Supporting Information

Chromic Properties of Dibenzo[*j,l*]fluoranthenes Exhibiting Different Resonance Contribution

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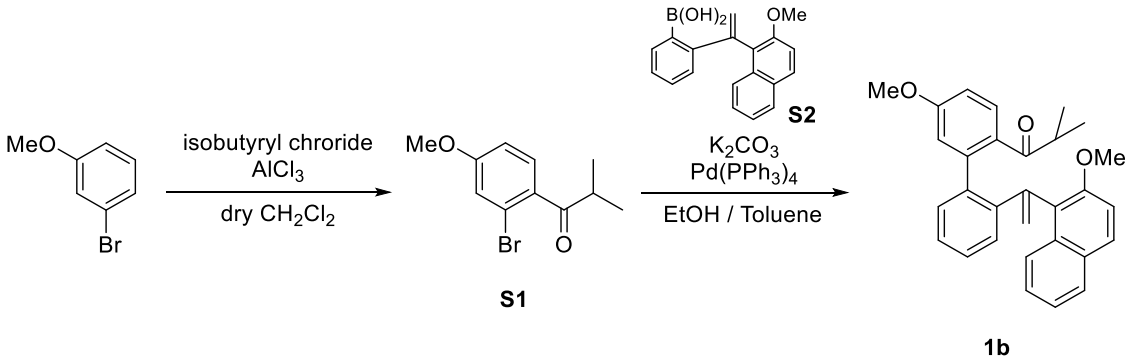
1. Synthesis of Hydroxydibenzofluoranthenes 2 and 3

General

All non-aqueous reactions were carried out in dried glassware under an atmosphere of dry argon unless otherwise noted. For reactions that require heating, oil bath was used as a heat source. *N*,*N*-Dimethylformamide (DMF) for reaction solvent was dried over molecular sieves 4Å prior to use. All other dehydrated solvents for the reactions were purchased and used without further desiccation. All reagents were purchased and used without further purifications. Analytical TLC was performed on pre-coated silica gel plate (Wako Silicagel 70 F_{254}). Column chromatography was performed on Wakogel 60 N unless otherwise stated. ^{1}H, ^{13}C NMR spectra were recorded on a JEOL JNM ECZ600R at 600 and 151 MHz, respectively. Chemical shifts (δ) and coupling constants (*J*) are presented in parts per million and hertz, respectively. Tetramethylsilane (δ 0.0 ppm), acetone-d6 (δ 2.04 ppm) and DMSO-d6 (δ 2.49 ppm) were used as internal standard for ^{1}H NMR. Residual $CDCl_3$ (δ 77.0 ppm), acetone-d6 (δ 29.8 ppm) and DMSO-d6 (δ 39.5 ppm) were used as internal standard for ^{13}C NMR. Multiplicities are indicated as s (singlet), d (doublet), t (triplet), sep (septet), m (multiplet), and br (broad). High-resolution mass spectra (HRMS) were recorded on a Shimadzu LCMS-IT-TOF fitted with an electrospray ionization (ESI) source. IR spectra were recorded on a Shimadzu IRAffinity-1, and the wave numbers of maximum absorption peaks are reported in cm^{-1}. X-Ray single crystal diffraction analyses were performed on a Rigaku XtaLAB P200 apparatus. UV-vis absorption spectra were recorded on a Shimazu UV-2600. Fluorescence spectra were recorded on a JASCO FP-8600.

Preparation of Substrate 1b



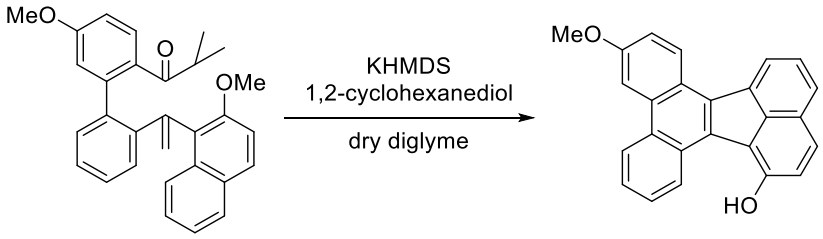
To a solution of 3-bromoanisole (12.5 mL, 99.6 mmol) and $AlCl_3$ (16.0 g, 120 mmol) in dry CH_2Cl_2 (110 mL) was added dropwise isobutyryl chloride (12.5 mL, 118 mmol) at 0 °C. After stirring for 18 h at room temperature, the reaction mixture was poured into ice/10% HCl aq. The mixture was extracted three times with Et_2O. The combined organic extracts were washed with water, sat. $NaHCO_3$ and brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography (hexane/EtOAc = 7/1–5/1) to afford **S1** (4.59 g, 18%) as pale yellow oil.

S1: R_f 0.58 (hexane/EtOAc = 3.5/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.18 (d, 6H, *J* = 7.2 Hz), 3.39 (sep, 1H, *J* = 7.2 Hz), 3.83 (s, 3H), 6.87 (dd, 1H, *J* = 8.4, 3.0 Hz), 7.14 (d, 1H, *J* = 3.0 Hz), 7.35 (d, 1H, *J* = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 18.4, 39.4, 55.6, 113.1, 119.0, 120.4, 130.0, 133.5, 161.2, 207.3 ppm; IR (film) 3970, 2936, 2870, 2839, 1693, 1593 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{11}H_{14}BrO_2$, 257.0172; found, 257.0156.

To a stirred solution of **S1** (1.30 g, 5.06 mmol), K_2CO_3 (2.98 g, 21.6 mmol), and $Pd(PPh_3)_4$ (637 mg, 551 μmol) in a mixture of toluene (10 mL) and EtOH (40 mL) was added **S2** [1] (1.67 g, 5.00 mmol). After stirring for 5 h at 95 °C, the reaction was quenched with water, phases were separated, and the aqueous layer was extracted three times with Et_2O. The combined organic layer was washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography (hexane/EtOAc = 5/1–4/1) to afford **1b** (1.83 g, 84%) as pale yellow amorphous.

1b: R_f 0.48 (hexane/EtOAc = 3.5/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 0.67–1.16 (m, 6H), 2.79 (brs, 1H), 3.45–3.85 (m, 6H), 5.36 (d, 1H, *J* = 1.0 Hz), 5.68 (brs, 1H), 6.28–7.01 (m, 2H), 7.04–7.60 (m, 8H), 7.60–7.81 (m, 2H), 7.95 (brs, 1H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 18.4, 19.9, 38.0, 55.1, 56.1, 112.1, 113.6, 116.3, 116.5, 123.0, 123.2, 125.5, 125.9, 126.0, 126.6, 127.3, 127.5, 128.9, 129.0, 130.1, 130.4, 131.7, 133.2, 139.2, 153.7, 160.2, 208.3 ppm (3 signals missing); IR (film) 3055, 3009, 2967, 2932, 2835, 1678, 1593 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{30}H_{29}O_3$, 437.2111; found, 437.2129.

Synthesis of 2b

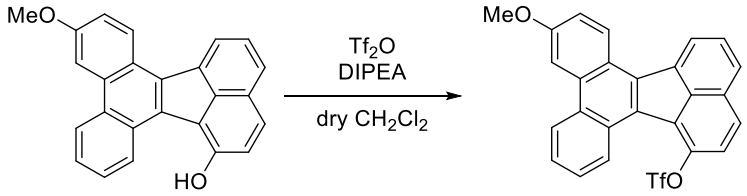


1b **2b**

To a stirred solution of **1b** (1.83 g, 4.20 mmol) and *cis*-1,2-cyclohexanediol (99.1 mg, 853 μmol) in dry diglyme (170 mL) was added KHMDS (1.0 M in THF, 12.5 mL, 12.5 mmol). The reaction mixture was evacuated for 15 min to degass the solvent, refilled with Ar and heated to reflux for 24 h with vigorous stirring. After cooling to room temperature, the reaction was quenched with 10% HCl aq. The aqueous layer was extracted three times with Et_2O and the combined organic layer was washed with water and brine, dried over Na_2SO_4 and evaporated. The residue was purified by silica gel column chromatography (hexanes/EtOAc = 3/1–1/1) to afford **2b** (900 mg, 62%) as yellow solids. Single crystals of **2b** suitable for X-ray crystallographic analysis were successfully grown by slow diffusion of hexane into the solution of **2b** in AcOEt at room temperature.

2b: R_f 0.10 (hexane/EtOAc = 4/1); mp. >250 °C; ^{1}H NMR (600 MHz, acetone-d6) δ 4.10 (s, 3H), 7.43 (dd, 1H, *J* = 8.4, 2.4 Hz), 7.48 (d, 1H, *J* = 8.4 Hz), 7.62–7.74 (m, 3H), 7.94 (d, 2H, *J* = 8.4 Hz), 8.34 (d, 1H, *J* = 1.8 Hz), 8.79 (d, 1H, *J* = 7.2 Hz), 8.88 (d, 1H, *J* = 7.2 Hz), 9.05 (d, 1H, *J* = 9.0 Hz), 10.18 (dd, 1H, *J* = 8.4, 1.2 Hz) , 10.40 (brs, 1H) ppm; ^{13}C NMR (151 MHz, acetone-d6) δ 55.8, 105.6, 118.3, 118.9, 122.7, 124.2, 125.3, 125.88, 125.94, 126.6, 127.2, 127.3, 127.4, 130.0, 130.6, 131.0, 131.6, 132.4, 133.2, 134.3, 134.4, 136.8, 153.7, 158.9 ppm (1 signal missing); IR (film) 3275, 2936, 1686, 1620 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{17}O_2$, 349.1223; found, 349.1236.

Synthesis of 5

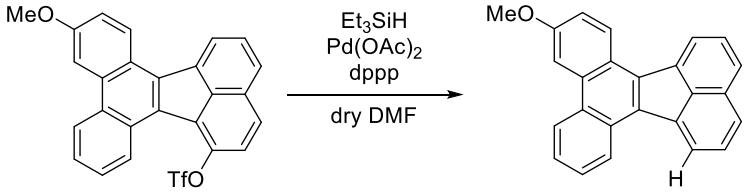


2b **5**

To a solution of **2b** (201 mg, 576 μmol) and DIPEA (150 μL, 859 μmol) in dry CH_2Cl_2 (15 mL) was added dropwise Tf_2O (140 μL, 864 μmol) at 0 °C. After stirring for 1 h at room temperature, the reaction was quenched with 10% HCl. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **5** (236 mg, 86%) as orange solids.

5: R_f 0.45 (hexane/EtOAc = 3.5/1); mp. 172–173 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.06 (s, 3H), 7.33 (dd, 1H, J = 9.0, 3.0 Hz), 7.54 (d, 1H, J = 9.0 Hz), 7.63–7.74 (m, 3H), 7.85 (d, 1H, J = 8.4 Hz), 7.89 (d, 1H, J = 9.0 Hz), 8.10 (d, 1H, J = 2.4 Hz), 8.49 (d, 1H, J = 7.2 Hz), 8.64 (d, 1H, J = 8.4 Hz), 8.72 (d, 1H, J = 9.0 Hz), 8.89 (d, 1H, J = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 55.5, 104.9, 117.4, 118.6 ($J_{C–F}$ = 322 Hz), 122.9, 123.4, 123.7, 126.1, 126.4, 126.5, 127.1, 127.2, 127.4, 128.26, 128.30, 128.70, 128.72, 129.9, 130.2, 130.9, 133.67, 133.73, 135.3, 138.1, 142.0, 158.6 ppm; IR (neat) 3001, 2936, 1612, 1412, 1207 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{26}H_{16}O_4S$, 481.0716; found, 481.0719.

Synthesis of S3

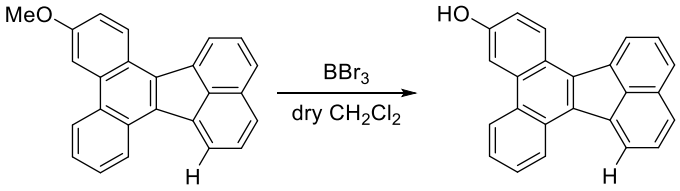


5 **S3**

To a solution of **5** (400 mg, 833 μmol), $Pd(OAc)_2$ (19.0 mg, 84.6 μmol) and dppp (34.8 mg, 84.4 μmol) in dry DMF (14 mL) was added Et_3SiH (350 μL, 2.20 mmol) at 60 °C and stirred for 2 h. After cooling to room temperature, the reaction was quenched with water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **S3** (251 mg, 91%) as yellow solids.

S3: R_f 0.65 (hexane/EtOAc = 3.5/1); mp. 137–139 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.04 (s, 3H), 7.32 (d, 1H, J = 7.8 Hz), 7.58–7.71 (m, 4H), 7.80 (d, 1H, J = 7.8 Hz), 7.83 (d, 1H, J = 7.8 Hz), 8.06 (s, 1H), 8.37–8.44 (m, 2H), 8.62 (d, 1H, J = 8.4 Hz), 8.71 (dd, 1H, J = 8.4, 4.8 Hz), 8.88 (dd, 1H, J = 8.4, 3.0 Hz) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 55.4, 104.9, 117.1, 123.6, 124.3, 124.4, 124.7, 124.9, 125.7, 126.3, 127.0, 127.2, 127.4, 127.8, 127.9, 129.3, 130.1, 131.5, 131.9, 132.5, 133.9, 137.8, 138.0, 157.9 ppm (1 signal missing); IR (neat) 2920, 2851, 1612 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{17}O$, 333.1274; found, 333.1278.

Synthesis of 3a

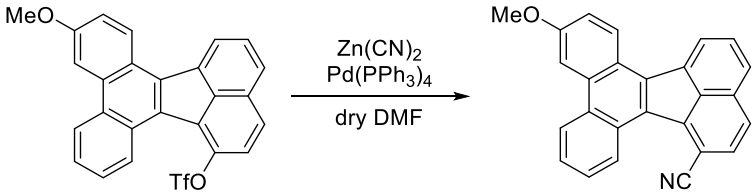


S3 **3a**

To a solution of **S3** (89.7 mg, 270 μmol) in dry CH_2Cl_2 (5.0 mL) was added dropwise BBr_3 (1.0 M in CH_2Cl_2, 0.54 mL, 0.54 mmol) at 0 °C. After stirring for 3.5 h at room temperature, the reaction was quenched with ice water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. Trituration (hexane) afforded **3a** (85.6 mg, 77%) as yellow solids.

3a: R_f 0.10 (hexane/EtOAc = 4/1); mp. >250 °C; ^{1}H NMR (600 MHz, acetone-d6) δ 7.40 (dd, 1H, *J* = 9.0, 3.0 Hz), 7.67 (td, 1H, *J* = 7.2, 1.2 Hz), 7.70–7.78 (m, 3H), 7.93 (d, 1H, *J* = 8.4 Hz), 7.96 (d, 1H, *J* = 7.8 Hz), 8.25 (d, 1H, *J* = 2.4 Hz), 8.64 (d, 1H, *J* = 7.8 Hz), 8.67 (d, 1H, *J* = 7.2 Hz), 8.73 (d, 1H, *J* = 7.8 Hz), 8.91 (d, 1H, *J* = 9.0 Hz), 8.94 (s, 1H), 8.95 (d, 1H, *J* = 7.2 Hz) ppm; ^{13}C NMR (151 MHz, acetone-d6) δ 108.5, 118.9, 124.4, 124.7, 125.4, 125.8, 125.9, 126.9, 127.6, 127.9, 128.4, 128.5, 128.9, 129.0, 130.4, 130.9, 131.0, 131.6, 132.5, 133.9, 134.8, 138.5, 138.7, 157.3 ppm; IR (neat) 3267, 3051, 1609 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{24}H_{15}O$, 319.1117; found, 319.1135.

Synthesis of S4

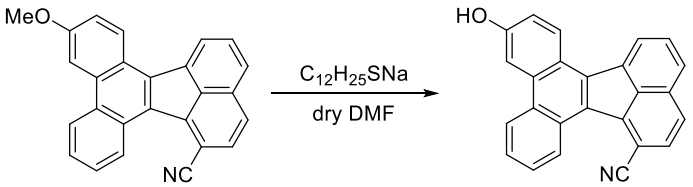


5 **S4**

The solution of **5** (480 mg, 1.00 mmol), $Pd(PPh_3)_4$ (116 mg, 100 μmol) and $Zn(CN)_2$ (353 mg, 3.01 mmol) in dry DMF (30 mL) was heated at 80 °C and stirred for 4 h. After cooling to room temperature, the reaction was quenched with water. The mixture was extracted three times with $CHCl_3$. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **S4** (284 mg, 80%) as red solids.

S4: R_f 0.52 ($CHCl_3$); mp. >250 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 4.06 (s, 3H), 7.40 (dd, 1H, *J* = 9.0, 3.0 Hz), 7.71 (td, 1H, *J* = 7.8, 1.2 Hz), 7.74 (td, 1H, *J* = 7.8, 1.8 Hz), 7.81 (t, 1H, *J* = 7.8 Hz), 7.97 (d, 1H, *J* = 8.4 Hz), 8.03 (d, 1H, *J* = 9.0 Hz), 8.10 (d, 1H, *J* = 8.4 Hz), 8.26 (d, 1H, *J* = 2.4 Hz), 8.71 (d, 1H, *J* = 6.6 Hz), 8.82 (d, 1H, *J* = 9.0 Hz), 8.92 (d, 1H, *J* = 8.4 Hz), 9.15 (d, 1H, *J* = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 55.6, 105.2, 118.4, 120.5, 122.6, 124.5, 126.6, 126.7, 127.1, 127.4, 127.7, 128.3, 128.5, 129.4, 129.9, 130.4, 130.9, 131.0, 131.7, 133.6, 135.7, 136.6, 140.4, 159.1 ppm (2 signals missing); IR (neat) 3009, 2967, 2843, 2210, 1609 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{26}H_{16}NO$, 358.1226; found, 358.1229.

Synthesis of 3c

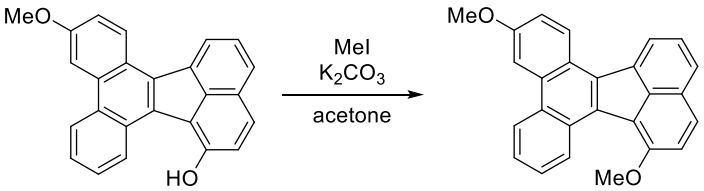


S4 **3c**

To a solution of **S4** (20.3 mg, 56.8 μmol) and sodium 1-dodecanethiolate [2] (64.8 mg, 284 μmol) in dry DMF (1 mL) was heated at 130 °C and stirred for 7.5 h. After cooling to room temperature, the reaction was quenched with 10% HCl. The mixture was extracted twice with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography (EtOAc) to give **3c** (15.2 mg, 78%) as dark purple solids.

3c: R_f 0.10 ($CHCl_3$); mp. >250 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 7.34 (dd, 1H, *J* = 9.0, 1.8 Hz), 7.70 (t, 1H, *J* = 6.6 Hz), 7.73 (td, 1H, *J* = 6.6, 1.2 Hz), 7.82 (t, 1H, *J* = 7.8 Hz), 7.96 (d, 1H, *J* = 7.8 Hz), 8.04 (d, 1H, *J* = 7.8 Hz) , 8.09 (d, 1H, *J* = 8.4 Hz), 8.13 (d, 1H, *J* = 2.4 Hz), 8.69 (d, 1H, *J* = 7.8 Hz), 8.75 (d, 1H, *J* = 7.8 Hz), 8.82 (d, 1H, *J* = 9.0 Hz), 9.15 (dd, 1H, *J* = 7.8, 1.2 Hz), 10.3 (brs, 1H) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 105.0, 107.5, 118.8, 120.6, 121.7, 124.0, 126.6, 126.68, 126.74, 127.3, 127.4, 127.7, 128.1, 128.5, 128.7, 129.7, 130.3, 131.0, 131.7, 133.8, 136.0, 136.8, 140.6, 157.7 ppm (1 signal missing); IR (neat) 3248, 3075, 3048, 2214, 1609 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{14}NO$, 344.1070; found, 344.1093.

Synthesis of 6

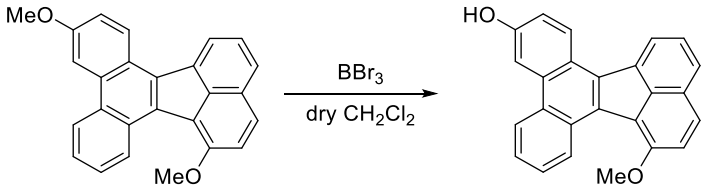


2b **6**

To a solution of **2b** (149 mg, 428 μmol) and K_2CO_3 (183 mg, 1.32 mmol) in acetone (15 mL) was added dropwise MeI (80.0 μL, 1.29 mmol) at room temperature. After refluxing for 1.5 h, the reaction was quenched with water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **6** (142 mg, 91%) as yellow solids.

6: R_f 0.70 ($CHCl_3$); mp. 164–166 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 4.05 (s, 3H), 4.28 (s, 3H), 7.42 (dd, 1H, *J* = 9.0, 2.4 Hz), 7.64–7.77 (m, 4H), 8.02 (d, 1H, *J* = 7.8 Hz), 8.13 (d, 1H, *J* = 9.0 Hz), 8.30 (s, 1H, *J* = 3.0 Hz), 8.81 (d, 1H, *J* = 7.2 Hz), 8.93 (d, 1H, *J* = 7.8 Hz), 8.99 (d, 1H, *J* = 9.0 Hz), 9.75 (d, 1H, *J* = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 55.5, 56.8, 105.1, 117.1, 117.8, 119.8, 123.6, 123.9, 124.8, 125.78, 125.82, 126.0, 126.5, 126.8, 127.2, 128.3, 129.1, 129.8, 131.3, 131.5, 132.0, 132.1, 132.5, 135.1, 154.7, 157.8 ppm; IR (neat) 3005, 2928, 2839, 1620 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{26}H_{19}O_2$, 363.1380; found, 363.1375.

Synthesis of 3b

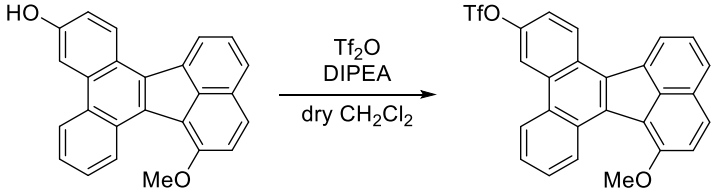


6 **3b**

To a solution of **6** (324 mg, 893 μmol) in dry CH_2Cl_2 (10 mL) was added dropwise BBr_3 (1.0 M in CH_2Cl_2, 1.20 mL, 1.20 mmol) at 0 °C. After stirring for 2.5 h at room temperature, the reaction was quenched with ice water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **3b** (158 mg, 51%) as orange solids.

3b: R_f 0.11 ($CHCl_3$); mp. 198–200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.26 (s, 3H),5.08 (brs, 1H), 7.30 (dd, 1H, J = 9.0, 3.0 Hz), 7.48 (d, 1H, J = 7.8 Hz), 7.62–7.67 (m, 2H), 7.70 (t, 1H, J = 7.8 Hz), 7.88 (d, 1H, J = 7.8 Hz), 8.14 (d, 1H, J = 9.0 Hz), 8.16 (d, 1H, J = 2.4 Hz), 8.62 (d, 1H, J = 7.2 Hz) , 8.64 (d, 1H, J = 7.8 Hz), 8.90 (d, 1H, J = 9.0 Hz), 9.77 (d, 1H, J = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 56.8, 107.8, 116.6, 117.0, 121.6, 123.1, 124.7, 125.2, 125.5, 125.7, 126.5, 126.66, 126.72, 128.8, 129.8, 130.0, 130.8, 132.2, 132.7, 133.1, 133.7, 136.4, 153.6, 154.6 ppm (1 signal missing); IR (neat) 3425, 3246, 2963, 2916, 2847, 1616 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{17}O_2$, 349.1223; found, 349.1247.

Synthesis of 7

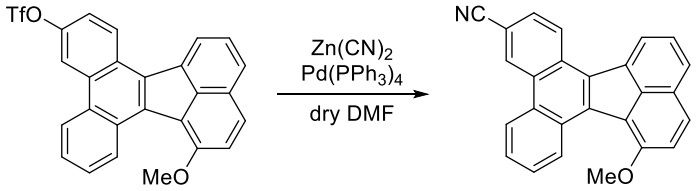


3b **7**

To a solution of **3b** (147 mg, 422 μmol) and DIPEA (110 μL, 631 μmol) in dry CH_2Cl_2 (10 mL) was added dropwise Tf_2O (110 μL, 655 μmol) at 0 °C. After stirring for 2.5 h at room temperature, the reaction was quenched with 10% HCl. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **7** (182 mg, 88%) as yellow solids.

7: R_f 0.85 ($CHCl_3$); mp. 150–151 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 4.28 (s, 3H), 7.66–7.72 (m, 2H), 7.73–7.82 (m, 3H), 8.04 (d, 1H, J = 8.4 Hz), 8.18 (d, 1H, J = 9.0 Hz), 8.80 (d, 1H, J = 7.8 Hz), 8.93 (d, 1H, J = 8.4 Hz), 9.02 (d, 1H, J = 2.4 Hz), 9.16 (d, 1H, J = 9.0 Hz), 9.75 (d, 1H, J = 7.8 Hz) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 56.7, 116.6, 116.8, 118.4 (J_{C-F} = 321 Hz), 118.9, 120.4, 124.0, 124.7, 125.8, 126.0, 126.9, 127.5, 127.6, 127.7, 128.5, 128.6, 129.1, 129.6, 130.2, 131.4, 131.9, 132.7, 134.2, 135.8, 147.3, 155.6 ppm; IR (neat) 2940, 2843, 1577, 1416, 1211, 1130 cm^{-1}; HRMS–ESI (*m/z*): $[M+K]^+$ calcd for $C_{26}H_{15}KO_4S$, 519.0275; found, 519.0302.

Synthesis of S5

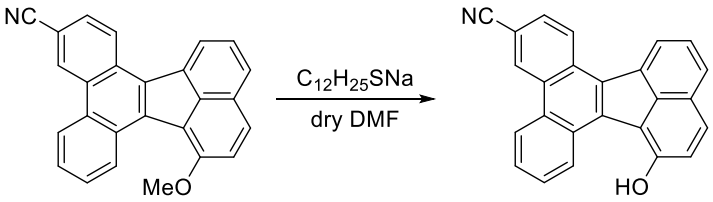


7 **S5**

The solution of **7** (177 mg, 368 μmol), $Pd(PPh_3)_4$ (43.0 mg, 37.2 μmol) and $Zn(CN)_2$ (129 mg, 1.10 mmol) in dry DMF (7.5 mL) was heated to 80 °C and stirred for 1 h. After cooling to room temperature, the reaction was quenched with water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **S5** (122 mg, 92%) as yellow solids.

S5: R_f 0.59 ($CHCl_3$); mp. >250 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 4.31 (s, 3H), 7.69–7.80 (m, 3H), 7.82 (t, 1H, *J* = 7.8 Hz), 8.04 (s, 1H, *J* = 8.4 Hz), 8.08 (d, 1H, *J* = 8.4 Hz), 8.24 (d, 1H, *J* = 9.0 Hz), 8.85 (d, 1H, *J* = 7.8 Hz), 9.04 (d, 1H, *J* = 7.8 Hz), 9.15 (d, 1H, *J* = 8.4 Hz), 9.47 (s, 1H), 9.78 (d, 1H, *J* = 8.4 Hz) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 56.9, 108.2, 116.9, 118.8, 119.5, 124.0, 124.7, 125.9, 126.0, 126.3, 127.3, 127.67, 127.71, 128.5, 129.0, 129.4, 129.6, 129.8, 130.1, 131.3, 132.0, 133.2, 134.0, 137.4, 156.1 ppm (1 signal missing); IR (neat) 3055, 2920, 2843, 2218, 1605 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{26}H_{16}NO$, 358.1226; found, 358.1214.

Synthesis of 2c

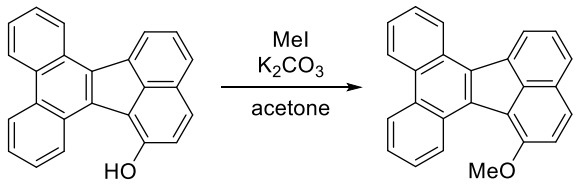


S5 **2c**

To a solution of **S5** (111 mg, 311 μmol) and sodium 1-dodecanethiolate (352 mg, 1.57 mmol) in dry DMF (6 mL) was heated at 120 °C and stirred for 4 h. After cooling to room temperature, the reaction was quenched with 10% HCl. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography (EtOAc) to give **2c** (104 mg, 98%) as yellow solids.

2c: R_f 0.09 ($CHCl_3$); mp. >250 °C; ^{1}H NMR (600 MHz, DMSO-d6) δ 7.48 (d, 1H, *J* = 8.4 Hz), 7.69 (t, 1H, *J* = 7.8 Hz), 7.77 (t, 1H, *J* = 7.8 Hz), 7.82 (t, 1H, *J* = 7.8 Hz), 8.02 (d, 1H, *J* = 7.8 Hz), 8.05 (d, 1H, *J* = 9.0 Hz), 8.07 (d, 1H, *J* = 9.0 Hz), 8.85 (d, 1H, *J* = 7.2 Hz), 9.05 (d, 1H, *J* = 8.4 Hz), 9.18 (d, 1H, *J* = 9.0 Hz), 9.49 (s, 1H), 10.14 (d, 1H, *J* = 7.8 Hz), 12.02 (brs, 1H) ppm; ^{13}C NMR (151 MHz, DMSO-d6) δ 107.9, 116.2, 119.6, 122.1, 123.9, 124.3, 125.2, 125.7, 125.9, 127.19, 127.24, 127.6, 128.9, 129.1, 129.39, 129.43, 129.6, 131.6, 132.6, 132.7, 133.7, 137.7, 155.3 ppm (2 signals missing); IR (neat) 3310, 2943, 2862, 2226, 1701, 1605 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{14}NO$, 344.1070; found, 344.1077.

