Supporting Information

1,4-Fullerenols C_{60}ArOH: Synthesis and Functionalization

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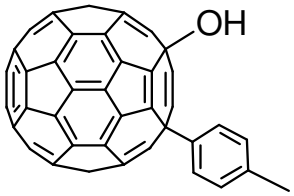
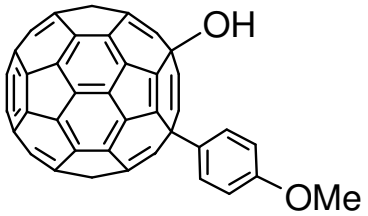
Synthesis of Fullerenols 2a-d from the Reactions of C_{60} with Phenylhydrazine Hydrochlorides 1a-d and Sodium Nitrite in the Presence of H_2O. A 50-mL round-bottomed flask containing a mixture of C_{60} (36.0 mg, 0.05 mmol), **1a** (**1b**, **1c** or **1d**, 0.1 mmol), and sodium nitrite (6.9 mg, 0.1 mmol) in toluene (25 mL) was ultrasonically treated to dissolve the reagents, and then 1 mL of H_2O was added. The resulting solution was stirred vigorously in an oil bath preset at 50 ^{o}C. The reaction was monitored by thin-layer chromatography (TLC) and stopped at the desired time. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60}, then with toluene/carbon disulfide as the eluent to afford fullerenol **2a** (**2b**, **2c** or **2d**).

The spectral data of fullerenols **2a-d** are listed below.

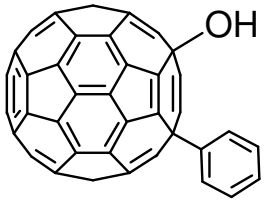


1-Hydroxyl-4-(4-methylphenyl)-1,4-dihydro[60]fullerene (**2a**): ^{1}H NMR (300 MHz, CS_2/$CDCl_3$) δ 2.50 (s, 3H), 3.77 (s, 1H), 7.40 (d, J = 8.1 Hz, 2H), 8.15 (d, J = 8.1 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation agent, all 1C unless indicated) δ 20.44 (CH$_3$), 60.03 (sp^3-C of C_{60}), 74.31 (sp^3-C of C_{60}), 126.96 (2C, aryl C), 129.10 (2C, aryl C), 136.19, 136.50, 136.58, 137.31, 137.36, 138.07, 139.42, 139.85, 140.88, 141.02, 141.06, 141.23, 141.56 (4C), 141.63, 141.76, 141.79 (2C), 141.82, 142.04, 142.12 (2C), 142.57 (3C), 142.70 (2C), 142.76, 142.89 (2C), 143.05, 143.08 (2C), 143.21, 143.28, 143.37, 143.70, 143.83, 144.09, 144.18, 144.31, 145.13, 145.19, 145.28, 145.55, 145.64, 145.67, 145.89, 146.26, 146.37, 146.46, 147.16, 147.48, 148.39, 149.54, 151.96, 152.62, 153.01; FT-IR ν/cm^{-1} (KBr) 2951, 2921, 1559, 1510, 1462, 1431, 1377, 1189, 1083, 1023, 934, 900, 820, 775, 764, 590, 565, 529; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 260 (5.08), 328 (4.56), 440 (3.84); HRMS (+ESI): calcd. for $C_{67}H_8NaO$ $[M+Na]^+$ 851.0473, found 851.0467.

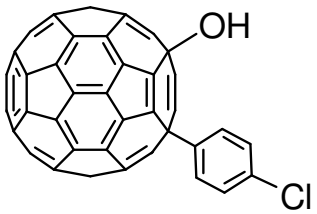


1-Hydroxy-4-(4-methoxylphenyl)-1,4-dihydro[60]fullerene (**2b**): ^{1}H NMR (300 MHz, CS_2/$CDCl_3$) δ 3.89 (s, 4H), 7.10 (d, J = 8.7 Hz, 2H), 8.17 (d, J = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation agent, all 1C unless indicated) δ 54.32 (OCH$_3$), 59.70 (sp^3-C of C_{60}), 74.28 (sp^3-C of C_{60}), 113.83 (2C, aryl C), 128.22 (2C, aryl C), 131.15 (aryl C), 136.58, 137.40, 137.42, 138.07, 139.47,

139.90, 140.92, 141.06, 141.11, 141.27, 141.57 (2C), 141.60, 141.62, 141.69 (2C), 141.78, 141.81, 141.86, 142.09, 142.16 (2C), 142.59, 142.60, 142.61, 142.74, 142.75, 142.80, 142.93, 142.94, 143.09, 143.11 (2C), 143.23, 143.32, 143.42, 143.72, 143.88, 144.14, 144.22, 144.36, 145.19, 145.22, 145.32, 145.59, 145.67, 145.71, 145.92, 146.19, 146.41, 146.50, 147.19, 147.51, 148.34, 149.66, 151.91, 152.81, 152.97, 158.30 (aryl *C*); FT-IR ν/cm^{-1} (KBr) 2949, 2921, 1604, 1507, 1460, 1429, 1300, 1251, 1180, 1081, 1026, 934, 899, 840, 825, 776, 644, 588, 545, 526; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.12), 328 (4.56), 441 (3.85); HRMS (+ESI): calcd. for $C_{67}H_8NaO_2$ $[M+Na]^+$ 867.0422, found 867.0412.



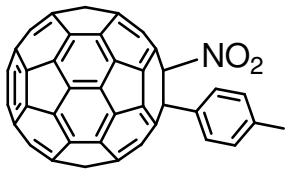
1-Hydroxyl-4-phenyl-1,4-dihydro[60]fullerene (**2c**): ^{1}H NMR (300 MHz, CS_2/$CDCl_3$) δ 3.88 (s, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.64 (t, J = 7.5 Hz, 2H), 8.32 (d, J = 7.5 Hz, 2H); ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 7.44 (t, J = 7.6 Hz, 1H), 7.58 (t, J = 7.6 Hz, 2H), 8.05 (s, 1H), 8.29 (d, J = 7.6 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation agent, all 1C unless indicated) δ 60.36 (sp^3-*C* of C_{60}), 74.46 (sp^3-*C* of C_{60}), 127.20 (2C, aryl *C*), 127.30 (aryl *C*), 128.56 (2C, aryl *C*), 136.78, 137.46, 137.64, 138.17, 139.14, 139.61, 140.01, 141.03, 141.19, 141.20, 141.39, 141.70, 141.71 (2C), 141.75 (2C), 141.94 (2C), 141.98, 142.04, 142.21, 142.27 (2C), 142.71 (3C), 142.83 (2C), 142.90, 142.99, 143.04, 143.19, 143.23 (2C), 143.37, 143.42, 143.49, 143.84, 144.03, 144.25, 144.35, 144.47, 145.27, 145.36, 145.44, 145.71, 145.79, 145.84, 146.03, 146.38, 146.51, 146.59, 147.33, 147.63, 148.52, 149.47, 152.03, 152.51, 152.81; FT-IR ν/cm^{-1} (KBr) 2950, 2920, 2850, 1598, 1492, 1461, 1446, 1429, 1187, 1154, 1102, 1091, 1080, 1021, 933, 898, 762, 734, 692, 579, 559, 545, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (5.08), 328 (4.56), 440 (3.83); HRMS (+ESI): calcd. for $C_{66}H_6NaO$ $[M+Na]^+$ 837.0316, found 837.0305.



1-(4-Chlorophenyl)-4-hydroxyl-1,4-dihydro[60]fullerene (**2d**): ^{1}H NMR (300 MHz, CS_2/$CDCl_3$) δ 3.91 (s, 1H), 7.57 (d, J = 8.4 Hz, 2H), 8.25 (d, J = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation agent, all 1C unless indicated) δ 59.14 (sp^3-*C* of C_{60}), 73.99 (sp^3-*C* of C_{60}), 128.27 (2C, aryl *C*), 128.42 (2C, aryl *C*), 136.47 (aryl *C*), 137.06, 137.35, 137.42, 137.58, 139.27, 139.60, 140.59, 140.76 (2C), 140.97, 141.22, 141.32 (4C), 141.41, 141.51, 141.56 (2C), 141.81 (2C), 141.87 (2C), 142.19, 142.30 (2C), 142.38 (2C), 142.47 (2C), 142.61, 142.72 (2C),

142.84, 142.93, 142.98 (2C), 143.39, 143.68, 143.84, 143.96, 144.08, 144.81, 144.97, 145.04, 145.31, 145.38, 145.45, 145.61, 145.78, 145.97, 146.09, 146.95, 147.22, 148.08, 148.50, 151.44, 151.62, 151.65; FT-IR ν/cm^{-1} (KBr) 2951, 2920, 2851, 1488, 1461, 1429, 1400, 1186, 1093, 1015, 897, 840, 822, 769, 622, 588, 561, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (4.96), 328 (4.43), 440 (3.66); HRMS (+ESI): calcd. for $C_{66}H_5NaClO$ $[M+Na]^+$ 870.9927, found 870.9911.

Synthesis of Intermediate 3a from the Reactions of C_{60} with 4-Methylphenylhydrazine Hydrochloride 1a and Sodium Nitrite in the Presence of H_2O. To a 50-mL round-bottomed flask was charged with C_{60} (36.0 mg, 0.05 mmol), 4-methylphenylhydrazine hydrochloride (31.7 mg, 0.1 mmol) and sodium nitrite (6.9 mg, 0.1 mmol). After they were dissolved in toluene (25 mL) by sonication, 1 mL of H_2O was added. The mixture was heated with slow stirring in an oil bath preset at 50 ^oC for 2 h. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} and intermediate **3a**.



1-(4-Methylphenyl)-2-nitro-1,2-dihydro[60]fullerene (**3a**): ^1H NMR (300 MHz, $CS_2/CDCl_3$) δ 2.52 (s, 3H), 7.46 (d, J = 8.1 Hz, 2H), 8.30 (d, J = 8.1 Hz, 2H); ^{13}C NMR (75 MHz, $CS_2/CDCl_3$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 21.06 (1C, *C*H_3), 69.29 (1C, sp^3-*C* of C_{60}), 106.46 (1C, sp^3-*C* of C_{60}), 129.25 (aryl *C*), 129.92 (aryl *C*), 134.68, 135.83 (1C, aryl *C*), 137.67, 138.84 (1C, aryl *C*), 138.97, 140.04, 140.92, 141.02, 141.20, 141.80 (4C), 141.94, 142.20, 142.42, 142.64, 143.63, 143.94, 144.06, 144.16, 144.30, 144.93 (6C), 145.13, 145.87 (4C), 146.11 (4C), 146.28, 147.42 (1C), 147.91 (1C), 152.33; FT-IR ν/cm^{-1} (KBr) 2917, 1556, 1507, 1431, 1341, 1187, 1021, 805, 780, 720, 577, 527, 476; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 255 (5.08), 320 (4.64), 420 (3.67), 688 (2.48); HRMS (+ESI): calcd. for $C_{67}H_7NaNO_2$ $[M+Na]^+$ 880.0374, found 880.0387.

Synthesis of Fullerenol 2a from the Reaction of Intermediate 3a with H_2O. Into a 25-mL round-bottomed flask was added intermediate **3a** (5.0 mg), H_2O (1 mL), and toluene (5 mL). The mixture was heated and stirred in an oil bath preset at 50 ^oC for 36 h. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with toluene/carbon disulfide as the eluent to afford fullerenol **2a** (2.1 mg, 43%).

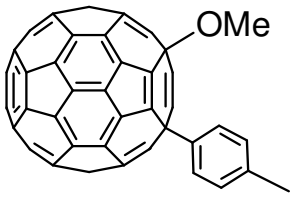
Acetylation of Fullerenols 2a-d in the Presence of *p*-Toluenesulfonic Acid. A mixture of fullerenol **2a** (**2b**, **2c** or **2d**, 10.0 mg), acetic anhydride (2 equiv.), and *p*-toluenesulfonic acid (2 equiv.) was dissolved in CS_2 (10 mL) and heated with stirring in an oil bath preset at 80 ^oC. The reaction was monitored by TLC and stopped

at the desired time. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to afford compound **6a** (**6b**, **6c** or **6d**, then with carbon disulfide/toluene as the eluent to afford unreacted fullerenol **2a** (**2b**, **2c** or **2d**). The spectral data were consistent with those previously reported by us.[1]

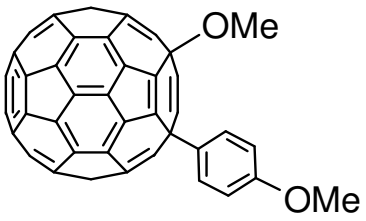
Methoxylation of Fullerenols 2a-d in the Presence of *p*-Toluenesulfonic Acid. To a 25-mL round-bottomed flask equipped with a reflux condenser were added fullerenol **2a** (**2b**, **2c** or **2d**, 10.0 mg), *p*-toluenesulfonic acid (5 equiv.), and a mixture of 1,4-dioxane-CS_2-MeOH (16 mL : 8 mL : 8 mL). The resulted solution was ultrasonically treated and stirred in an oil bath preset at 100 ^oC. The reaction was monitored by TLC and stopped at the desired time. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to afford compound **7a** (**7b**, **7c** or **7d**), then with carbon disulfide/toluene as the eluent to afford unreacted fullerenol **2a** (**2b**, **2c** or **2d**).

Synthesis of Methoxylated Fullerene 7a from the Reaction of Intermediate 3a with Methanol. Into a 25-mL round-bottomed flask was added intermediate **3a** (5.0 mg), MeOH (1 mL), and anhydrous toluene (5 mL). The mixture was heated and stirred in an oil bath preset at 50 ^oC for 36 h. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to afford methoxylated fullerene **7a** (3.5 mg, 71%).

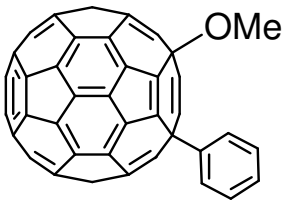
The spectral data of compounds **7a-d** are listed below.



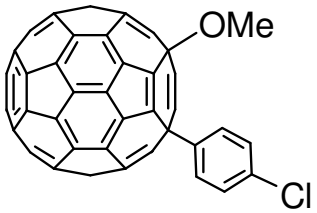
1-Methoxy-4-(4-methylphenyl)-1,4-dihydro[60]fullerene (**7a**): ^1H NMR (300 MHz, CS_2/DMSO-d_6) δ 2.58 (s, 3H), 4.23 (s, 3H), 7.47 (d, J = 8.0 Hz, 2H), 8.18 (d, J = 8.0 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6, all 1C unless indicated) δ 20.80 (CH_3), 53.81 (OCH_3), 60.54 (sp^3-*C* of C_{60}), 80.38 (sp^3-*C* of C_{60}), 127.04 (2C, aryl *C*), 129.60 (2C, aryl *C*), 136.33 (aryl *C*), 136.78, 137.21 (aryl *C*), 137.29, 138.89, 139.33, 139.50, 140.08, 140.27, 141.39, 141.52, 141.63, 141.72, 141.90 (2C), 142.07, 142.08, 142.14, 142.30, 142.34, 142.49 (3C), 142.57, 142.62, 142.67, 143.15, 143.29, 143.31, 143.35, 143.38, 143.40, 143.46, 143.47, 143.51, 143.64, 143.70, 143.89, 144.04, 144.25, 144.76, 144.92 (2C), 145.70, 145.77, 145.88, 145.91, 146.13, 146.16, 146.19, 146.35, 146.39, 146.53, 147.03, 147.63, 148.12, 148.48, 151.97, 153.42, 153.64; FT-IR ν/cm^{-1} (KBr) 2921, 1508, 1454, 1431, 1187, 1092, 1061, 984, 763, 582, 562, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 255 (5.05), 327 (4.51), 439 (3.81), 690 (2.25); HRMS (MALDI-TOF): calcd. for $C_{67}H_7$ [M-CH_3O] 811.0548, found 811.0546.



1-Methoxy-4-(4-methoxyphenyl)-1,4-dihydro[60]fullerene (**7b**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 3.97 (s, 3H), 4.24 (s, 3H), 7.17 (d, J = 8.7 Hz, 2H), 8.20 (d, J = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent, all 1C unless indicated) δ 53.27 (O*C*H$_3$), 54.19 (O*C*H$_3$), 59.31 (sp^3-*C* of C_{60}), 79.47 (sp^3-*C* of C_{60}), 113.65 (2C, aryl *C*), 127.45 (2C, aryl *C*), 130.33 (aryl *C*), 135.86, 136.39, 137.99, 138.50 (2C), 139.18, 139.38, 140.50, 140.63, 140.75, 140.83, 141.03 (2C), 141.15, 141.18, 141.26, 141.41, 141.43, 141.60 (3C), 141.67, 141.73, 141.79, 142.26, 142.42, 142.44, 142.47, 142.50 (2C), 142.57 (2C), 142.63, 142.74, 142.81, 143.02, 143.14, 143.36, 143.86, 144.04 (2C), 144.80, 144.90, 144.99 (2C), 145.24, 145.26, 145.30, 145.46, 145.50, 145.56, 146.15, 146.74, 147.23, 147.54, 151.16, 152.70, 152.76, 158.02 (aryl *C*); FT-IR v/cm^{-1} (KBr) 2921, 1603, 1505, 1457, 1430, 1299, 1250, 1178, 1091, 1059, 1034, 982, 924, 898, 838, 823, 762, 643, 583, 565, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.08), 327 (4.55), 439 (3.83), 688 (2.44); HRMS (MALDI-TOF): calcd. for $C_{67}H_7O$ [M-CH_3O] 827.0497, found 827.0496.



