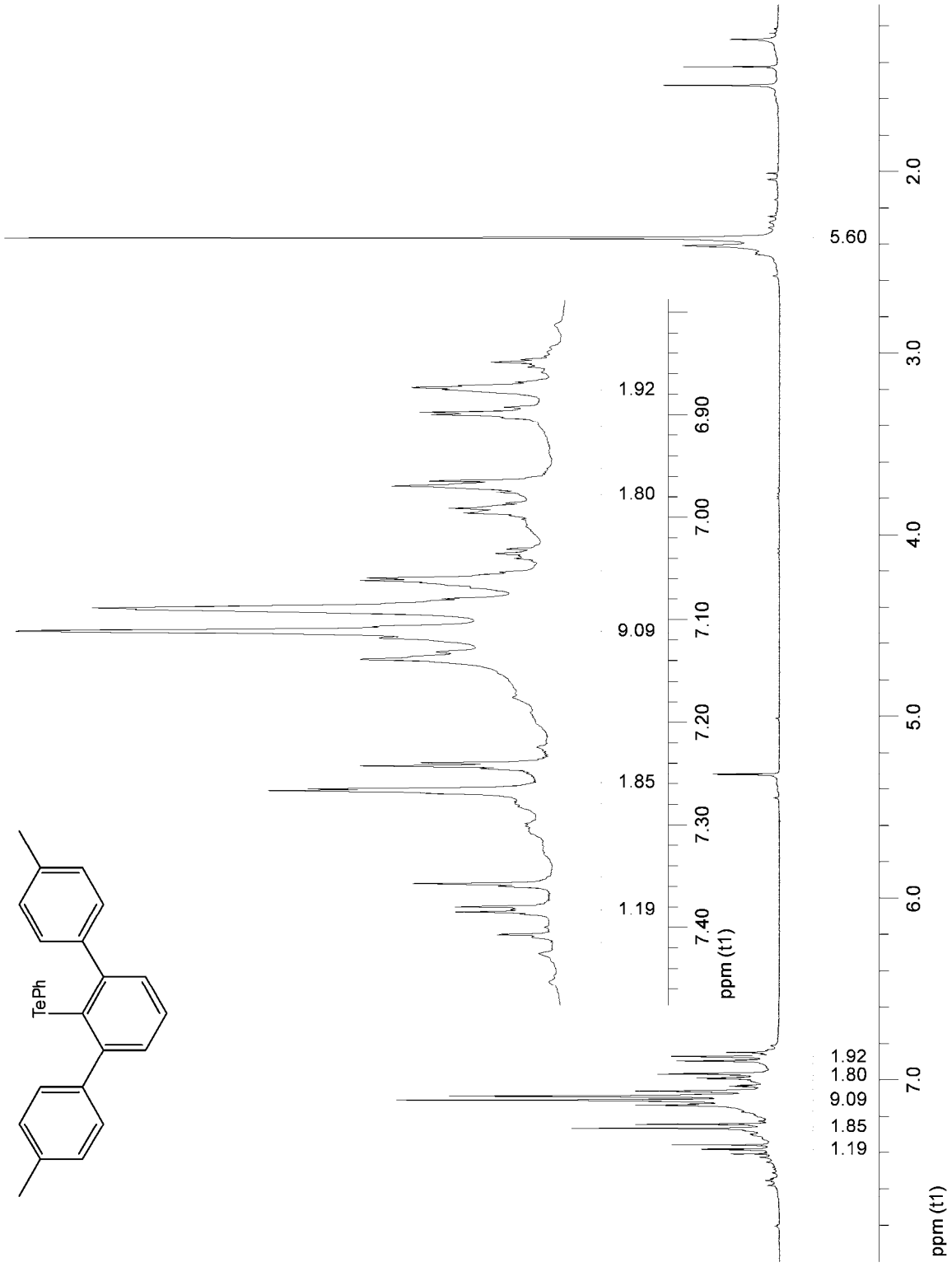


Figure S50. ^{1}H NMR spectrum of **3f**.