Synthesis of 4



2a **4**

To a solution of **2a** (50.5 mg, 159 μmol) and K_2CO_3 (67.0 mg, 485 μmol) in acetone (6.0 mL) was added dropwise MeI (30.0 μL, 483 μmol) at room temperature. After refluxing for 3 h, the reaction was quenched with water. The mixture was extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography ($CHCl_3$) to give **4** (51.9 mg, 98%) as yellow solids.

4: R_f 0.79 ($CHCl_3$); mp. 190–192 °C; ^{1}H NMR (600 MHz,$CDCl_3$) δ 4.27 (s, 3H), 7.49 (d, 1H, J = 9.0 Hz), 7.64–7.75 (m, 5H), 7.89 (d, 1H, J = 7.8 Hz), 7.99 (d, 1H, J = 8.4 Hz), 8.70 (d, 1H, J = 7.2 Hz), 8.81 (t, 2H, J = 7.2 Hz), 9.00 (d, 1H, J = 8.4 Hz), 9.80 (dd, 1H, J = 7.8, 1.8 Hz) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 56.8, 116.5, 121.5, 123.0, 123.5, 124.9, 125.2, 125.4, 125.6, 125.7, 126.1, 126.3, 126.7, 127.0, 128.7, 129.4, 129.9, 130.9, 131.3, 132.1, 133.2, 135.7, 136.5, 155.0 ppm (1 signal missing); IR (neat) 3005, 2962, 2936, 2839, 1574 cm^{-1}; HRMS–ESI (*m/z*): $[M+H]^+$ calcd for $C_{25}H_{17}O$, 333.1274; found, 333.1261.

2. X-ray crystallographic data

CCDC2251568 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Table S1. Summary of crystallographic data

Empirical formula	$C_{25}H_{16}O_2$
Formula weight	348.38
Temperature/K	93.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.6918(3)
b/Å	5.05931(11)
c/Å	21.7368(5)
α/°	90
β/°	108.000(2)
γ/°	90
Volume/Å^3	1641.22(6)
Z	4
ρ_{calc}g/cm^3	1.410
μ/mm^{-1}	0.699
F(000)	728.0
Crystal size/mm^3	0.02 × 0.02 × 0.01
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.554 to 146.784
Index ranges	-19 ≤ h ≤ 19, -6 ≤ k ≤ 3, -27 ≤ l ≤ 22
Reflections collected	11768
Independent reflections	3238 [R_{int} = 0.0333, R_{sigma} = 0.0362]
Data/restraints/parameters	3238/0/247
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.1067
Final R indexes [all data]	R_1 = 0.0433, wR_2 = 0.1095
Largest diff. peak/hole / e Å^{-3}	0.26/-0.20

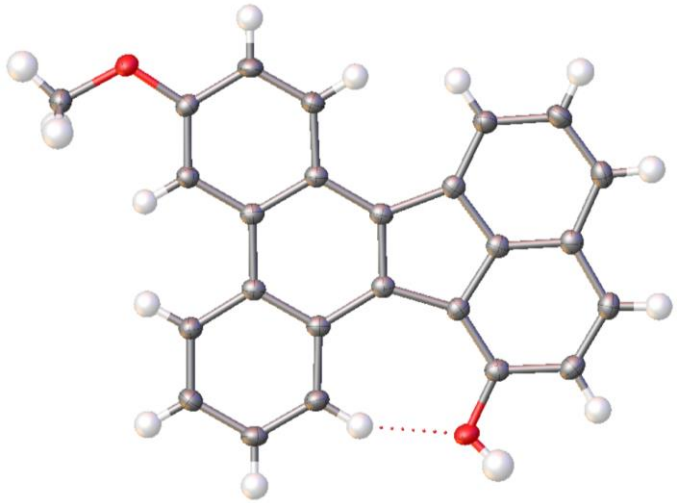


Fig. S1 X-ray crystallographic structure of **2b**

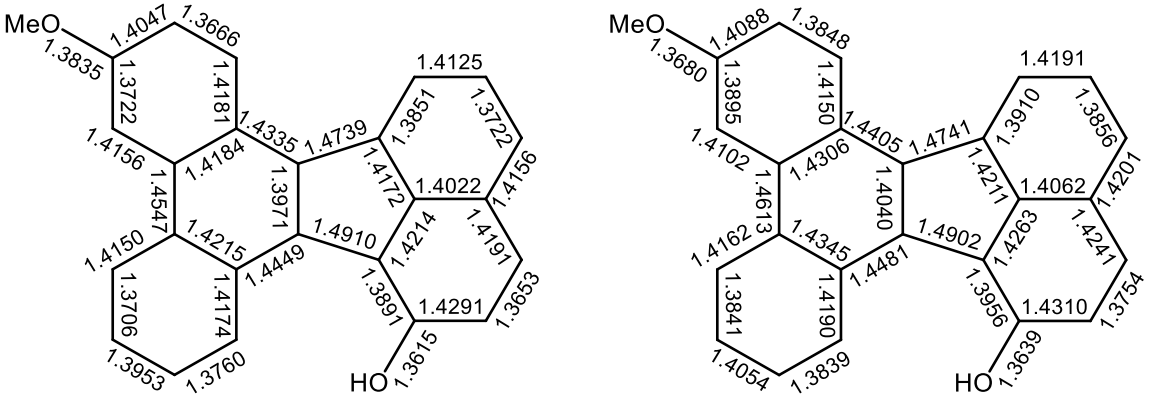


Fig. S2 Comparison with bond lengths of **2b** from crystallographic data (left) and calculation (right, see Fig. S12).

3. UV-vis absorption spectra of 2 and 3 in CH_2Cl_2 under acidic conditions

The UV-vis spectra of **2** and **3** in CH_2Cl_2 was unchanged under acidic conditions (left, blue line) with the addition of an excess amount of trifluoroacetic acid (TFA) compared to neutral conditions (right, black line). The spectra of **2a**, **2b**, **2c**, **3a**, **3b**, and **3c** are shown in Figs. S3-S8, respectively.

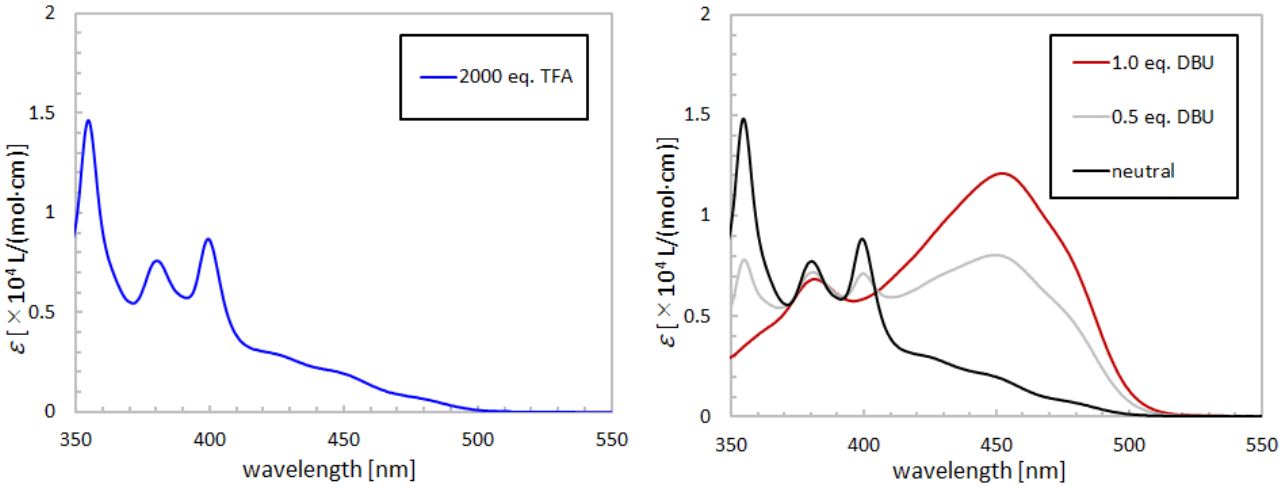


Fig. S3 UV-vis absorption spectra of **2a** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

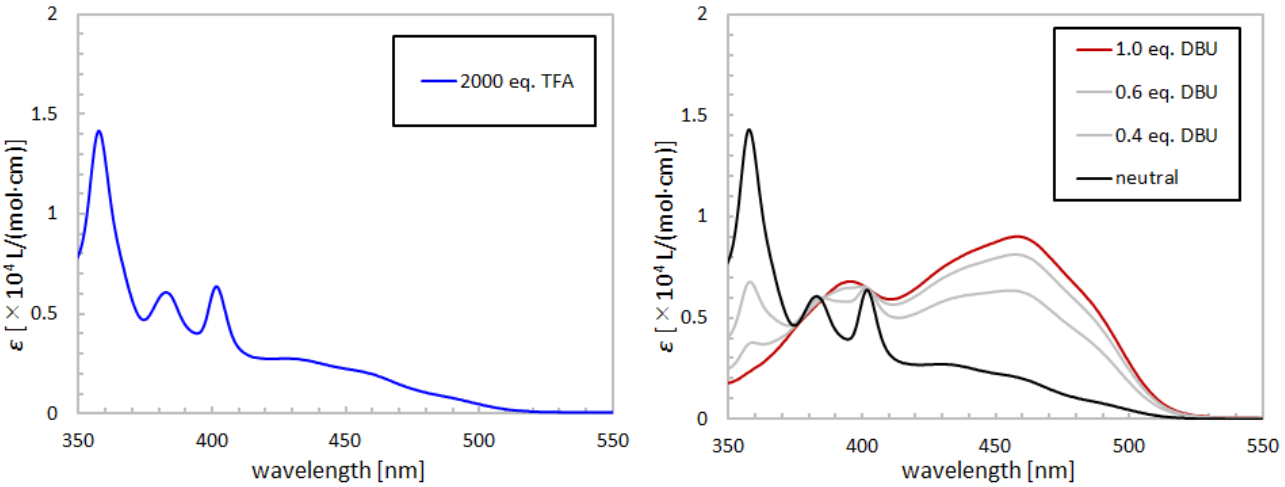


Fig. S4 UV-vis absorption spectra of **2b** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

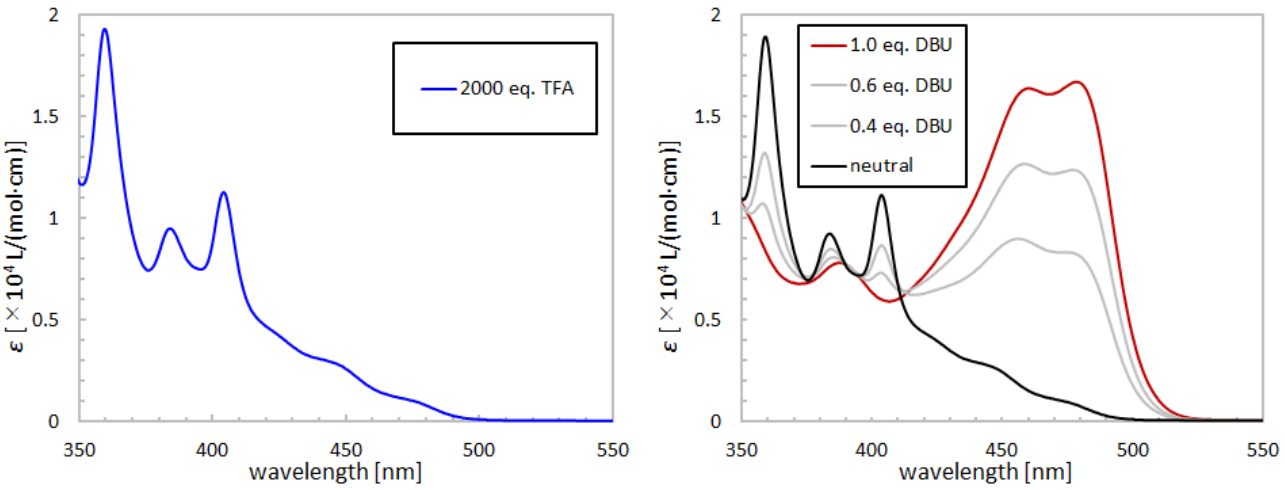


Fig. S5 UV-vis absorption spectra of **2c** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

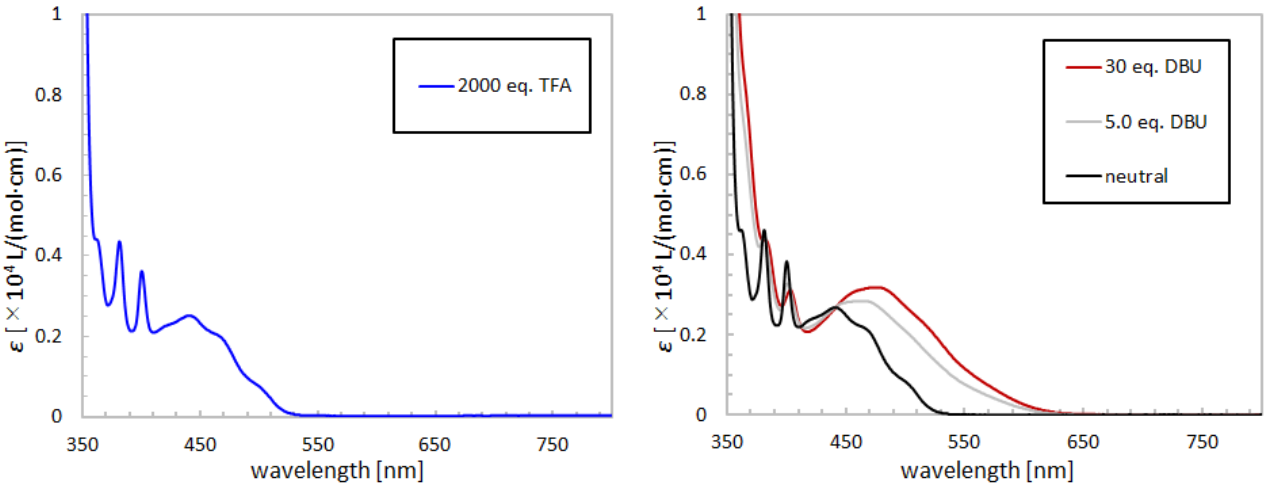


Fig. S6 UV-vis absorption spectra of **3a** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

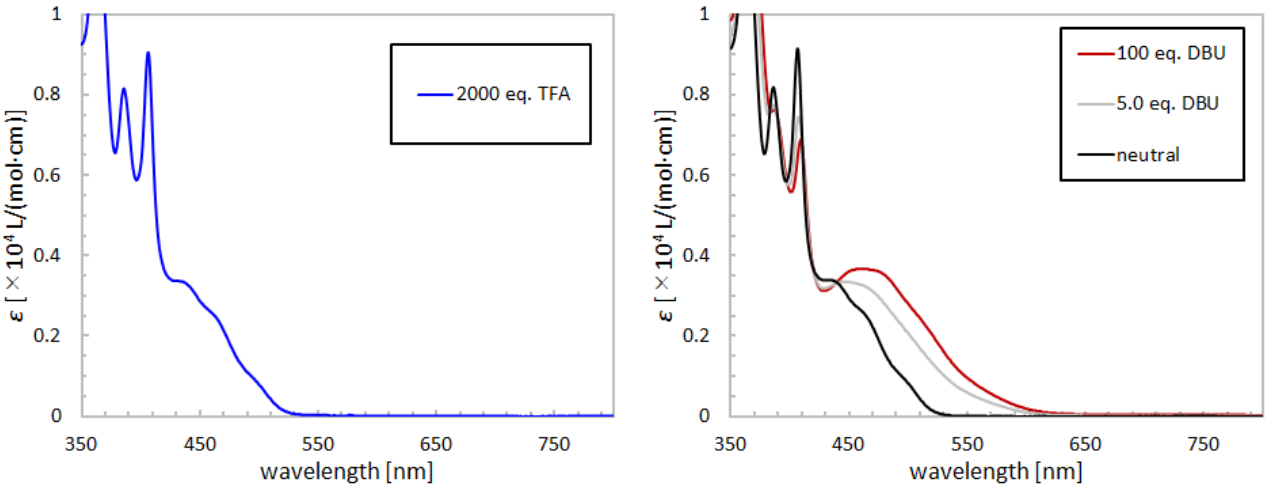


Fig. S7 UV-vis absorption spectra of **3b** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

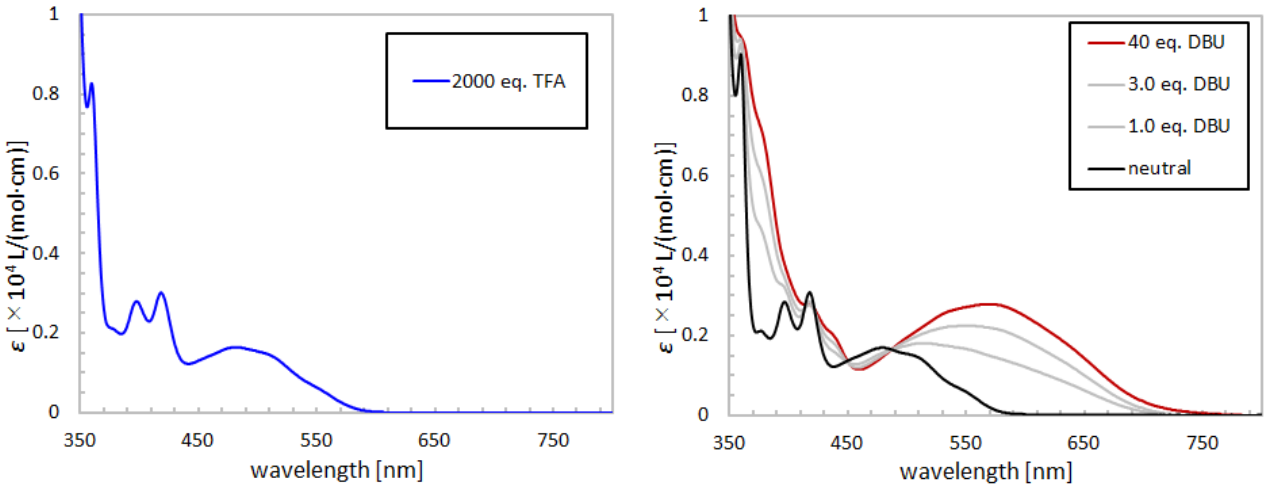


Fig. S8 UV-vis absorption spectra of **3c** (5.0×10^{-5}M) at 296 K, added with TFA (left) or DBU (right).

4. Solvatochromic properties of 2c and 3c in EtOH

The effect of solvent on halochromism was investigated for compounds **2c** and **3c**. CH_2Cl_2 as a nonpolar solvent, dimethylsulfoxide (DMSO) as an aprotic polar solvent, and EtOH as a protic polar solvent were selected (Fig. S9). The chromic properties (UV-vis spectra) of **2c** and **3c** in CH_2Cl_2 and DMSO were depicted in the main text. The chromic properties of **2c** and **3c** in EtOH were similar to those in DMSO.

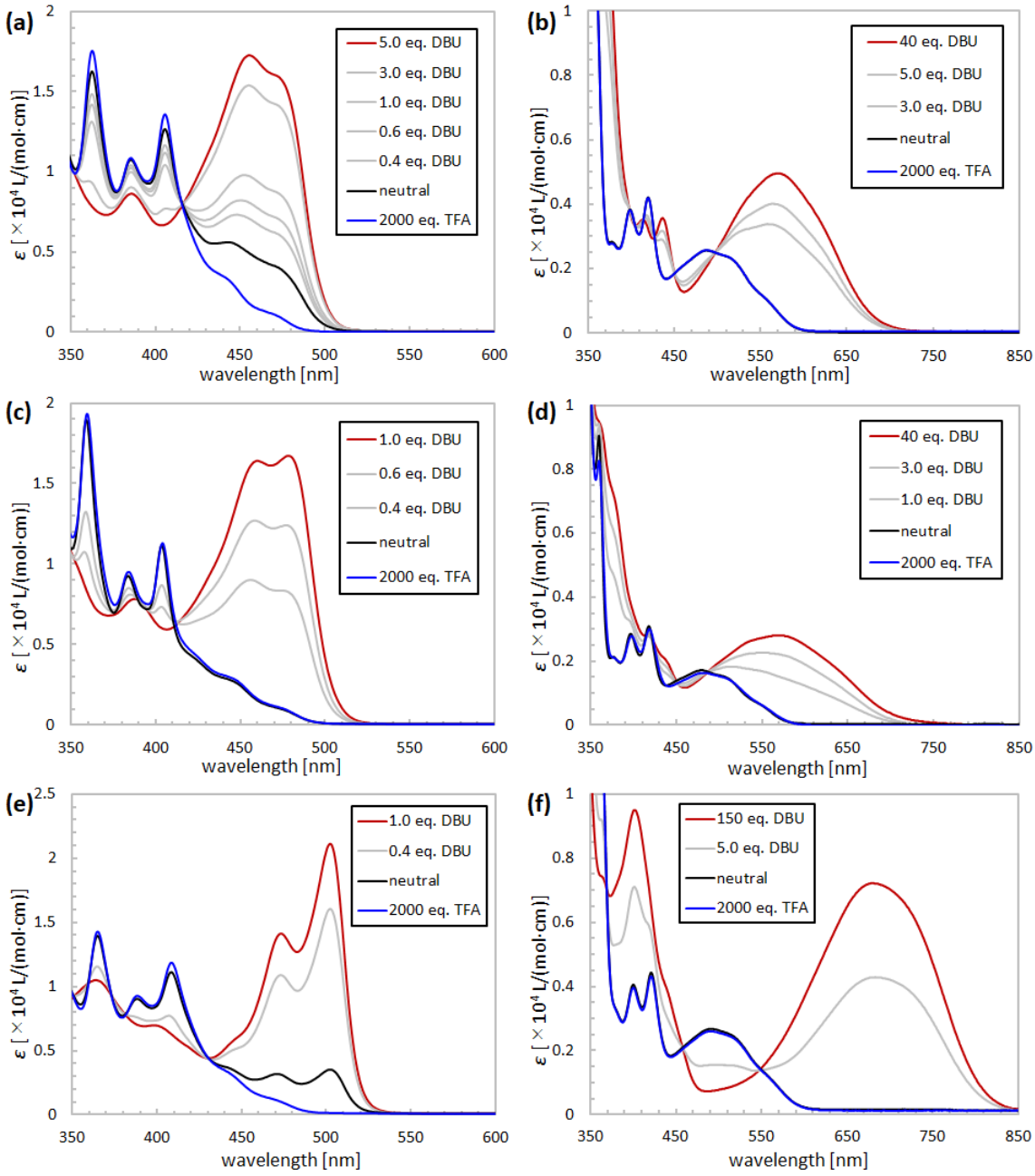


Fig. S9 UV-vis absorption spectra of **2c** and **3c** (5.0×10^{-5}M) in EtOH, CH_2Cl_2 or DMSO at 296 K, added with TFA or DBU. (a) 2c in EtOH, (b) **3c** in EtOH, (c) **2c** in CH_2Cl_2, (d) **3c** in CH_2Cl_2, (e) **2c** in DMSO, (d) **3c** in DMSO.

Table S2. Photophysical properties of hydroxydibenzofluoranthenes **2c** and **3c** in EtOH.[a]

	Compound	λ_{Abs} [nm] (ε [10^3 L/(mol cm)])
2c	Neutral form (no additive)	443 (5.60)
	Anionic form (in the presence of DBU) [b]	455 (17.3)
3c	Neutral form	488 (2.58)
	Anionic form	680 (4.96)

a) Absorption spectra was recorded in solution at room temperature at $c = 5.0 \times 10^{-5}$ M. b) Each hydroxydibenzofluoranthene (anionic form) was studied in the presence of DBU (for **2c**: 5.0 eq.; **3c:** 40 eq.)

Table S3. Photophysical properties of hydroxydibenzofluoranthenes **2c** and **3c** in DMSO.[a]

	Compound	λ_{Abs} [nm] (ε [10^3 L/(mol cm)])
2c	Neutral form (no additive)	471 (3.14), 503 (3.48)
	Anionic form (in the presence of DBU) [b]	503 (21.1)
3c	Neutral form	421 (4.42), 492 (2.66)
	Anionic form	680 (7.22)

a) Absorption spectra was recorded in solution at room temperature at $c = 5.0 \times 10^{-5}$ M. b) Each hydroxydibenzofluoranthene (anionic form) was studied in the presence of DBU (for **2c**: 1.0 eq.; **3c:** 150 eq.)

5. HOMA Calculation

Harmonic Oscillator Model of Aromaticity (HOMA) [3] values for **2b** was calculated from a following equation:

$$\mathrm{HOMA} = 1 - \frac{1}{n}\{\alpha_{\mathrm{CC}} \sum [(R(\mathrm{CC})_{\mathrm{opt}} - R_{\mathrm{i}})]^2$$

where n is the number of bonds taken into summation, α is an empirical constant, R_{opt} is an optimal bond length, R_{i} is an experimental bond length from X-ray crystallographic structure.

For HOMA, α_{CC} = 257.7, $R(\mathrm{CC})_{\mathrm{opt}}$ = 1.388 Å were used.

Table S4. HOMA values for **2b**

Ring	A	B	C	D	E	F
HOMA	0.846	0.506	0.862	–0.0328	0.885	0.807

6. Computational results

All the calculations were performed using Gaussian 16 program.[3] Electronic transitions were simulated by time-dependent DFT (TD-DFT) calculations at the B3LYP/CPCM(DCM)/6-31+G(d,p) level of theory for the structure optimized at the B3LYP/CPCM(DCM)/6-31+G(d,p) level of theory. NICS values were calculated using the standard GIAO (GIAO=NMR) at the level of B3LYP/6-31+G(d,p) for the structure optimized at the B3LYP/6-31+G(d,p) theoretical level.

6-1. Frontier molecular orbitals and energy levels of 2b and 3b

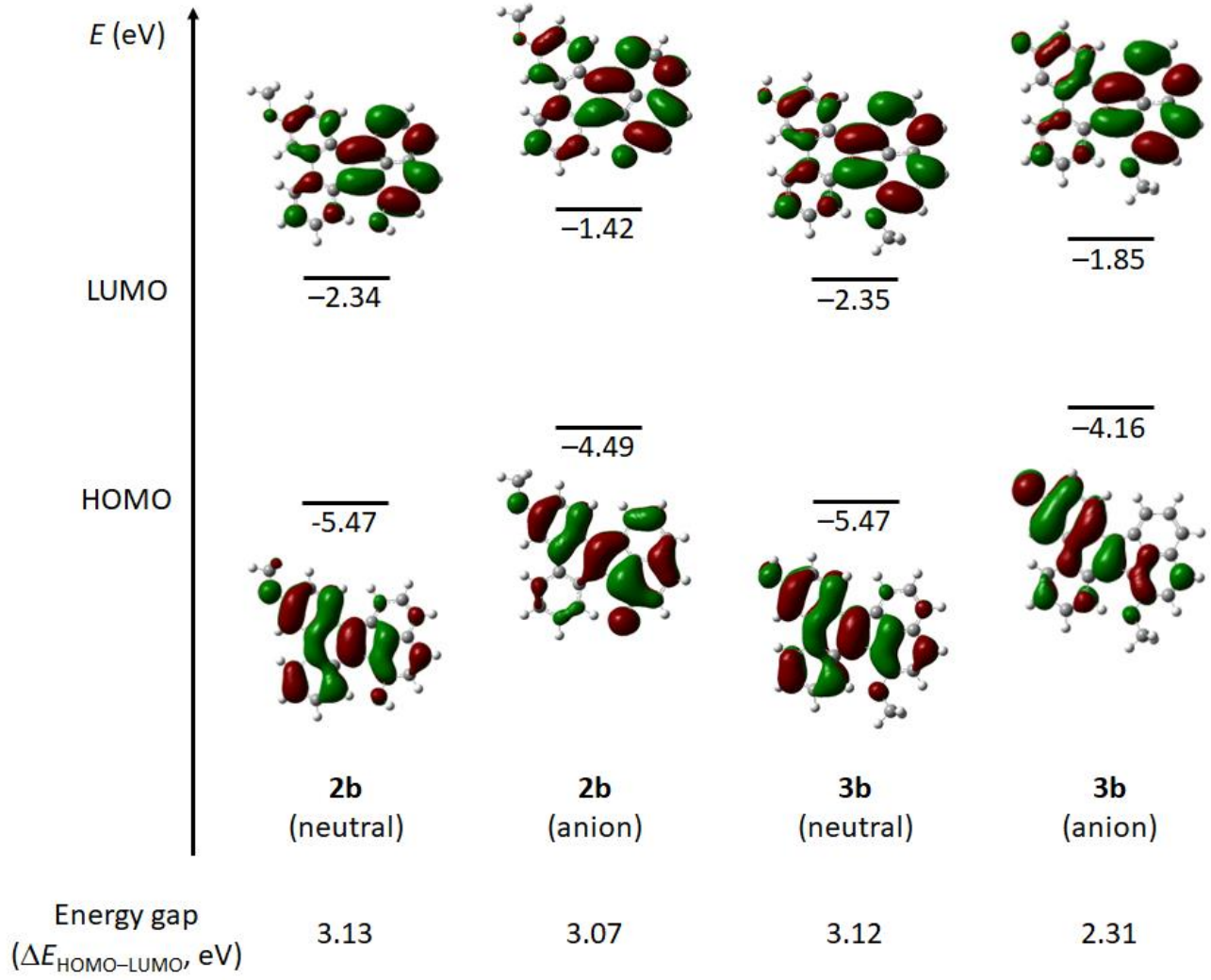


Fig. S10 Calculated frontier molecular orbitals and energy levels of **2b** (neutral, anion) and **3b** (neutral, anion) at the B3LYP/6-31+G(d,p)-CPCM(DCM).