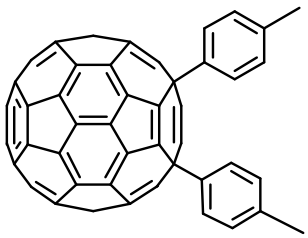
1-Methoxy-4-phenyl-1,4-dihydro[60]fullerene (**7c**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 4.25 (s, 3H), 7.56 (t, J = 7.5 Hz, 1H), 7.69 (t, J = 7.5 Hz, 2H), 8.32 (d, J = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6, all 1C unless indicated) δ 53.84 (O*C*H$_3$), 60.79 (sp^3-*C* of C_{60}), 80.43 (sp^3-*C* of C_{60}), 127.12 (2C, aryl *C*), 127.83 (aryl *C*), 129.00 (2C, aryl *C*), 136.86, 137.45, 138.90, 139.15, 139.38, 139.68, 140.14, 140.30, 141.43, 141.56, 141.65, 141.76, 141.90, 141.91, 142.13, 142.14, 142.18, 142.34, 142.39, 142.53 (3C), 142.60, 142.65, 142.71, 143.17, 143.32, 143.33, 143.38, 143.41, 143.44, 143.49, 143.50 (2C), 143.69, 143.72, 143.90, 144.07, 144.32, 144.80, 144.96 (2C), 145.75, 145.79, 145.92, 145.97, 146.16, 146.21, 146.23, 146.39, 146.43, 146.54, 147.04, 147.68, 148.16, 148.46, 151.80, 153.24, 153.40; FT-IR v/cm^{-1} (KBr) 2919, 1491, 1429, 1186, 1152, 1096, 1060, 983, 924, 897, 763, 734, 692, 584, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 256 (5.05), 327 (4.52), 438 (3.81), 690 (2.20); HRMS (MALDI-TOF): calcd. for $C_{66}H_5$ [M-CH_3O] 797.0391, found 797.0395.



1-(4-Chlorophenyl)-4-methoxy-1,4-dihydro[60]fullerene (**7d**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 4.27 (s, 3H), 7.67 (d, J = 8.4 Hz, 2H), 8.31 (d, J = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6, all 1C unless indicated) δ 53.88 (O*C*H$_3$), 60.00 (sp^3-*C* of C_{60}), 80.37 (sp^3-*C* of C_{60}), 128.64 (2C, aryl *C*), 129.10 (2C, aryl *C*), 133.90 (aryl *C*), 136.97, 137.63, 137.78 (aryl *C*), 138.76, 139.46, 139.92, 140.24, 140.32, 141.41, 141.58, 141.64, 141.77, 141.86, 141.90, 142.18, 142.22 (2C), 142.34, 142.45, 142.47, 142.51, 142.55 (2C), 142.67, 142.74, 143.15, 143.30, 143.32, 143.39 (2C), 143.44 (3C), 143.47, 143.71, 143.72, 143.77, 144.04, 144.41, 144.85, 144.98, 145.00, 145.75, 145.79, 145.92, 145.95, 146.19, 146.25, 146.27, 146.34 (2C), 146.39, 146.96, 147.74, 148.18, 148.23, 151.21, 152.57, 152.75; FT-IR ν/cm^{-1} (KBr) 2920, 1486, 1456, 1428, 1185, 1094, 1060, 1014, 982, 924, 896, 841, 822, 763, 621, 585, 561, 526; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 256 (5.09), 327 (4.55), 443 (3.83), 685 (2.48); HRMS (MALDI-TOF): calcd. for $C_{66}H_4Cl$ [M-CH_3O] 831.0002, found 831.0001.

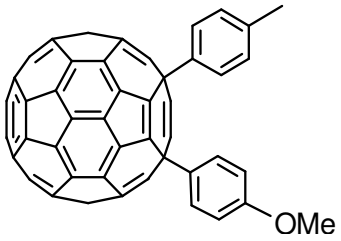
Arylation of Fullerenols 2a-d in the Presence of *p*-Toluenesulfonic Acid. Into a 25-mL round-bottomed flask was added fullerenol **2a** (**2b**, **2c** or **2d**, 10.0 mg), *p*-toluenesulfonic acid (5 equiv.), and 20 mL of toluene. The mixture was heated and stirred in an oil bath preset at 80 ^{o}C. The reaction was monitored by TLC and stopped at the desired time. After the solvent was evaporated *in vacuo*, the residue was separated on a silica gel column with carbon disulfide as the eluent to afford compound **8a** (**8b**, **8c** or **8d**), then with carbon disulfide/toluene as the eluent to afford unreacted fullerenol **2a** (**2b**, **2c** or **2d**).

The spectral data of compounds **8a-d** are listed below.

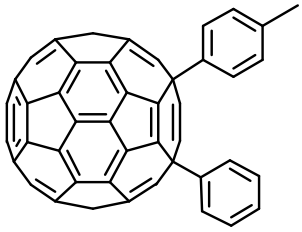


1,4-Bis(4-methylphenyl)-1,4-dihydro[60]fullerene (**8a**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 2.61 (s, 6H), 7.42 (d, J = 8.1 Hz, 4H), 8.06 (d, J = 8.1 Hz, 4H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 20.28 (*C*H$_3$), 60.00 (sp^3-*C* of C_{60}), 126.13 (4C, aryl *C*), 128.82 (4C, aryl *C*), 135.88, 135.94, 136.38, 137.37, 139.54 (aryl *C*), 140.63 (1C), 140.83, 141.12, 141.18, 141.29 (1C), 141.56 (1C), 141.67, 141.70, 141.75, 142.45, 142.52, 142.56, 142.77, 142.88, 142.91, 143.31, 143.46 (1C), 143.60, 143.74, 144.08, 145.36, 145.48,

145.52, 145.65, 147.06, 147.17, 149.63, 155.42; FT-IR ν/cm^{-1} (KBr) 2921, 1507, 1428, 1186, 1120, 1020, 810, 772, 761, 587, 563, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 261 (5.08), 328 (4.55), 444 (3.84), 686 (2.54); HRMS (MALDI-TOF): calcd. for $C_{74}H_{14}$ [M] 902.1096, found 902.1071.

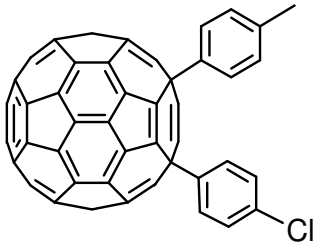


1-(4-Methoxyphenyl)-4-(4-methylphenyl)-1,4-dihydro[60]fullerene (**8b**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 2.61 (s, 3H), 4.00 (s, 3H), 7.11 (d, J = 8.7 Hz, 2H), 7.42 (d, J = 7.8 Hz, 2H), 8.04-8.08 (m, 4H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 20.48 (CH_3), 54.14 (OCH_3), 59.90 (sp^3-*C* of C_{60}), 60.25 (sp^3-*C* of C_{60}), 113.74 (2C, aryl *C*), 126.38 (2C, aryl *C*), 127.53 (2C, aryl *C*), 129.06 (2C, aryl *C*), 131.05 (aryl *C*), 136.06, 136.17, 136.22, 136.66, 137.61 (2C), 139.79, 140.89, 141.10, 141.11, 141.41 (2C), 141.44 (2C), 141.56, 141.93, 141.94, 141.97 (2C), 142.01 (2C), 142.71, 142.74, 142.77, 142.80, 142.82 (2C), 143.03, 143.05, 143.15 (2C), 143.18 (4C), 143.57 (2C), 143.71, 143.85, 143.87, 143.96, 144.07, 144.35 (2C), 145.63 (2C), 145.69, 145.76, 145.79 (2C), 145.90, 145.91, 147.27, 147.34, 147.44 (2C), 149.89, 150.03, 155.66, 155.74, 158.35 (aryl *C*); FT-IR ν/cm^{-1} (KBr) 2922, 1604, 1506, 1458, 1431, 1300, 1251, 1179, 1035, 824, 765, 584, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.99), 328 (4.46), 444 (3.75), 680 (2.41); HRMS (MALDI-TOF): calcd. for $C_{74}H_{14}O$ [M] 918.1045, found 918.1039.



1-(4-Methylphenyl)-4-phenyl-1,4-dihydro[60]fullerene (**8c**): ^{1}H NMR (300 MHz, CS_2/DMSO-d_6) δ 2.55 (s, 3H), 7.36 (t, J = 8.1 Hz, 2H), 7.51-7.60 (m, 3H), 8.00 (t, J = 8.1 Hz, 2H), 8.14 (t, J = 8.1 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 20.48 (CH_3), 60.33 (sp^3-*C* of C_{60}), 60.51 (sp^3-*C* of C_{60}), 126.39 (2C, aryl *C*), 126.46 (2C, aryl *C*), 127.30 (aryl *C*), 128.41 (2C, aryl *C*), 129.07 (2C, aryl *C*), 136.20 (2C), 136.30, 136.71, 137.65, 137.74, 139.11, 139.90, 140.96, 141.15 (2C), 141.42 (2C), 141.50 (2C), 141.62, 141.88 (2C), 142.02, 142.04, 142.07 (2C), 142.73, 142.78, 142.84, 142.88 (3C), 143.08, 143.11, 143.16, 143.18, 143.23 (2C), 143.24, 143.25, 143.62 (2C), 143.78, 143.83, 143.93, 143.97, 144.21, 144.42 (2C), 145.70 (2C), 145.78 (2C), 145.84 (2C), 145.98 (2C), 147.33, 147.37, 147.50, 147.51, 149.75, 149.97, 155.50, 155.69; FT-IR ν/cm^{-1} (KBr)

2919, 1596, 1490, 1427, 1266, 1229, 1186, 1029, 897, 759, 733, 691, 583, 558, 526; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (4.97), 329 (4.51), 444 (3.79), 678 (2.52); HRMS (MALDI-TOF): calcd. for $C_{73}H_{12}$ [M] 888.0939, found 888.0934.

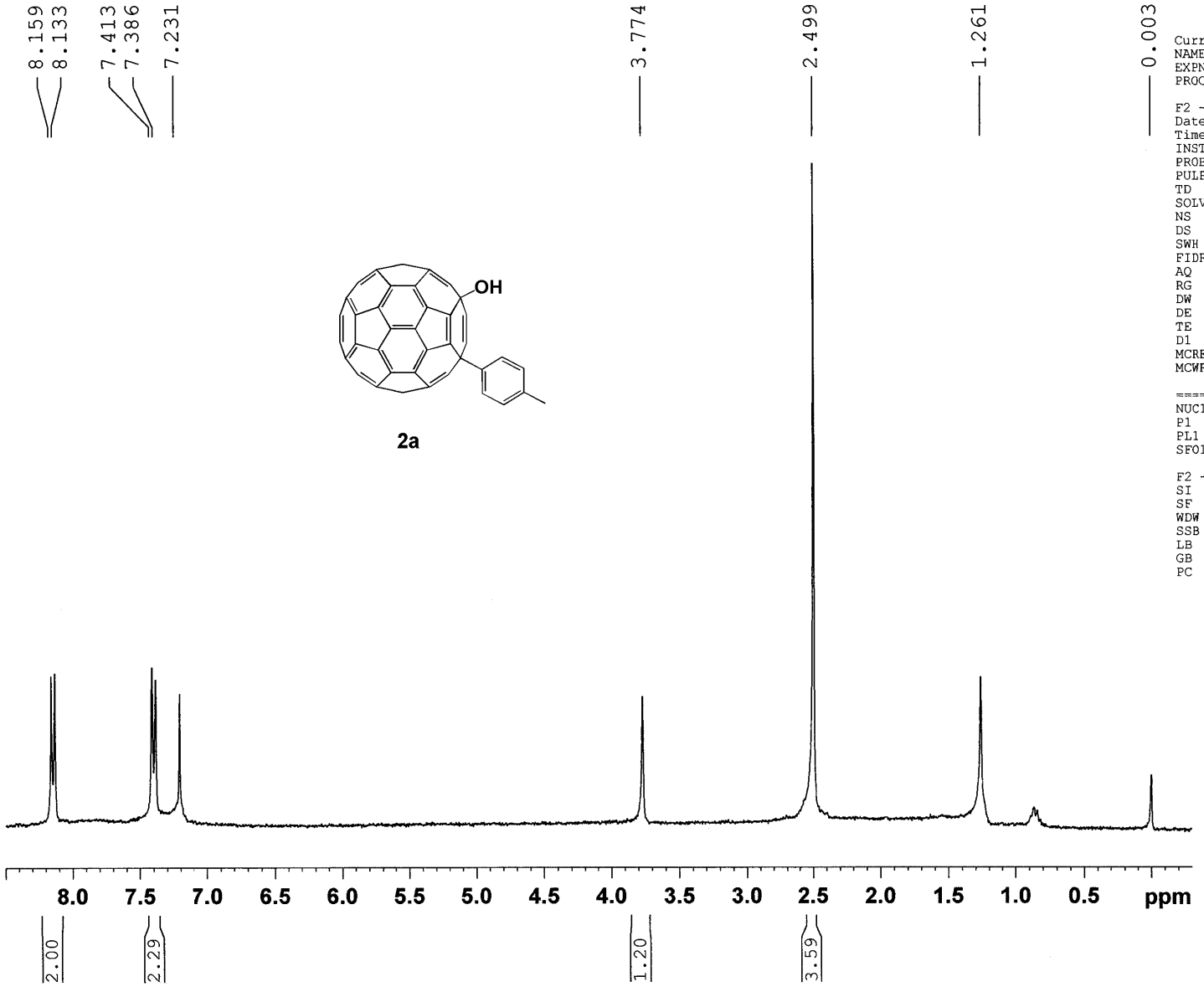


1-(4-Chlorophenyl)-4-(4-methylphenyl)-1,4-dihydro[60]fullerene (**8d**): ^{1}H NMR (300 MHz, CS_2/$CDCl_3$) δ 2.51 (s, 3H), 7.36 (d, J = 8.1 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.99 (d, J = 8.1 Hz, 2H), 8.07 (d, J = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 20.40 (CH$_3$), 59.58 (sp^3-C of C_{60}), 60.16 (sp^3-C of C_{60}), 126.17 (2C, aryl C), 127.81 (2C, aryl C), 128.41 (2C, aryl C), 129.09 (2C, aryl C), 133.28 (aryl C), 135.86, 135.98, 136.26, 136.81, 137.35, 137.57, 137.73, 139.83, 140.78, 140.98, 141.03, 141.22, 141.26, 141.36 (2C), 141.49, 141.72 (3C), 141.87, 141.91 (1C), 141.93, 142.46, 142.66, 142.70 (3C), 142.80, 142.88 (3C), 142.98, 143.04, 143.06, 143.09, 143.13, 143.44 (3C), 143.56, 143.77, 143.88, 144.30 (2C), 144.34, 145.50, 145.56 (2C), 145.57, 145.68, 145.71, 145.84, 145.86, 147.01, 147.13, 147.35, 147.41, 149.11, 149.78, 154.64, 155.47; FT-IR v/cm^{-1} (KBr) 2918, 1507, 1486, 1458, 1428, 1400, 1267, 1228, 1185, 1094, 1014, 896, 837, 817, 763, 621, 584, 559, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.97), 327 (4.51), 444 (3.76), 677 (2.40); HRMS (MALDI-TOF): calcd. for $C_{73}H_{11}Cl$ [M] 922.0549, found 922.0554.

References:

1. Chen, Z.-X.; Wang, G.-W. *J. Org. Chem.* **2005**, *70*, 2380.

^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 2a

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
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Time                10.37
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PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     48
DS                      1
SWH              8992.806 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                   456.1
DW                  55.600 use
DE                   6.00 use
TE                  300.0 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 use
PL1                 -3.00 dB
SFO1          300.1321009 MHz

F2 - Processing parameters
SI                  16384
SF            300.1300219 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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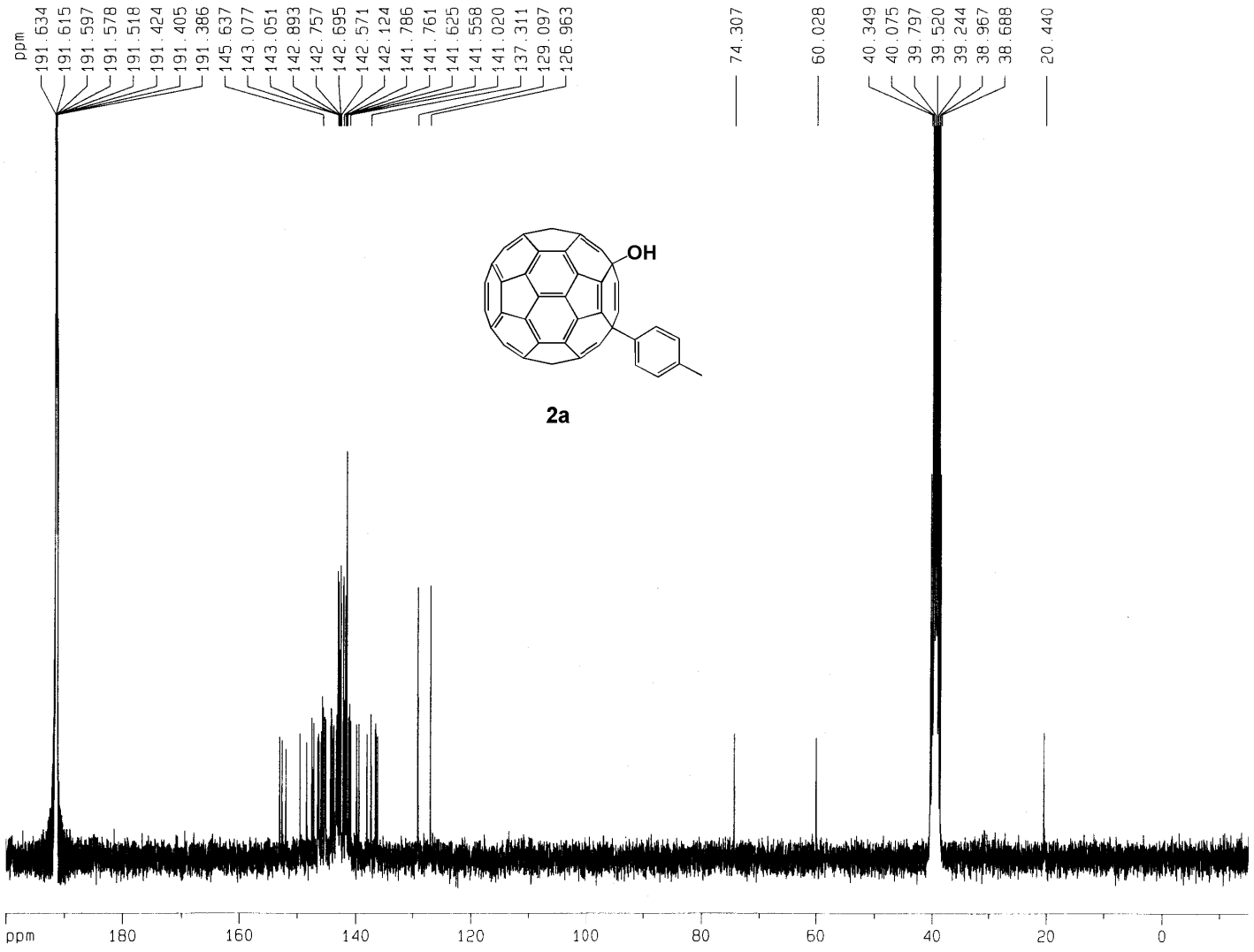
^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 2a