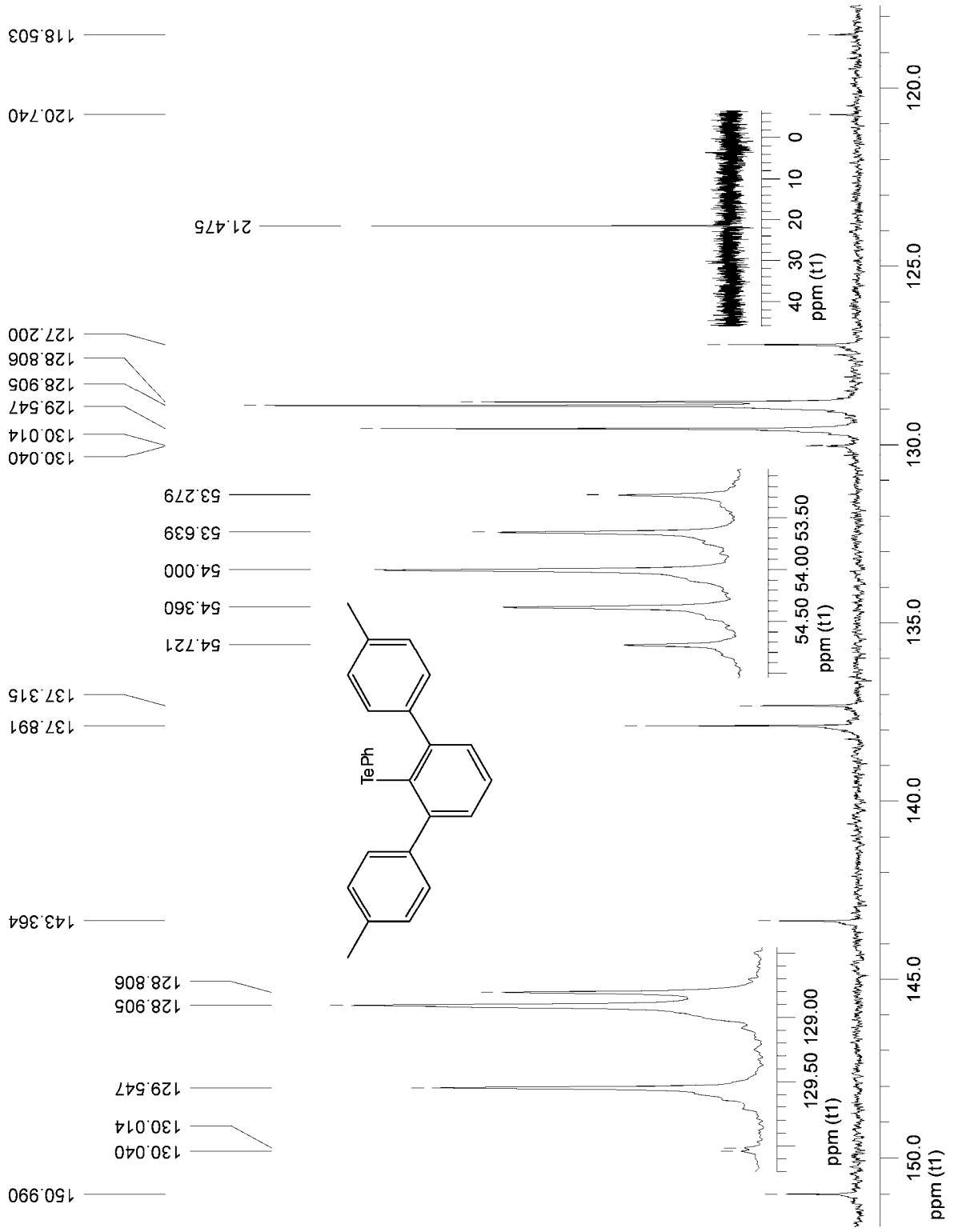


Figure S51. ^{13}C NMR spectrum of **3f**.

27. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Takajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M. Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision E.01, and Gaussian 09, Revision A.02 Wallingford, CT, 2003, Gaussian, Inc.