6-2. TD-DFT calculations

Table S5. Major theoretical electronic transitions of **2a** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.7350	453.33	0.0920	H → L (0.69246)
2	3.1955	388.00	0.2430	H–1 → L (0.67573) H → L+1 (0.16702)
3	3.5506	349.20	0.1494	H–2 → L (0.63426) H–1 → L (0.12719) H → L+1 (–0.25744)

Table S6. Major theoretical electronic transitions of **2a** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.6916	460.64	0.2392	H → L (0.69029)
2	3.0581	405.42	0.1073	H–1 → L (0.64837) H → L+1 (–0.25335)
3	3.2242	384.54	0.1755	H–1 → L (0.24434) H → L+1 (0.64787)

Table S7. Major theoretical electronic transitions of **2b** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.5942	477.93	0.1133	H → L (0.69523)
2	3.2079	386.49	0.2274	H–1 → L (0.67714) H → L+1 (–0.22317)
3	3.4950	354.75	0.2374	H–2 → L (0.45751) H–1 → L (0.20340) H → L+1 (0.48061)

Table S8. Major theoretical electronic transitions of **2b** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.6069	475.60	0.2245	H → L (0.69253)
2	3.0125	411.56	0.0484	H–1 → L (0.56199) H → L+1 (–0.41699)
3	3.1230	411.56	0.0484	H–1 → L (0.41074) H → L+1 (0.56026)

Table S9. Major theoretical electronic transitions of **2c** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.7470	451.34	0.1319	H → L (0.68950)
2	3.1460	394.10	0.3123	H–1 → L (0.67675) H → L+1 (0.15874)
3	3.5131	352.92	0.1795	H–2 → L (0.58354) H–1 → L (0.14905) H → L+1 (–0.29864) H → L+2 (–0.17114)

Table S10. Major theoretical electronic transitions of **2c** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.6422	469.25	0.4327	H → L (0.69146)
2	2.9798	416.08	0.0665	H–1 → L (0.65007) H → L+1 (–0.24816)
3	3.1481	393.84	0.1867	H–1 → L (0.24310) H → L+1 (0.63015) H → L+2 (–0.15109)

Table S11. Major theoretical electronic transitions of **3a** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.5635	483.65	0.0912	H → L (0.69633)
2	3.2232	384.66	0.1817	H–2 → L (0.11089) H–1 → L (0.63200) H → L+1 (0.27733)
3	3.5218	352.04	0.3411	H–2 → L (0.43514) H–1 → L (–0.27657) H → L+1 (0.46801)

Table S12. Major theoretical electronic transitions of **3a** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	1.9012	652.15	0.2027	H → L (0.70014)
2	2.9292	423.27	0.0088	H–2 → L (–0.26954) H → L+1 (0.64752)
3	3.0910	401.11	0.0000	H–1 → L (0.70127)

Table S13. Major theoretical electronic transitions of **3b** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.5884	479.01	0.1098	H → L (0.69431)
2	3.1547	393.01	0.2559	H–1 → L (0.66952) H → L+1 (0.18404)
3	3.4694	357.37	0.1949	H–2 → L (0.42991) H–1 → L (–0.16862) H → L+1 (0.51965)

Table S14. Major theoretical electronic transitions of **3b** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	1.8902	655.93	0.1877	H → L (0.70123)
2	2.9583	419.10	0.0027	H–2 → L (0.11956) H–1 → L (–0.32687) H → L+1 (0.21909)
3	3.1089	398.80	0.2693	H–1 → L (0.57851) H → L+1 (0.31021) H → L+2 (0.21909)

Table S15. Major theoretical electronic transitions of **3c** (neutral).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	2.2528	550.35	0.0936	H → L (0.69573)
2	2.9551	419.56	0.1842	H–1 → L (0.67867) H → L+1 (–0.16235)
3	3.2907	376.78	0.1120	H–2 → L (0.68838) H → L+2 (–0.11204)

Table S16. Major theoretical electronic transitions of **3c** (anion).

Excited states	Energy (eV)	Wavelength (nm)	Oscillator strength (*f*)	description
1	1.7179	721.71	0.2833	H → L (0.69659)
2	2.7672	448.05	0.0233	H–2 → L (–0.13334) H–1 → L (0.48521) H → L+1 (0.48180)
3	2.8245	438.96	0.0009	H–2 → L (0.61892) H–1 → L (0.30295) H → L+1 (–0.13193)

6-3. NICS calculations

Table S17. NICS values of **2a** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	–10.01	–6.77	–9.74	+0.25	–8.85	–7.94
NICS (0)	–7.68	–4.51	–7.91	+3.63	–7.13	–7.15
NICS (–1)	–9.33	–7.12	–10.22	+0.22	–9.03	–7.74

Table S18. NICS values of **2a** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–9.07	–6.58	–9.98	–6.02	–9.96	–3.07
NICS (0)	–7.25	–4.09	–7.91	–4.71	–8.83	–0.17
NICS (–1)	–9.07	–6.58	–9.98	–6.02	–9.96	–3.07

Table S19. NICS values of **2b** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	–10.08	–6.24	–9.76	+0.32	–8.82	–7.87
NICS (0)	–8.95	–3.98	–7.91	+3.67	–7.15	–7.10
NICS (–1)	–9.51	–6.65	–10.18	+0.31	–9.07	–7.66

Table S20. NICS values of **2b** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–9.53	–6.27	–9.92	+6.00	–9.97	–3.13
NICS (0)	–8.92	–3.75	–7.85	+4.75	–8.83	–6.25
NICS (–1)	–9.53	–6.27	–9.92	+6.00	–9.97	–3.13

Table S21. NICS values of **2c** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	–9.92	–6.74	–9.93	–0.26	–8.84	–7.97
NICS (0)	–8.24	–4.34	–8.07	+3.09	–7.13	–7.12
NICS (–1)	–9.29	–7.03	–10.40	–0.20	–9.09	–7.72

Table S22. NICS values of **2c** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–8.61	–6.30	–10.12	–6.23	–10.04	–2.84
NICS (0)	–7.40	–3.69	–8.02	–4.85	–8.85	+0.24
NICS (–1)	–8.61	–6.30	–10.12	–6.23	–10.04	–2.84

Table S23. NICS values of **3a** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	9.54	–6.82	–9.69	+2.23	–8.50	–8.35
NICS (0)	8.94	–4.56	–7.72	+6.44	–6.55	–6.41
NICS (–1)	9.54	–6.82	–9.69	+2.23	–8.50	–8.35

Table S24. NICS values of **3a** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–5.63	–4.70	–8.81	+3.39	–8.35	–6.53
NICS (0)	–2.92	–2.51	–6.91	+7.62	–6.50	–4.46
NICS (–1)	–5.63	–4.70	–8.81	+3.39	–8.35	–6.53

Table S25. NICS values of **3b** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	–9.80	–6.43	–9.62	+0.46	–8.83	–8.23
NICS (0)	–8.85	–4.13	–7.85	+3.77	–7.14	–7.12
NICS (–1)	–9.16	–6.81	–10.20	+0.39	–9.03	–7.87

Table S26. NICS values of **3b** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–5.91	–4.59	–8.56	+2.41	–8.55	–7.13
NICS (0)	–2.86	–2.47	–6.81	+5.98	–6.93	–6.04
NICS (–1)	–5.30	–5.03	–9.11	+2.29	–8.79	–6.76

Table S27. NICS values of **3c** (neutral).

Ring	A	B	C	D	E	F
NICS (1)	–9.59	–6.21	–9.32	+3.20	–7.79	–8.56
NICS (0)	–8.58	–4.01	–7.74	+7.83	–5.61	–6.91
NICS (–1)	–9.05	–6.69	–10.27	+3.33	–7.75	–7.98

Table S28. NICS values of **3c** (anion).

Ring	A	B	C	D	E	F
NICS (1)	–4.94	–3.70	–8.47	+3.86	–7.43	–5.20
NICS (0)	–1.50	–1.59	–6.82	+8.39	–5.51	–3.43
NICS (–1)	–4.43	–4.33	–9.18	+4.02	–7.66	–4.95

6-4. Calculated bond lengths

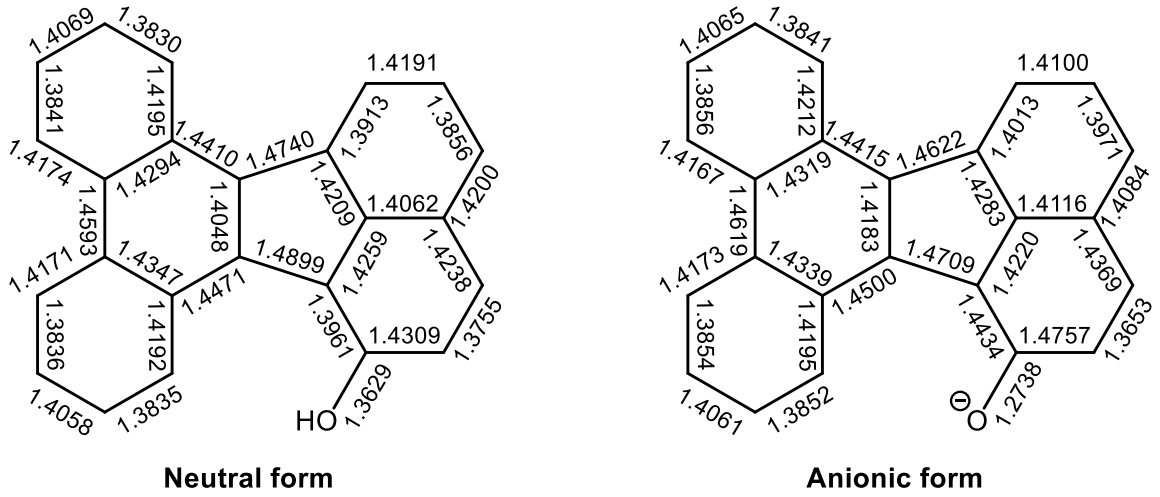


Fig. S11 Calculated bond lengths of neutral (left) and anionic (right) form for **2a**.

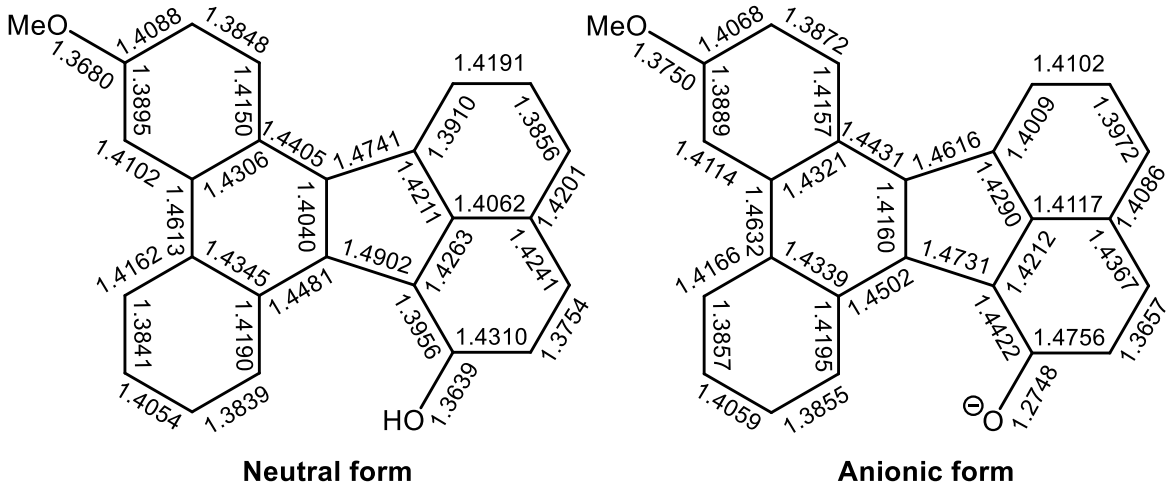


Fig. S12 Calculated bond lengths of neutral (left) and anionic (right) form for **2b**.

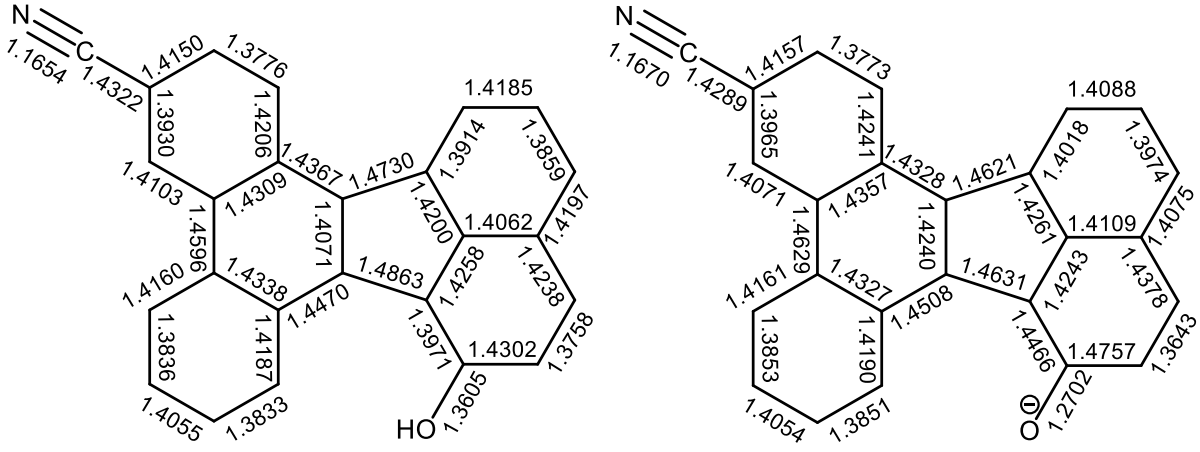


Fig. S13 Calculated bond lengths of neutral (left) and anionic (right) form for **2c**.

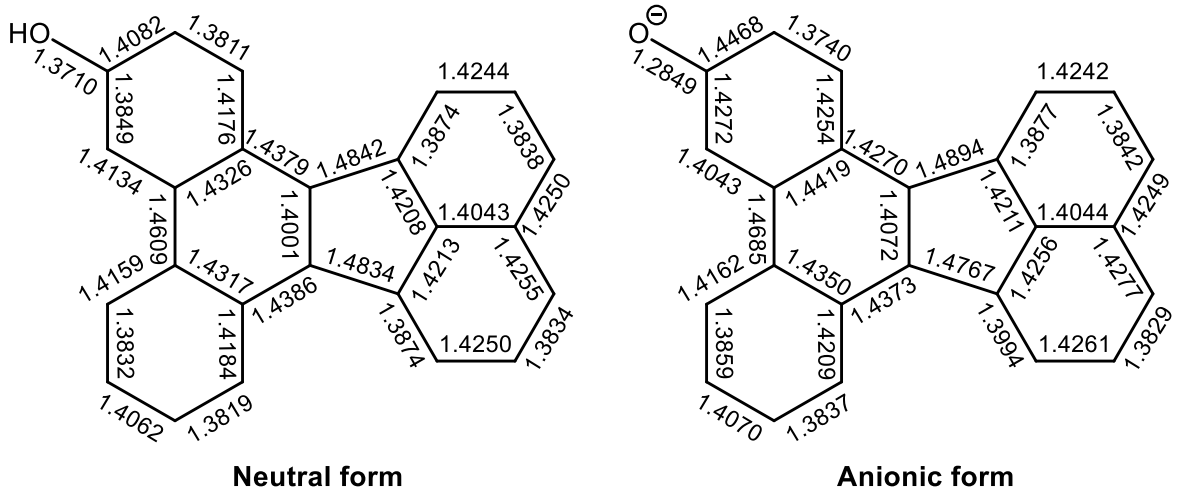


Fig. S14 Calculated bond lengths of neutral (left) and anionic (right) form for **3a**.

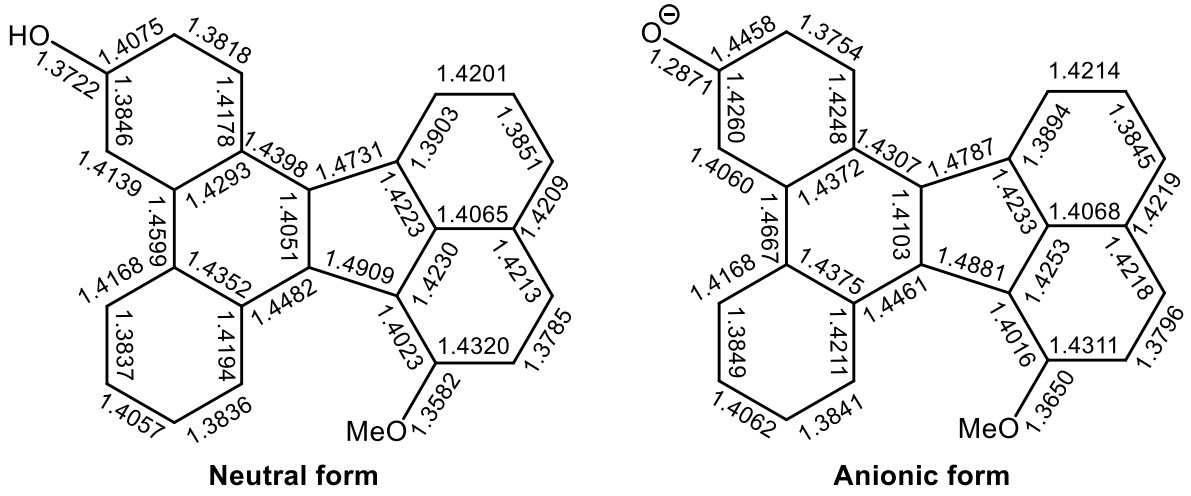


Fig. S15 Calculated bond lengths of neutral (left) and anionic (right) form for **3b**.

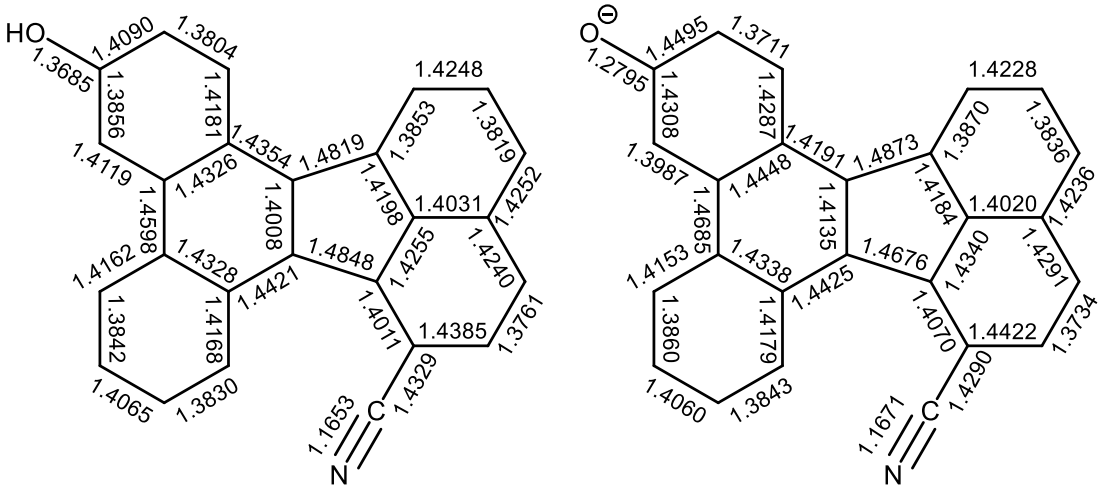


Fig. S16 Calculated bond lengths of neutral (left) and anionic (right) form for **3c**.

Optimized structure for 2a (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	3.93805200	-2.67873700	0.21707800
C	3.81931300	-1.30217800	0.13588800
C	2.55702300	-0.66356500	0.04683800
C	1.38298300	-1.47885900	0.04278900
C	1.53510000	-2.88675900	0.14037900
C	2.78165400	-3.47995700	0.22284800
C	2.42935200	0.78731600	-0.04320700
C	1.13328400	1.40250700	-0.04909300
C	-0.04020400	0.55838100	0.01871000
C	0.09297700	-0.83962400	-0.01916100
C	3.57171700	1.61991700	-0.14305000
C	3.46992400	2.99527600	-0.25477200
C	2.19937100	3.59632000	-0.27930100
C	1.06272100	2.81391300	-0.17988700
C	-2.17260200	-0.36717400	-0.03717700
C	-3.56727800	-0.54502700	-0.06140800
C	-4.05955600	-1.87036200	-0.19410500
C	-3.16829500	-2.92710500	-0.28729800
C	-1.76393200	-2.72966100	-0.23733200
C	-1.24866600	-1.44498100	-0.09702900
C	-1.49368400	0.88282700	0.06220800
C	-2.31580200	2.00000200	0.22063500
C	-3.73889300	1.85238800	0.20030900
C	-4.35848300	0.63288500	0.05567800
H	4.92130600	-3.13417300	0.28705000
O	-1.80735100	3.24855800	0.42080900
H	4.72617100	-0.71036400	0.15196200
H	0.66066900	-3.51905500	0.17750300
H	2.86297400	-4.55993000	0.30266800
H	4.56102100	1.17957300	-0.14662900
H	4.36808700	3.60071800	-0.33323600
H	2.10488400	4.67358500	-0.38188300
H	0.09502200	3.28883400	-0.20578800
H	-5.13096900	-2.04812800	-0.22509500
H	-3.54579300	-3.93909200	-0.39854100
H	-1.13347100	-3.60499600	-0.32478500
H	-4.34211800	2.75032200	0.31076800

H	-5.44275100	0.57057800	0.04314000
H	-2.52268500	3.89720400	0.49315900

Optimized structure for 2a (neutral, B3LYP/6-31+G(d,p))

C	3.93448600	-2.67786700	0.22492100
C	3.81670900	-1.30292900	0.13156100
C	2.55601900	-0.66304500	0.04283600
C	1.38238600	-1.47739700	0.04922200
C	1.53277900	-2.88337300	0.16360200
C	2.77795600	-3.47724300	0.24650000
C	2.42875300	0.78661900	-0.05241900
C	1.13389400	1.40291200	-0.04753100
C	-0.03773200	0.55862400	0.02319400
C	0.09439300	-0.83754200	-0.01641300
C	3.56958800	1.61812200	-0.16448400
C	3.46767900	2.99266600	-0.27377000
C	2.19824500	3.59446100	-0.28223400
C	1.06258300	2.81378700	-0.17310800
C	-2.17211300	-0.36673900	-0.03639100
C	-3.56572200	-0.54598300	-0.06414100
C	-4.05610200	-1.87125900	-0.20782700
C	-3.16415500	-2.92417000	-0.30984800
C	-1.75994800	-2.72448000	-0.25587800
C	-1.24684200	-1.44272900	-0.10074600
C	-1.49208100	0.88221000	0.06845300
C	-2.31444300	1.99544800	0.23061300
C	-3.73623100	1.84746100	0.20880700
C	-4.35720800	0.62943000	0.05829700
H	4.91766600	-3.13384100	0.29493600
O	-1.81070100	3.25002700	0.43443900
H	4.72343400	-0.71064300	0.14049600
H	0.65562800	-3.51095000	0.21917300
H	2.85888000	-4.55625400	0.34077000
H	4.55792300	1.17559600	-0.18050500
H	4.36540600	3.59771000	-0.36213500
H	2.10358500	4.67219400	-0.38059900
H	0.09571300	3.28973200	-0.18770100
H	-5.12737000	-2.05077000	-0.24176600

H	-3.54012800	-3.93567300	-0.43207000
H	-1.12499900	-3.59551400	-0.35533200
H	-4.34024600	2.74624600	0.32063700
H	-5.44174200	0.56726000	0.04359000
H	-2.53550500	3.88279400	0.52569600

Optimized structure for 2a (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	-3.92868100	-2.69284300	-0.03226800
C	-3.80515900	-1.31283900	-0.01641700
C	-2.54329000	-0.66899000	-0.00402500
C	-1.36230400	-1.47870100	-0.00740700
C	-1.52192600	-2.89079300	-0.02733900
C	-2.76971500	-3.48973600	-0.03891600
C	-2.41984800	0.78762600	0.00990800
C	-1.12559400	1.40471800	0.00471000
C	0.06160200	0.57236500	-0.00550800
C	-0.07020700	-0.83972000	0.00237000
C	-3.56276600	1.62561200	0.02943300
C	-3.46156400	3.00723500	0.04262800
C	-2.19112400	3.60966100	0.03692400
C	-1.05162600	2.82225300	0.01846000
C	2.18033900	-0.32577800	0.00348100
C	3.58100300	-0.50086400	0.00835700
C	4.08693000	-1.81502600	0.03054300
C	3.20796800	-2.90079500	0.04752500
C	1.80986700	-2.71836300	0.03969000
C	1.26931700	-1.42580100	0.01457800
C	1.49130900	0.91805200	-0.01174400
C	2.28213900	2.12528200	-0.03669400
C	3.74339000	1.91956100	-0.03059200
C	4.36412600	0.70370000	-0.00916800
O	1.85974500	3.32664500	-0.06507400
H	-4.91348000	-3.15086100	-0.04214600
H	-4.71296400	-0.72126000	-0.01601500
H	-0.64816200	-3.52515800	-0.03931700
H	-2.84858900	-4.57332000	-0.05532400
H	-4.55374200	1.18764600	0.03620500
H	-4.36190700	3.61547800	0.05792400

H	-2.09963000	4.69280000	0.04739500
H	-0.06393900	3.27379300	0.01170700
H	5.16190500	-1.98123200	0.03587300
H	3.60449400	-3.91223700	0.06745200
H	1.19117600	-3.60726500	0.05748200
H	4.33096400	2.83455500	-0.04566300
H	5.45080700	0.63900600	-0.00614200

Optimized structure for 2a (anion, B3LYP/6-31+G(d,p))

C	3.93786700	-2.68351400	0.00000400
C	3.80557900	-1.30374700	0.00000000
C	2.54387600	-0.66331800	-0.00000100
C	1.36374000	-1.47697700	0.00000200
C	1.53237300	-2.88882300	0.00000800
C	2.78151700	-3.48354500	0.00000900
C	2.41524000	0.79286700	-0.00000300
C	1.11882900	1.40446800	0.00000000
C	-0.06513100	0.56878000	0.00000200
C	0.07185300	-0.84647300	0.00000000
C	3.55363500	1.63590200	-0.00000700
C	3.44546700	3.01679600	-0.00000700
C	2.17220600	3.61212900	-0.00000400
C	1.03554900	2.82142300	0.00000000
C	-2.17565700	-0.33093100	0.00000000
C	-3.57639500	-0.50656000	-0.00000100
C	-4.08106500	-1.81837000	-0.00000600
C	-3.20285200	-2.90692900	-0.00001000
C	-1.80651400	-2.72458800	-0.00000800
C	-1.26427400	-1.43241500	-0.00000200
C	-1.48732700	0.91052500	0.00000300
C	-2.27634500	2.12654800	0.00000500
C	-3.74293900	1.91589400	0.00000500
C	-4.35954300	0.70084000	0.00000200
O	-1.86117400	3.31830200	0.00000800
H	4.92571100	-3.13715200	0.00000400
H	4.70989400	-0.70573200	-0.00000300
H	0.65835800	-3.52334900	0.00001400
H	2.86344500	-4.56805300	0.00001400

H	4.54678200	1.20094500	-0.00001000
H	4.34402900	3.62997700	-0.00001000
H	2.07278900	4.69513700	-0.00000400
H	0.04480000	3.26985800	0.00000200
H	-5.15719200	-1.98396600	-0.00000700
H	-3.60122300	-3.91887100	-0.00001400
H	-1.18559100	-3.61300000	-0.00001300
H	-4.32314200	2.83557100	0.00000700
H	-5.44739300	0.63233600	0.00000200

Optimized structure for 2b (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.10015700	-0.81289400	0.09644200
C	3.45281600	0.41548600	0.04321700
C	2.04734300	0.51488000	-0.01510800
C	1.27202200	-0.68738400	-0.01729700
C	1.96170700	-1.92093700	0.05242800
C	3.34311500	-2.00100100	0.10579900
C	1.36898800	1.80762300	-0.07770800
C	-0.06372000	1.87638900	-0.05704800
C	-0.82426300	0.64593100	0.01056300
C	-0.16494700	-0.59221800	-0.04853000
C	2.10268500	3.01492700	-0.17631900
C	1.47997900	4.24810500	-0.26079100
C	0.07622200	4.31495100	-0.25745600
C	-0.67152000	3.15454100	-0.15944700
C	-2.43855400	-1.02800000	-0.03081000
C	-3.65741400	-1.72912300	-0.03993300
C	-3.60291700	-3.14121100	-0.18075900
C	-2.37510800	-3.77282600	-0.29653700
C	-1.15449400	-3.04975500	-0.26308600
C	-1.17193800	-1.66669600	-0.11557000
C	-2.29038800	0.38665600	0.07421800
C	-3.47691600	1.09951600	0.25195600
C	-4.73397500	0.41581800	0.24682800
C	-4.83975800	-0.94741900	0.09840500
O	-3.48809000	2.44798600	0.45593000
O	5.46663800	-0.77310800	0.14801600
C	6.18712700	-2.00640100	0.21271900