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Current Data Parameters
NAME                  lym070705
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070706
Time                       6.53
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                   zgdc
TD                       32768
SOLVENT                   DMSO
NS                        17408
DS                            4
SWH                22675.736 Hz
FIDRES             0.692009 Hz
AQ                 0.7225844 sec
RG                         8192
DW                    22.050 usec
DE                     6.00 usec
TE                     302.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                    3.00 usec
PL1                  -1.00 dB
SF01              75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL2                   -3.00 dB
PL12                  16.00 dB
SF02             300.1315007 MHz

F2 - Processing parameters
SI                       131072
SF                75.4678556 MHz
WDW                        EM
SSB                         0
LB                     0.50 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                    22.00 cm
CY                     0.00 cm
F1P                  200.045 ppm
F1                  15096.99 Hz
F2P                  -15.063 ppm
F2                  -1136.78 Hz
PPMCM                9.77765 ppm/cm
HZCM               737.89850 Hz/cm
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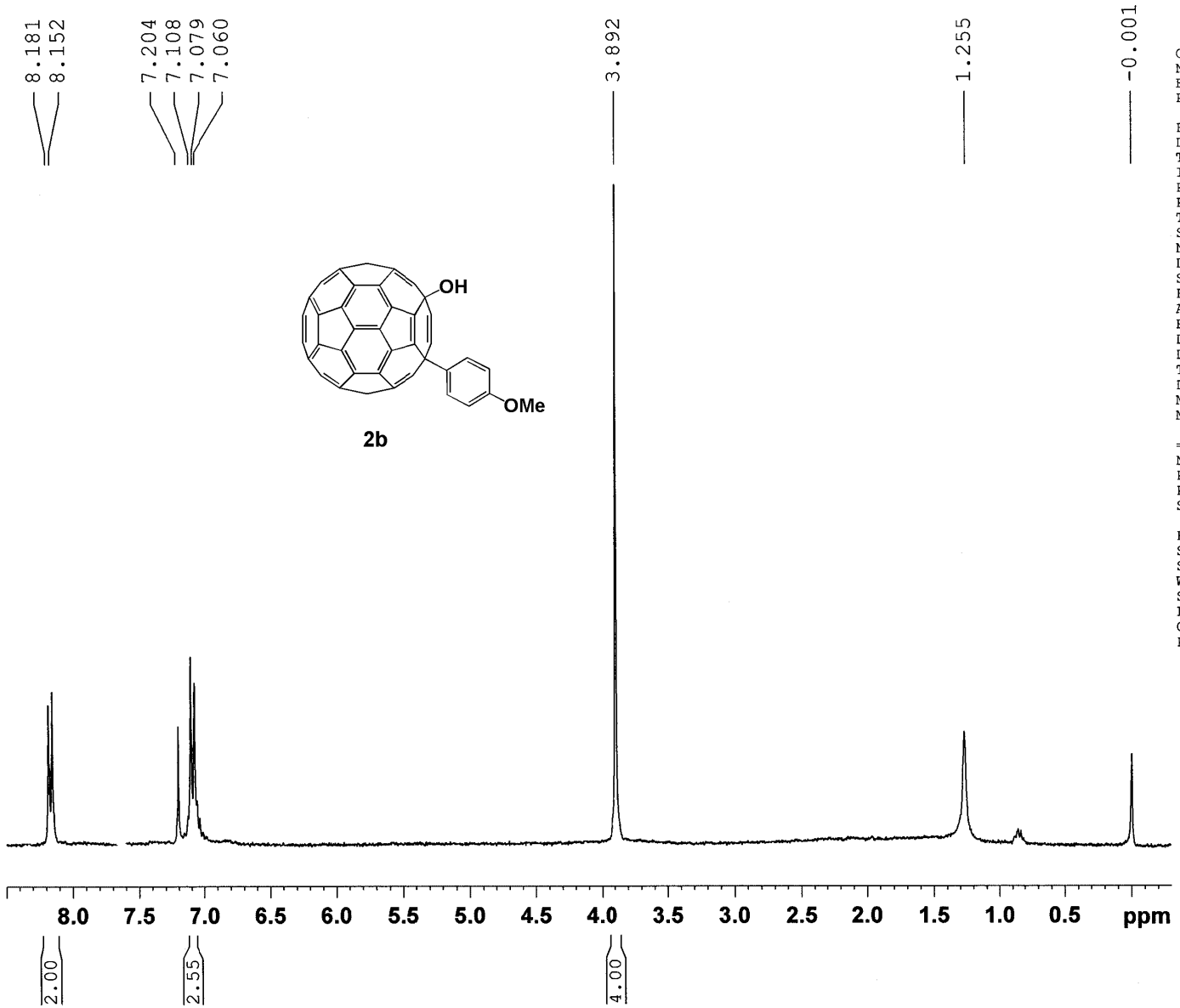
^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 2b

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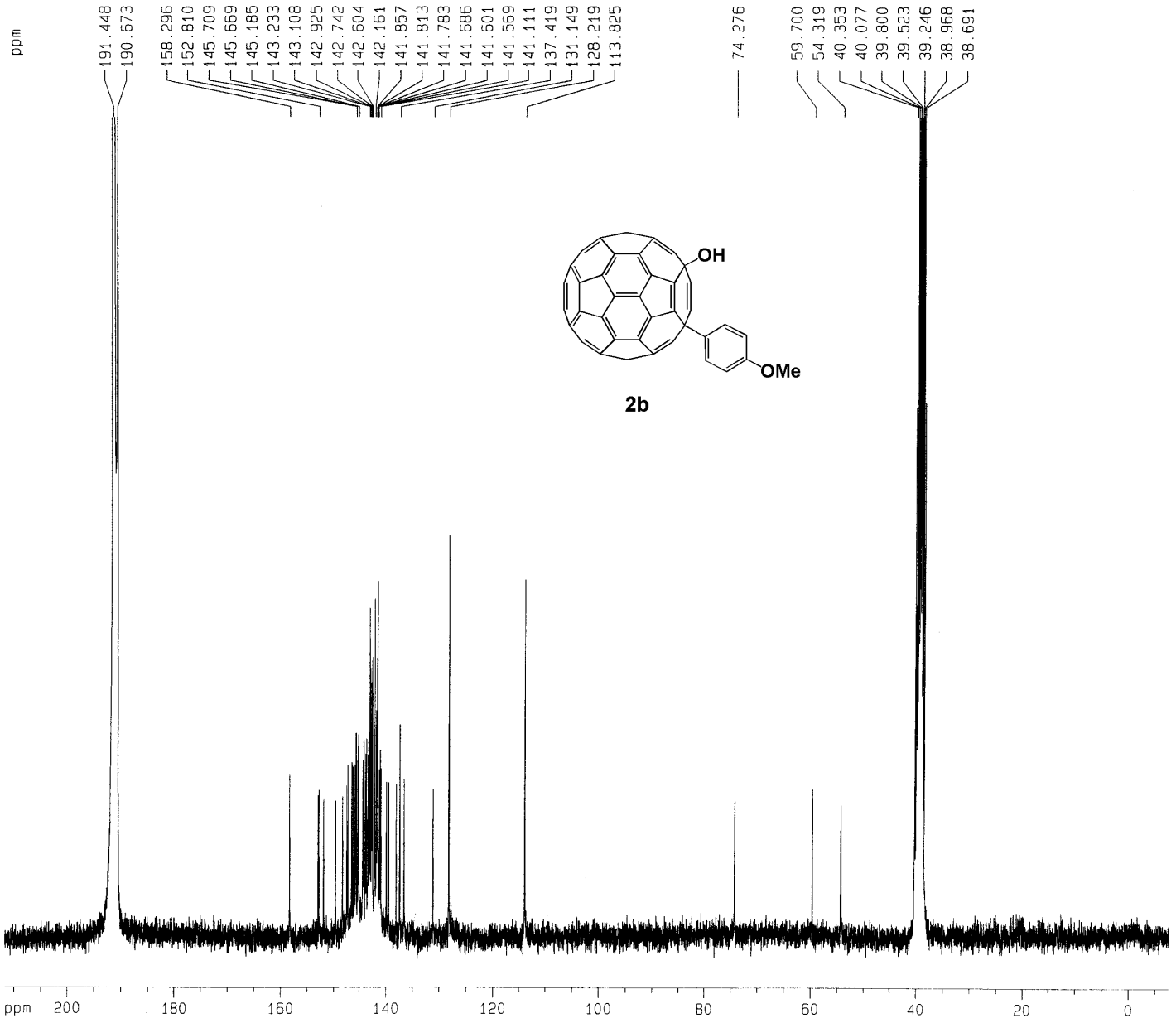
Current Data Parameters
NAME          lym07122701
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20071227
Time                10.30
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      1
SWH              8992.806 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                  456.1
DW                 55.600 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.50 usec
PL1                 -3.00 dB
SFO1          300.1321009 MHz

F2 - Processing parameters
SI                   16384
SF            300.1300238 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound **2b**

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Current Data Parameters
NAME            czx031223c
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20031224
Time                 8.16
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                  17302
DS                      2
SWH           16556.291 Hz
FIDRES         0.505258 Hz
AQ            0.9896436 sec
RG                 5792.6
DW                30.200 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 5.30 usec
PL1                -6.00 dB
SFO1         75.4755588 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                -3.00 dB
PL12               16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4678527 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                22.00 cm
CY              3000.00 cm
F1P              211.803 ppm
F1             15984.29 Hz
F2P               -7.579 ppm
F2              -572.00 Hz
PPMCM            9.97191 ppm/cm
HZCM           752.55872 Hz/cm
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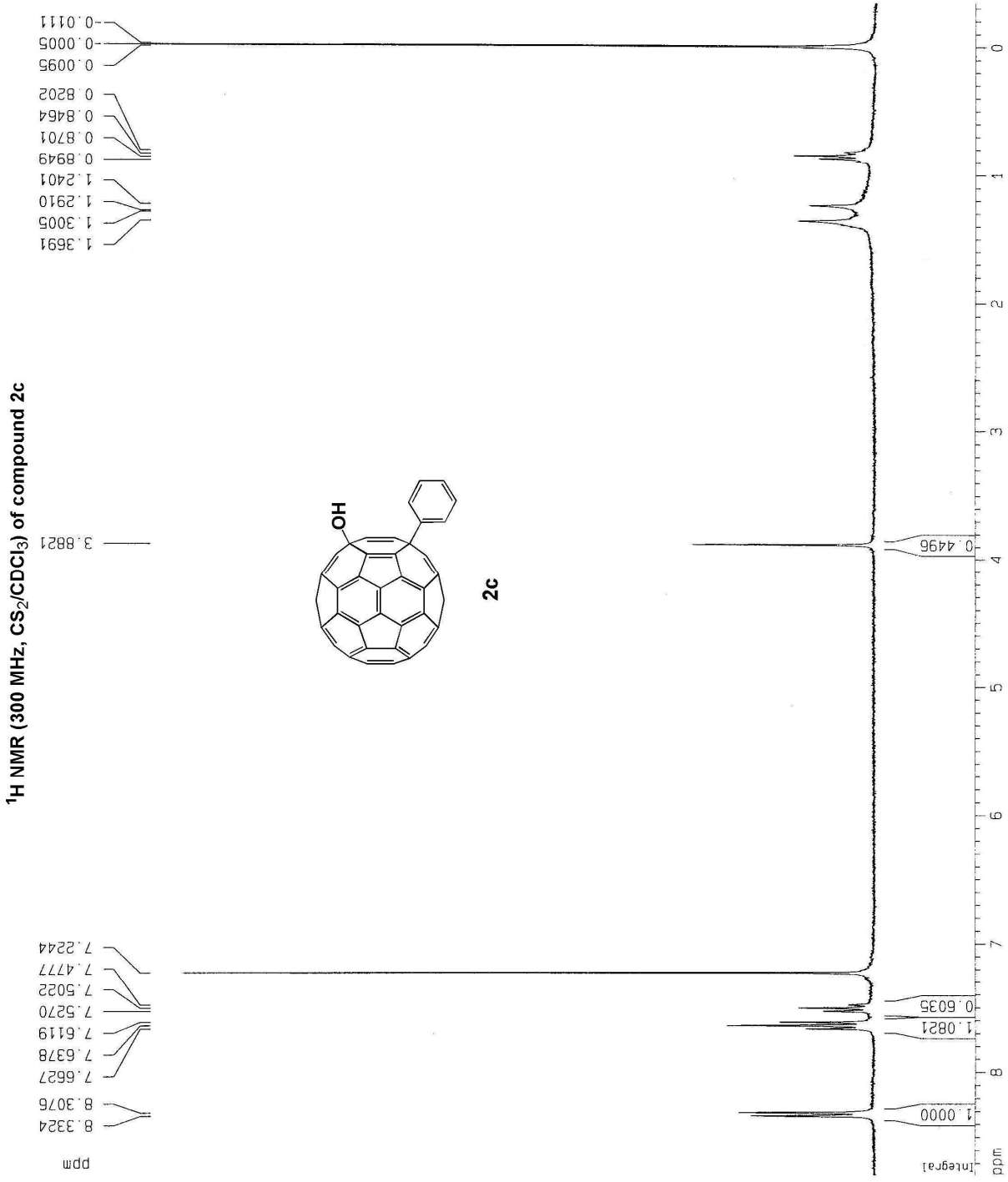
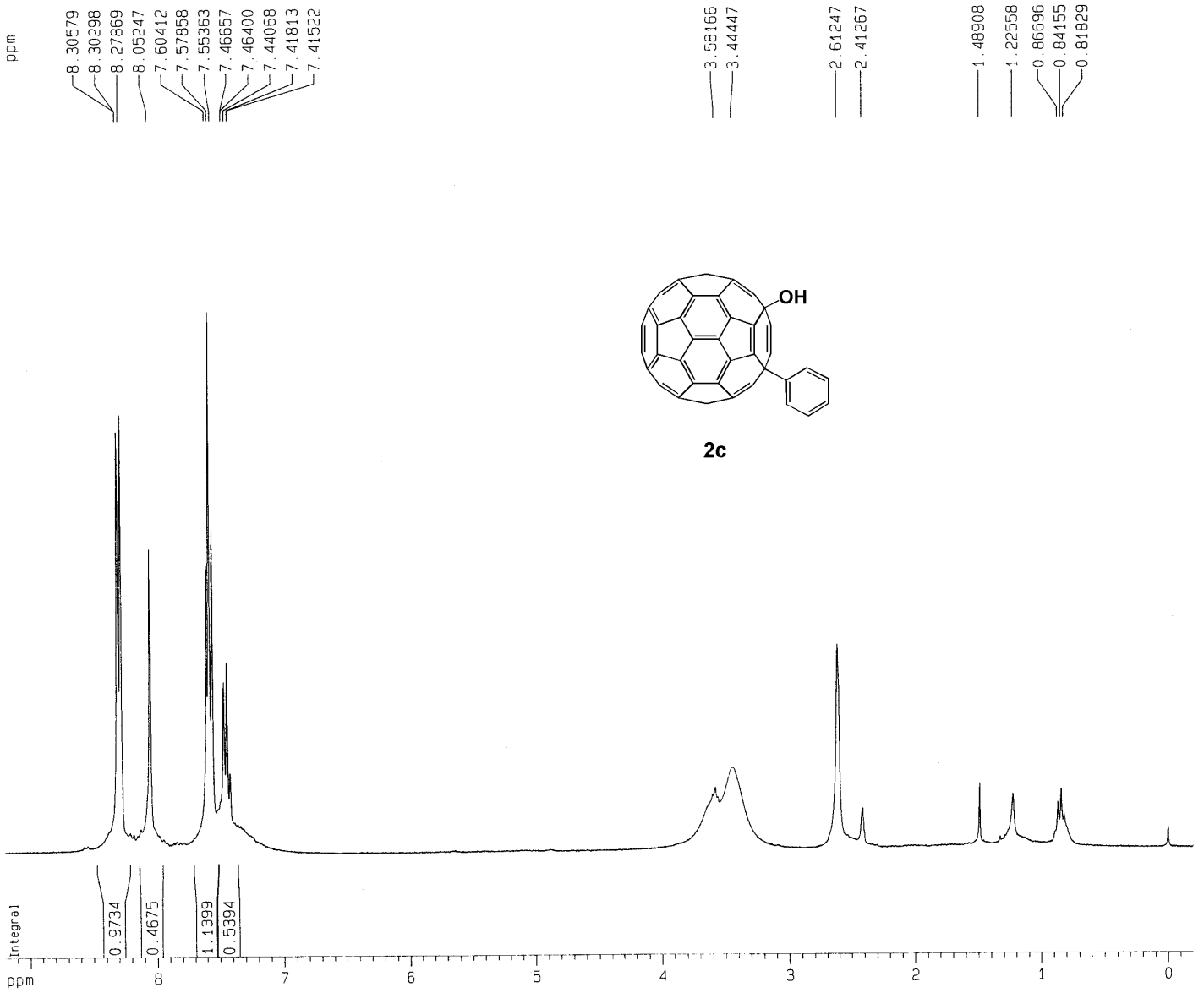
^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 2c



^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 2c



2c

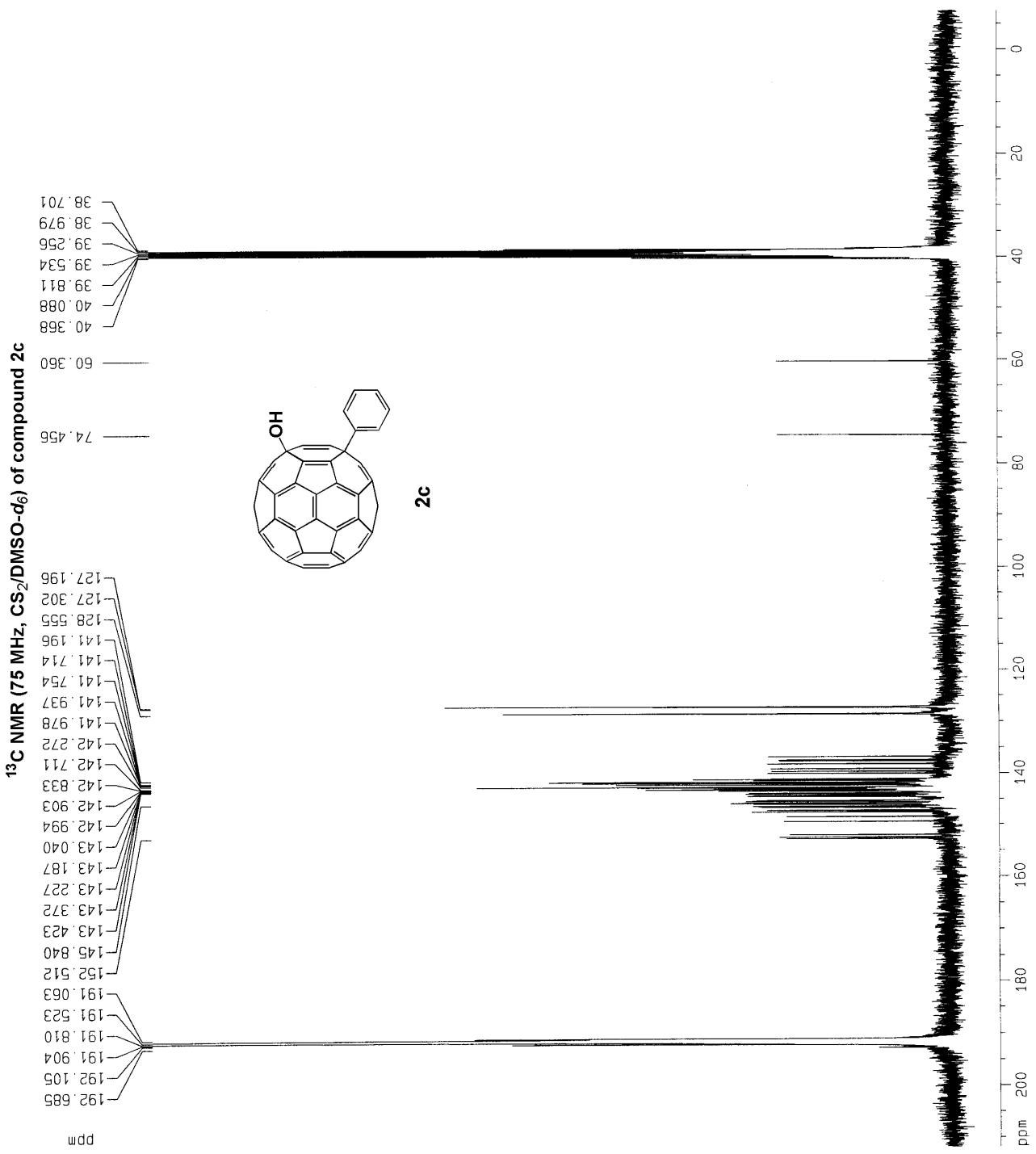
```
Current Data Parameters
NAME                 czx031127
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20031127
Time                     16.07
INSTRUM                  av300
PROBHD     5 mm BBO BB-1H
PULPROG                    zg
TD                      32768
SOLVENT                  DMSO
NS                        200
DS                          2
SWH                  5995.204 Hz
FIDRES               0.182959 Hz
AQ                   2.7329011 sec
RG                       203.2
DW                      83.400 usec
DE                       6.00 usec
TE                      300.0 K
D1                   2.00000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       7.50 usec
PL1                     -3.00 dB
SFO1                300.1321009 MHz

F2 - Processing parameters
SI                       16384
SF                  300.1300280 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       22.00 cm
CY                        0.00 cm
F1P                       9.196 ppm
F1                     2759.88 Hz
F2P                      -0.198 ppm
F2                     -59.30 Hz
PPMCM                 0.42696 ppm/cm
HZCM                128.14424 Hz/cm
```


13C NMR (75 MHz, CS2/DMSO-d6) of compound 2c
Current Data Parameters
NAME czx031127
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20031127
Time 17.46
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 1703
DS 2
SWH 16556.291 Hz
FIDRES 0.505256 Hz
AQ 0.9896436 sec
RG 3649.1
DW 30.200 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.40 usec
PL1 -6.00 dB
SFO1 75.4755588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1315007 MHz
F2 - Processing parameters
SI 131072
SF 75.4678444 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 211.913 ppm
F1 15992.63 Hz
F2P -7.469 ppm
F2 -563.66 Hz
PPMCM 9.97191 ppm/cm
HZCM 752.55865 Hz/cm
OH
2c
ppm
192.685
192.105
191.904
191.810
191.523
191.063
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145.840
143.423
143.372
143.227
143.187
143.040
142.994
142.903
142.833
142.711
142.272
141.978
141.937
141.754
141.714
141.196
128.555
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127.196
74.456
60.360
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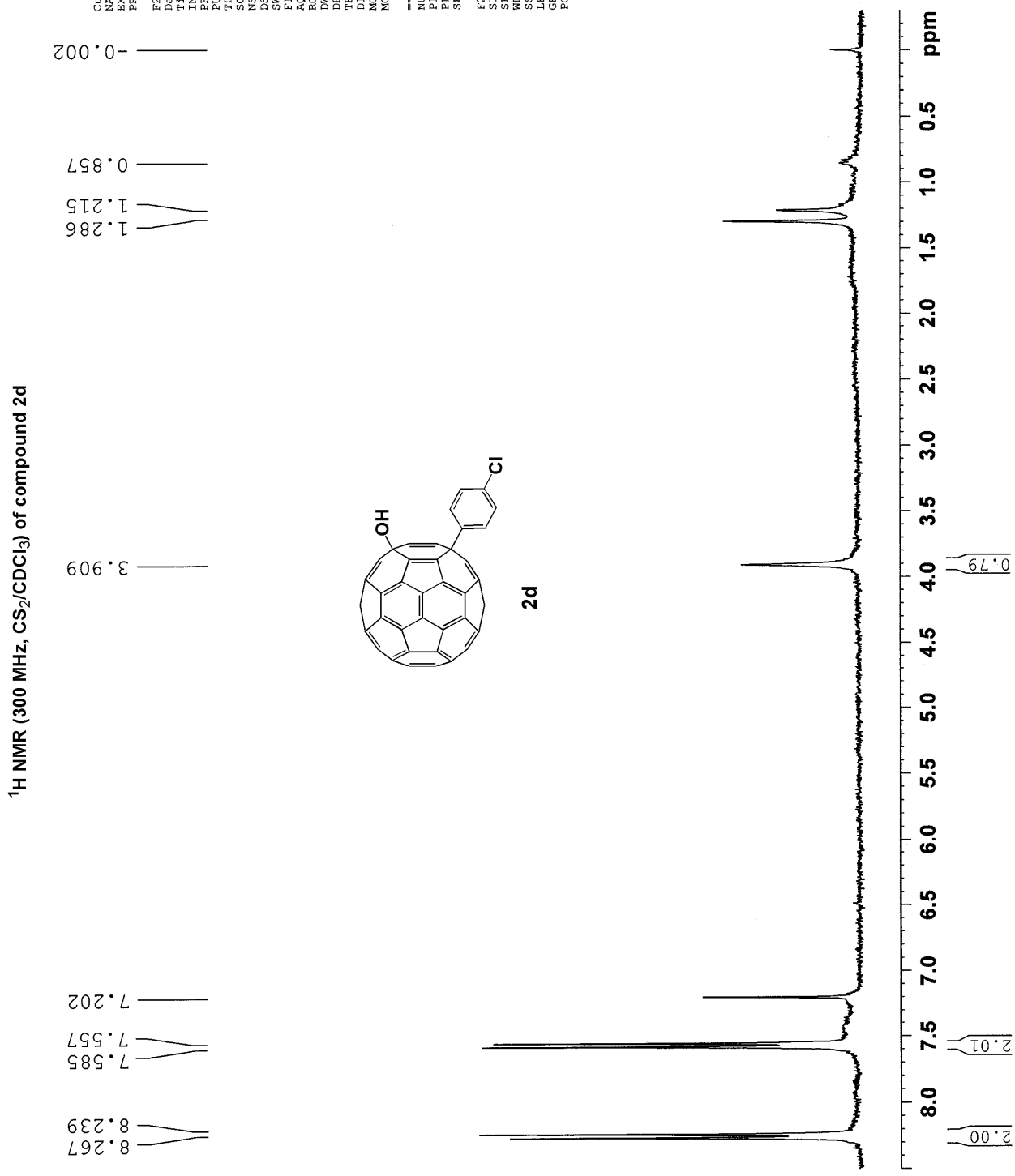
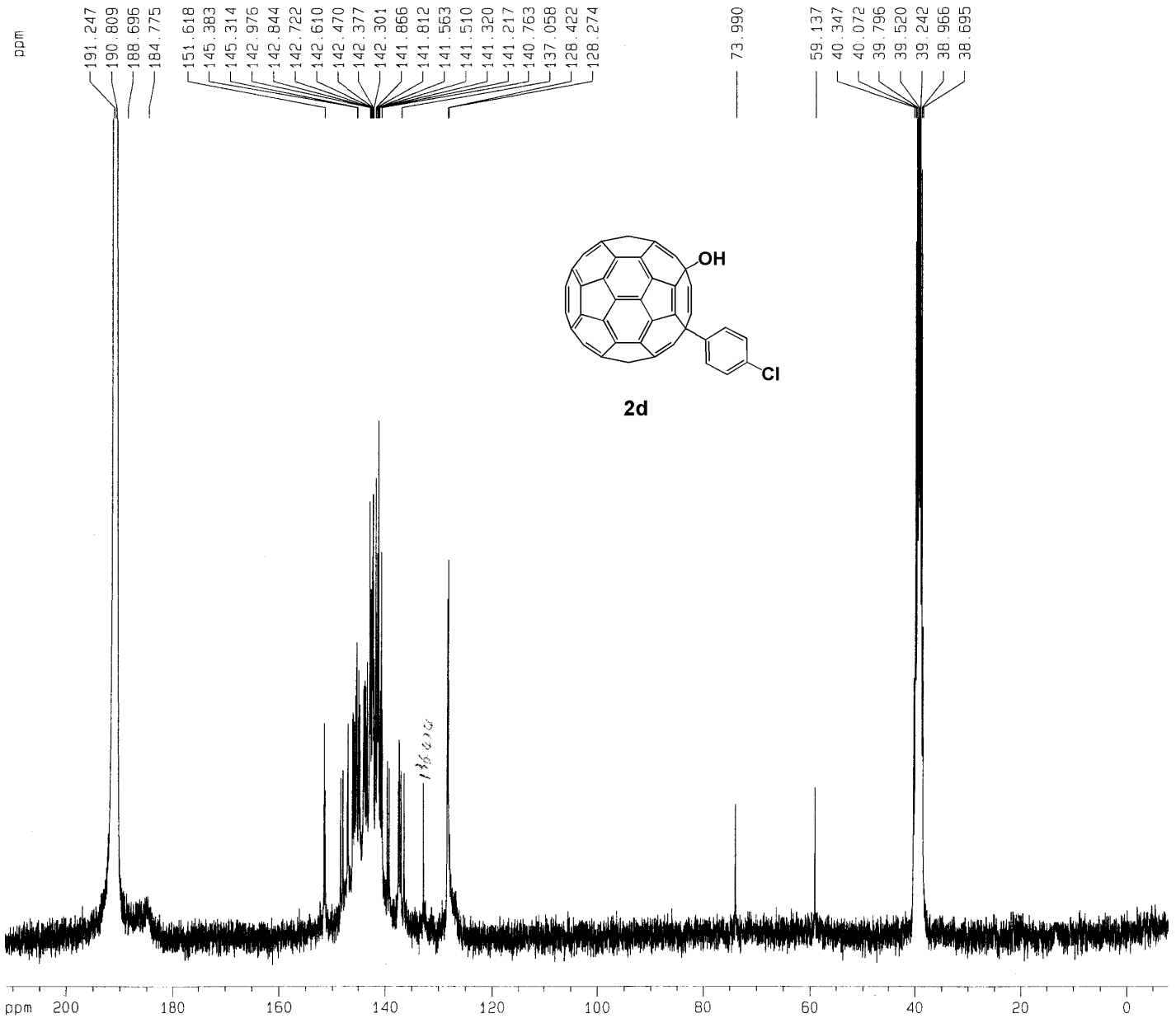
39.811
39.534
39.256
38.979
38.701
ppm



^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 2d

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 2d

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Current Data Parameters
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EXPNO                  2
PROCNO                 1

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Time                7.58
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zgdc
TD                 32768
SOLVENT             DMSO
NS                 17777
DS                     2
SWH           16556.291 Hz
FIDRES        0.505258 Hz
AQ            0.9896436 sec
RG                  4096
DW               30.200 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                2.40 usec
PL1              -6.00 dB
SFO1         75.4755588 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2             120.00 dB
PL12             16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4678762 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