H	4.07851000	1.29885900	0.05743800
H	1.40629900	-2.84614000	0.09050400
H	3.81762100	-2.97274800	0.16509300
H	3.18513800	2.98684500	-0.20004200
H	2.07584100	5.15265000	-0.33892500
H	-0.42668400	5.27452900	-0.33740100
H	-1.74770800	3.22236300	-0.16371500
H	-4.52324100	-3.71842900	-0.20029600
H	-2.33559500	-4.85161600	-0.41365900
H	-0.23698000	-3.61436800	-0.36799600
H	-5.63375600	1.01354100	0.37190600
H	-5.81679300	-1.42177800	0.09791900
H	-4.39831400	2.76679400	0.54216600
H	7.24134900	-1.73069000	0.24074700
H	5.93297600	-2.56763700	1.11886700
H	5.99546000	-2.62493400	-0.67122400

Optimized structure for 2b (neutral, B3LYP/6-31+G(d,p))

C	4.09586200	-0.81730800	0.10113900
C	3.45108700	0.41058800	0.03844500
C	2.04695900	0.51237400	-0.02094100
C	1.27044200	-0.68867800	-0.01626200
C	1.95654200	-1.92194200	0.06675200
C	3.33774800	-2.00355200	0.12185600
C	1.37033700	1.80490100	-0.08790900
C	-0.06124800	1.87623900	-0.05828700
C	-0.82112800	0.64679400	0.01267600
C	-0.16505300	-0.59066500	-0.05023800
C	2.10441900	3.00975000	-0.19736000
C	1.48303800	4.24256900	-0.28126100
C	0.08038800	4.31150600	-0.26549500
C	-0.66832100	3.15371800	-0.15829600
C	-2.43928700	-1.02553900	-0.03113700
C	-3.65749400	-1.72581900	-0.04149500
C	-3.60392100	-3.13694100	-0.19447300
C	-2.37821700	-3.76642600	-0.32175000
C	-1.15751600	-3.04300300	-0.28592400
C	-1.17316100	-1.66354000	-0.12318900

C	-2.28755000	0.38813200	0.08070700
C	-3.47117800	1.09886800	0.26732600
C	-4.72795600	0.41680300	0.26282800
C	-4.83763600	-0.94516600	0.10644400
O	-3.48433400	2.45026600	0.47886600
O	5.46345700	-0.77666300	0.15269300
C	6.18020700	-2.00217600	0.22917900
H	4.08075500	1.29081500	0.04898800
H	1.39596600	-2.84364700	0.11945600
H	3.81140000	-2.97528000	0.19332500
H	3.18651600	2.97795100	-0.23100300
H	2.07943400	5.14616700	-0.36820000
H	-0.42176500	5.27174900	-0.34348200
H	-1.74386900	3.22352300	-0.15384600
H	-4.52469600	-3.71383700	-0.21538900
H	-2.33958200	-4.84413800	-0.45053400
H	-0.23861600	-3.60311300	-0.40431900
H	-5.62829100	1.01480000	0.39354600
H	-5.81544500	-1.41860200	0.10577800
H	-4.39503700	2.75543500	0.58577300
H	7.23548100	-1.72732500	0.25458600
H	5.92909700	-2.55861100	1.14110300
H	5.99148600	-2.63360700	-0.64827100

Optimized structure for 2b (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	-4.09019100	-0.81995100	0.00000100
C	-3.43997700	0.40737000	0.00000000
C	-2.03228400	0.50919400	0.00000000
C	-1.25171500	-0.69145000	0.00000000
C	-1.94866400	-1.92374300	0.00000100
C	-3.33342100	-2.00590100	0.00000100
C	-1.35610900	1.80681700	0.00000000
C	0.07606500	1.87615300	0.00000000
C	0.85254200	0.65129300	0.00000000
C	0.18843400	-0.59932100	0.00000000
C	-2.08840800	3.01943400	0.00000000
C	-1.46342000	4.25613400	-0.00000100
C	-0.05903600	4.32192100	-0.00000100

C	0.68968100	3.15617800	-0.00000100
C	2.46374300	-0.99248100	0.00000000
C	3.68820400	-1.69513200	0.00000000
C	3.64671000	-3.10310600	0.00000000
C	2.41650100	-3.76542600	0.00000000
C	1.19715300	-3.05694400	0.00000000
C	1.19815500	-1.65606900	0.00000000
C	2.30741400	0.42011200	0.00000000
C	3.50139200	1.22911100	-0.00000100
C	4.77026900	0.47583400	-0.00000100
C	4.87528400	-0.88577500	0.00000000
O	3.57508500	2.50175200	-0.00000100
O	-5.46458100	-0.77973300	0.00000100
C	-6.17908500	-2.01493600	0.00000200
H	-4.06499000	1.29189600	0.00000000
H	-1.39520100	-2.85108700	0.00000100
H	-3.80760100	-2.98006100	0.00000100
H	-3.17178700	2.99588200	0.00000000
H	-2.06002100	5.16431600	-0.00000100
H	0.44280200	5.28625800	-0.00000100
H	1.77536400	3.19228500	-0.00000100
H	4.57382800	-3.67208000	0.00000000
H	2.39171800	-4.85175100	0.00000000
H	0.28272700	-3.63785200	0.00000000
H	5.66499800	1.09394400	-0.00000100
H	5.85332800	-1.36384900	0.00000000
H	-7.23614400	-1.74699100	0.00000200
H	-5.95423700	-2.60647300	-0.89531200
H	-5.95423700	-2.60647300	0.89531500

Optimized structure for 2b (anion, B3LYP/6-31+G(d,p))

C	4.08954100	-0.81541000	-0.00000100
C	3.43790400	0.40870100	0.00000200
C	2.03066200	0.50949700	0.00000200
C	1.25087100	-0.69356600	-0.00000100
C	1.95212500	-1.92302900	-0.00000700
C	3.33809300	-2.00221600	-0.00000700
C	1.35216200	1.80533600	0.00000300

C	-0.07975700	1.87096400	0.00000000
C	-0.85399900	0.64557100	-0.00000100
C	-0.18636900	-0.60700000	0.00000000
C	2.08096500	3.01914800	0.00000700
C	1.45175600	4.25326800	0.00000600
C	0.04748400	4.31380000	0.00000300
C	-0.69958800	3.14780300	-0.00000100
C	-2.45947100	-0.99342300	-0.00000100
C	-3.68494500	-1.69449700	0.00000000
C	-3.64581600	-3.09954100	0.00000500
C	-2.41633200	-3.76700900	0.00000900
C	-1.19741700	-3.06161300	0.00000800
C	-1.19409600	-1.66042100	0.00000200
C	-2.30056600	0.41613400	-0.00000300
C	-3.49482400	1.23606600	-0.00000500
C	-4.76831900	0.47829600	-0.00000500
C	-4.87182000	-0.88055600	-0.00000300
O	-3.56862900	2.49642100	-0.00000700
O	5.47427800	-0.77038700	0.00000000
C	6.17718700	-1.99707700	-0.00000400
H	4.06259200	1.29352800	0.00000500
H	1.39599900	-2.84905300	-0.00001300
H	3.81382600	-2.97659900	-0.00001200
H	3.16499200	2.99665600	0.00001000
H	2.04621100	5.16423300	0.00000900
H	-0.45988800	5.27581800	0.00000200
H	-1.78675100	3.18194200	-0.00000300
H	-4.57537200	-3.66652100	0.00000600
H	-2.39527800	-4.85438600	0.00001400
H	-0.28210000	-3.64275600	0.00001300
H	-5.65715700	1.10482100	-0.00000700
H	-5.85012500	-1.36126100	-0.00000200
H	7.23844700	-1.73778800	-0.00000200
H	5.95341900	-2.59614100	0.89412200
H	5.95342100	-2.59613400	-0.89413500

Optimized structure for 2c (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.09484800	-1.29228600	0.13313300

C	3.57567000	-0.00141600	0.06586700
C	2.18689900	0.23216300	-0.01025500
C	1.30411100	-0.89394400	-0.01441700
C	1.86371800	-2.19706300	0.06786300
C	3.22344500	-2.40705800	0.13705900
C	1.64129400	1.58368700	-0.08802300
C	0.22228200	1.78809900	-0.07116100
C	-0.64890300	0.63547600	0.00768300
C	-0.11348900	-0.66417200	-0.05671400
C	2.48700600	2.71380700	-0.20068800
C	1.98114600	3.99746600	-0.30448000
C	0.58991700	4.19681900	-0.30858300
C	-0.26450100	3.11479400	-0.19566900
C	-2.41492800	-0.87336300	-0.03455100
C	-3.69779500	-1.44908400	-0.04185800
C	-3.78530400	-2.85778200	-0.19485800
C	-2.62682300	-3.60789700	-0.32149900
C	-1.34035500	-3.01129400	-0.28642200
C	-1.21965600	-1.63420800	-0.12789100
C	-2.12879200	0.51865100	0.08133600
C	-3.23644800	1.34590600	0.28309600
C	-4.55459900	0.79090100	0.27740200
C	-4.79413600	-0.55379100	0.11236000
O	-3.10554200	2.68051200	0.51239800
C	5.51143900	-1.48765100	0.21152000
N	6.66323500	-1.65373100	0.27464100
H	4.27179400	0.82636300	0.08385500
H	1.21439200	-3.05825900	0.10359600
H	3.62432800	-3.41225600	0.20551100
H	3.56225000	2.58732800	-0.22329900
H	2.65909700	4.84085700	-0.39377000
H	0.18094200	5.19813800	-0.40653600
H	-1.32943900	3.28313600	-0.20644300
H	-4.75869100	-3.33987900	-0.21502200
H	-2.69564100	-4.68399000	-0.44808500
H	-0.48450300	-3.66413100	-0.40019500
H	-5.39058100	1.47218500	0.41596900
H	-5.81342000	-0.92882600	0.11306400

H	-3.97510200	3.09079000	0.62819000

Optimized structure for 2c (neutral, B3LYP/6-31+G(d,p))

C	4.09714400	-1.29147600	0.13103200
C	3.57545500	-0.00327200	0.05612600
C	2.18621300	0.23274900	-0.01374400
C	1.30334800	-0.89165100	-0.00725900
C	1.86258600	-2.19309500	0.08829600
C	3.22262800	-2.40269600	0.15272700
C	1.64047300	1.58333000	-0.09136000
C	0.22204300	1.78966500	-0.06598700
C	-0.64833900	0.63740700	0.01016000
C	-0.11369600	-0.66032500	-0.05150600
C	2.48583700	2.71256800	-0.20700700
C	1.98157600	3.99647600	-0.30176900
C	0.59146200	4.19756000	-0.29182600
C	-0.26337100	3.11718400	-0.17793600
C	-2.41582000	-0.87383300	-0.03112200
C	-3.69638800	-1.45298500	-0.04003500
C	-3.78033600	-2.86195200	-0.19541500
C	-2.62160500	-3.60725100	-0.32638100
C	-1.33691100	-3.00616200	-0.29081000
C	-1.21880100	-1.63152700	-0.12498100
C	-2.13041300	0.51864000	0.08187000
C	-3.23955400	1.34167600	0.27452300
C	-4.55526800	0.78351800	0.27246700
C	-4.79409200	-0.56171500	0.11270800
O	-3.11910700	2.68448100	0.48960500
C	5.51557600	-1.48829600	0.20155300
N	6.66689000	-1.65429600	0.25778900
H	4.27283800	0.82380800	0.06472800
H	1.21011900	-3.05140600	0.14270900
H	3.62555800	-3.40657500	0.23226800
H	3.56062700	2.58303200	-0.23825700
H	2.66007800	4.83937500	-0.39335900
H	0.18312400	5.20019700	-0.37963100
H	-1.32747000	3.28765400	-0.17811800
H	-4.75254400	-3.34685000	-0.21565300

H	-2.68773900	-4.68309600	-0.45766600
H	-0.47771000	-3.65333400	-0.41315500
H	-5.39402200	1.46394500	0.40763200
H	-5.81293500	-0.93870000	0.11416900
H	-3.99378100	3.07895700	0.60702300

Optimized structure for 2c (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	-4.08679300	-1.30250900	-0.00000300
C	-3.55965300	-0.00936500	0.00000000
C	-2.17268100	0.22798600	0.00000100
C	-1.27999600	-0.89640800	-0.00000100
C	-1.84998100	-2.20141400	-0.00000500
C	-3.21070100	-2.41460400	-0.00000600
C	-1.62867100	1.58591900	0.00000300
C	-0.21101100	1.79261600	0.00000100
C	0.67849400	0.64652400	-0.00000100
C	0.13470000	-0.66951700	0.00000100
C	-2.47528200	2.72107900	0.00000700
C	-1.97111200	4.01141200	0.00000800
C	-0.58021900	4.21251900	0.00000600
C	0.27743800	3.12484800	0.00000200
C	2.43308000	-0.83967500	0.00000000
C	3.72097700	-1.41570800	0.00000000
C	3.82094500	-2.81967800	0.00000500
C	2.66277800	-3.60157900	0.00000800
C	1.37996200	-3.01915400	0.00000700
C	1.24214400	-1.62414700	0.00000200
C	2.13868700	0.55390200	-0.00000300
C	3.25245900	1.47709200	-0.00000600
C	4.58893100	0.85132400	-0.00000600
C	4.82340400	-0.49266900	-0.00000300
O	3.20021900	2.74623900	-0.00001000
C	-5.50217500	-1.49828500	-0.00000400
N	-6.65711800	-1.66531500	-0.00000400
H	-4.25670400	0.81841100	0.00000200
H	-1.20280100	-3.06475100	-0.00000900
H	-3.61054200	-3.42307900	-0.00001000
H	-3.55152300	2.59683800	0.00000900

H	-2.65230900	4.85769700	0.00001100
H	-0.17391300	5.22053600	0.00000700
H	1.35388100	3.26625500	0.00000000
H	4.80023200	-3.29276500	0.00000500
H	2.74651100	-4.68476400	0.00001200
H	0.52936100	-3.68957400	0.00001100
H	5.41878100	1.55382300	-0.00000800
H	5.84273500	-0.87438800	-0.00000300

Optimized structure for 2c (anion, B3LYP/6-31+G(d,p))

C	4.09594400	-1.29351400	0.00000700
C	3.55724300	-0.00364400	-0.00000200
C	2.17138500	0.23160100	-0.00000300
C	1.27914300	-0.89569700	0.00000300
C	1.85805800	-2.19802600	0.00001700
C	3.21924900	-2.40553300	0.00001900
C	1.62209400	1.58788900	-0.00000800
C	0.20412300	1.79002600	-0.00000100
C	-0.68209700	0.64206600	0.00000300
C	-0.13232300	-0.67567000	-0.00000100
C	2.46347900	2.72608600	-0.00001800
C	1.95364400	4.01390900	-0.00001900
C	0.56238700	4.20860100	-0.00001000
C	-0.29215300	3.11912900	-0.00000100
C	-2.42875800	-0.84399000	0.00000100
C	-3.71637900	-1.42030300	-0.00000100
C	-3.81554400	-2.82183500	-0.00001300
C	-2.65746000	-3.60602800	-0.00002400
C	-1.37627100	-3.02405100	-0.00002100
C	-1.23729200	-1.62925600	-0.00000600
C	-2.13415000	0.54776400	0.00000700
C	-3.24916000	1.47902300	0.00001500
C	-4.58915000	0.84709600	0.00001500
C	-4.81976600	-0.49481500	0.00000700
O	-3.20058400	2.73748600	0.00002200
C	5.51190800	-1.48564400	0.00000700
N	6.66762900	-1.65164900	0.00000700
H	4.25080200	0.82772000	-0.00000800

H	1.21013100	-3.06140100	0.00003100
H	3.62414100	-3.41280000	0.00003000
H	3.54067900	2.60423300	-0.00002500
H	2.63225900	4.86357800	-0.00002700
H	0.14936000	5.21437300	-0.00001000
H	-1.37034900	3.25725700	0.00000600
H	-4.79583700	-3.29495000	-0.00001500
H	-2.74268200	-4.68990800	-0.00003600
H	-0.52329300	-3.69261000	-0.00003400
H	-5.41384800	1.55537700	0.00002100
H	-5.83901900	-0.88030400	0.00000700

Optimized structure for 3a (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	-3.86417800	-1.91478600	0.00001300
C	-3.57568600	-0.56030700	0.00001000
C	-2.24276700	-0.09010000	0.00000600
C	-1.17601800	-1.04636800	0.00000500
C	-1.51162900	-2.42364700	0.00000700
C	-2.82157400	-2.86130800	0.00001100
C	-1.93670500	1.33838600	0.00000200
C	-0.57357600	1.77886900	-0.00000400
C	0.47608000	0.79400100	-0.00000500
C	0.18236000	-0.57496300	0.00000200
C	-2.95902100	2.31937100	0.00000400
C	-2.67333300	3.67368600	0.00000000
C	-1.33405700	4.10533500	-0.00000600
C	-0.31219900	3.17379900	-0.00000800
C	2.49003200	-0.35362400	-0.00000500
C	3.86301100	-0.64850300	-0.00000700
C	4.22225100	-2.02749500	0.00000000
C	3.23113700	-2.99325900	0.00001000
C	1.84537400	-2.66398300	0.00001100
C	1.45926700	-1.33140300	0.00000300
C	1.95005800	0.96112200	-0.00001100
C	2.84995900	2.01709200	-0.00002000
C	4.24935200	1.74808100	-0.00002300
C	4.75754500	0.46139700	-0.00001700
O	-5.18433900	-2.28453900	0.00001800

H	2.54139300	3.05495000	-0.00002500
H	-4.41316600	0.12558600	0.00001100
H	-0.72881300	-3.16772600	0.00000400
H	-3.04405400	-3.92498200	0.00001100
H	-3.99915900	2.01708600	0.00000800
H	-3.48255300	4.39764300	0.00000100
H	-1.10018300	5.16580000	-0.00000900
H	0.70911500	3.52550400	-0.00001200
H	5.26982700	-2.31572600	-0.00000100
H	3.50937500	-4.04300200	0.00001600
H	1.13785900	-3.48360400	0.00002000
H	4.93356000	2.59146100	-0.00003000
H	5.83103100	0.29387300	-0.00001900
H	-5.26362400	-3.24892100	0.00002000

Optimized structure for 3a (neutral, B3LYP/6-31+G(d,p))

C	3.86304000	-1.91399400	0.00011200
C	3.57415700	-0.56087800	0.00005100
C	2.24222500	-0.09079100	0.00000300
C	1.17514900	-1.04637900	0.00000600
C	1.51029900	-2.42256700	0.00010200
C	2.82051100	-2.85911700	0.00015000
C	1.93637200	1.33692400	-0.00004500
C	0.57411300	1.77727300	-0.00003300
C	-0.47520700	0.79311200	0.00002000
C	-0.18246300	-0.57485900	-0.00003500
C	2.95798100	2.31727100	-0.00010700
C	2.67350100	3.67088400	-0.00016600
C	1.33516600	4.10252200	-0.00018300
C	0.31391900	3.17160200	-0.00012200
C	-2.49014300	-0.35313400	0.00000500
C	-3.86247700	-0.64708600	0.00001200
C	-4.22195200	-2.02519900	-0.00014300
C	-3.23221400	-2.99089700	-0.00029400
C	-1.84709300	-2.66170100	-0.00027800
C	-1.45960200	-1.33056000	-0.00010300
C	-1.94898600	0.96056900	0.00010100
C	-2.84820900	2.01569300	0.00027800

C	-4.24723300	1.74838100	0.00030900
C	-4.75568800	0.46296500	0.00017000
O	5.18397800	-2.28338900	0.00014900
H	-2.53677800	3.05277600	0.00041300
H	4.41361500	0.12209600	0.00004900
H	0.72546100	-3.16460200	0.00017100
H	3.04311700	-3.92388300	0.00023200
H	3.99752000	2.01298500	-0.00011500
H	3.48311400	4.39457700	-0.00021300
H	1.10179600	5.16327700	-0.00025500
H	-0.70792800	3.52177000	-0.00017300
H	-5.26987800	-2.31308000	-0.00015000
H	-3.51168500	-4.04056200	-0.00042900
H	-1.13826700	-3.48050800	-0.00042700
H	-4.93143100	2.59207100	0.00044600
H	-5.82954800	0.29641600	0.00018900
H	5.25807900	-3.24643700	0.00020400

Optimized structure for 3a (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	-3.92334800	-2.04316700	0.00000300
C	-3.59607200	-0.65398900	0.00000200
C	-2.28240600	-0.15775500	0.00000100
C	-1.17933900	-1.08634900	0.00000100
C	-1.49512600	-2.47629000	0.00000300
C	-2.78838800	-2.94045600	0.00000400
C	-1.99389900	1.28214000	0.00000000
C	-0.63845700	1.75342200	-0.00000100
C	0.43246300	0.79477900	0.00000000
C	0.15668900	-0.58510800	0.00000000
C	-3.03298600	2.24441100	-0.00000100
C	-2.78052900	3.60709700	-0.00000200
C	-1.45098100	4.06744200	-0.00000200
C	-0.40999500	3.15583300	-0.00000200
C	2.46696400	-0.31790900	-0.00000100
C	3.84563900	-0.58540600	-0.00000100
C	4.23101500	-1.95720700	-0.00000200
C	3.25895200	-2.94262600	-0.00000300
C	1.86714600	-2.64039100	-0.00000200

C	1.45473200	-1.31540600	-0.00000100
C	1.89643000	0.98849300	0.00000000
C	2.78062100	2.06026900	0.00000000
C	4.18580200	1.81669400	0.00000000
C	4.72173100	0.54183800	-0.00000100
O	-5.13164600	-2.48029700	0.00000300
H	-4.44198000	0.02502700	0.00000100
H	-0.69285100	-3.20209300	0.00000400
H	-2.98650100	-4.01015100	0.00000600
H	-4.06527900	1.91541500	-0.00000100
H	-3.60674300	4.31227800	-0.00000200
H	-1.23826100	5.13292300	-0.00000300
H	0.60439900	3.52918300	-0.00000200
H	5.28436300	-2.22499400	-0.00000200
H	3.55823300	-3.98693200	-0.00000300
H	1.17355000	-3.47168200	-0.00000300
H	2.45266500	3.09247600	0.00000000
H	4.85327300	2.67414600	0.00000000
H	5.79834300	0.39462700	-0.00000100

Optimized structure for 3a (anion, B3LYP/6-31+G(d,p))

C	3.92305900	-2.05323600	0.00000600
C	3.58950000	-0.65312900	0.00000700
C	2.28586600	-0.15829800	0.00000200
C	1.17334700	-1.08825100	-0.00000200
C	1.48901800	-2.48302500	-0.00000400
C	2.77560800	-2.95001700	0.00000000
C	1.99293900	1.28401900	0.00000000
C	0.63744600	1.75646400	-0.00000200
C	-0.43296300	0.80041200	0.00000000
C	-0.15059500	-0.58599200	-0.00000300
C	3.03062700	2.24365700	-0.00000200
C	2.78387200	3.60840000	-0.00000600
C	1.45631400	4.07012400	-0.00000900
C	0.41392300	3.15953000	-0.00000700
C	-2.46384800	-0.31745500	-0.00000100
C	-3.84281400	-0.58292300	0.00000100
C	-4.22760400	-1.95353400	-0.00000400

C	-3.25650300	-2.94023500	-0.00000800
C	-1.86623800	-2.63963400	-0.00000800
C	-1.45212300	-1.31477300	-0.00000500
C	-1.88612100	0.99051800	0.00000300
C	-2.77618500	2.06236900	0.00001100
C	-4.17898900	1.81780600	0.00001300
C	-4.71996600	0.54498400	0.00000700
O	5.11125500	-2.48546100	0.00001000
H	4.44343600	0.01513700	0.00001100
H	0.68175600	-3.20383000	-0.00000800
H	2.98158100	-4.01803500	-0.00000100
H	4.06043000	1.90655900	-0.00000100
H	3.61331900	4.31099600	-0.00000700
H	1.24385500	5.13679600	-0.00001300
H	-0.60088000	3.53296300	-0.00001200
H	-5.28225000	-2.22033400	-0.00000300
H	-3.55805900	-3.98496400	-0.00001100
H	-1.16894500	-3.46771400	-0.00001100
H	-2.44559200	3.09386800	0.00001800
H	-4.84674400	2.67673900	0.00001900
H	-5.79737400	0.39882400	0.00000800

Optimized structure for 3b (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.56613000	-1.06231900	0.24517900
C	3.93711500	0.16638000	0.13689100
C	2.53167500	0.26660500	0.01970100
C	1.75193100	-0.93127600	0.02114700
C	2.43087800	-2.16948700	0.14738800
C	3.80639600	-2.24709000	0.25368500
C	1.86203900	1.55724100	-0.11081300
C	0.42900900	1.63303900	-0.12916900
C	-0.34001300	0.40974200	-0.03266700
C	0.31767900	-0.83175500	-0.05586900
C	2.60521000	2.75591100	-0.24544600
C	1.99210900	3.98611000	-0.40489600
C	0.58883400	4.05870100	-0.44525200
C	-0.16763600	2.90793700	-0.31175300
C	-1.95687900	-1.25751300	-0.08397900

C	-3.17784100	-1.95518900	-0.10910800
C	-3.12575100	-3.36909900	-0.23966700
C	-1.89865500	-4.00563600	-0.32679500
C	-0.67541400	-3.28636200	-0.27172400
C	-0.69048800	-1.90291900	-0.13506300
C	-1.80815500	0.15434500	0.01265200
C	-2.99432300	0.88164000	0.18684300
C	-4.25309600	0.19942700	0.15894400
C	-4.35475100	-1.16673300	0.00576100
O	5.93389300	-1.07256400	0.35468900
O	-2.94212300	2.22096100	0.40615000
C	-4.14286900	2.97901600	0.60007100
H	4.56397200	1.04875100	0.15626800
H	1.86881100	-3.09043000	0.19040300
H	4.29461500	-3.21252700	0.35649900
H	3.68772900	2.72145800	-0.24233300
H	2.59481500	4.88331500	-0.51052000
H	0.09398400	5.01519600	-0.58801000
H	-1.24339700	2.97561200	-0.34816000
H	-4.04772200	-3.94313100	-0.27325800
H	-1.86046300	-5.08530700	-0.43615700
H	0.24210000	-3.85516400	-0.35308300
H	-5.16244100	0.77632900	0.26650700
H	-5.33415600	-1.63645200	-0.01241100
H	6.25594700	-1.98142500	0.43512800
H	-3.81063000	4.00548000	0.75448200
H	-4.78815200	2.93247100	-0.28271900
H	-4.68798000	2.63435800	1.48429000

Optimized structure for 3b (neutral, B3LYP/6-31+G(d,p))

C	4.55877400	-1.07033300	0.26064900
C	3.93432900	0.15802900	0.13768900
C	2.53064500	0.26202400	0.01674200
C	1.74738000	-0.93311600	0.02647600
C	2.41969600	-2.17122200	0.17304700
C	3.79456100	-2.25105700	0.28444500
C	1.86484200	1.55275300	-0.12275300
C	0.43283100	1.63297100	-0.13886200

C	-0.33801700	0.41239800	-0.03827100
C	0.31523500	-0.82919500	-0.05895500
C	2.61084700	2.74739800	-0.26596700
C	2.00168900	3.97772900	-0.43061100
C	0.59943700	4.05425600	-0.46740900
C	-0.16019700	2.90771200	-0.32597200
C	-1.95999700	-1.25195700	-0.09063100
C	-3.18080800	-1.94784200	-0.11628600
C	-3.13008700	-3.36130400	-0.25507900
C	-1.90530800	-3.99709900	-0.35047300
C	-0.68148900	-3.27839400	-0.29259800
C	-0.69458000	-1.89813100	-0.14401100
C	-1.80724800	0.15909500	0.00870200
C	-2.99055700	0.88527500	0.18738400
C	-4.24974200	0.20623100	0.16342200
C	-4.35496900	-1.15923200	0.00564200
O	5.92705900	-1.08285000	0.37179200
O	-2.93716100	2.22970500	0.40338800
C	-4.12548800	2.97080900	0.66680900
H	4.56642500	1.03634700	0.15081900
H	1.85026300	-3.08699600	0.23344500
H	4.27871800	-3.21773900	0.40540100
H	3.69318500	2.70749800	-0.26617400
H	2.60688800	4.87255600	-0.54338000
H	0.10759800	5.01176000	-0.61507600
H	-1.23529000	2.97756400	-0.36175100
H	-4.05288000	-3.93436300	-0.28985200
H	-1.86854800	-5.07606600	-0.46903000
H	0.23746800	-3.84371900	-0.38476700
H	-5.15825600	0.78450200	0.27394100
H	-5.33539300	-1.62759800	-0.01190700
H	6.24135400	-1.99140600	0.46434800
H	-3.79370300	3.99486700	0.84290100
H	-4.80952800	2.95382300	-0.18967700
H	-4.63816000	2.59735000	1.56055100

Optimized structure for 3b (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.66075900	-1.13866800	0.27034100