1D NMR plot parameters
CX               22.00 cm
CY                0.00 cm
F1P             211.491 ppm
F1             15960.80 Hz
F2P              -7.891 ppm
F2             -595.49 Hz
PPMCM          9.97191 ppm/cm
HZCM          752.55872 Hz/cm
```
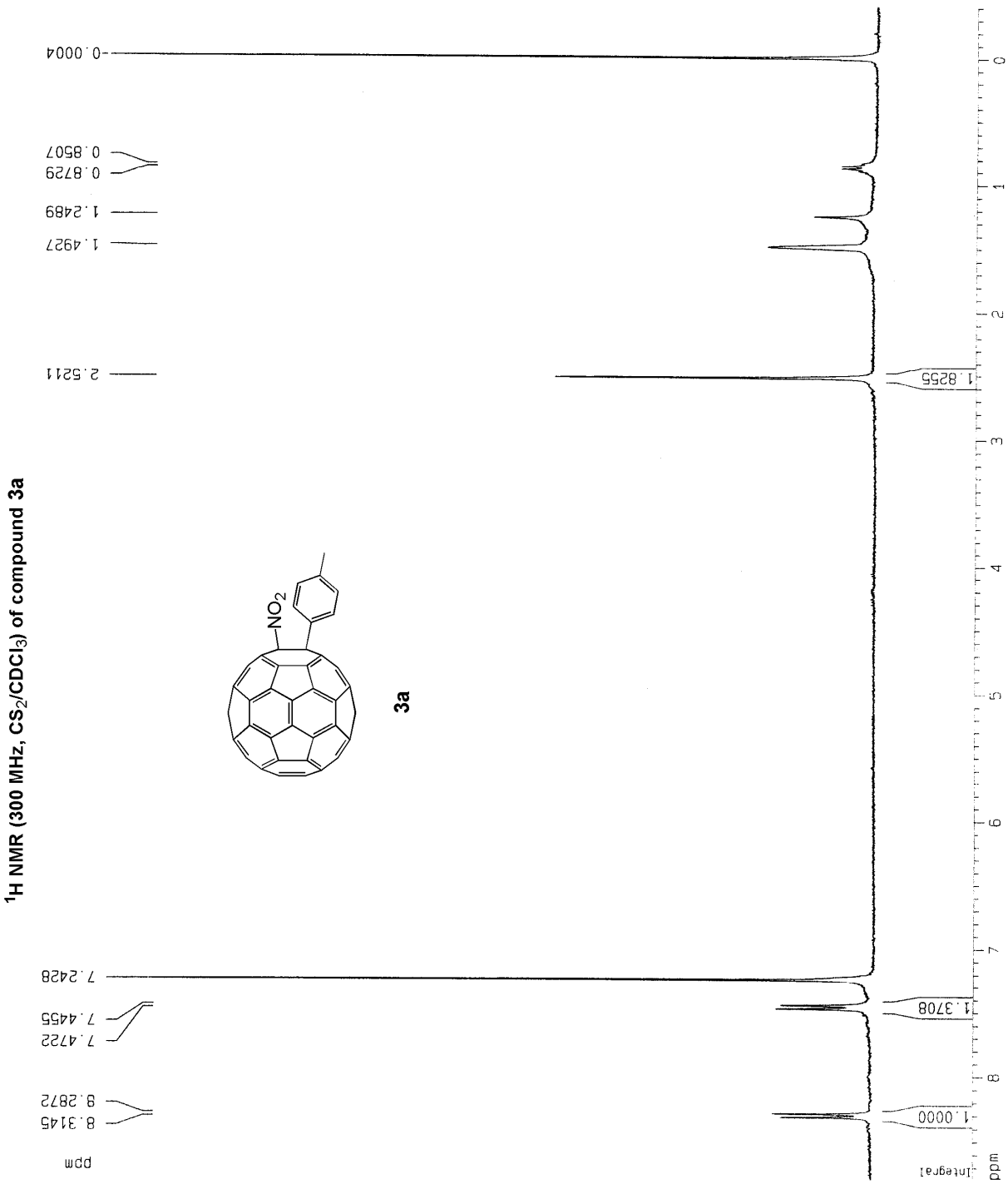
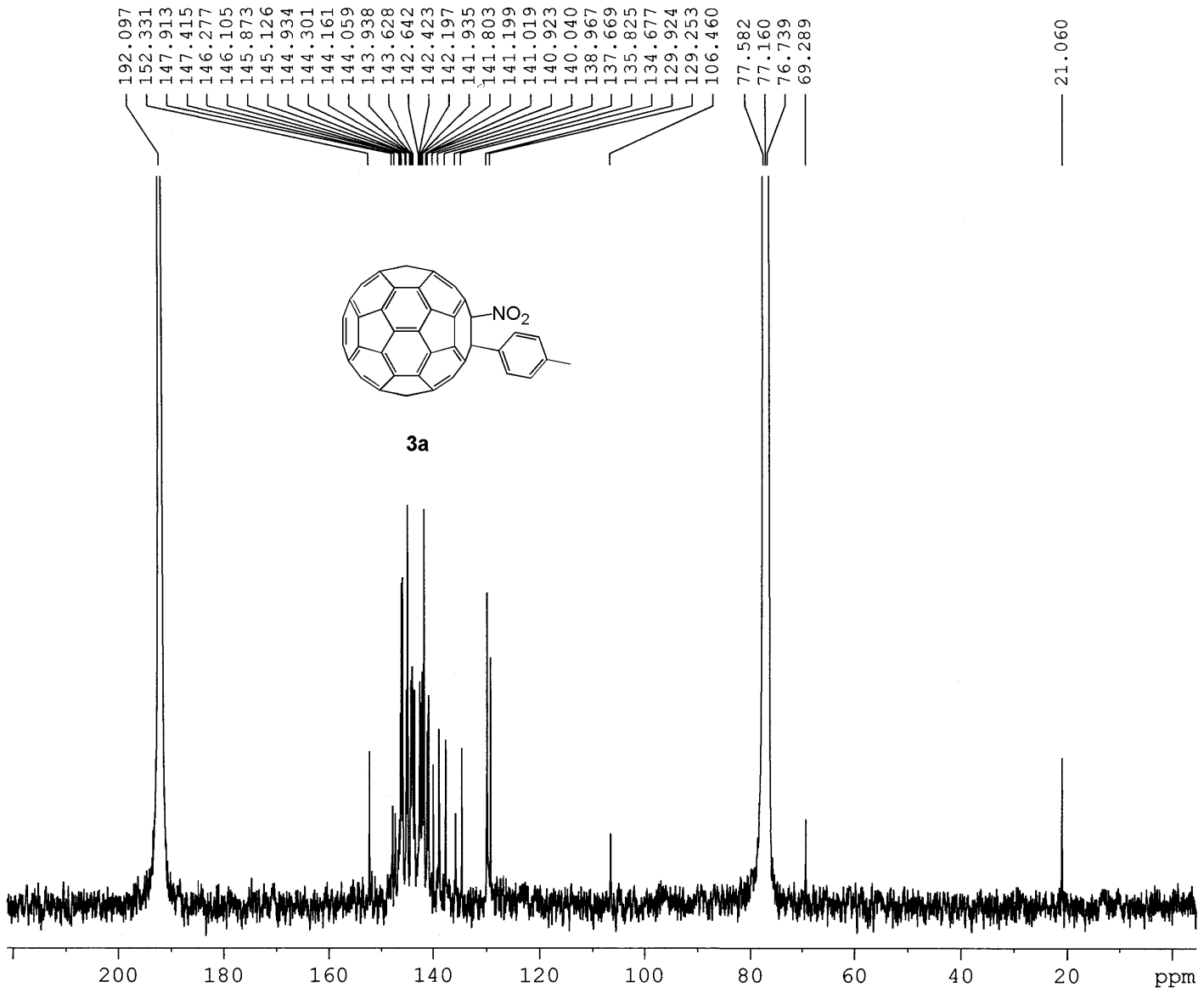

^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 3a



^{13}C NMR (75 MHz, CS_2/$CDCl_3$) of compound 3a



3a

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Current Data Parameters
NAME                 lym08012101
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
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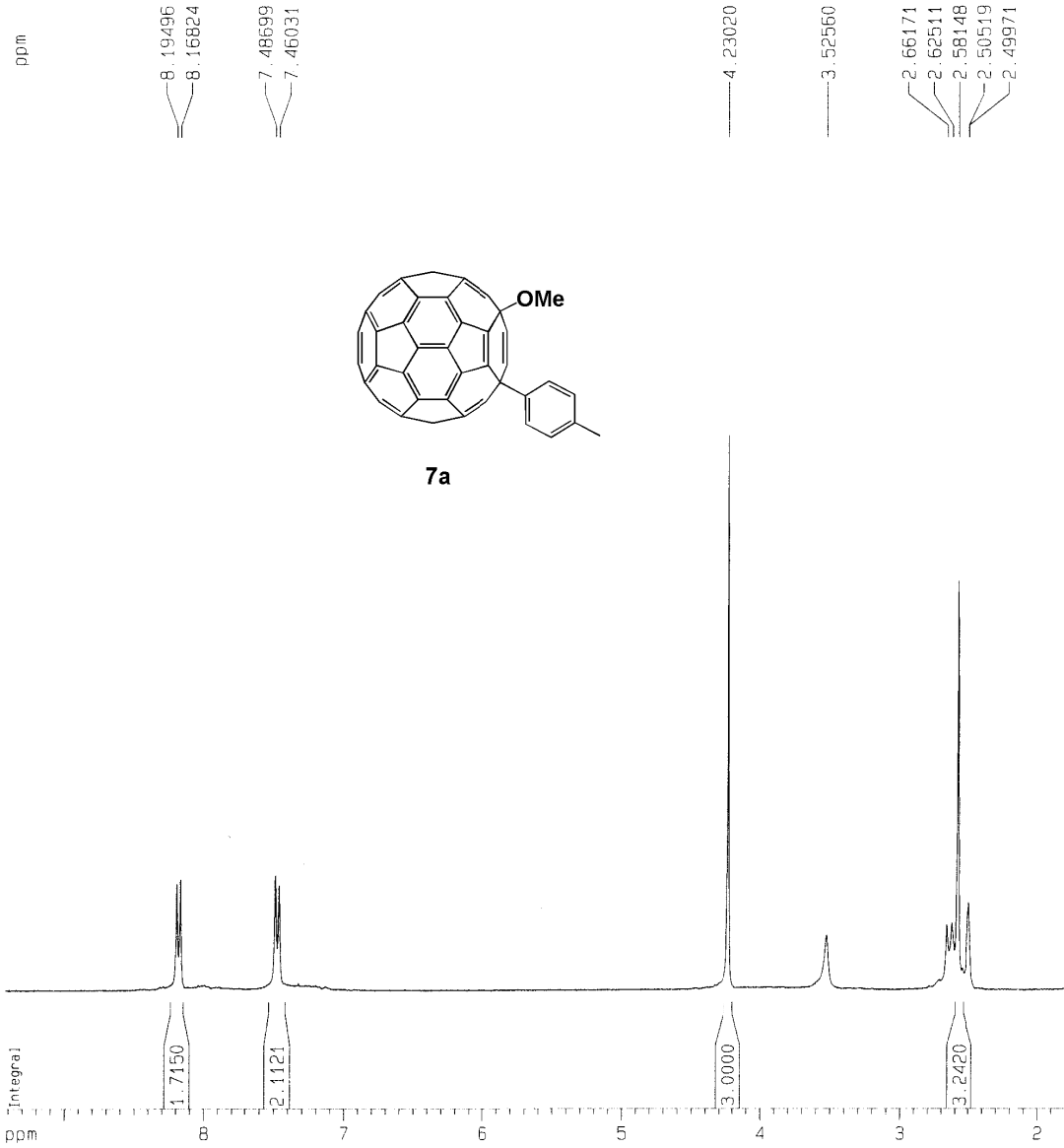
Time                        8.05
INSTRUM                    av300
PROBHD    5 mm BBO BB-1H
PULPROG                     zgdc
TD                         32768
SOLVENT                    CDCl3
NS                         20868
DS                             4
SWH                  37878.789 Hz
FIDRES               1.155969 Hz
AQ                   0.4325876 sec
RG                          6502
DW                     13.200 usec
DE                      6.00 usec
TE                        300.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                      3.00 usec
PL1                       -1.00 dB
SFO1                75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                  80.00 usec
PL2                       -3.00 dB
PL12                      16.00 dB
SFO2                300.1315007 MHz

F2 - Processing parameters
SI                        131072
SF                  75.4677936 MHz
WDW                           EM
SSB                            0
LB                      4.00 Hz
GB                             0
PC                          1.40
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 7a



7a

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Current Data Parameters
NAME                lym060707
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20060707
Time                     9.26
INSTRUM                 av300
PROBHD   5 mm BBO BB-1H
PULPROG                    zg
TD                      65536
SOLVENT                 DMSO
NS                         64
DS                          1
SWH                 5995.204 Hz
FIDRES              0.091480 Hz
AQ                  5.4657526 sec
RG                        512
DW                   83.400 usec
DE                    6.00 usec
TE                    300.0 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    7.50 usec
PL1                  -3.00 dB
SFO1             300.1321009 MHz

F2 - Processing parameters
SI                      16384
SF                300.1300029 MHz
WDW                        no
SSB                         0
LB                    0.00 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                     22.00 cm
CY                      0.00 cm
F1P                     9.422 ppm
F1                   2827.94 Hz
F2P                    -0.565 ppm
F2                   -169.66 Hz
PPMCM                0.45399 ppm/cm
HZCM               136.25462 Hz/cm
```
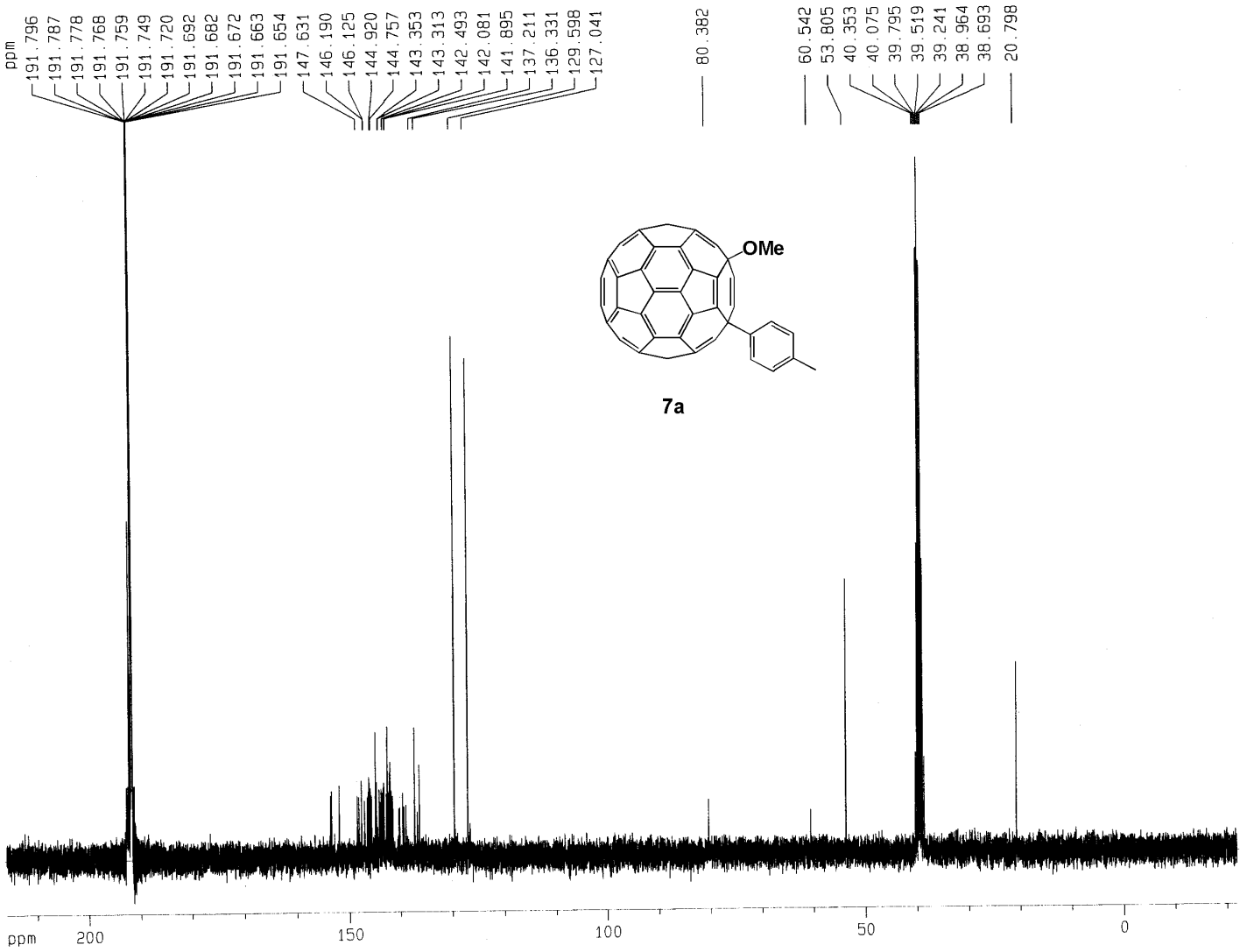
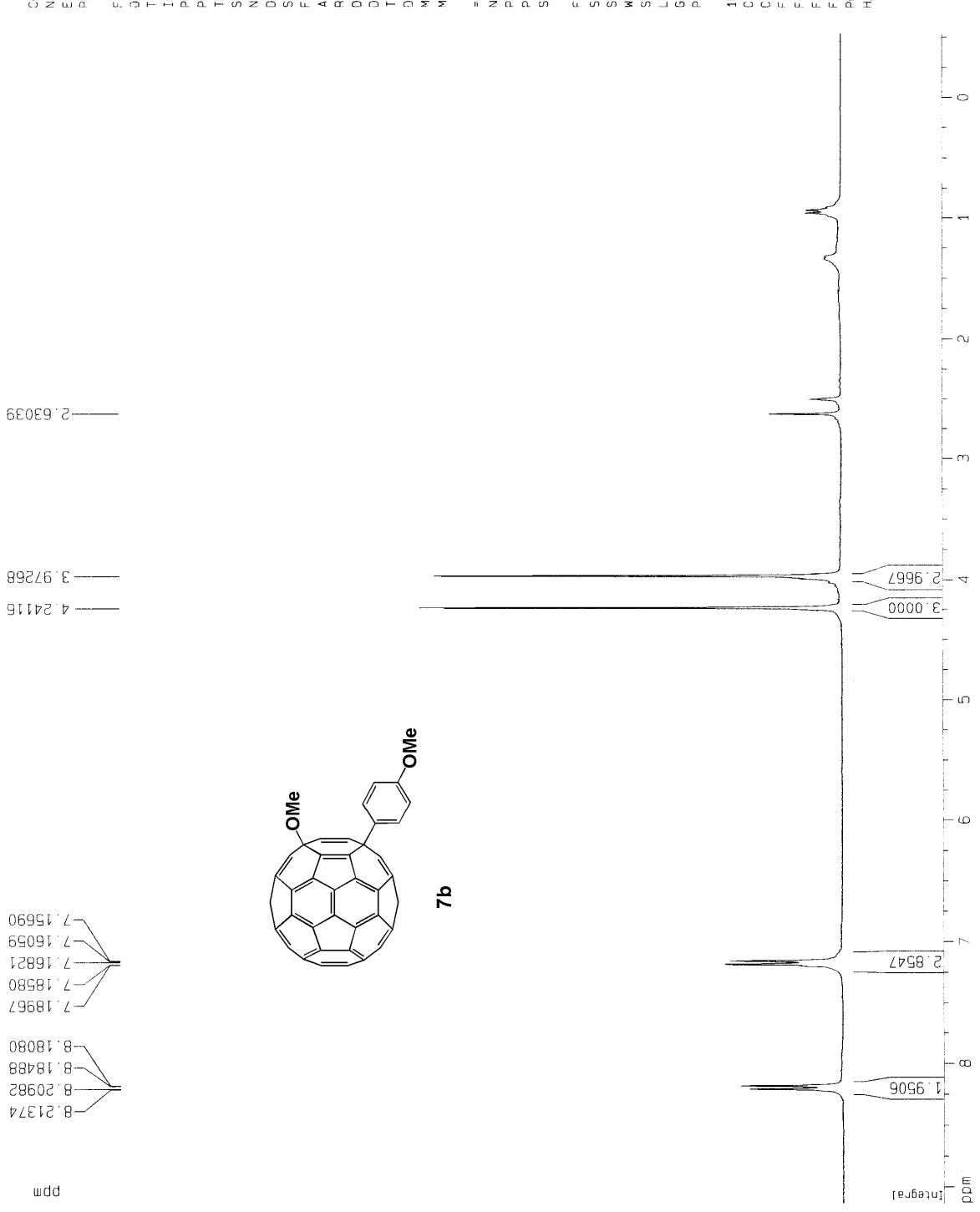