C	3.97486400	0.10656100	0.15873700
C	2.57941100	0.22474000	0.03343400
C	1.76864400	-0.96186800	0.02528400
C	2.44177200	-2.21144600	0.15016900
C	3.80905100	-2.30688900	0.26438300
C	1.91447300	1.52438100	-0.10801600
C	0.48048000	1.62126300	-0.13101800
C	-0.30609500	0.41182400	-0.03167300
C	0.34527600	-0.83886000	-0.05161300
C	2.67013100	2.71442900	-0.24961900
C	2.07758400	3.95488100	-0.41766000
C	0.67509000	4.04698700	-0.46108500
C	-0.09602300	2.90580900	-0.32376300
C	-1.94244800	-1.23976600	-0.08594100
C	-3.17218800	-1.92248200	-0.11420800
C	-3.13495100	-3.33755900	-0.24821900
C	-1.91533700	-3.98715900	-0.33463400
C	-0.68300400	-3.28140800	-0.27526500
C	-0.68206300	-1.89905700	-0.13524300
C	-1.77411800	0.17212800	0.01276000
C	-2.95347300	0.90848700	0.18984900
C	-4.22007100	0.24302900	0.15830900
C	-4.34167200	-1.12205400	0.00038400
O	5.93966200	-1.23242400	0.38088200
O	-2.88416600	2.25238300	0.41882800
C	-4.07599500	3.01795900	0.61292500
H	4.60262300	0.99092500	0.18376600
H	1.86440600	-3.12536800	0.18783600
H	4.28193300	-3.28115600	0.36960500
H	3.75204700	2.65979300	-0.24442400
H	2.69452800	4.84229400	-0.52847400
H	0.19237100	5.00924700	-0.61076400
H	-1.17123500	2.98771400	-0.36414700
H	-4.06355800	-3.90123200	-0.28456800
H	-1.88904300	-5.06729300	-0.44625700
H	0.22952400	-3.85826200	-0.35436300
H	-5.12219100	0.83164400	0.26695200
H	-5.32671900	-1.57985900	-0.02134300

H	-3.73752100	4.04167500	0.77498400
H	-4.72159700	2.98406600	-0.27115900
H	-4.63010200	2.67457000	1.49297300

Optimized structure for 3b (anion, B3LYP/6-31+G(d,p))

C	4.65285000	-1.15498000	0.30909500
C	3.96278700	0.10078700	0.18301100
C	2.57989800	0.22276600	0.03990400
C	1.75804700	-0.96630800	0.02802400
C	2.42603500	-2.22208000	0.17206900
C	3.78560900	-2.32444900	0.30291600
C	1.91437600	1.52296600	-0.12407000
C	0.48106600	1.62552900	-0.15378700
C	-0.30802000	0.42080000	-0.04613200
C	0.34843000	-0.83515500	-0.06284500
C	2.67436100	2.70543400	-0.28203600
C	2.09072800	3.94785900	-0.46899800
C	0.68961800	4.04550600	-0.51729500
C	-0.08724700	2.90995000	-0.36749800
C	-1.94370900	-1.23380800	-0.09693600
C	-3.17583400	-1.91166600	-0.12609900
C	-3.13943300	-3.32615000	-0.27366100
C	-1.92206500	-3.97539200	-0.37417700
C	-0.68793000	-3.27286000	-0.31304300
C	-0.68455000	-1.89387700	-0.15356300
C	-1.76436000	0.18092000	0.00640000
C	-2.94603100	0.91226400	0.19544700
C	-4.21084200	0.25434500	0.16734500
C	-4.34378800	-1.11155100	-0.00082400
O	5.90876900	-1.25241200	0.43066500
O	-2.87062500	2.26705800	0.43122900
C	-4.04054000	3.00006700	0.73963900
H	4.60263600	0.97568100	0.21480900
H	1.83777900	-3.12931000	0.21969100
H	4.26164200	-3.29464800	0.42745800
H	3.75568300	2.63800300	-0.27560000
H	2.71414300	4.83003800	-0.59286400
H	0.21046700	5.00802400	-0.68418900

H	-1.16154800	2.99599000	-0.41765900
H	-4.06997200	-3.88843400	-0.31071600
H	-1.89868900	-5.05514100	-0.49934900
H	0.22687600	-3.84353400	-0.40838400
H	-5.11090000	0.84677800	0.28345900
H	-5.33105600	-1.56597000	-0.02245300
H	-3.70428600	4.01967100	0.94029100
H	-4.75046800	3.01569000	-0.09896900
H	-4.54419800	2.60449100	1.63200300

Optimized structure for 3c (neutral, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.32923500	-1.40999600	0.31195100
C	3.81333600	-0.12882700	0.20048200
C	2.42889800	0.09319000	0.03471600
C	1.54929300	-1.03696700	-0.00039800
C	2.11382800	-2.33218300	0.12109200
C	3.47212600	-2.52755200	0.27065000
C	1.88162100	1.43630300	-0.13143800
C	0.46371600	1.62934300	-0.20428400
C	-0.40026800	0.48306000	-0.06619600
C	0.13470200	-0.81125800	-0.09234900
C	2.72249500	2.56715600	-0.27179400
C	2.21224100	3.83159700	-0.51008100
C	0.82361200	4.00805700	-0.64711500
C	-0.02472700	2.92554100	-0.50200700
C	-2.17387200	-1.01659900	-0.10954600
C	-3.46143100	-1.57400900	-0.11791800
C	-3.55560400	-2.98716300	-0.27725900
C	-2.40212300	-3.74021200	-0.38721400
C	-1.10458000	-3.15446800	-0.32981700
C	-0.98076600	-1.78292600	-0.17969600
C	-1.87809800	0.37152200	0.02362300
C	-2.97350700	1.20475000	0.28631300
C	-4.30445900	0.65908700	0.27390900
C	-4.55333400	-0.67670500	0.05656500
O	5.68255400	-1.53807600	0.46939300
C	-2.90465700	2.57937900	0.68497800
N	-2.95252600	3.68111400	1.06150300

H	4.51271100	0.69595100	0.25123300
H	1.47267700	-3.20139200	0.12501600
H	3.87470200	-3.53201200	0.36927600
H	3.79791700	2.45024000	-0.21801400
H	2.88597100	4.67600100	-0.61884700
H	0.41562100	4.98669100	-0.88125300
H	-1.08304000	3.07481800	-0.65260000
H	-4.53094900	-3.46377700	-0.30802000
H	-2.47592100	-4.81619600	-0.51177100
H	-0.25127900	-3.81496800	-0.41569100
H	-5.12953200	1.33892000	0.45695200
H	-5.57400500	-1.04660300	0.05001100
H	5.92631800	-2.47158100	0.54504200

Optimized structure for 3c (neutral, B3LYP/6-31+G(d,p))

C	4.33678800	-1.39641800	0.29799600
C	3.81761400	-0.11866700	0.17915400
C	2.43187600	0.10067100	0.02589000
C	1.55401000	-1.03015300	0.00688800
C	2.11983800	-2.32199500	0.14345400
C	3.47998600	-2.51357100	0.28241400
C	1.87972700	1.44148900	-0.13434400
C	0.46084400	1.63374000	-0.18845000
C	-0.40083800	0.48417700	-0.05678400
C	0.13922600	-0.80710300	-0.08409800
C	2.71768700	2.57287800	-0.27772900
C	2.20439200	3.83936000	-0.49192600
C	0.81457500	4.01807900	-0.59758500
C	-0.03100300	2.93418800	-0.45562500
C	-2.16729400	-1.02720400	-0.09762400
C	-3.44936900	-1.59579600	-0.10887000
C	-3.53265100	-3.00800700	-0.27354200
C	-2.37464100	-3.75151400	-0.39297300
C	-1.08327300	-3.15504200	-0.33676000
C	-0.96910000	-1.78444700	-0.17305200
C	-1.88115700	0.36431900	0.03123900
C	-2.98358000	1.19135200	0.28047300
C	-4.30881600	0.63112600	0.27151200

C	-4.54779800	-0.70679800	0.06372700
O	5.69323500	-1.52001400	0.44072800
C	-2.94195900	2.57863300	0.64063600
N	-3.02515000	3.69168600	0.97362800
H	4.51813900	0.70529600	0.21800000
H	1.47651200	-3.18940200	0.17359500
H	3.88332500	-3.51732900	0.39533400
H	3.79370100	2.45378200	-0.24265500
H	2.87660100	4.68520500	-0.60071100
H	0.39976200	5.00071600	-0.80024700
H	-1.09136100	3.09163700	-0.57338400
H	-4.50464300	-3.49221900	-0.30410700
H	-2.44139600	-4.82727100	-0.52621900
H	-0.22278300	-3.80436900	-0.43854500
H	-5.13768300	1.30846100	0.44772100
H	-5.56595700	-1.08481700	0.05858400
H	5.93545500	-2.45116800	0.52729300

Optimized structure for 3c (anion, B3LYP/CPCM(DCM)/6-31+G(d,p))

C	4.39943900	-1.51965600	0.34659300
C	3.83667600	-0.20940700	0.22978700
C	2.47188700	0.03739100	0.04885000
C	1.55358200	-1.07683700	-0.00261400
C	2.10473700	-2.38962500	0.11523900
C	3.44799900	-2.61102000	0.27801500
C	1.93781000	1.39361500	-0.12975600
C	0.52314700	1.61567600	-0.20140800
C	-0.36665900	0.48850100	-0.06527900
C	0.16043200	-0.82276400	-0.09358300
C	2.79888500	2.50637600	-0.28227800
C	2.31893500	3.78389600	-0.52434500
C	0.93403400	3.98948900	-0.65291400
C	0.06424000	2.92332800	-0.50115200
C	-2.15560000	-0.99052800	-0.10271100
C	-3.45241500	-1.52327200	-0.11606100
C	-3.57117400	-2.93258000	-0.27840300
C	-2.43122100	-3.70833200	-0.39294800
C	-1.12520500	-3.14657700	-0.33754700

C	-0.97744700	-1.77656900	-0.17975200
C	-1.82858000	0.39948900	0.02811900
C	-2.91865800	1.25113500	0.28509800
C	-4.26073300	0.72352000	0.26660800
C	-4.53456300	-0.60513500	0.05236700
O	5.65155700	-1.72799100	0.50715800
C	-2.83192600	2.61930400	0.68835800
N	-2.86452300	3.72198700	1.06943700
H	4.54391400	0.61062100	0.29106300
H	1.44251100	-3.24489100	0.10699900
H	3.83086900	-3.62400600	0.37785800
H	3.87146300	2.36069400	-0.23451100
H	3.01215500	4.61175400	-0.64172300
H	0.54390800	4.97593000	-0.88732800
H	-0.99211000	3.09511100	-0.64577600
H	-4.55538300	-3.39154900	-0.30975000
H	-2.52617500	-4.78248900	-0.52182500
H	-0.28193300	-3.81860700	-0.43156800
H	-5.07460700	1.41948400	0.44259200
H	-5.56112900	-0.95854000	0.04095600

Optimized structure for 3c (anion, B3LYP/6-31+G(d,p))

C	4.42005000	-1.49155300	0.32605100
C	3.83991500	-0.17651800	0.20539900
C	2.48034400	0.06093300	0.04277600
C	1.56191400	-1.06223200	0.01011600
C	2.12234700	-2.37548000	0.14266100
C	3.46291900	-2.59142200	0.28945800
C	1.92855400	1.41405800	-0.13063200
C	0.51209800	1.62902100	-0.17720800
C	-0.37260800	0.49438300	-0.05064600
C	0.17741900	-0.81734200	-0.08051300
C	2.78117800	2.52908500	-0.29203600
C	2.29433100	3.80955200	-0.50505100
C	0.90754900	4.01301800	-0.58861100
C	0.04484600	2.94107900	-0.43667900
C	-2.13529600	-1.01454000	-0.08177100
C	-3.42361900	-1.56704600	-0.10576000

C	-3.52107400	-2.97470100	-0.27391300
C	-2.37065500	-3.73594900	-0.39761700
C	-1.07660200	-3.15591700	-0.34294000
C	-0.94862200	-1.78430600	-0.16600000
C	-1.82209300	0.38720200	0.04035700
C	-2.93619000	1.22701300	0.27209200
C	-4.26583600	0.66937900	0.24935900
C	-4.52287300	-0.66360000	0.05014100
O	5.65728800	-1.68989600	0.46367600
C	-2.90428100	2.60845600	0.63255100
N	-3.00708300	3.72381700	0.96430400
H	4.55155100	0.63992500	0.25392100
H	1.45760000	-3.22888400	0.16651100
H	3.85974200	-3.59710100	0.40494700
H	3.85430600	2.38028600	-0.26996300
H	2.98415100	4.64069100	-0.62673500
H	0.50403800	5.00335300	-0.78279800
H	-1.01496900	3.11874800	-0.53631000
H	-4.50018100	-3.44673800	-0.30785700
H	-2.45251100	-4.81085600	-0.53748200
H	-0.21971100	-3.80724200	-0.45771900
H	-5.09045700	1.35773200	0.40936300
H	-5.54456900	-1.03289900	0.03510300

Input geometry for NICS(1) calculation of 2a (neutral)

C	3.93450000	-2.67790000	0.22490000
C	3.81670000	-1.30290000	0.13160000
C	2.55600000	-0.66300000	0.04280000
C	1.38240000	-1.47740000	0.04920000
C	1.53280000	-2.88340000	0.16360000
C	2.77800000	-3.47720000	0.24650000
C	2.42880000	0.78660000	-0.05240000
C	1.13390000	1.40290000	-0.04750000
C	-0.03770000	0.55860000	0.02320000
C	0.09440000	-0.83750000	-0.01640000
C	3.56960000	1.61810000	-0.16450000
C	3.46770000	2.99270000	-0.27380000
C	2.19820000	3.59450000	-0.28220000

C	1.06260000	2.81380000	-0.17310000
C	-2.17210000	-0.36670000	-0.03640000
C	-3.56570000	-0.54600000	-0.06410000
C	-4.05610000	-1.87130000	-0.20780000
C	-3.16420000	-2.92420000	-0.30980000
C	-1.75990000	-2.72450000	-0.25590000
C	-1.24680000	-1.44270000	-0.10070000
C	-1.49210000	0.88220000	0.06850000
C	-2.31440000	1.99540000	0.23060000
C	-3.73620000	1.84750000	0.20880000
C	-4.35720000	0.62940000	0.05830000
H	4.91770000	-3.13380000	0.29490000
O	-1.81070000	3.25000000	0.43440000
H	4.72340000	-0.71060000	0.14050000
H	0.65560000	-3.51090000	0.21920000
H	2.85890000	-4.55630000	0.34080000
H	4.55790000	1.17560000	-0.18050000
H	4.36540000	3.59770000	-0.36210000
H	2.10360000	4.67220000	-0.38060000
H	0.09570000	3.28970000	-0.18770000
H	-5.12740000	-2.05080000	-0.24180000
H	-3.54010000	-3.93570000	-0.43210000
H	-1.12500000	-3.59550000	-0.35530000
H	-4.34020000	2.74620000	0.32060000
H	-5.44170000	0.56730000	0.04360000
H	-2.53550000	3.88280000	0.52570000
Bq	2.66670000	-2.08030000	0.14310000
Bq	2.63090000	-2.01250000	1.14020000
Bq	2.70260000	-2.14810000	-0.85400000
Bq	1.25960000	-0.03830000	-0.00020000
Bq	2.31010000	2.20140000	-0.16560000
Bq	-0.97090000	-0.24120000	-0.01240000
Bq	-2.66080000	-1.64590000	-0.16250000
Bq	-2.93960000	0.74030000	0.07760000
Bq	1.27990000	-0.00370000	0.99900000
Bq	1.23940000	-0.07290000	-0.99940000
Bq	2.34650000	2.28770000	0.83000000
Bq	2.27380000	2.11520000	-1.16120000

Bq	-0.95900000	-0.16400000	-1.00930000
Bq	-0.98270000	-0.31850000	0.98460000
Bq	-2.64490000	-1.54390000	-1.15710000
Bq	-2.67670000	-1.74790000	0.83220000
Bq	-2.93550000	0.86090000	-0.91510000
Bq	-2.94370000	0.61970000	1.07030000

Input geometry for NICS(1) calculation of 2a (anion)

C	3.93790000	-2.68350000	0.00000000
C	3.80560000	-1.30370000	0.00000000
C	2.54390000	-0.66330000	0.00000000
C	1.36370000	-1.47700000	0.00000000
C	1.53240000	-2.88880000	0.00000000
C	2.78150000	-3.48350000	0.00000000
C	2.41520000	0.79290000	0.00000000
C	1.11880000	1.40450000	0.00000000
C	-0.06510000	0.56880000	0.00000000
C	0.07190000	-0.84650000	0.00000000
C	3.55360000	1.63590000	0.00000000
C	3.44550000	3.01680000	0.00000000
C	2.17220000	3.61210000	0.00000000
C	1.03550000	2.82140000	0.00000000
C	-2.17570000	-0.33090000	0.00000000
C	-3.57640000	-0.50660000	0.00000000
C	-4.08110000	-1.81840000	0.00000000
C	-3.20290000	-2.90690000	0.00000000
C	-1.80650000	-2.72460000	0.00000000
C	-1.26430000	-1.43240000	0.00000000
C	-1.48730000	0.91050000	0.00000000
C	-2.27630000	2.12650000	0.00000000
C	-3.74290000	1.91590000	0.00000000
C	-4.35950000	0.70080000	0.00000000
O	-1.86120000	3.31830000	0.00000000
H	4.92570000	-3.13720000	0.00000000
H	4.70990000	-0.70570000	0.00000000
H	0.65840000	-3.52330000	0.00000000
H	2.86340000	-4.56810000	0.00000000
H	4.54680000	1.20090000	0.00000000

H	4.34400000	3.63000000	0.00000000
H	2.07280000	4.69510000	0.00000000
H	0.04480000	3.26990000	0.00000000
H	-5.15720000	-1.98400000	0.00000000
H	-3.60120000	-3.91890000	0.00000000
H	-1.18560000	-3.61300000	0.00000000
H	-4.32310000	2.83560000	0.00000000
H	-5.44740000	0.63230000	0.00000000
Bq	2.66080000	-2.08330000	0.00000000
Bq	1.24140000	-0.03680000	0.00000000
Bq	2.29010000	2.21390000	0.00000000
Bq	-0.98410000	-0.22610000	0.00000000
Bq	-2.68450000	-1.62000000	0.00000000
Bq	-2.93640000	0.80270000	0.00000000
Bq	2.66080000	-2.08330000	-1.00000000
Bq	2.66080000	-2.08330000	-1.00000000
Bq	2.66080000	-2.08330000	1.00000000
Bq	1.24140000	-0.03680000	-1.00000000
Bq	1.24140000	-0.03680000	1.00000000
Bq	2.29010000	2.21390000	-1.00000000
Bq	2.29010000	2.21390000	1.00000000
Bq	-0.98410000	-0.22610000	-1.00000000
Bq	-0.98410000	-0.22610000	1.00000000
Bq	-2.68450000	-1.62000000	-1.00000000
Bq	-2.68450000	-1.62000000	1.00000000
Bq	-2.93640000	0.80270000	-1.00000000
Bq	-2.93640000	0.80270000	1.00000000

Input geometry for NICS(1) calculation of 2b (neutral)

C	4.09590000	-0.81730000	0.10110000
C	3.45110000	0.41060000	0.03840000
C	2.04700000	0.51240000	-0.02090000
C	1.27040000	-0.68870000	-0.01630000
C	1.95650000	-1.92190000	0.06680000
C	3.33770000	-2.00360000	0.12190000
C	1.37030000	1.80490000	-0.08790000
C	-0.06120000	1.87620000	-0.05830000
C	-0.82110000	0.64680000	0.01270000

C	-0.16510000	-0.59070000	-0.05020000
C	2.10440000	3.00970000	-0.19740000
C	1.48300000	4.24260000	-0.28130000
C	0.08040000	4.31150000	-0.26550000
C	-0.66830000	3.15370000	-0.15830000
C	-2.43930000	-1.02550000	-0.03110000
C	-3.65750000	-1.72580000	-0.04150000
C	-3.60390000	-3.13690000	-0.19450000
C	-2.37820000	-3.76640000	-0.32170000
C	-1.15750000	-3.04300000	-0.28590000
C	-1.17320000	-1.66350000	-0.12320000
C	-2.28750000	0.38810000	0.08070000
C	-3.47120000	1.09890000	0.26730000
C	-4.72800000	0.41680000	0.26280000
C	-4.83760000	-0.94520000	0.10640000
O	-3.48430000	2.45030000	0.47890000
O	5.46350000	-0.77670000	0.15270000
C	6.18020000	-2.00220000	0.22920000
H	4.08080000	1.29080000	0.04900000
H	1.39600000	-2.84360000	0.11950000
H	3.81140000	-2.97530000	0.19330000
H	3.18650000	2.97800000	-0.23100000
H	2.07940000	5.14620000	-0.36820000
H	-0.42180000	5.27170000	-0.34350000
H	-1.74390000	3.22350000	-0.15380000
H	-4.52470000	-3.71380000	-0.21540000
H	-2.33960000	-4.84410000	-0.45050000
H	-0.23860000	-3.60310000	-0.40430000
H	-5.62830000	1.01480000	0.39350000
H	-5.81540000	-1.41860000	0.10580000
H	-4.39500000	2.75540000	0.58580000
H	7.23550000	-1.72730000	0.25460000
H	5.92910000	-2.55860000	1.14110000
H	5.99150000	-2.63360000	-0.64830000
Bq	2.69310000	-0.75140000	0.04850000
Bq	0.60670000	0.59350000	-0.03680000
Bq	0.71810000	3.06640000	-0.17480000
Bq	-1.37720000	-0.44900000	-0.02220000

Bq	-3.57020000	-0.29880000	0.10740000
Bq	-2.40160000	-2.39350000	-0.16630000
Bq	2.73720000	-0.78370000	-0.95000000
Bq	2.64900000	-0.71910000	1.04700000
Bq	0.57080000	0.55800000	-1.03550000
Bq	0.64270000	0.62890000	0.96190000
Bq	0.70110000	2.98510000	-1.17130000
Bq	0.73510000	3.14770000	0.82180000
Bq	-1.43410000	-0.38830000	-1.01880000
Bq	-1.32030000	-0.50960000	0.97430000
Bq	-2.44890000	-2.29660000	-1.16050000
Bq	-2.35430000	-2.49050000	0.82780000
Bq	-3.62990000	-0.18020000	-0.88370000
Bq	-3.51050000	-0.41740000	1.09860000

Input geometry for NICS(1) calculation of 2b (anion)

C	4.08950000	-0.81540000	0.00000000
C	3.43790000	0.40870000	0.00000000
C	2.03070000	0.50950000	0.00000000
C	1.25090000	-0.69360000	0.00000000
C	1.95210000	-1.92300000	0.00000000
C	3.33810000	-2.00220000	0.00000000
C	1.35220000	1.80530000	0.00000000
C	-0.07980000	1.87100000	0.00000000
C	-0.85400000	0.64560000	0.00000000
C	-0.18640000	-0.60700000	0.00000000
C	2.08100000	3.01910000	0.00000000
C	1.45180000	4.25330000	0.00000000
C	0.04750000	4.31380000	0.00000000
C	-0.69960000	3.14780000	0.00000000
C	-2.45950000	-0.99340000	0.00000000
C	-3.68490000	-1.69450000	0.00000000
C	-3.64580000	-3.09950000	0.00000000
C	-2.41630000	-3.76700000	0.00000000
C	-1.19740000	-3.06160000	0.00000000
C	-1.19410000	-1.66040000	0.00000000
C	-2.30060000	0.41610000	0.00000000
C	-3.49480000	1.23610000	0.00000000

C	-4.76830000	0.47830000	0.00000000
C	-4.87180000	-0.88060000	0.00000000
O	-3.56860000	2.49640000	0.00000000
O	5.47430000	-0.77040000	0.00000000
C	6.17720000	-1.99710000	0.00000000
H	4.06260000	1.29350000	0.00000000
H	1.39600000	-2.84910000	0.00000000
H	3.81380000	-2.97660000	0.00000000
H	3.16500000	2.99670000	0.00000000
H	2.04620000	5.16420000	0.00000000
H	-0.45990000	5.27580000	0.00000000
H	-1.78680000	3.18190000	0.00000000
H	-4.57540000	-3.66650000	0.00000000
H	-2.39530000	-4.85440000	0.00000000
H	-0.28210000	-3.64280000	0.00000000
H	-5.65720000	1.10480000	0.00000000
H	-5.85010000	-1.36130000	0.00000000
H	7.23840000	-1.73780000	0.00000000
H	5.95340000	-2.59610000	0.89410000
H	5.95340000	-2.59610000	-0.89410000
Bq	2.68320000	-0.75270000	0.00000000
Bq	0.58560000	0.58850000	0.00000000
Bq	0.69220000	3.06840000	0.00000000
Bq	-1.39890000	-0.43980000	0.00000000
Bq	-2.43300000	-2.37940000	0.00000000
Bq	-3.59660000	-0.23970000	0.00000000
Bq	2.68320000	-0.75270000	1.00000000
Bq	2.68320000	-0.75270000	-1.00000000
Bq	0.58560000	0.58850000	-1.00000000
Bq	0.58560000	0.58850000	1.00000000
Bq	0.69220000	3.06840000	-1.00000000
Bq	0.69220000	3.06840000	1.00000000
Bq	-1.39890000	-0.43980000	-1.00000000
Bq	-1.39890000	-0.43980000	1.00000000
Bq	-2.43300000	-2.37940000	-1.00000000
Bq	-2.43300000	-2.37940000	1.00000000
Bq	-3.59660000	-0.23970000	-1.00000000
Bq	-3.59660000	-0.23970000	1.00000000

Input geometry for NICS(1) calculation of 2c (neutral)

C	4.09710000	-1.29150000	0.13100000
C	3.57550000	-0.00330000	0.05610000
C	2.18620000	0.23270000	-0.01370000
C	1.30330000	-0.89170000	-0.00730000
C	1.86260000	-2.19310000	0.08830000
C	3.22260000	-2.40270000	0.15270000
C	1.64050000	1.58330000	-0.09140000
C	0.22200000	1.78970000	-0.06600000
C	-0.64830000	0.63740000	0.01020000
C	-0.11370000	-0.66030000	-0.05150000
C	2.48580000	2.71260000	-0.20700000
C	1.98160000	3.99650000	-0.30180000
C	0.59150000	4.19760000	-0.29180000
C	-0.26340000	3.11720000	-0.17790000
C	-2.41580000	-0.87380000	-0.03110000
C	-3.69640000	-1.45300000	-0.04000000
C	-3.78030000	-2.86200000	-0.19540000
C	-2.62160000	-3.60730000	-0.32640000
C	-1.33690000	-3.00620000	-0.29080000
C	-1.21880000	-1.63150000	-0.12500000
C	-2.13040000	0.51860000	0.08190000
C	-3.23960000	1.34170000	0.27450000
C	-4.55530000	0.78350000	0.27250000
C	-4.79410000	-0.56170000	0.11270000
O	-3.11910000	2.68450000	0.48960000
C	5.51560000	-1.48830000	0.20160000
N	6.66690000	-1.65430000	0.25780000
H	4.27280000	0.82380000	0.06470000
H	1.21010000	-3.05140000	0.14270000
H	3.62560000	-3.40660000	0.23230000
H	3.56060000	2.58300000	-0.23830000
H	2.66010000	4.83940000	-0.39340000
H	0.18310000	5.20020000	-0.37960000
H	-1.32750000	3.28770000	-0.17810000
H	-4.75250000	-3.34680000	-0.21570000
H	-2.68770000	-4.68310000	-0.45770000

H	-0.47770000	-3.65330000	-0.41320000
H	-5.39400000	1.46390000	0.40760000
H	-5.81290000	-0.93870000	0.11420000
H	-3.99380000	3.07900000	0.60700000
Bq	2.70790000	-1.09160000	0.06790000
Bq	0.76500000	0.44850000	-0.03660000
Bq	1.10970000	2.89950000	-0.18930000
Bq	-1.30540000	-0.40190000	-0.02310000
Bq	-3.47190000	-0.04080000	0.11180000
Bq	-2.51160000	-2.23900000	-0.16810000
Bq	2.75520000	-1.13440000	-0.93010000
Bq	2.66060000	-1.04880000	1.06580000
Bq	0.72690000	0.41120000	-1.03520000
Bq	0.80310000	0.48580000	0.96200000
Bq	1.08750000	2.81200000	-1.18520000
Bq	1.13180000	2.98700000	0.80660000
Bq	-1.33520000	-0.31500000	-1.01890000
Bq	-1.27560000	-0.48880000	0.97270000
Bq	-2.54500000	-2.12740000	-1.16130000
Bq	-2.47820000	-2.35050000	0.82510000
Bq	-3.52260000	0.08590000	-0.87890000
Bq	-3.42130000	-0.16750000	1.10240000

Input geometry for NICS(1) calculation of 2c (anion)

C	4.09590000	-1.29350000	0.00000000
C	3.55720000	-0.00360000	0.00000000
C	2.17140000	0.23160000	0.00000000
C	1.27910000	-0.89570000	0.00000000
C	1.85810000	-2.19800000	0.00000000
C	3.21920000	-2.40550000	0.00000000
C	1.62210000	1.58790000	0.00000000
C	0.20410000	1.79000000	0.00000000
C	-0.68210000	0.64210000	0.00000000
C	-0.13230000	-0.67570000	0.00000000
C	2.46350000	2.72610000	0.00000000
C	1.95360000	4.01390000	0.00000000
C	0.56240000	4.20860000	0.00000000
C	-0.29220000	3.11910000	0.00000000

C	-2.42880000	-0.84400000	0.00000000
C	-3.71640000	-1.42030000	0.00000000
C	-3.81550000	-2.82180000	0.00000000
C	-2.65750000	-3.60600000	0.00000000
C	-1.37630000	-3.02410000	0.00000000
C	-1.23730000	-1.62930000	0.00000000
C	-2.13410000	0.54780000	0.00000000
C	-3.24920000	1.47900000	0.00000000
C	-4.58920000	0.84710000	0.00000000
C	-4.81980000	-0.49480000	0.00000000
O	-3.20060000	2.73750000	0.00000000
C	5.51190000	-1.48560000	0.00000000
N	6.66760000	-1.65160000	0.00000000
H	4.25080000	0.82770000	0.00000000
H	1.21010000	-3.06140000	0.00000000
H	3.62410000	-3.41280000	0.00000000
H	3.54070000	2.60420000	0.00000000
H	2.63230000	4.86360000	0.00000000
H	0.14940000	5.21440000	0.00000000
H	-1.37030000	3.25730000	0.00000000
H	-4.79580000	-3.29500000	0.00000000
H	-2.74270000	-4.68990000	0.00000000
H	-0.52330000	-3.69260000	0.00000000
H	-5.41380000	1.55540000	0.00000000
H	-5.83900000	-0.88030000	0.00000000
Bq	2.69680000	-1.09410000	0.00000000
Bq	0.74370000	0.44670000	0.00000000
Bq	1.08560000	2.90760000	0.00000000
Bq	-1.32290000	-0.39180000	0.00000000
Bq	-3.48960000	0.01910000	0.00000000
Bq	-2.53860000	-2.22420000	0.00000000
Bq	2.69680000	-1.09410000	-1.00000000
Bq	2.69680000	-1.09410000	1.00000000
Bq	0.74370000	0.44670000	-1.00000000
Bq	0.74370000	0.44670000	1.00000000
Bq	1.08560000	2.90760000	-1.00000000
Bq	1.08560000	2.90760000	1.00000000
Bq	-1.32290000	-0.39180000	1.00000000

Bq	-1.32290000	-0.39180000	-1.00000000
Bq	-2.53860000	-2.22420000	-1.00000000
Bq	-2.53860000	-2.22420000	1.00000000
Bq	-3.48960000	0.01910000	1.00000000
Bq	-3.48960000	0.01910000	-1.00000000

Input geometry for NICS(1) calculation of 3a (neutral)

C	3.86300000	-1.91400000	0.00010000
C	3.57420000	-0.56090000	0.00010000
C	2.24220000	-0.09080000	0.00000000
C	1.17510000	-1.04640000	0.00000000
C	1.51030000	-2.42260000	0.00010000
C	2.82050000	-2.85910000	0.00010000
C	1.93640000	1.33690000	0.00000000
C	0.57410000	1.77730000	0.00000000
C	-0.47520000	0.79310000	0.00000000
C	-0.18250000	-0.57490000	0.00000000
C	2.95800000	2.31730000	-0.00010000
C	2.67350000	3.67090000	-0.00020000
C	1.33520000	4.10250000	-0.00020000
C	0.31390000	3.17160000	-0.00010000
C	-2.49010000	-0.35310000	0.00000000
C	-3.86250000	-0.64710000	0.00000000
C	-4.22200000	-2.02520000	-0.00010000
C	-3.23220000	-2.99090000	-0.00030000
C	-1.84710000	-2.66170000	-0.00030000
C	-1.45960000	-1.33060000	-0.00010000
C	-1.94900000	0.96060000	0.00010000
C	-2.84820000	2.01570000	0.00030000
C	-4.24720000	1.74840000	0.00030000
C	-4.75570000	0.46300000	0.00020000
O	5.18400000	-2.28340000	0.00010000
H	-2.53680000	3.05280000	0.00040000
H	4.41360000	0.12210000	0.00000000
H	0.72550000	-3.16460000	0.00020000
H	3.04310000	-3.92390000	0.00020000
H	3.99750000	2.01300000	-0.00010000
H	3.48310000	4.39460000	-0.00020000

H	1.10180000	5.16330000	-0.00030000
H	-0.70790000	3.52180000	-0.00020000
H	-5.26990000	-2.31310000	-0.00010000
H	-3.51170000	-4.04060000	-0.00040000
H	-1.13830000	-3.48050000	-0.00040000
H	-4.93140000	2.59210000	0.00040000
H	-5.82950000	0.29640000	0.00020000
H	5.25810000	-3.24640000	0.00020000
Bq	2.53090000	-1.48230000	0.00010000
Bq	0.87830000	0.36590000	0.00000000
Bq	1.63190000	2.72940000	-0.00010000
Bq	-1.31130000	-0.10100000	0.00000000
Bq	-3.35880000	0.69790000	0.00020000
Bq	-2.85230000	-1.66810000	-0.00010000
Bq	2.53090000	-1.48230000	-0.99990000
Bq	2.53080000	-1.48230000	1.00010000
Bq	0.87830000	0.36590000	-1.00000000
Bq	0.87830000	0.36590000	1.00000000
Bq	1.63180000	2.72930000	-1.00010000
Bq	1.63190000	2.72950000	0.99990000
Bq	-1.31130000	-0.10090000	-1.00000000
Bq	-1.31130000	-0.10110000	1.00000000
Bq	-2.85230000	-1.66800000	-1.00010000
Bq	-2.85220000	-1.66820000	0.99990000
Bq	-3.35880000	0.69800000	-0.99980000
Bq	-3.35870000	0.69780000	1.00010000

Input geometry for NICS(1) calculation of 3a (anion)

C	3.92310000	-2.05320000	0.00000000
C	3.58950000	-0.65310000	0.00000000
C	2.28590000	-0.15830000	0.00000000
C	1.17330000	-1.08830000	0.00000000
C	1.48900000	-2.48300000	0.00000000
C	2.77560000	-2.95000000	0.00000000
C	1.99290000	1.28400000	0.00000000
C	0.63740000	1.75650000	0.00000000
C	-0.43300000	0.80040000	0.00000000
C	-0.15060000	-0.58600000	0.00000000

C	3.03060000	2.24370000	0.00000000
C	2.78390000	3.60840000	0.00000000
C	1.45630000	4.07010000	0.00000000
C	0.41390000	3.15950000	0.00000000
C	-2.46380000	-0.31750000	0.00000000
C	-3.84280000	-0.58290000	0.00000000
C	-4.22760000	-1.95350000	0.00000000
C	-3.25650000	-2.94020000	0.00000000
C	-1.86620000	-2.63960000	0.00000000
C	-1.45210000	-1.31480000	0.00000000
C	-1.88610000	0.99050000	0.00000000
C	-2.77620000	2.06240000	0.00000000
C	-4.17900000	1.81780000	0.00000000
C	-4.72000000	0.54500000	0.00000000
O	5.11130000	-2.48550000	0.00000000
H	4.44340000	0.01510000	0.00000000
H	0.68180000	-3.20380000	0.00000000
H	2.98160000	-4.01800000	0.00000000
H	4.06040000	1.90660000	0.00000000
H	3.61330000	4.31100000	0.00000000
H	1.24390000	5.13680000	0.00000000
H	-0.60090000	3.53300000	0.00000000
H	-5.28230000	-2.22030000	0.00000000
H	-3.55810000	-3.98500000	0.00000000
H	-1.16890000	-3.46770000	0.00000000
H	-2.44560000	3.09390000	0.00000000
H	-4.84670000	2.67670000	0.00000000
H	-5.79740000	0.39880000	0.00000000
Bq	-2.85150000	-1.62480000	0.00000000
Bq	-3.31130000	0.75260000	0.00000000
Bq	-1.27710000	-0.08550000	0.00000000
Bq	0.91760000	0.33470000	0.00000000
Bq	1.71920000	2.68700000	0.00000000
Bq	2.53940000	-1.56430000	0.00000000
Bq	2.53940000	-1.56430000	-1.00000000
Bq	2.53940000	-1.56430000	1.00000000
Bq	0.91760000	0.33470000	-1.00000000
Bq	0.91760000	0.33470000	1.00000000

Bq	1.71920000	2.68700000	-1.00000000
Bq	1.71920000	2.68700000	1.00000000
Bq	-1.27710000	-0.08550000	-1.00000000
Bq	-1.27710000	-0.08550000	1.00000000
Bq	-2.85150000	-1.62480000	1.00000000
Bq	-2.85150000	-1.62480000	-1.00000000
Bq	-3.31130000	0.75260000	1.00000000
Bq	-3.31130000	0.75260000	-1.00000000

Input geometry for NICS(1) calculation of 3b (neutral)

C	4.09590000	-0.81730000	0.10110000
C	3.45110000	0.41060000	0.03840000
C	2.04700000	0.51240000	-0.02090000
C	1.27040000	-0.68870000	-0.01630000
C	1.95650000	-1.92190000	0.06680000
C	3.33770000	-2.00360000	0.12190000
C	1.37030000	1.80490000	-0.08790000
C	-0.06120000	1.87620000	-0.05830000
C	-0.82110000	0.64680000	0.01270000
C	-0.16510000	-0.59070000	-0.05020000
C	2.10440000	3.00970000	-0.19740000
C	1.48300000	4.24260000	-0.28130000
C	0.08040000	4.31150000	-0.26550000
C	-0.66830000	3.15370000	-0.15830000
C	-2.43930000	-1.02550000	-0.03110000
C	-3.65750000	-1.72580000	-0.04150000
C	-3.60390000	-3.13690000	-0.19450000
C	-2.37820000	-3.76640000	-0.32170000
C	-1.15750000	-3.04300000	-0.28590000
C	-1.17320000	-1.66350000	-0.12320000
C	-2.28750000	0.38810000	0.08070000
C	-3.47120000	1.09890000	0.26730000
C	-4.72800000	0.41680000	0.26280000
C	-4.83760000	-0.94520000	0.10640000
O	-3.48430000	2.45030000	0.47890000
O	5.46350000	-0.77670000	0.15270000
C	6.18020000	-2.00220000	0.22920000
H	4.08080000	1.29080000	0.04900000

H	1.39600000	-2.84360000	0.11950000
H	3.81140000	-2.97530000	0.19330000
H	3.18650000	2.97800000	-0.23100000
H	2.07940000	5.14620000	-0.36820000
H	-0.42180000	5.27170000	-0.34350000
H	-1.74390000	3.22350000	-0.15380000
H	-4.52470000	-3.71380000	-0.21540000
H	-2.33960000	-4.84410000	-0.45050000
H	-0.23860000	-3.60310000	-0.40430000
H	-5.62830000	1.01480000	0.39350000
H	-5.81540000	-1.41860000	0.10580000
H	-4.39500000	2.75540000	0.58580000
H	7.23550000	-1.72730000	0.25460000
H	5.92910000	-2.55860000	1.14110000
H	5.99150000	-2.63360000	-0.64830000
Bq	2.69310000	-0.75140000	0.04850000
Bq	0.60670000	0.59350000	-0.03680000
Bq	0.71810000	3.06640000	-0.17480000
Bq	-1.37720000	-0.44900000	-0.02220000
Bq	-3.57020000	-0.29880000	0.10740000
Bq	-2.40160000	-2.39350000	-0.16630000
Bq	2.73720000	-0.78370000	-0.95000000
Bq	2.64900000	-0.71910000	1.04700000
Bq	0.57080000	0.55800000	-1.03550000
Bq	0.64270000	0.62890000	0.96190000
Bq	0.70110000	2.98510000	-1.17130000
Bq	0.73510000	3.14770000	0.82180000
Bq	-1.43410000	-0.38830000	-1.01880000
Bq	-1.32030000	-0.50960000	0.97430000
Bq	-2.44890000	-2.29660000	-1.16050000
Bq	-2.35430000	-2.49050000	0.82780000
Bq	-3.62990000	-0.18020000	-0.88370000
Bq	-3.51050000	-0.41740000	1.09860000

Input geometry for NICS(1) calculation of 3b (anion)

C	4.08950000	-0.81540000	0.00000000
C	3.43790000	0.40870000	0.00000000
C	2.03070000	0.50950000	0.00000000

C	1.25090000	-0.69360000	0.00000000
C	1.95210000	-1.92300000	0.00000000
C	3.33810000	-2.00220000	0.00000000
C	1.35220000	1.80530000	0.00000000
C	-0.07980000	1.87100000	0.00000000
C	-0.85400000	0.64560000	0.00000000
C	-0.18640000	-0.60700000	0.00000000
C	2.08100000	3.01910000	0.00000000
C	1.45180000	4.25330000	0.00000000
C	0.04750000	4.31380000	0.00000000
C	-0.69960000	3.14780000	0.00000000
C	-2.45950000	-0.99340000	0.00000000
C	-3.68490000	-1.69450000	0.00000000
C	-3.64580000	-3.09950000	0.00000000
C	-2.41630000	-3.76700000	0.00000000
C	-1.19740000	-3.06160000	0.00000000
C	-1.19410000	-1.66040000	0.00000000
C	-2.30060000	0.41610000	0.00000000
C	-3.49480000	1.23610000	0.00000000
C	-4.76830000	0.47830000	0.00000000
C	-4.87180000	-0.88060000	0.00000000
O	-3.56860000	2.49640000	0.00000000
O	5.47430000	-0.77040000	0.00000000
C	6.17720000	-1.99710000	0.00000000
H	4.06260000	1.29350000	0.00000000
H	1.39600000	-2.84910000	0.00000000
H	3.81380000	-2.97660000	0.00000000
H	3.16500000	2.99670000	0.00000000
H	2.04620000	5.16420000	0.00000000
H	-0.45990000	5.27580000	0.00000000
H	-1.78680000	3.18190000	0.00000000
H	-4.57540000	-3.66650000	0.00000000
H	-2.39530000	-4.85440000	0.00000000
H	-0.28210000	-3.64280000	0.00000000
H	-5.65720000	1.10480000	0.00000000
H	-5.85010000	-1.36130000	0.00000000
H	7.23840000	-1.73780000	0.00000000
H	5.95340000	-2.59610000	0.89410000

H	5.95340000	-2.59610000	-0.89410000
Bq	2.68320000	-0.75270000	0.00000000
Bq	0.58560000	0.58850000	0.00000000
Bq	0.69220000	3.06840000	0.00000000
Bq	-1.39890000	-0.43980000	0.00000000
Bq	-2.43300000	-2.37940000	0.00000000
Bq	-3.59660000	-0.23970000	0.00000000
Bq	2.68320000	-0.75270000	1.00000000
Bq	2.68320000	-0.75270000	-1.00000000
Bq	0.58560000	0.58850000	-1.00000000
Bq	0.58560000	0.58850000	1.00000000
Bq	0.69220000	3.06840000	-1.00000000
Bq	0.69220000	3.06840000	1.00000000
Bq	-1.39890000	-0.43980000	-1.00000000
Bq	-1.39890000	-0.43980000	1.00000000
Bq	-2.43300000	-2.37940000	-1.00000000
Bq	-2.43300000	-2.37940000	1.00000000
Bq	-3.59660000	-0.23970000	-1.00000000
Bq	-3.59660000	-0.23970000	1.00000000

Input geometry for NICS(1) calculation of 3c (neutral)

C	4.09710000	-1.29150000	0.13100000
C	3.57550000	-0.00330000	0.05610000
C	2.18620000	0.23270000	-0.01370000
C	1.30330000	-0.89170000	-0.00730000
C	1.86260000	-2.19310000	0.08830000
C	3.22260000	-2.40270000	0.15270000
C	1.64050000	1.58330000	-0.09140000
C	0.22200000	1.78970000	-0.06600000
C	-0.64830000	0.63740000	0.01020000
C	-0.11370000	-0.66030000	-0.05150000
C	2.48580000	2.71260000	-0.20700000
C	1.98160000	3.99650000	-0.30180000
C	0.59150000	4.19760000	-0.29180000
C	-0.26340000	3.11720000	-0.17790000
C	-2.41580000	-0.87380000	-0.03110000
C	-3.69640000	-1.45300000	-0.04000000
C	-3.78030000	-2.86200000	-0.19540000

C	-2.62160000	-3.60730000	-0.32640000
C	-1.33690000	-3.00620000	-0.29080000
C	-1.21880000	-1.63150000	-0.12500000
C	-2.13040000	0.51860000	0.08190000
C	-3.23960000	1.34170000	0.27450000
C	-4.55530000	0.78350000	0.27250000
C	-4.79410000	-0.56170000	0.11270000
O	-3.11910000	2.68450000	0.48960000
C	5.51560000	-1.48830000	0.20160000
N	6.66690000	-1.65430000	0.25780000
H	4.27280000	0.82380000	0.06470000
H	1.21010000	-3.05140000	0.14270000
H	3.62560000	-3.40660000	0.23230000
H	3.56060000	2.58300000	-0.23830000
H	2.66010000	4.83940000	-0.39340000
H	0.18310000	5.20020000	-0.37960000
H	-1.32750000	3.28770000	-0.17810000
H	-4.75250000	-3.34680000	-0.21570000
H	-2.68770000	-4.68310000	-0.45770000
H	-0.47770000	-3.65330000	-0.41320000
H	-5.39400000	1.46390000	0.40760000
H	-5.81290000	-0.93870000	0.11420000
H	-3.99380000	3.07900000	0.60700000
Bq	2.70790000	-1.09160000	0.06790000
Bq	0.76500000	0.44850000	-0.03660000
Bq	1.10970000	2.89950000	-0.18930000
Bq	-1.30540000	-0.40190000	-0.02310000
Bq	-3.47190000	-0.04080000	0.11180000
Bq	-2.51160000	-2.23900000	-0.16810000
Bq	2.75520000	-1.13440000	-0.93010000
Bq	2.66060000	-1.04880000	1.06580000
Bq	0.72690000	0.41120000	-1.03520000
Bq	0.80310000	0.48580000	0.96200000
Bq	1.08750000	2.81200000	-1.18520000
Bq	1.13180000	2.98700000	0.80660000
Bq	-1.33520000	-0.31500000	-1.01890000
Bq	-1.27560000	-0.48880000	0.97270000
Bq	-2.54500000	-2.12740000	-1.16130000

Bq	-2.47820000	-2.35050000	0.82510000
Bq	-3.52260000	0.08590000	-0.87890000
Bq	-3.42130000	-0.16750000	1.10240000

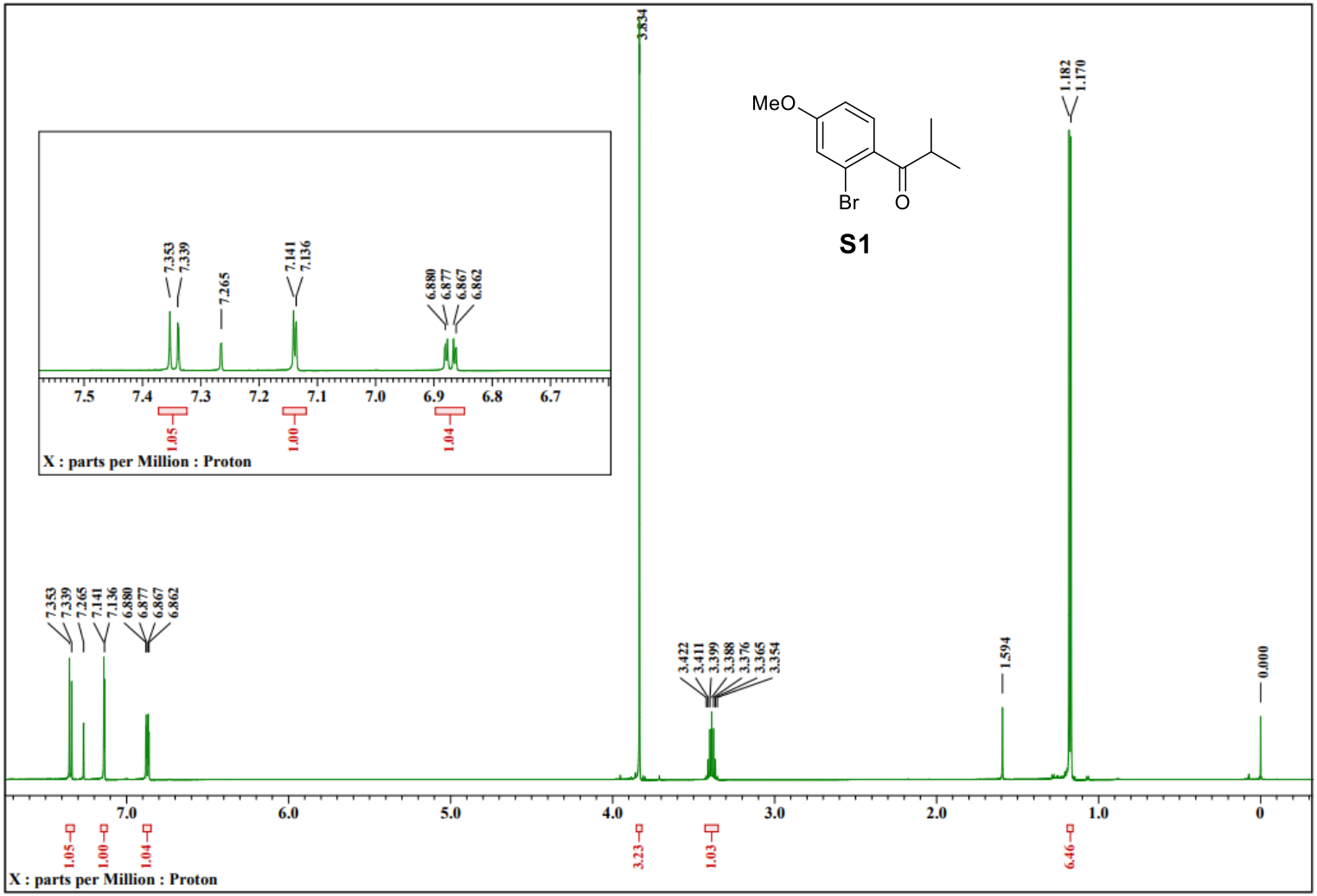
Input geometry for NICS(1) calculation of 3c (anion)

C	4.09590000	-1.29350000	0.00000000
C	3.55720000	-0.00360000	0.00000000
C	2.17140000	0.23160000	0.00000000
C	1.27910000	-0.89570000	0.00000000
C	1.85810000	-2.19800000	0.00000000
C	3.21920000	-2.40550000	0.00000000
C	1.62210000	1.58790000	0.00000000
C	0.20410000	1.79000000	0.00000000
C	-0.68210000	0.64210000	0.00000000
C	-0.13230000	-0.67570000	0.00000000
C	2.46350000	2.72610000	0.00000000
C	1.95360000	4.01390000	0.00000000
C	0.56240000	4.20860000	0.00000000
C	-0.29220000	3.11910000	0.00000000
C	-2.42880000	-0.84400000	0.00000000
C	-3.71640000	-1.42030000	0.00000000
C	-3.81550000	-2.82180000	0.00000000
C	-2.65750000	-3.60600000	0.00000000
C	-1.37630000	-3.02410000	0.00000000
C	-1.23730000	-1.62930000	0.00000000
C	-2.13410000	0.54780000	0.00000000
C	-3.24920000	1.47900000	0.00000000
C	-4.58920000	0.84710000	0.00000000
C	-4.81980000	-0.49480000	0.00000000
O	-3.20060000	2.73750000	0.00000000
C	5.51190000	-1.48560000	0.00000000
N	6.66760000	-1.65160000	0.00000000
H	4.25080000	0.82770000	0.00000000
H	1.21010000	-3.06140000	0.00000000
H	3.62410000	-3.41280000	0.00000000
H	3.54070000	2.60420000	0.00000000
H	2.63230000	4.86360000	0.00000000
H	0.14940000	5.21440000	0.00000000

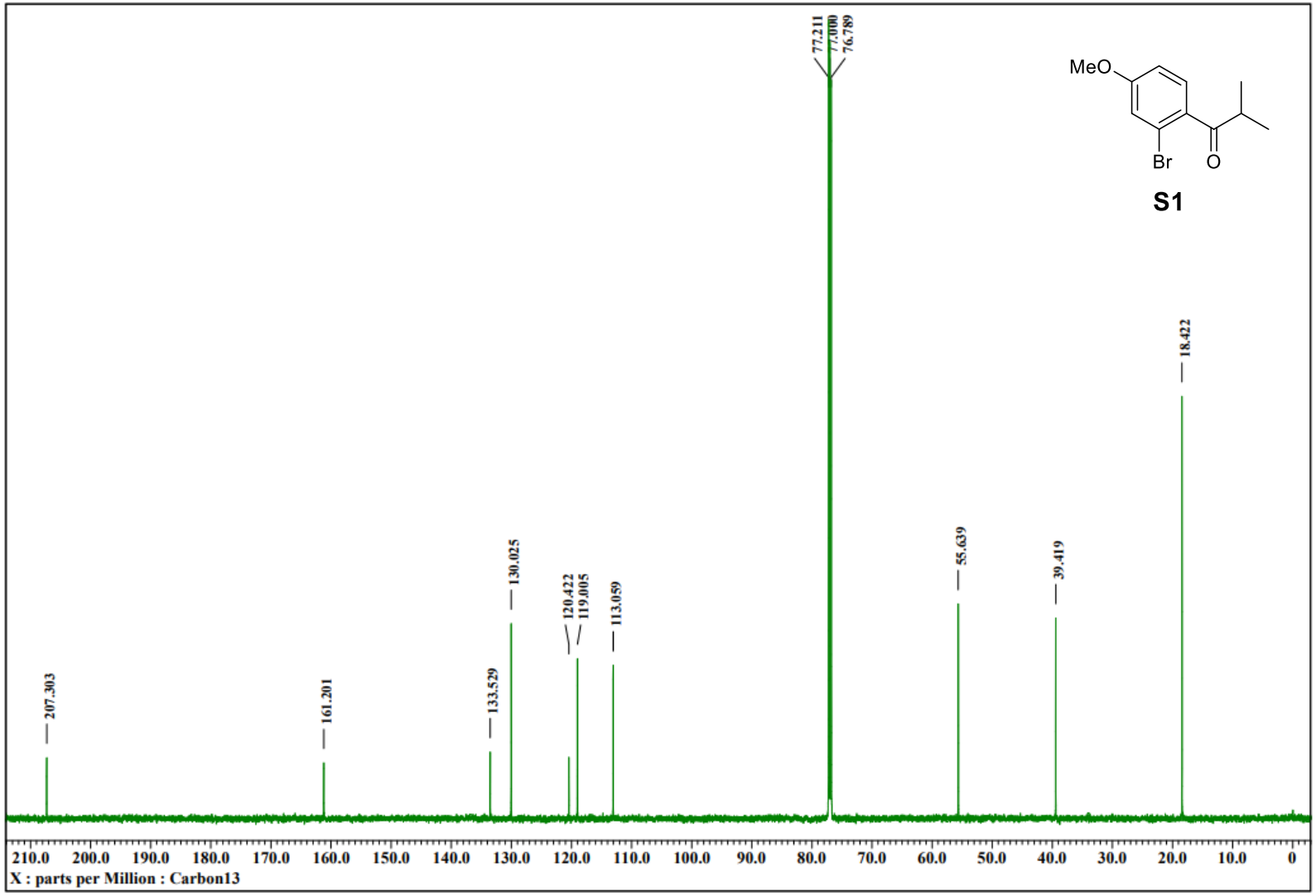
H	-1.37030000	3.25730000	0.00000000
H	-4.79580000	-3.29500000	0.00000000
H	-2.74270000	-4.68990000	0.00000000
H	-0.52330000	-3.69260000	0.00000000
H	-5.41380000	1.55540000	0.00000000
H	-5.83900000	-0.88030000	0.00000000
Bq	2.69680000	-1.09410000	0.00000000
Bq	0.74370000	0.44670000	0.00000000
Bq	1.08560000	2.90760000	0.00000000
Bq	-1.32290000	-0.39180000	0.00000000
Bq	-3.48960000	0.01910000	0.00000000
Bq	-2.53860000	-2.22420000	0.00000000
Bq	2.69680000	-1.09410000	-1.00000000
Bq	2.69680000	-1.09410000	1.00000000
Bq	0.74370000	0.44670000	-1.00000000
Bq	0.74370000	0.44670000	1.00000000
Bq	1.08560000	2.90760000	-1.00000000
Bq	1.08560000	2.90760000	1.00000000
Bq	-1.32290000	-0.39180000	1.00000000
Bq	-1.32290000	-0.39180000	-1.00000000
Bq	-2.53860000	-2.22420000	-1.00000000
Bq	-2.53860000	-2.22420000	1.00000000
Bq	-3.48960000	0.01910000	1.00000000
Bq	-3.48960000	0.01910000	-1.00000000