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 7a

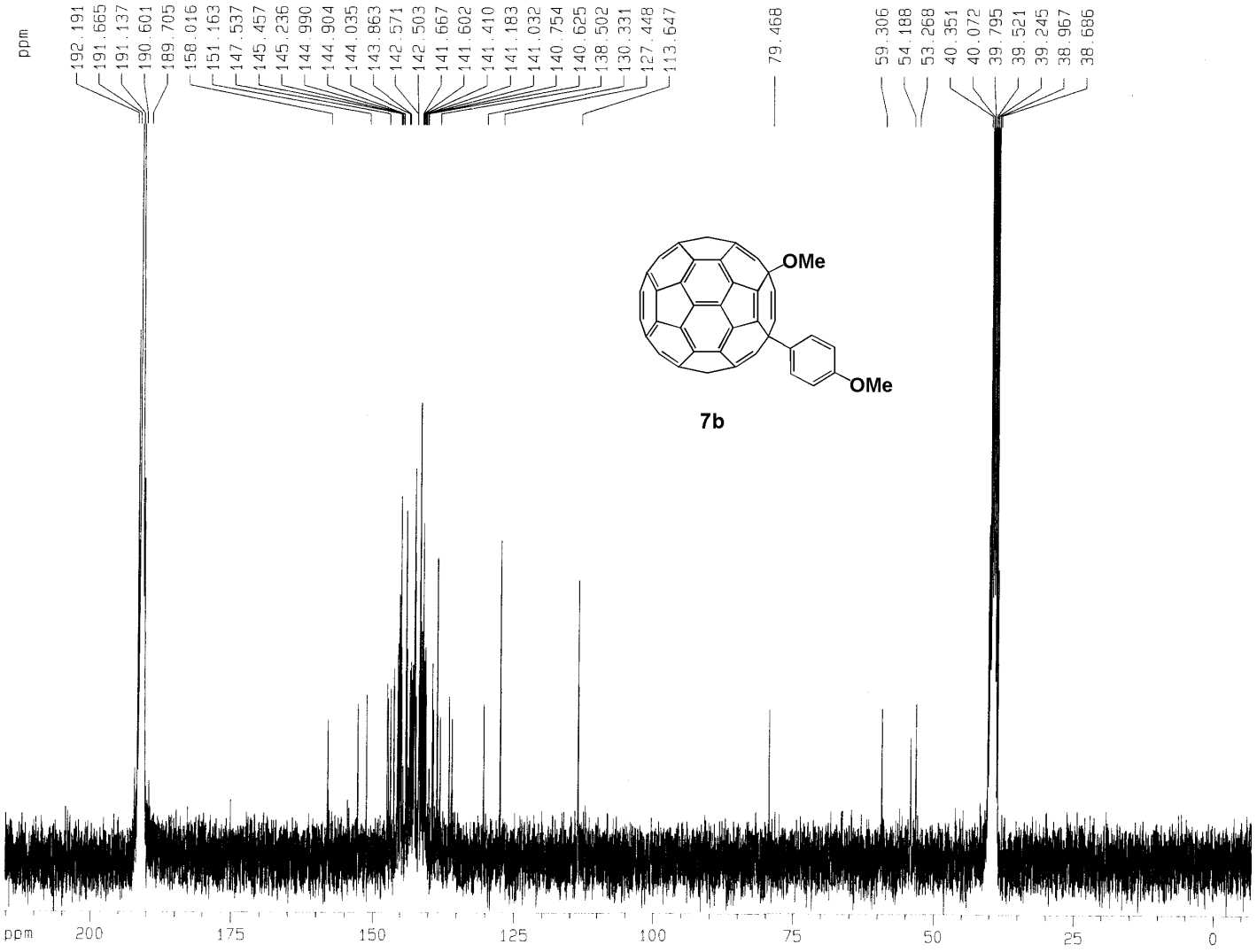



```
Current Data Parameters
NAME                  lym070312
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070313
Time                       7.54
INSTRUM                   av300
PROBHD    5 mm BBO BB-1H
PULPROG                   zgdc
TD                       65536
SOLVENT                   DMSO
NS                        14633
DS                            4
SWH                22675.736 Hz
FIDRES             0.346004 Hz
AQ                 1.4451188 sec
RG                      3649.1
DW                     22.050 usec
DE                      6.00 usec
TE                     300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                        3.00 usec
PL1                      -1.00 dB
SFO1               75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -3.00 dB
PL12                     16.00 dB
SFO2              300.1315007 MHz

F2 - Processing parameters
SI                       131072
SF                 75.4678212 MHz
WDW                        EM
SSB                         0
LB                       0.50 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      22.00 cm
CY                       0.00 cm
F1P                    215.993 ppm
F1                   16300.49 Hz
F2P                   -21.817 ppm
F2                  -1646.48 Hz
PPMCM                10.80953 ppm/cm
HZCM                815.77130 Hz/cm
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 7b



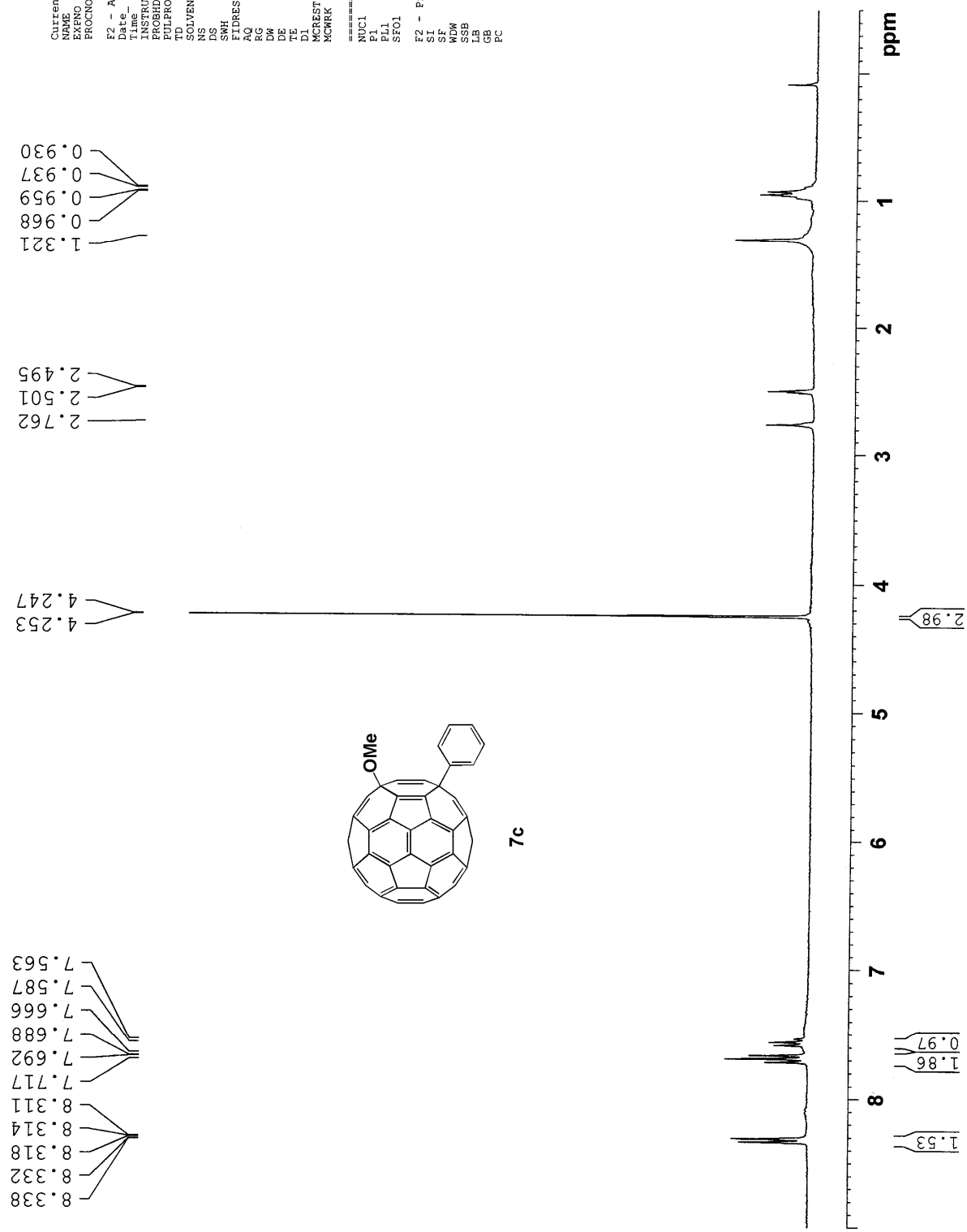
^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 7b



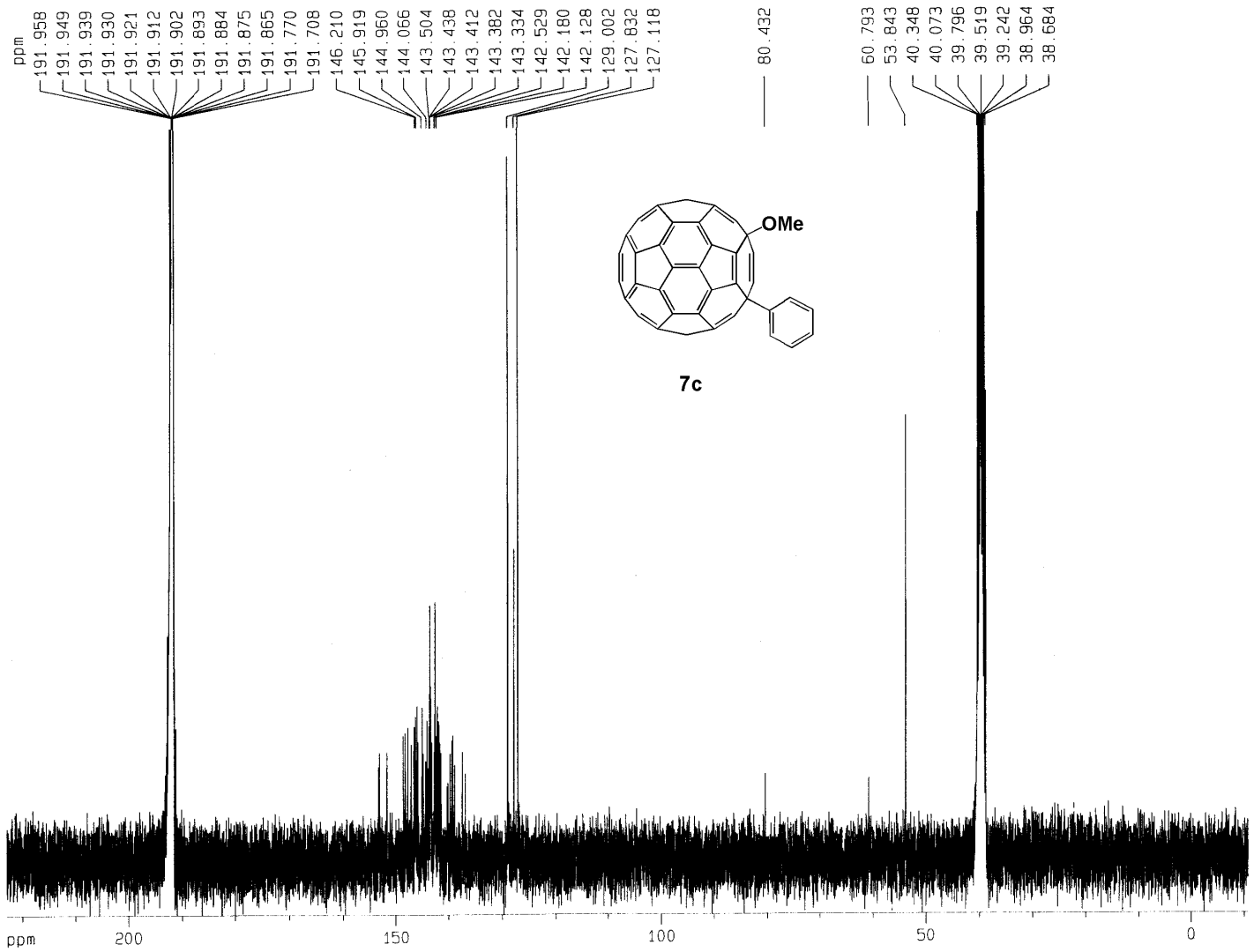
7b

```
Current Data Parameters
NAME            lym060706
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060707
Time                8.04
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zgdc
TD                  65536
SOLVENT              DMSO
NS                   15093
DS                       4
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ            1.4451188 sec
RG                   13004
DW              22.050 usec
DE               6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1               3.00 usec
PL1              -1.00 dB
SF01          75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2           80.00 usec
PL2              -3.00 dB
PL12             16.00 dB
SF02         300.1315007 MHz

F2 - Processing parameters
SI                  131072
SF            75.4678890 MHz
WDW                   EM
SSB                    0
LB                0.50 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                22.00 cm
CY                 0.00 cm
F1P             215.212 ppm
F1             16241.56 Hz
F2P              -6.726 ppm
F2              -507.56 Hz
PPMCM          10.08805 ppm/cm
HZCM          761.32373 Hz/cm
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 7c



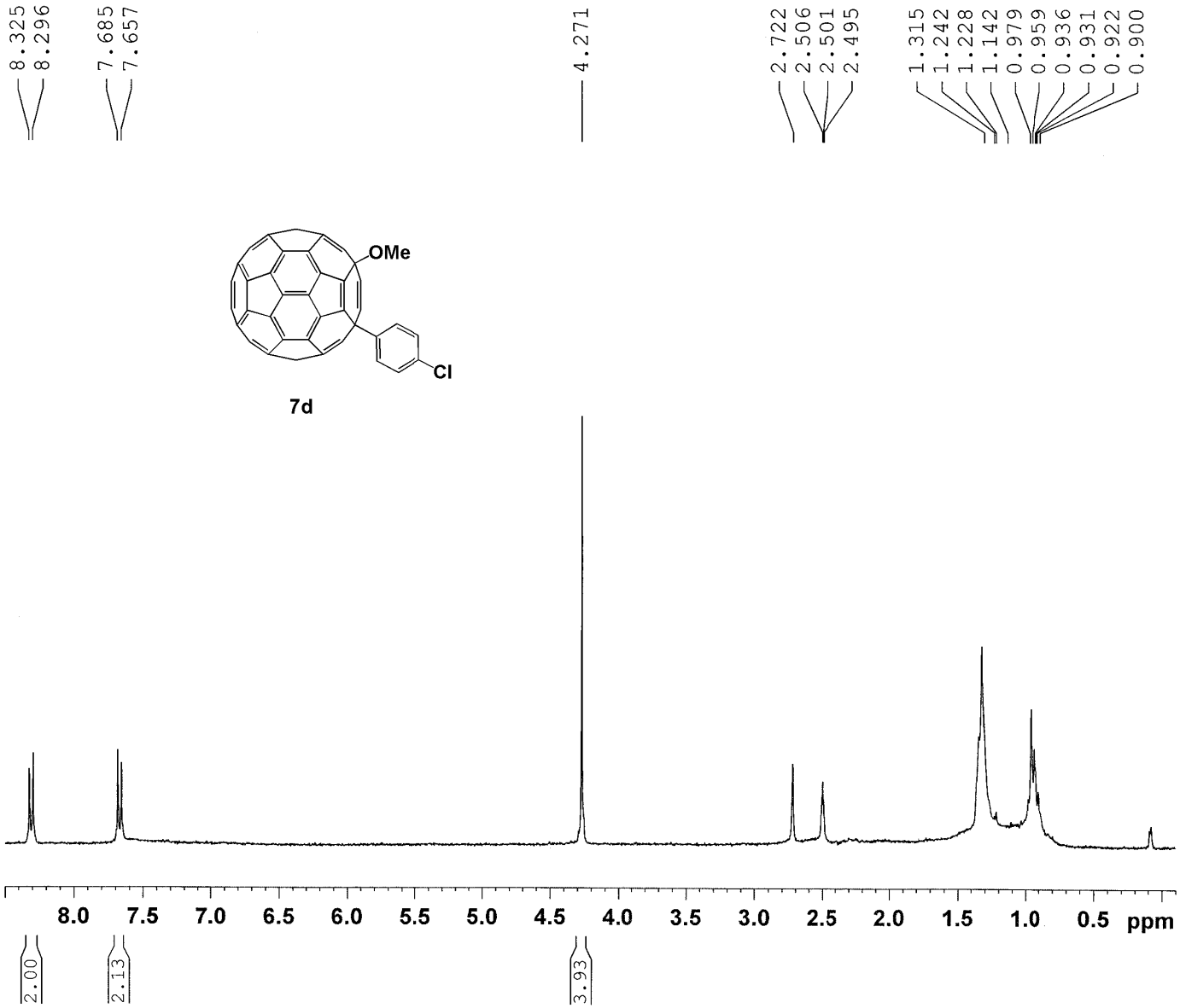
^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 7c



7c

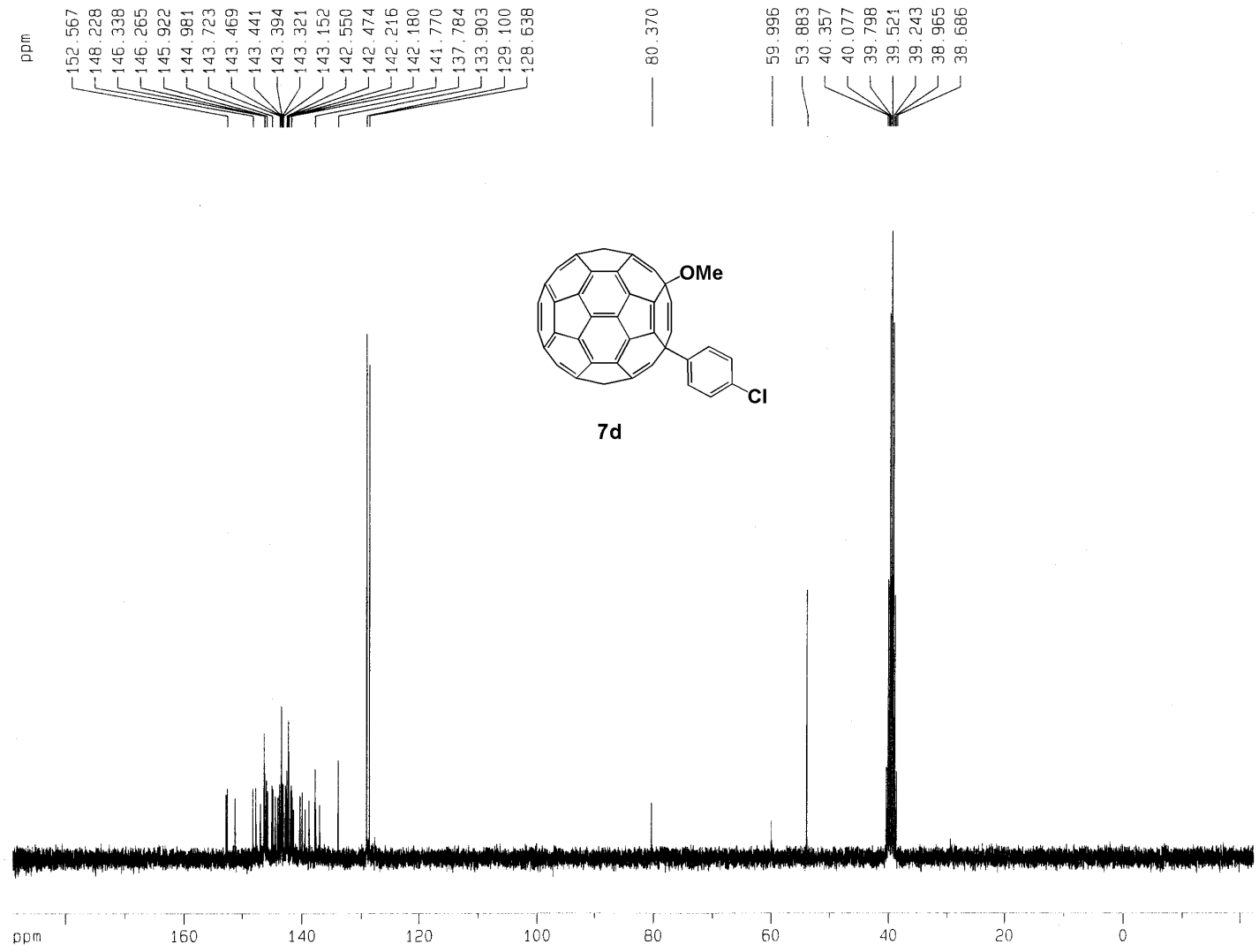

```
Current Data Parameters
NAME                  lym070212
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070214
Time                      18.50
INSTRUM                   av300
PROBHD    5 mm BBO BB-1H
PULPROG                   zgdc
TD                        65536
SOLVENT                     DMSO
NS                        51200
DS                            4
SWH                   22675.736 Hz
FIDRES                0.346004 Hz
AQ                    1.4451188 sec
RG                       11585.2
DW                        22.050 usec
DE                         6.00 usec
TE                        673.2 K
D1                    2.00000000 sec
d11                   0.03000000 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         3.00 usec
PL1                       -1.00 dB
SFO1                 75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                       -3.00 dB
PL12                      16.00 dB
SFO2                300.1315007 MHz

F2 - Processing parameters
SI                        131072
SF                   75.4678191 MHz
WDW                           EM
SSB                            0
LB                         0.50 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                        22.00 cm
CY                      4000.00 cm
F1P                      222.967 ppm
F1                     16826.81 Hz
F2P                      -10.677 ppm
F2                      -805.79 Hz
PPMCM                  10.62018 ppm/cm
HZCM                  801.48151 Hz/cm
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 7d