7. ^{1}H and ^{13}C NMR spectra

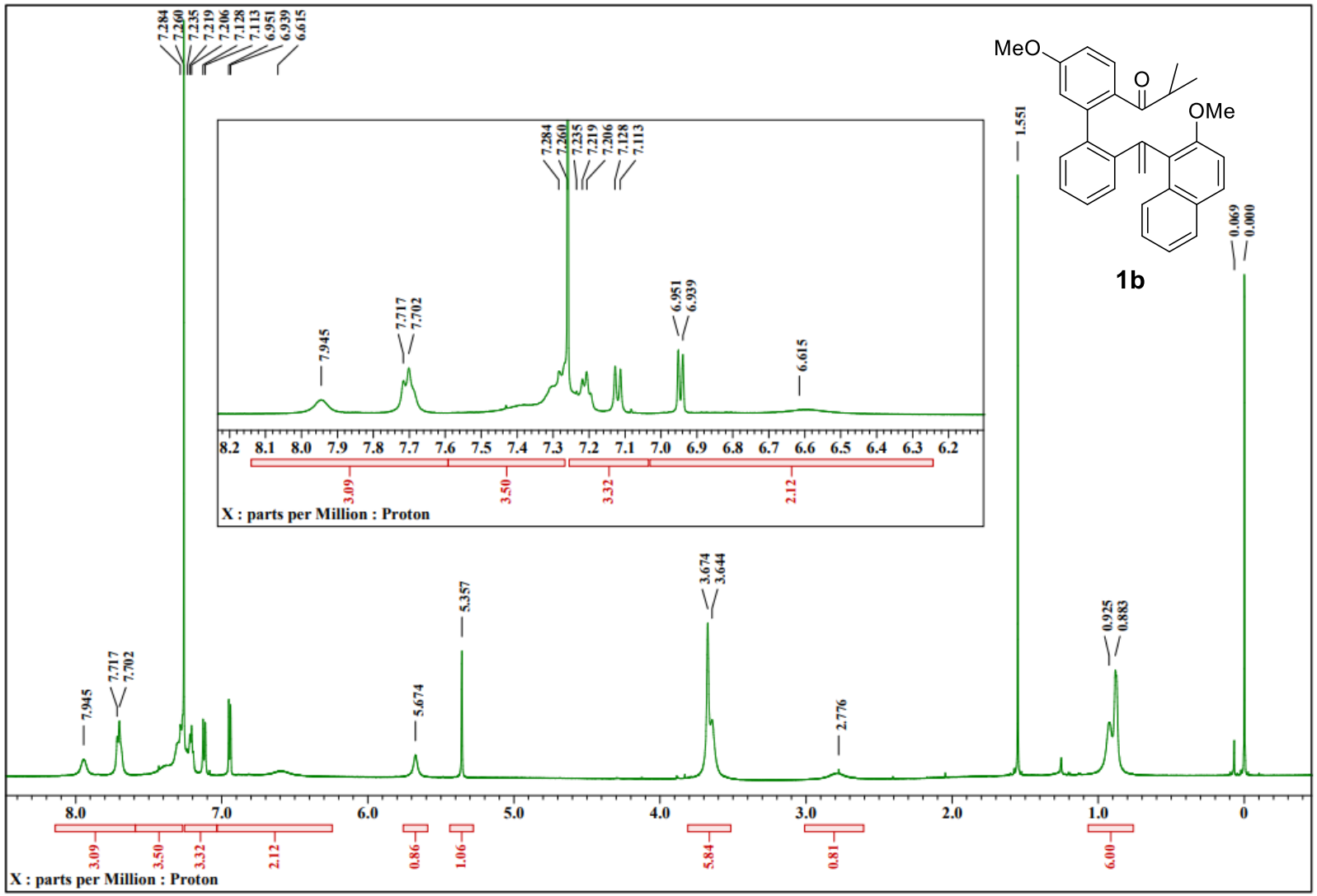
S1: ^{1}H NMR, $CDCl_3$, 600 MHz



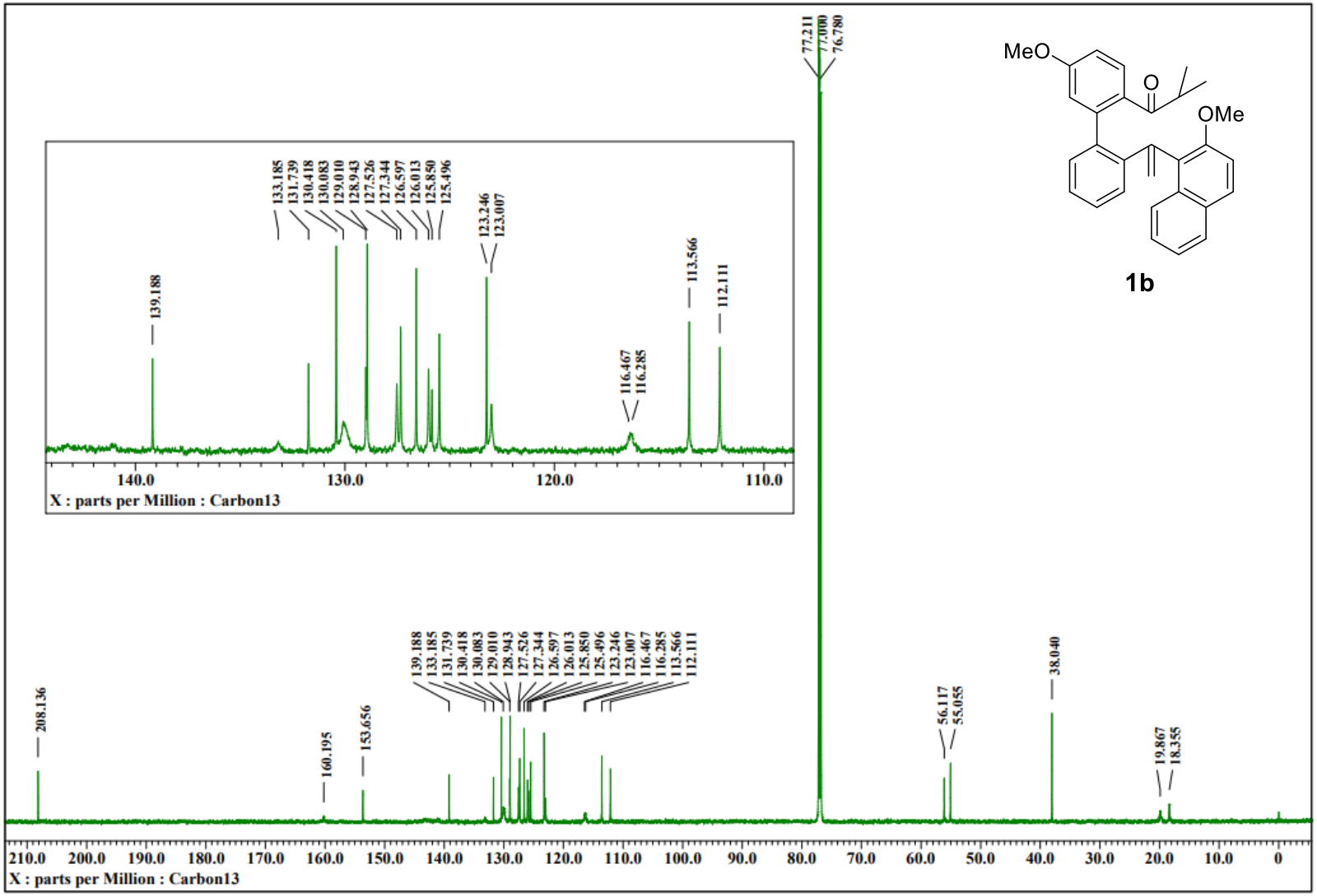
S1: ^{13}C NMR, $CDCl_3$, 151 MHz



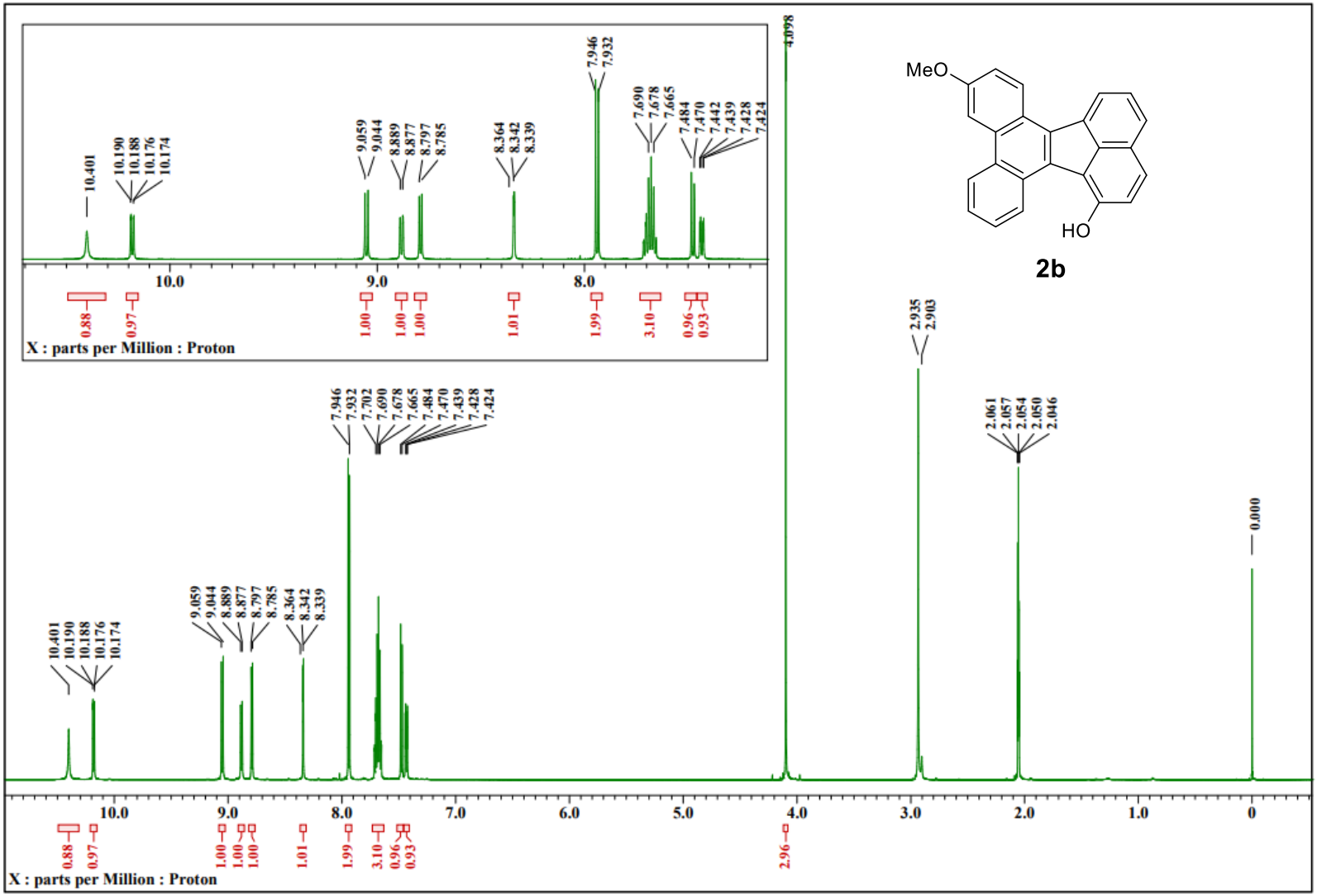
1b: ^{1}H NMR, $CDCl_3$, 600 MHz



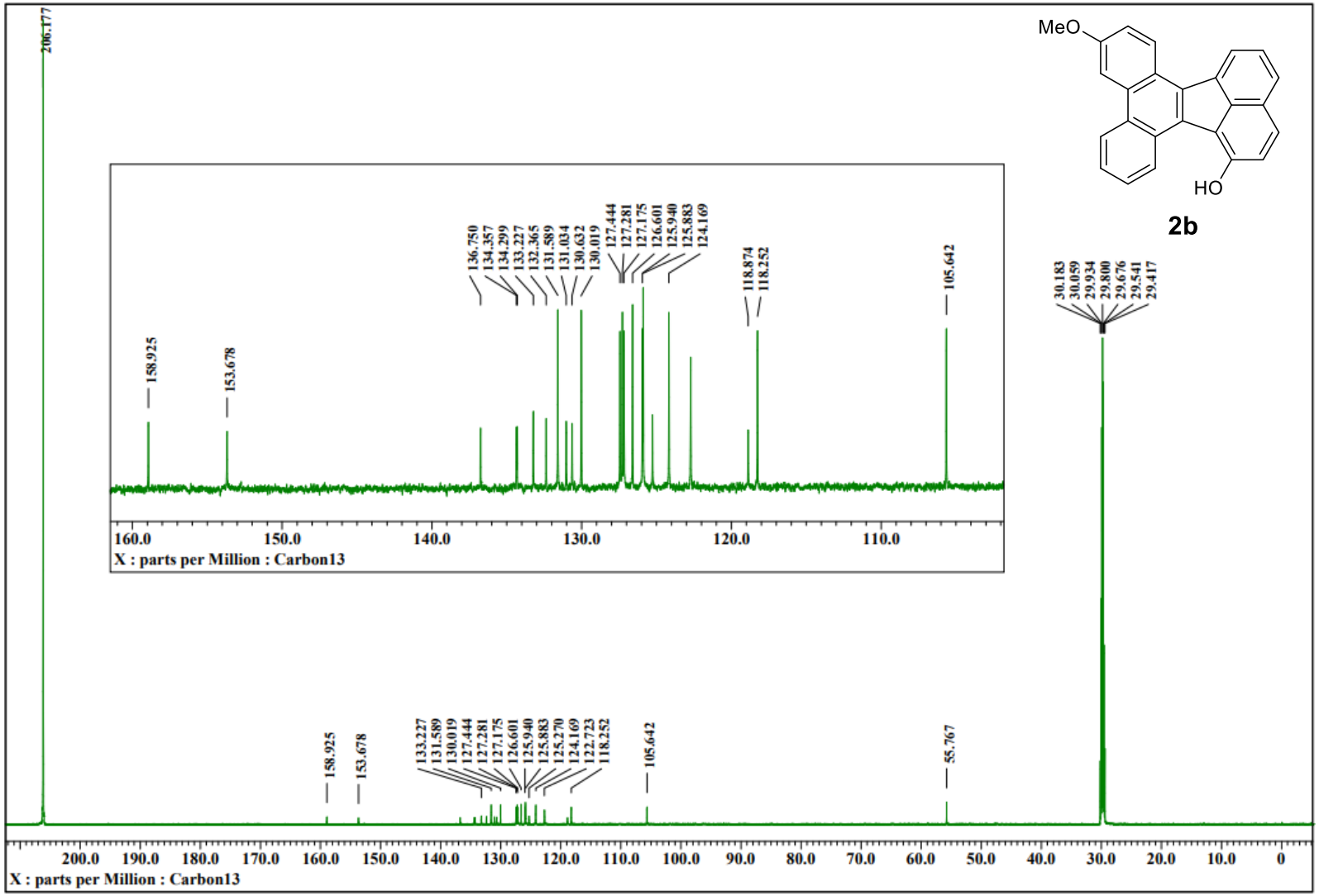
1b: ^{13}C NMR, $CDCl_3$, 151 MHz



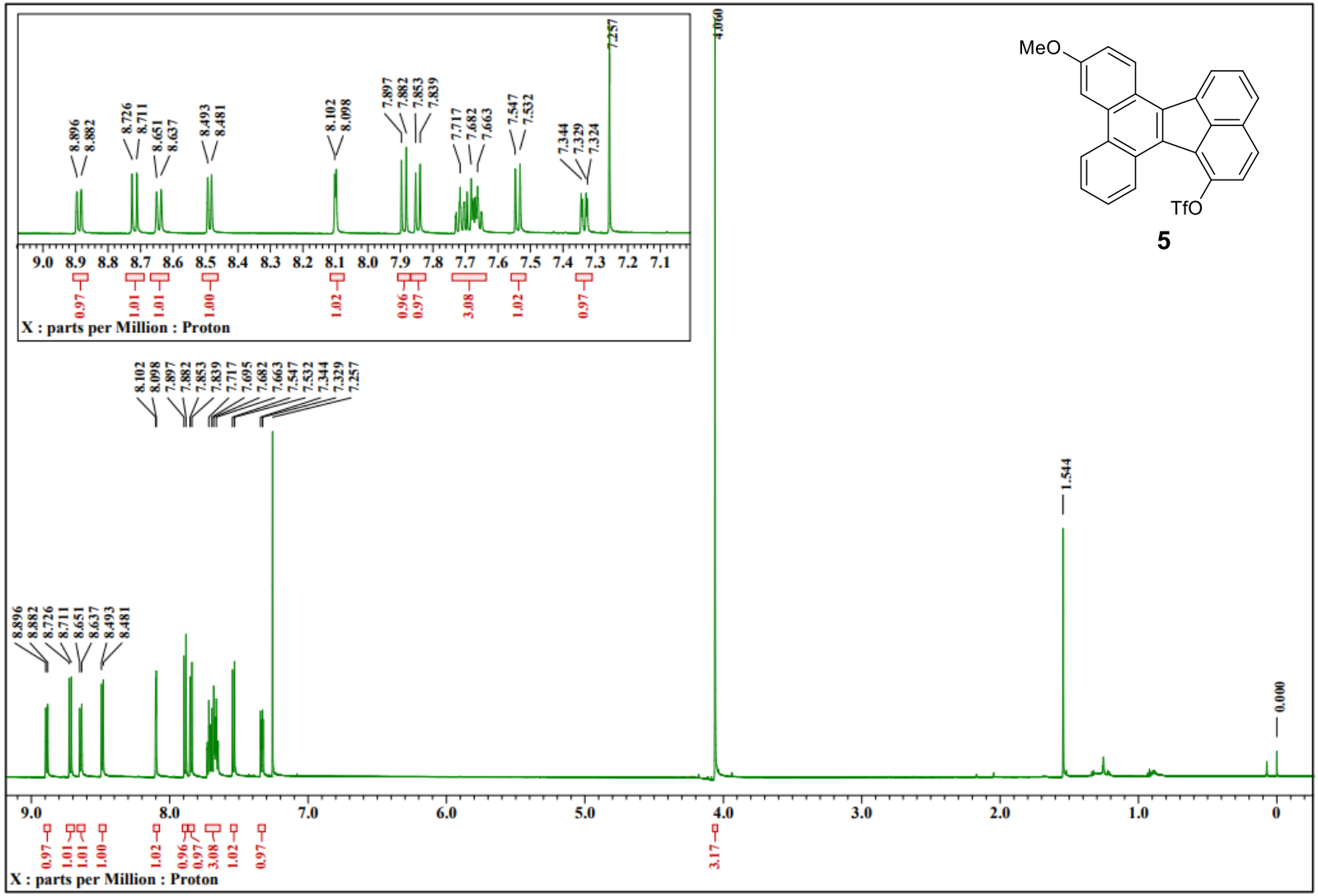
2b: ^{1}H NMR, acetone-d6, 600 MHz



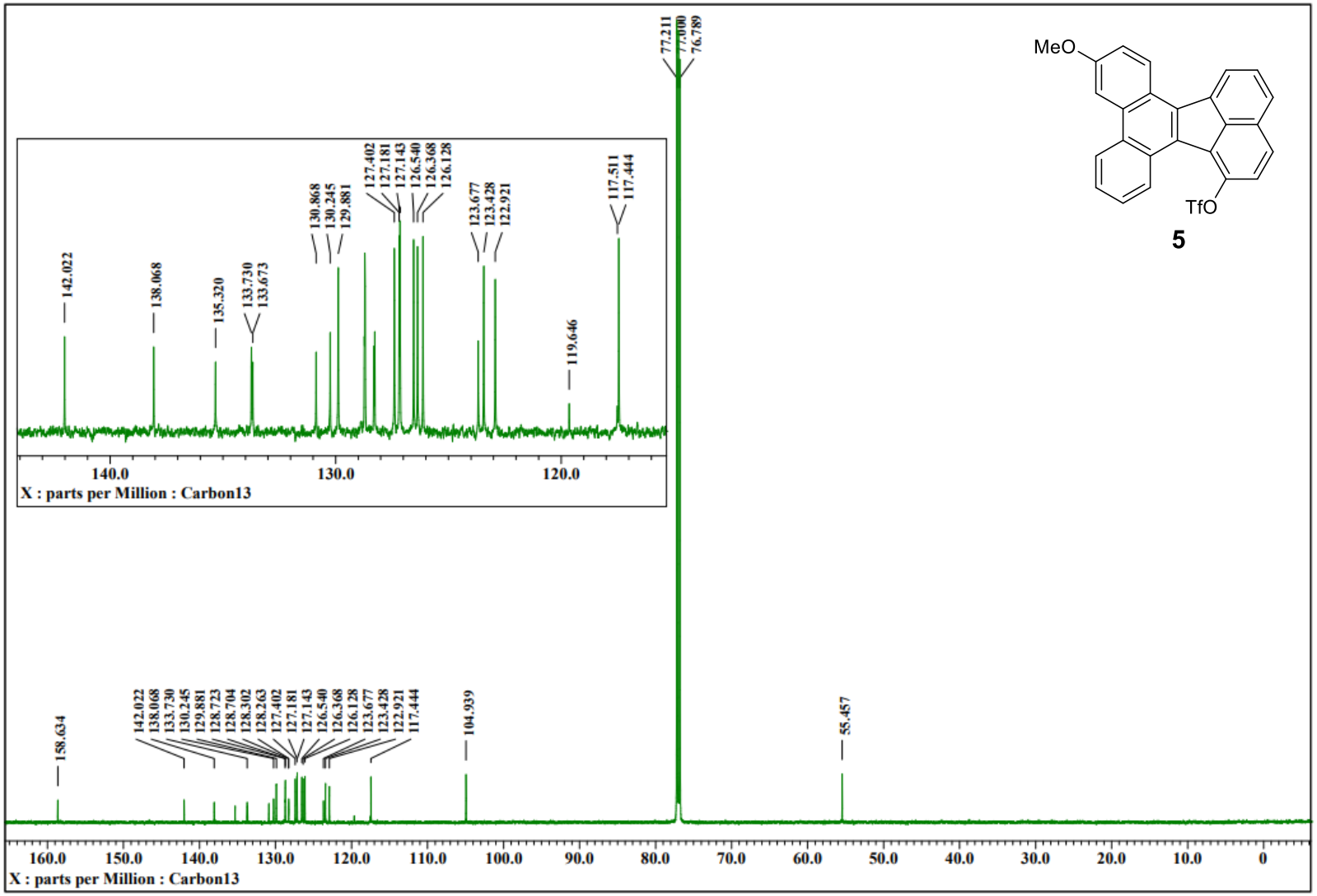
2b: ^{13}C NMR, acetone-d6, 151 MHz



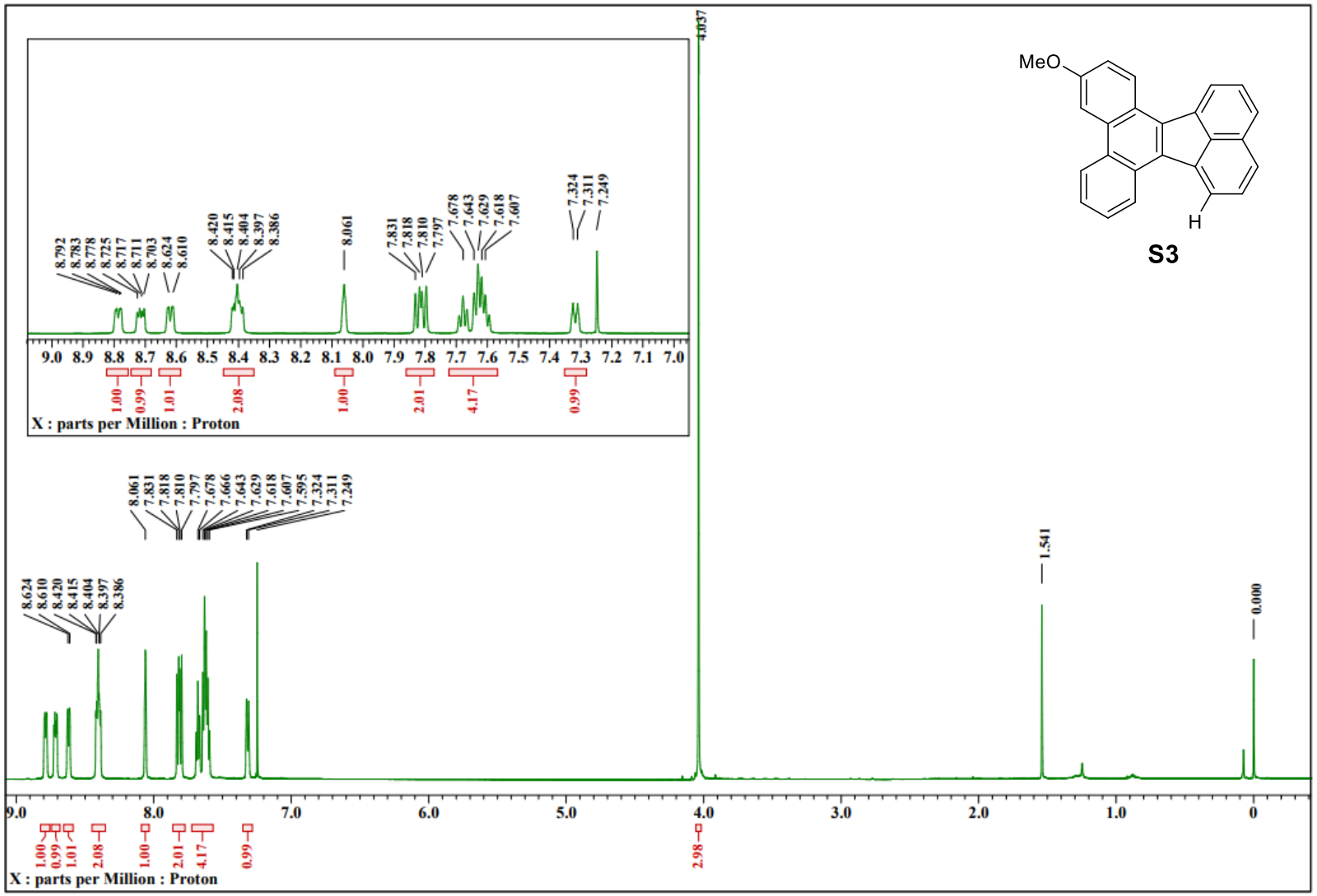
5: ^{1}H NMR, $CDCl_3$, 600 MHz



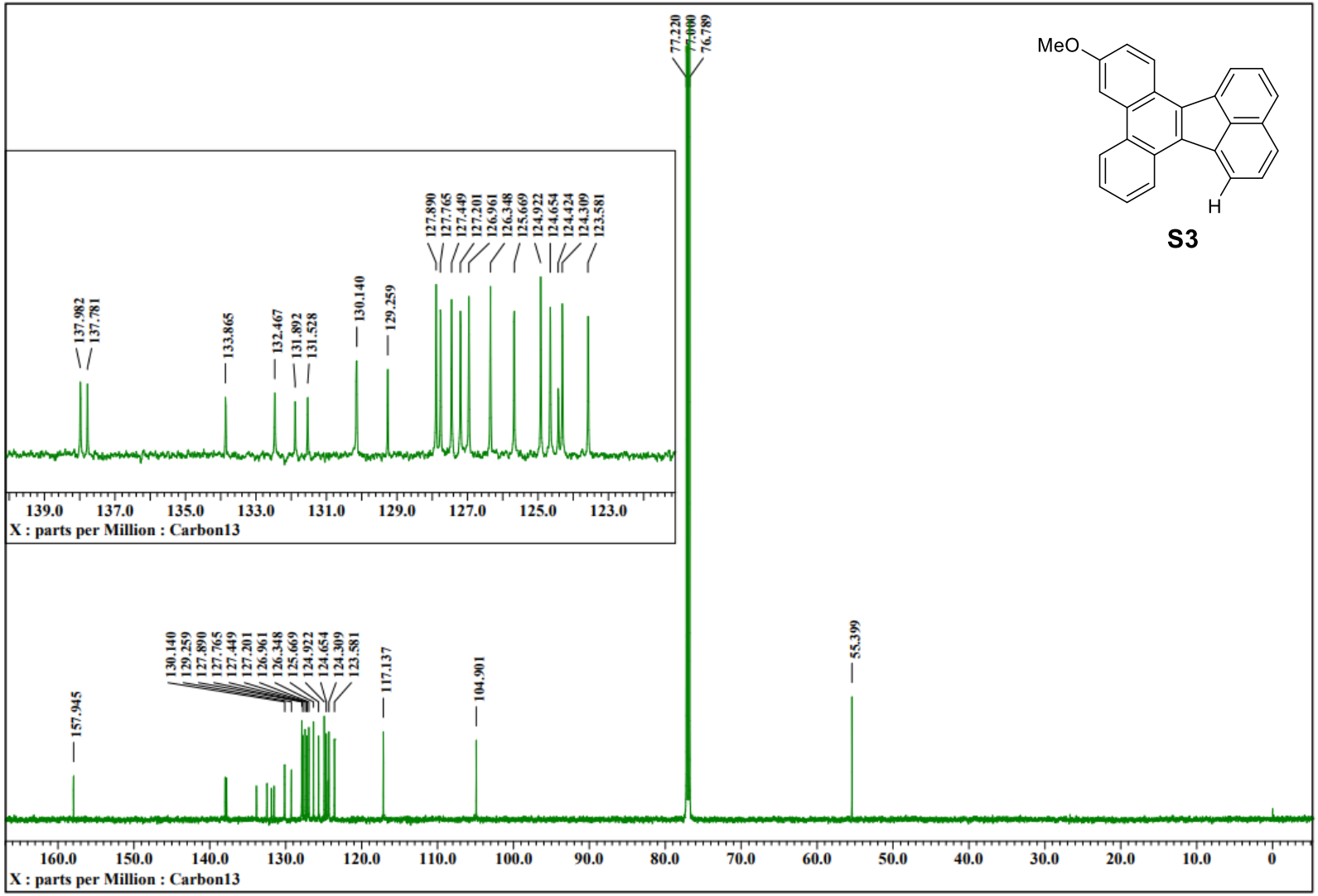
5: ^{13}C NMR, $CDCl_3$, 151 MHz