```
Current Data Parameters
NAME                 lym070115
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20070115
Time                      9.18
INSTRUM                 av300
PROBHD     5 mm BBO BB-1H
PULPROG                     zg
TD                       65536
SOLVENT                  DMSO
NS                         24
DS                          1
SWH                  8992.806 Hz
FIDRES               0.137219 Hz
AQ                   3.6438515 sec
RG                         362
DW                    55.600 usec
DE                     6.00 usec
TE                     300.0 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                     7.50 usec
PL1                    -3.00 dB
SFO1             300.1321009 MHz

F2 - Processing parameters
SI                       16384
SF               300.1300023 MHz
WDW                         no
SSB                          0
LB                    0.00 Hz
GB                           0
PC                        1.00
```

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 7d



Current Data Parameters
NAME lym070326
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070327
Time 7.52
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT DMSO
NS 14776
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 3649.1
DW 22.050 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

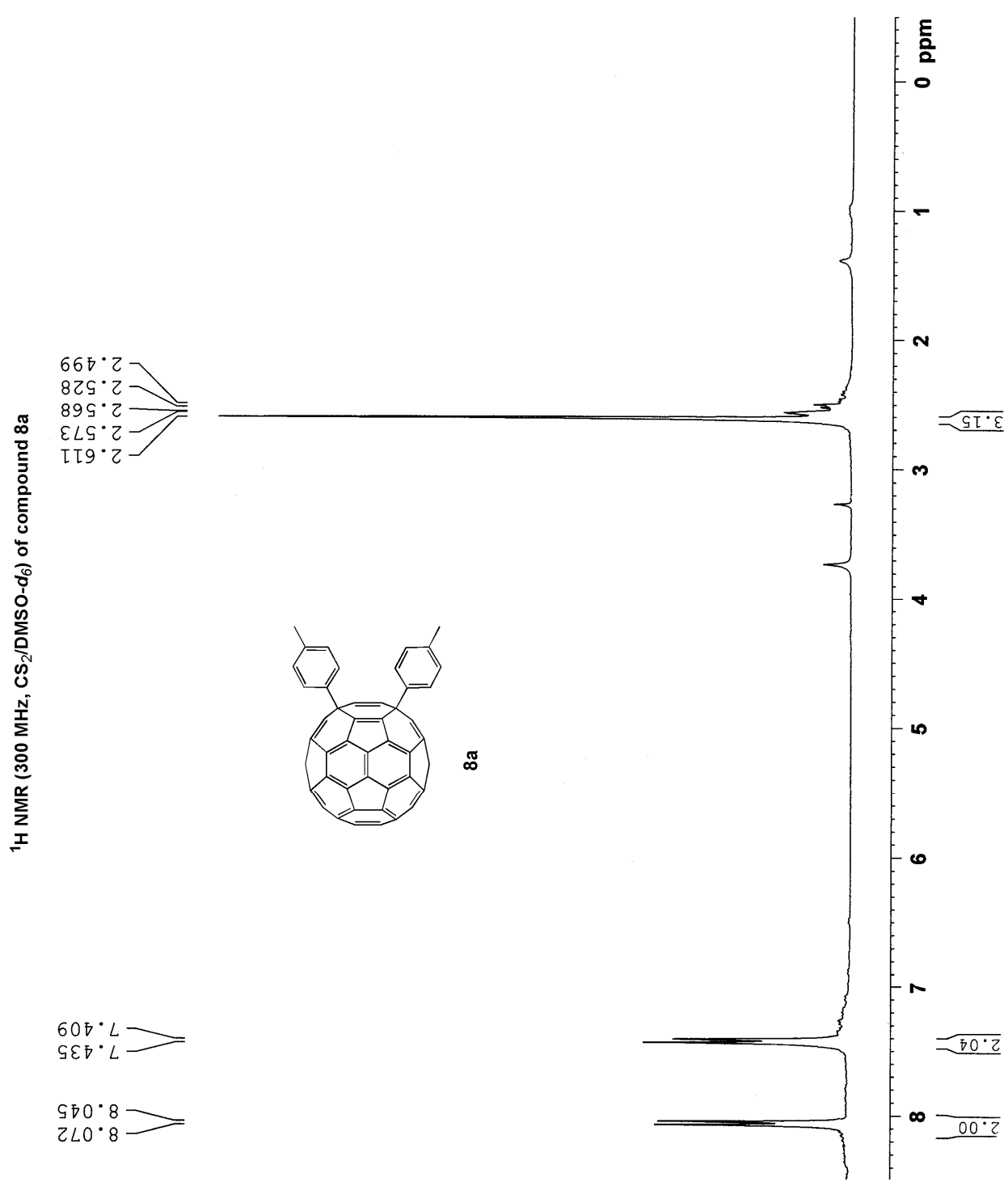
======== CHANNEL f1 ========
NUC1 13C
P1 3.00 usec
PL1 -1.00 dB
SFO1 75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SFO2 300.1315007 MHz

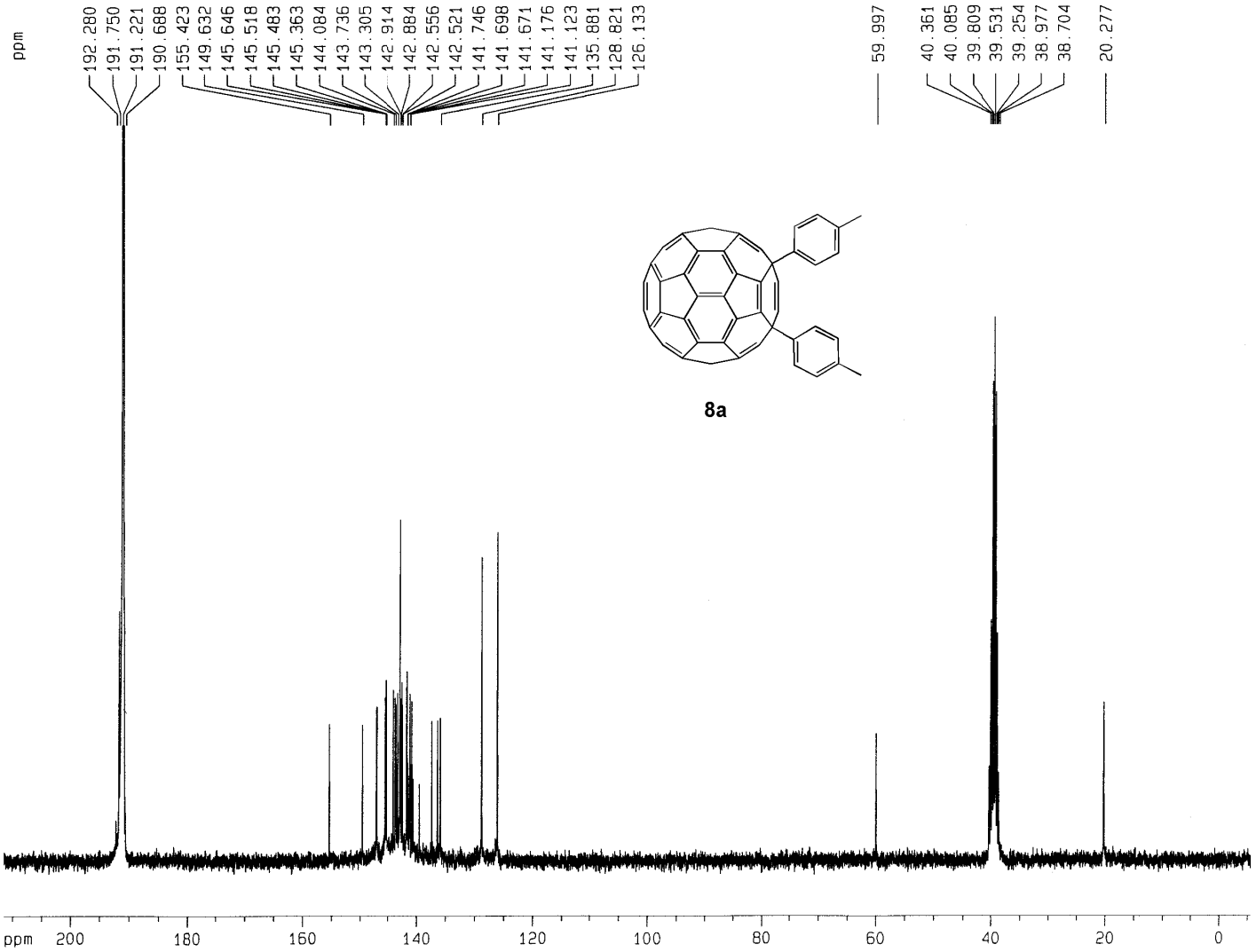
F2 - Processing parameters
SI 131072
SF 75.4678183 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 188.896 ppm
F1 14255.54 Hz
F2P -22.271 ppm
F2 -1680.78 Hz
PPMCM 9.59850 ppm/cm
HZCM 724.37787 Hz/cm

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 8a



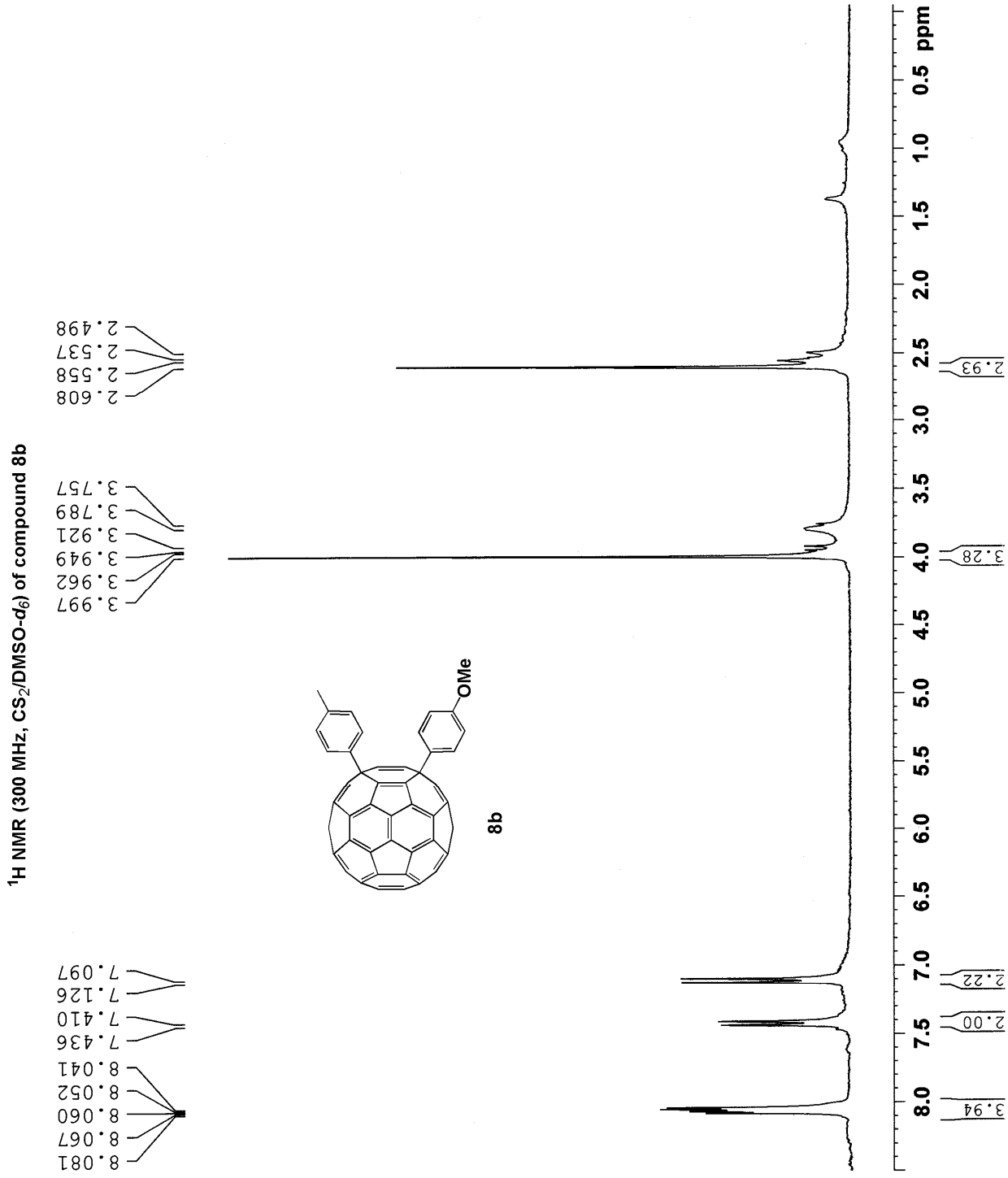
^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 8a



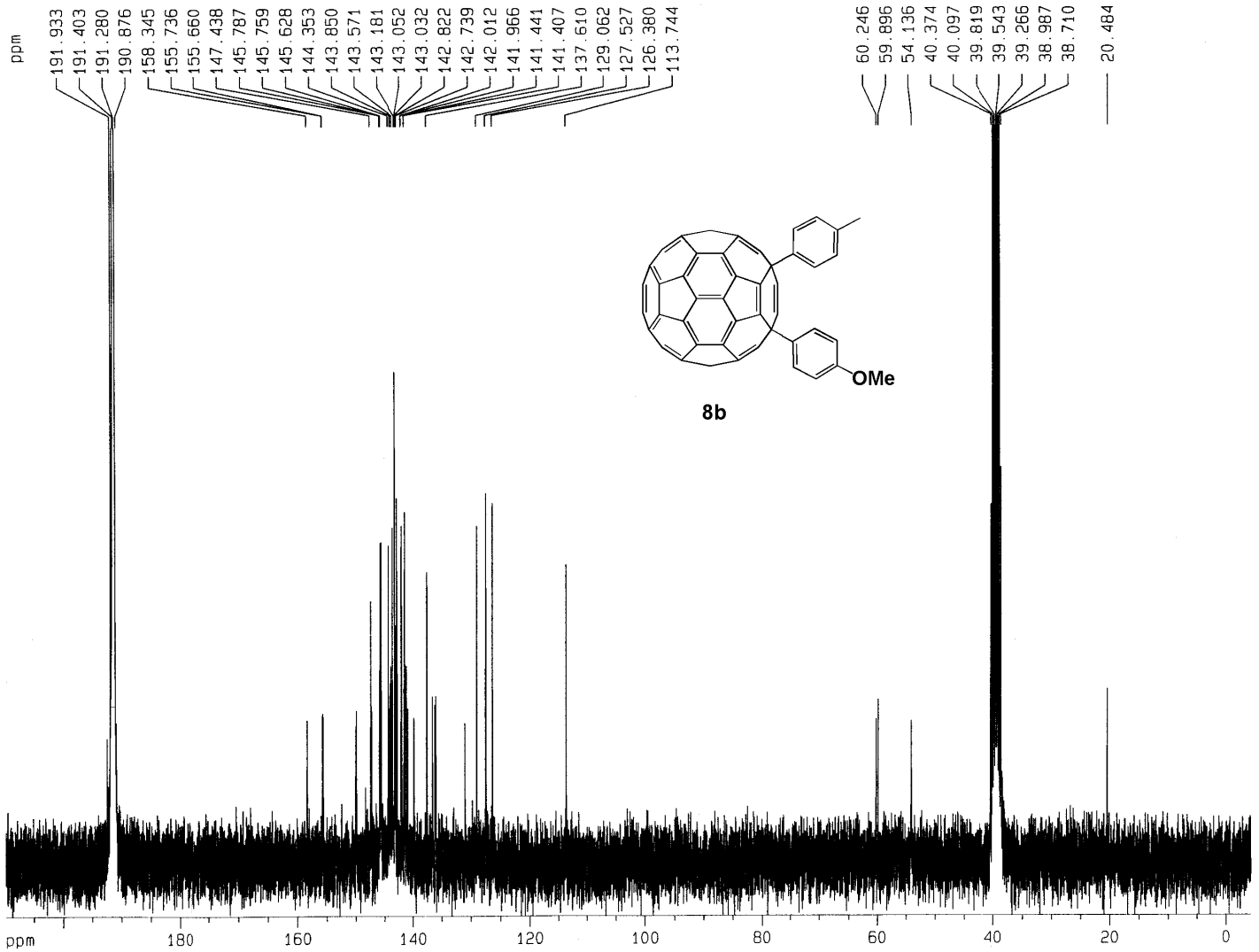
8a

```
Current Data Parameters
NAME                  lym060419
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20060421
Time                       8.12
INSTRUM                   av300
PROBHD    5 mm BBO BB-1H
PULPROG                    zgdc
TD                        65536
SOLVENT                     DMSO
NS                        14832
DS                            4
SWH                22675.736 Hz
FIDRES              0.346004 Hz
AQ                  1.4451188 sec
RG                     9195.2
DW                     22.050 usec
DE                      6.00 usec
TE                     300.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                      3.00 usec
PL1                    -1.00 dB
SFO1               75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -3.00 dB
PL12                   16.00 dB
SFO2              300.1315007 MHz

F2 - Processing parameters
SI                        131072
SF                 75.4678736 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                     22.00 cm
CY                      0.00 cm
F1P                   211.513 ppm
F1                  15962.47 Hz
F2P                    -5.546 ppm
F2                  -418.54 Hz
PPMCM                 9.86634 ppm/cm
HZCM                744.59137 Hz/cm
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 8b



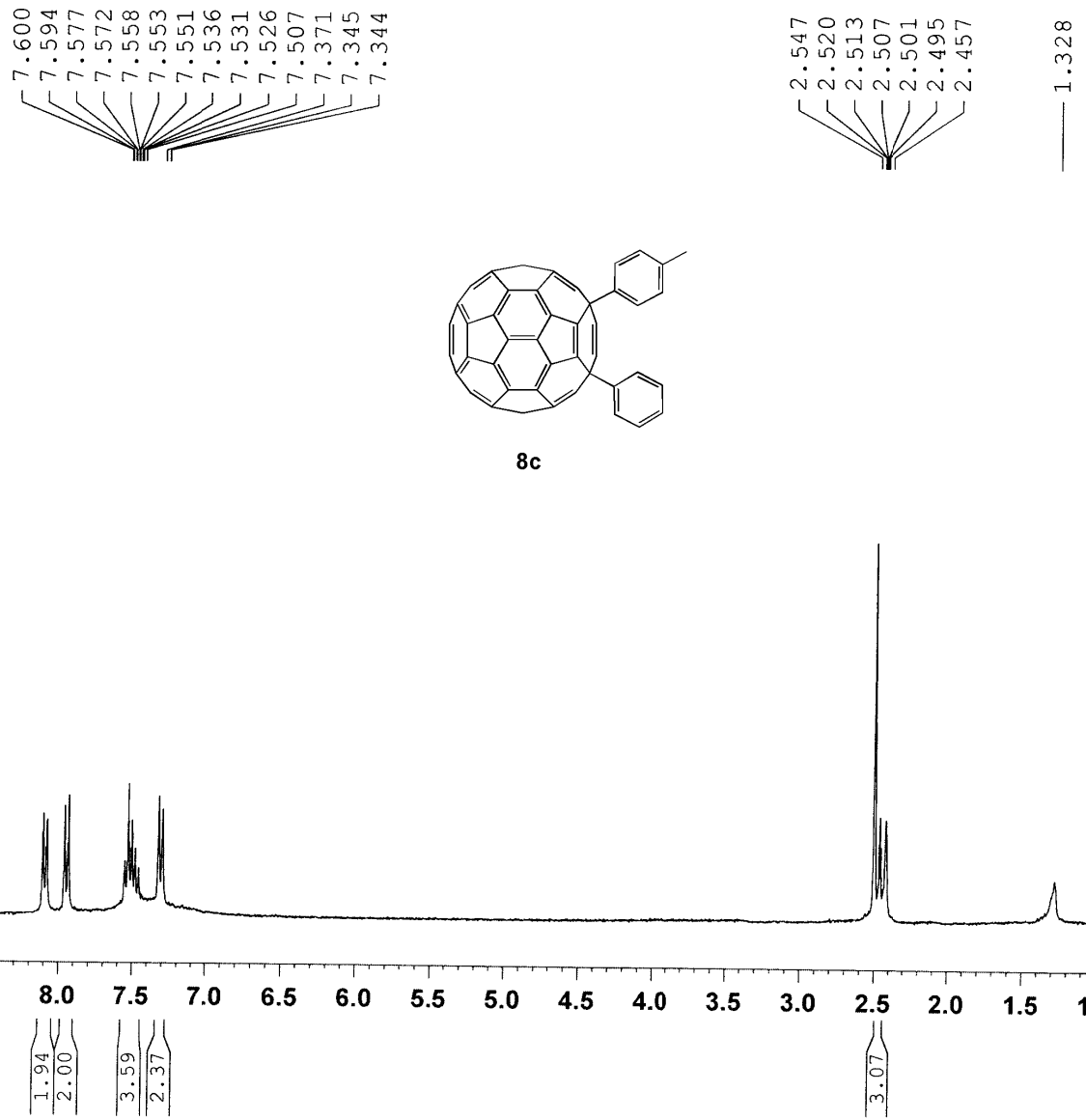
^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 8b



8b

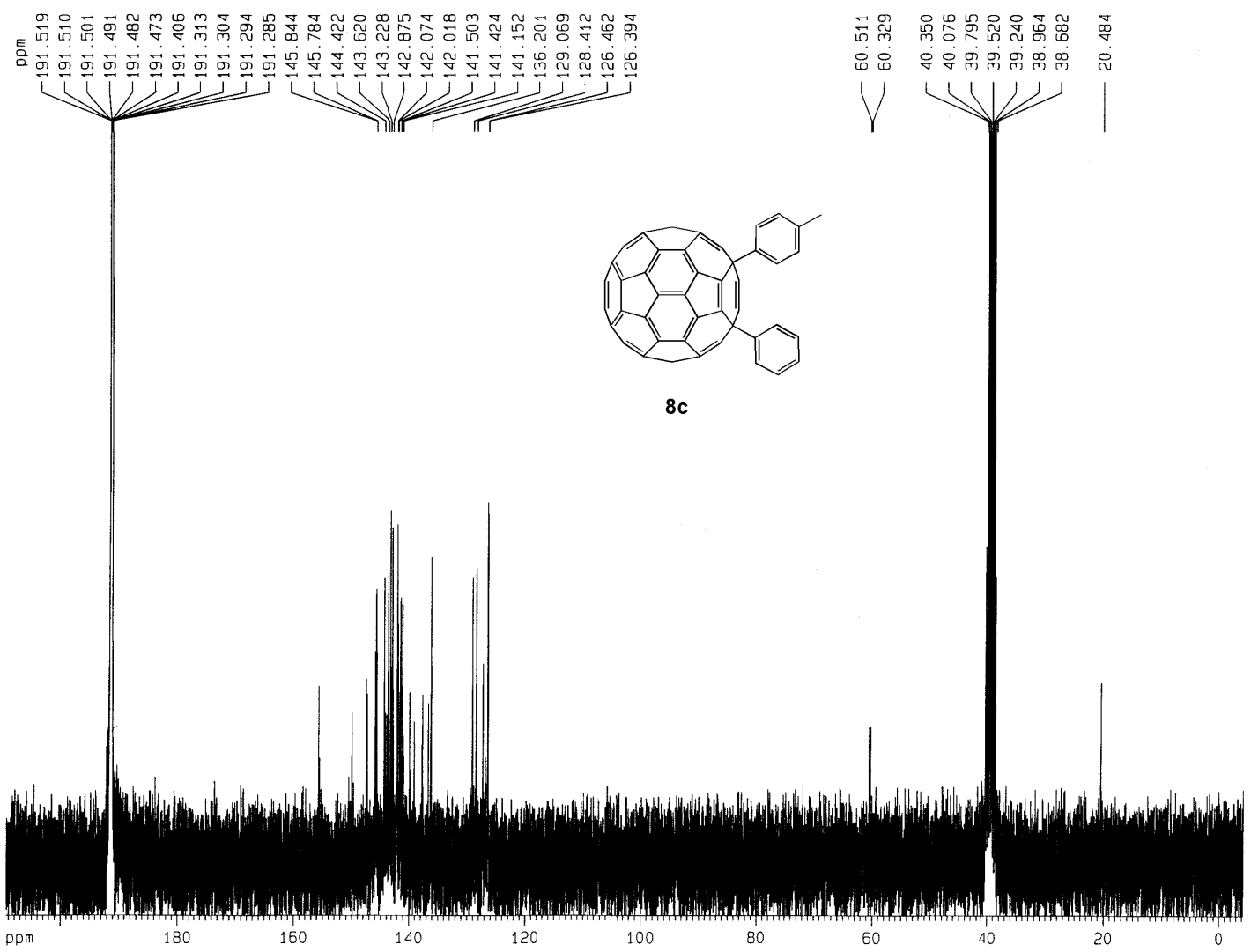

```
Current Data Parameters
NAME                  lym060421
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20060425
Time                       8.03
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                   zgdc
TD                       65536
SOLVENT                   DMSO
NS                        14944
DS                            4
SWH                   22675.736 Hz
FIDRES                0.346004 Hz
AQ                    1.4451188 sec
RG                       4597.6
DW                       22.050 usec
DE                        6.00 usec
TE                       300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                        3.00 usec
PL1                      -1.00 dB
SF01                 75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                      -3.00 dB
PL12                     16.00 dB
SF02                300.1315007 MHz

F2 - Processing parameters
SI                         131072
SF                   75.4678539 MHz
WDW                          EM
SSB                           0
LB                        0.50 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        22.00 cm
CY                         0.00 cm
F1P                      209.883 ppm
F1                     15839.39 Hz
F2P                       -4.266 ppm
F2                      -321.97 Hz
PPMCM                    9.73404 ppm/cm
HZCM                   734.60712 Hz/cm
```

^{1}H NMR (300 MHz, CS_2/DMSO-d_6) of compound 8c




```
Current Data Parameters
NAME          lym06053001
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060530
Time                11.00
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  65536
SOLVENT              DMSO
NS                     32
DS                      1
SWH              5995.204 Hz
FIDRES           0.091480 Hz
AQ               5.4657526 sec
RG                  645.1
DW                 83.400 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.50 usec
PL1                 -3.00 dB
SFO1          300.1321009 MHz

F2 - Processing parameters
SI                   16384
SF            300.1300152 MHz
WDW                     no
SSB                      0
LB                  0.00 Hz
GB                       0
PC                    1.00
```

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 8c



8c

Current Data Parameters
NAME lym060428
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060429
Time 8.12
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT DMSO
NS 14838
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 7298.2
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

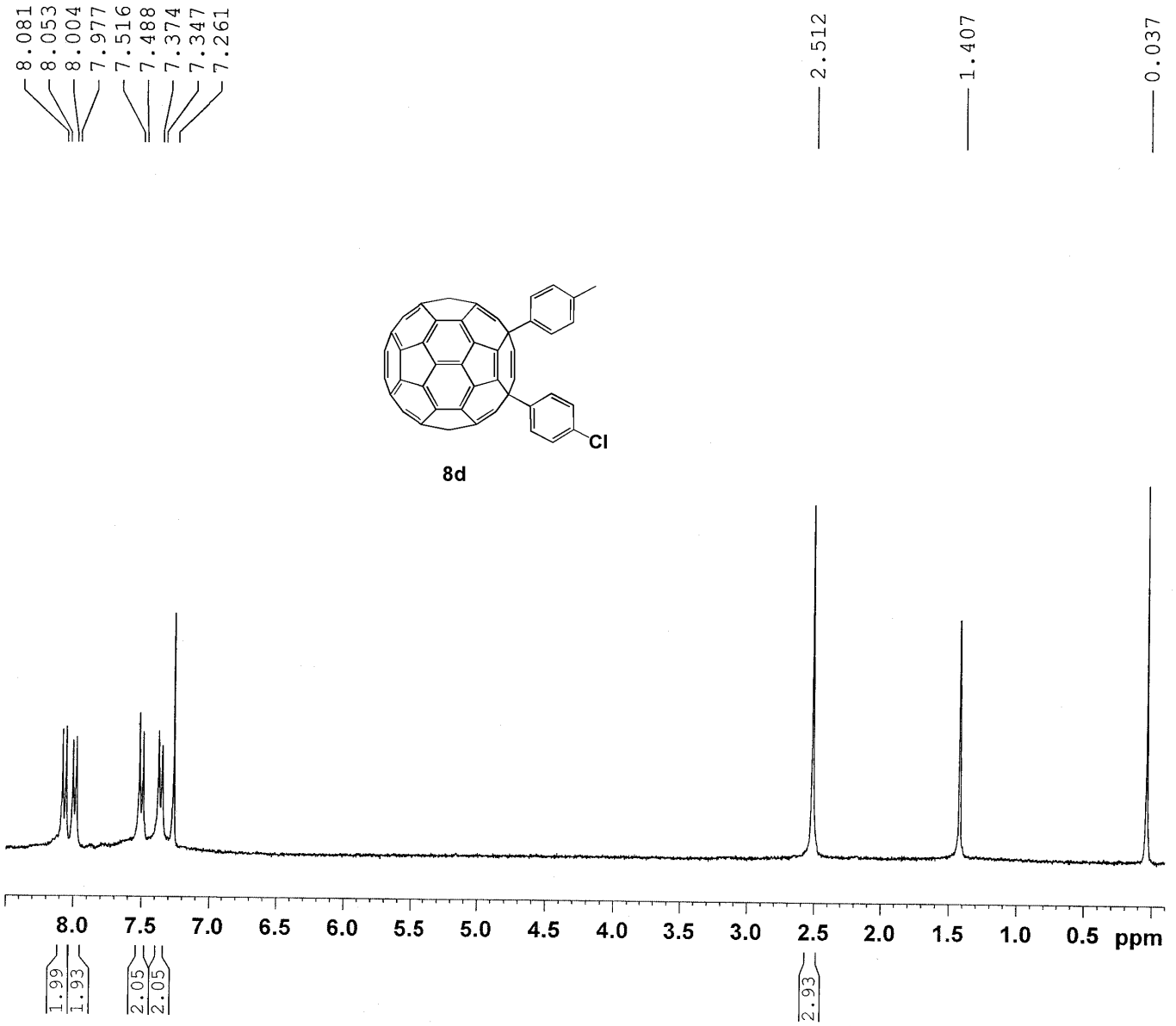
======== CHANNEL f1 ========
NUC1 13C
P1 3.00 usec
PL1 -1.00 dB
SFO1 75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SFO2 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4678501 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.40

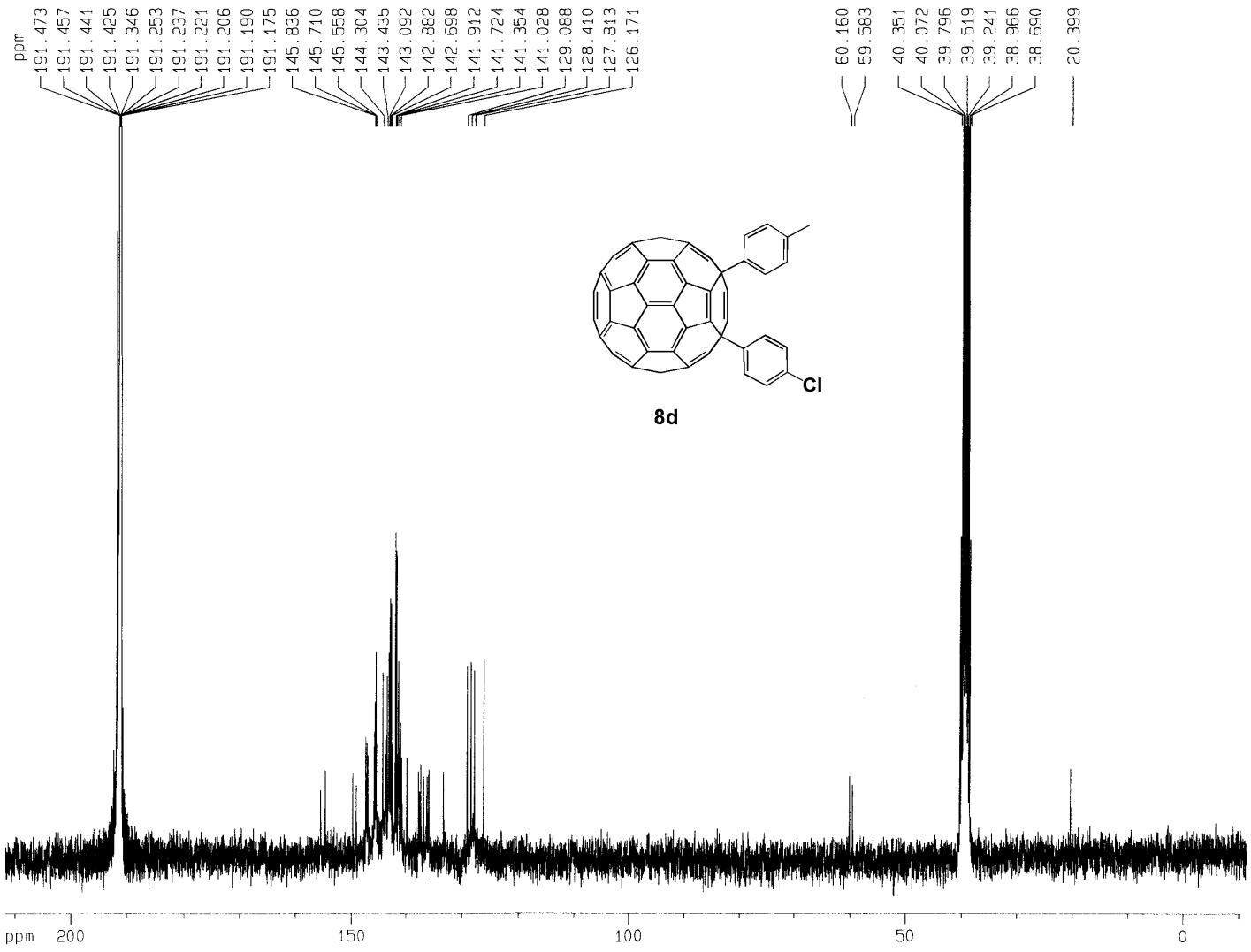
1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 209.461 ppm
F1 15807.60 Hz
F2P -4.216 ppm
F2 -318.16 Hz
PPMCM 9.71260 ppm/cm
HZCM 732.98907 Hz/cm

^{1}H NMR (300 MHz, CS_2/$CDCl_3$) of compound 8d




```
Current Data Parameters
NAME            lym060410
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060410
Time                17.17
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              5995.204 Hz
FIDRES           0.091480 Hz
AQ               5.4657526 sec
RG                   456.1
DW                  83.400 usec
DE                   6.00 usec
TE                  300.1 K
D1              2.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                 -3.00 dB
SFO1          300.1321009 MHz

F2 - Processing parameters
SI                  16384
SF            300.1300066 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

^{13}C NMR (75 MHz, CS_2/DMSO-d_6) of compound 8d




```
Current Data Parameters
NAME          tym06052201
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_              20060523
Time                   7.01
INSTRUM               av300
PROBHD    5 mm BBO BB-1H
PULPROG               zgdc
TD                   65536
SOLVENT               DMSO
NS                   16384
DS                       4
SWH             37878.789 Hz
FIDRES          0.577984 Hz
AQ              0.8651252 sec
RG                10321.3
DW                13.200 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  3.00 usec
PL1                -1.00 dB
SF01          75.4768051 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               16.00 dB
SF02         300.1315007 MHz

F2 - Processing parameters
SI                  131072
SF            75.4678616 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 22.00 cm
CY                  0.00 cm
F1P               211.721 ppm
F1              15978.17 Hz
F2P               -11.354 ppm
F2              -856.85 Hz
PPMCM           10.13979 ppm/cm
HZCM           765.22815 Hz/cm
```