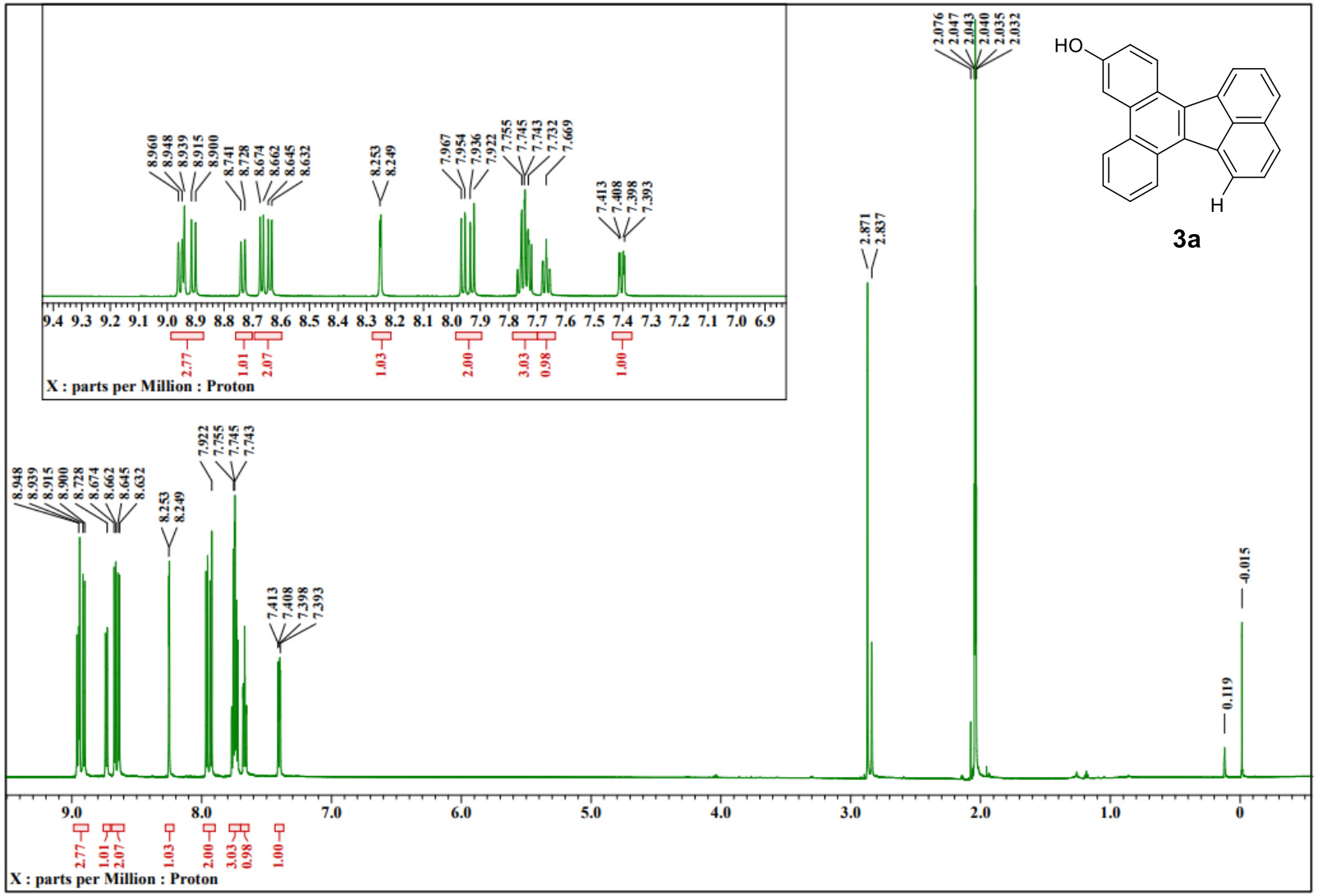
S3: ^{1}H NMR, $CDCl_3$, 600 MHz



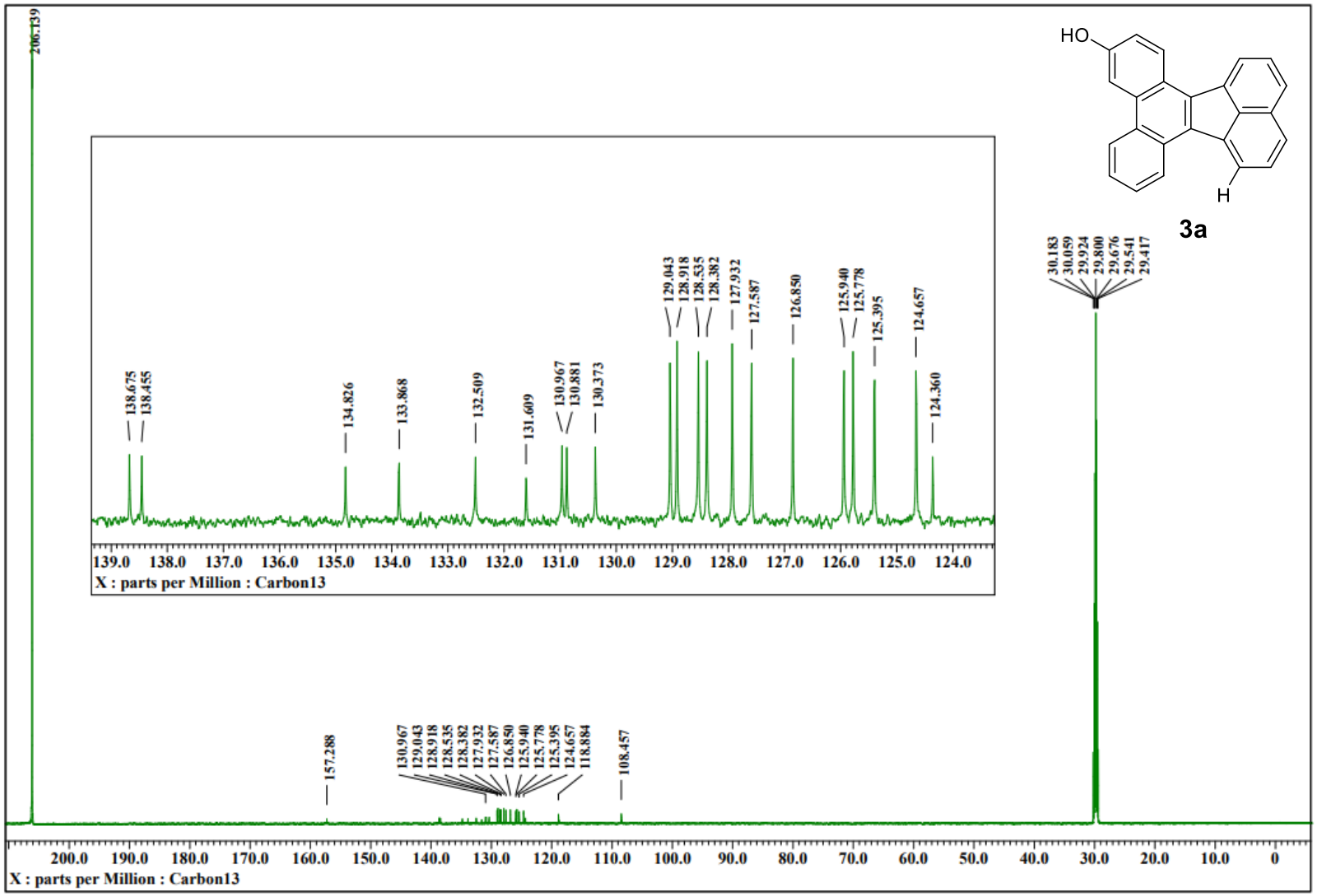
S3: ^{13}C NMR, $CDCl_3$, 151 MHz



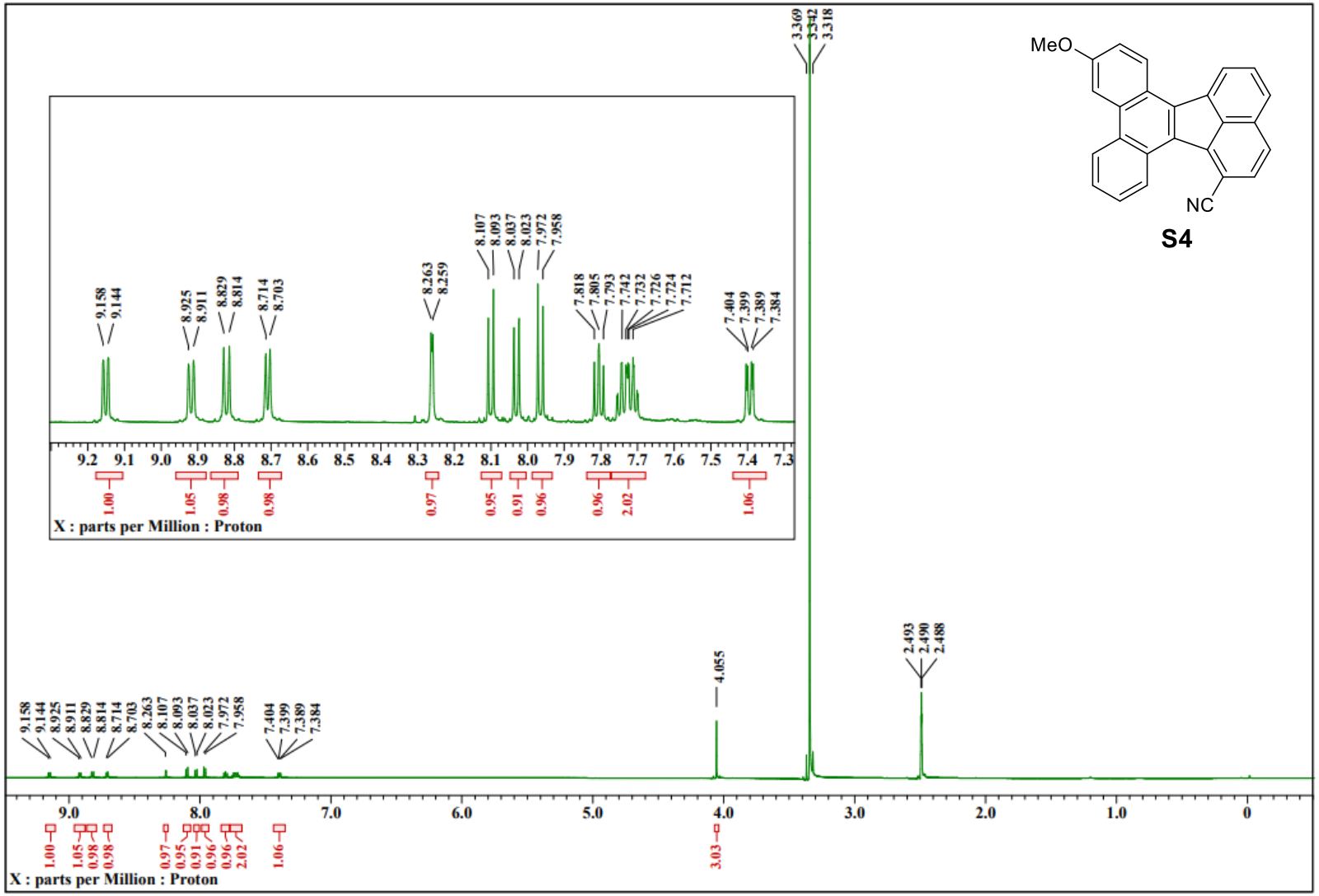
3a: ^{1}H NMR, acetone-d6, 600 MHz



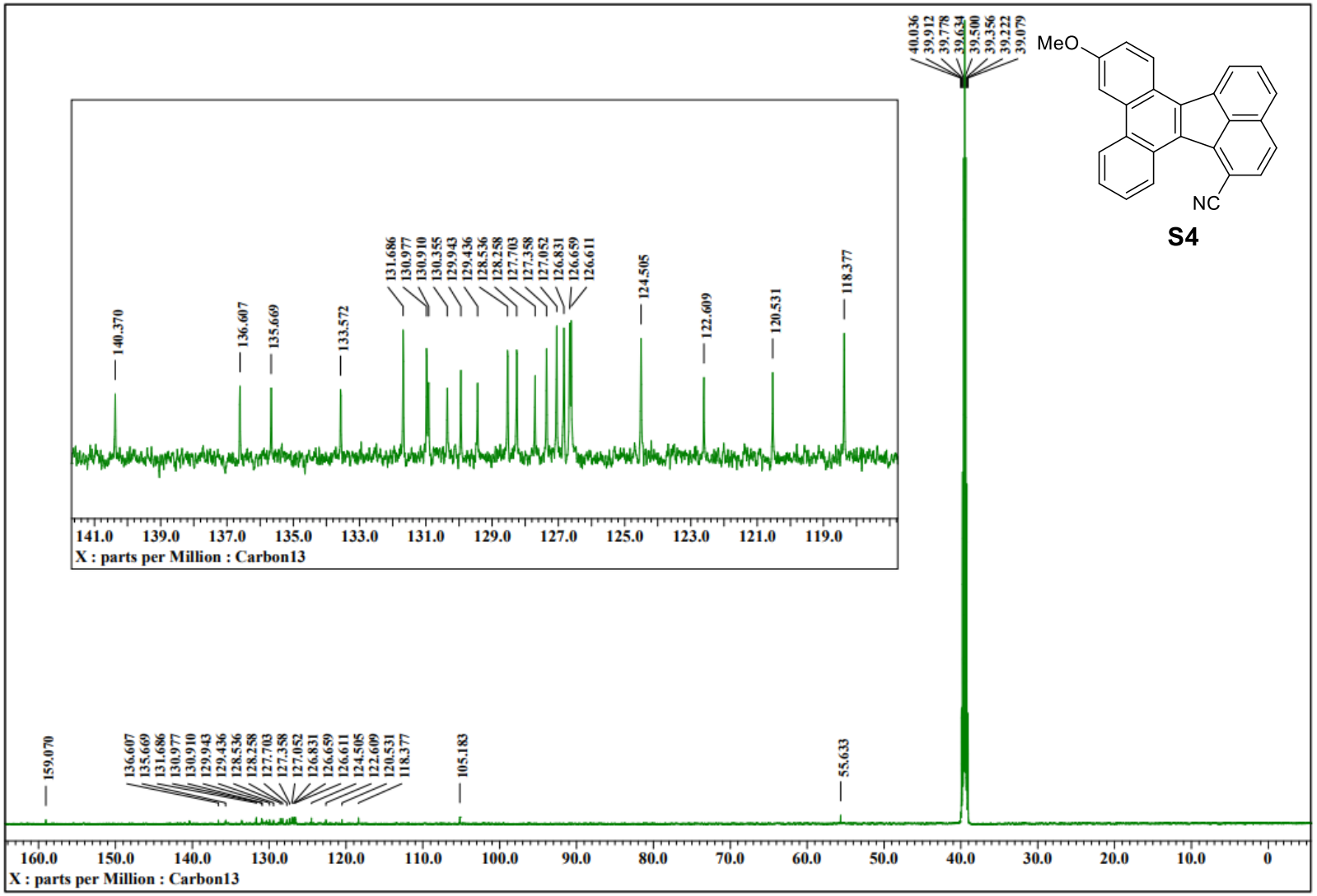
3a: ^{13}C NMR, acetone-d6, 151 MHz



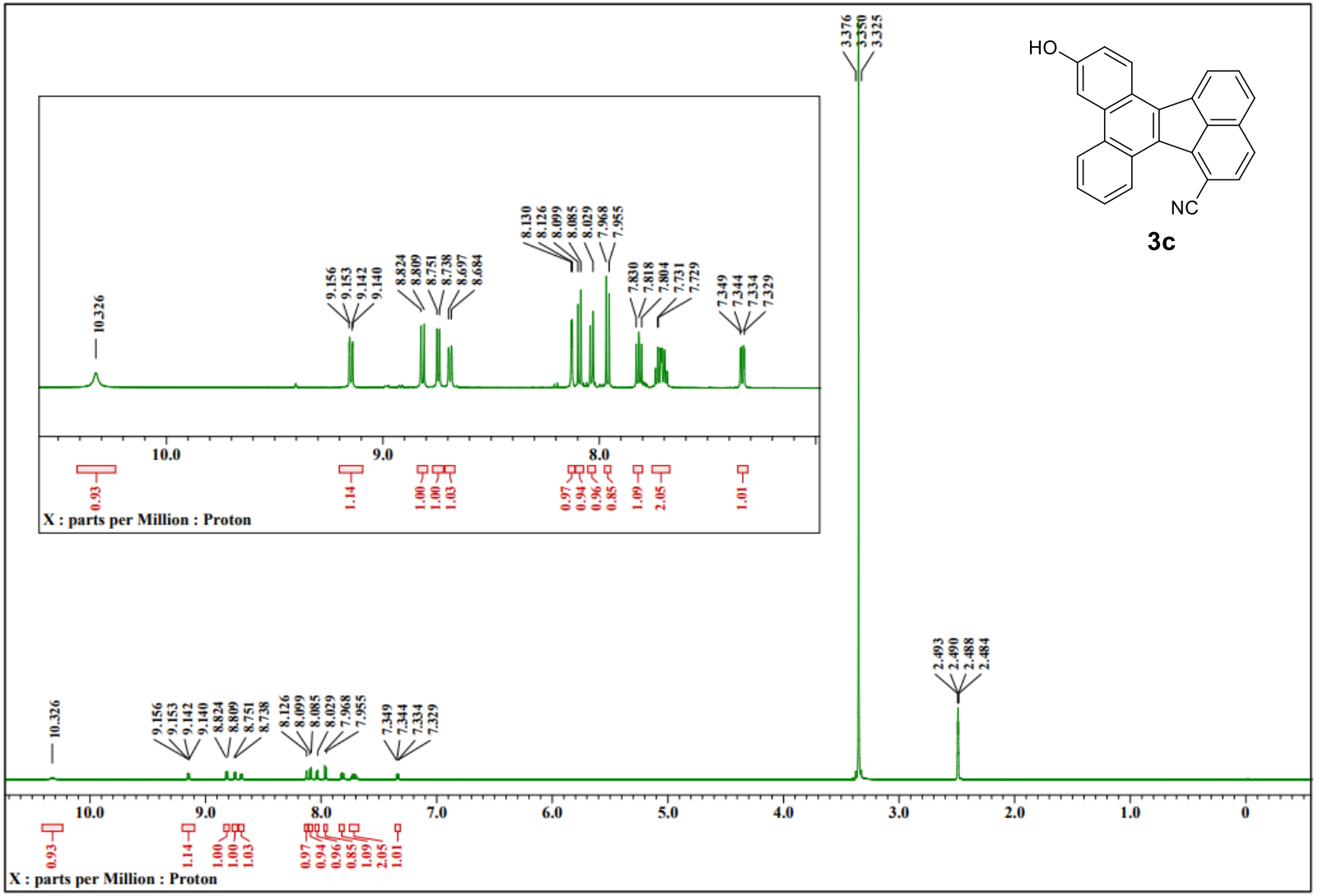
S4: ^{1}H NMR, DMSO-d6, 600 MHz



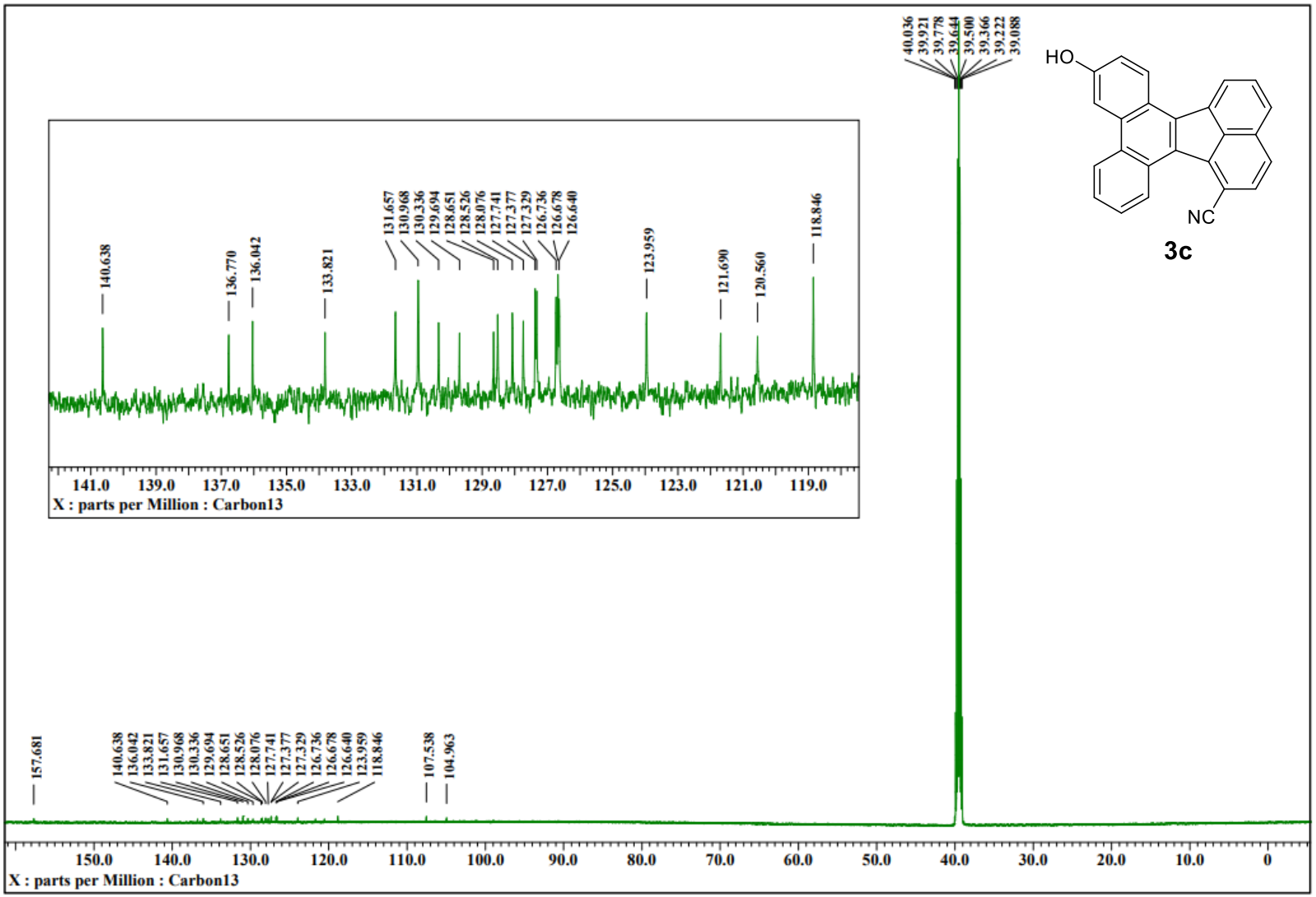
S4: ^{13}C NMR, DMSO-d6, 151 MHz



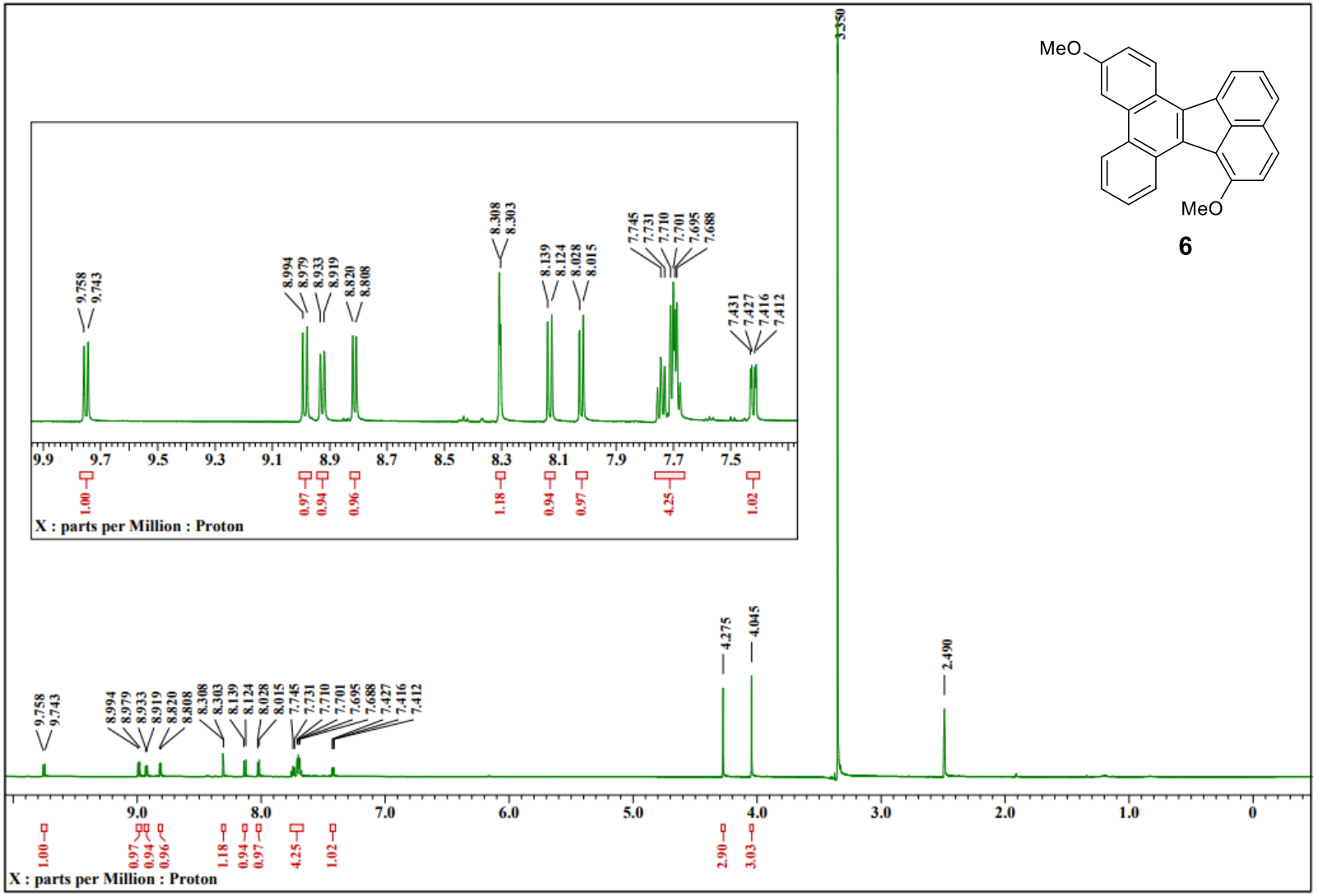
3c: ^{1}H NMR, DMSO-d6, 600 MHz



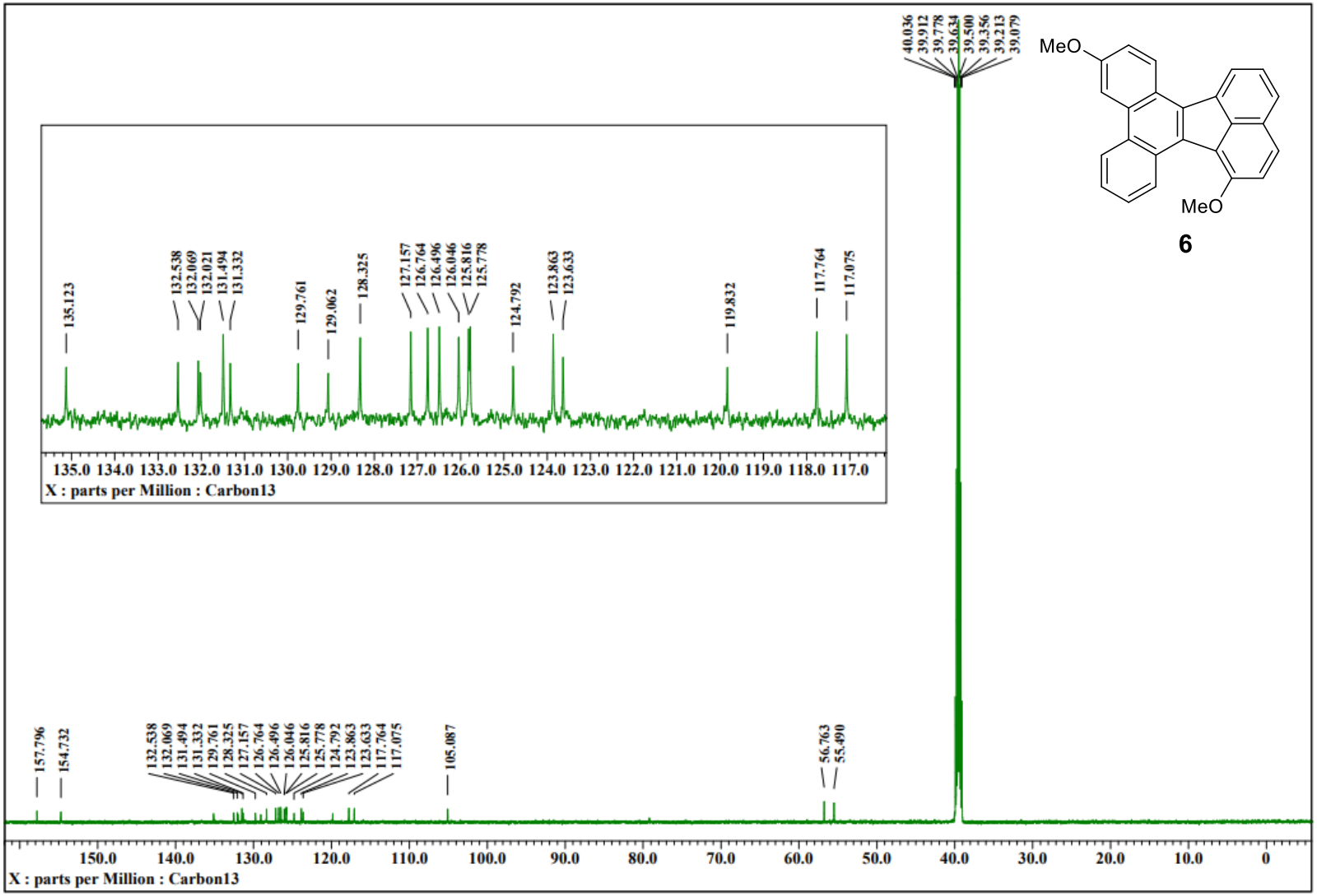
3c: ^{13}C NMR, DMSO-d6, 151 MHz



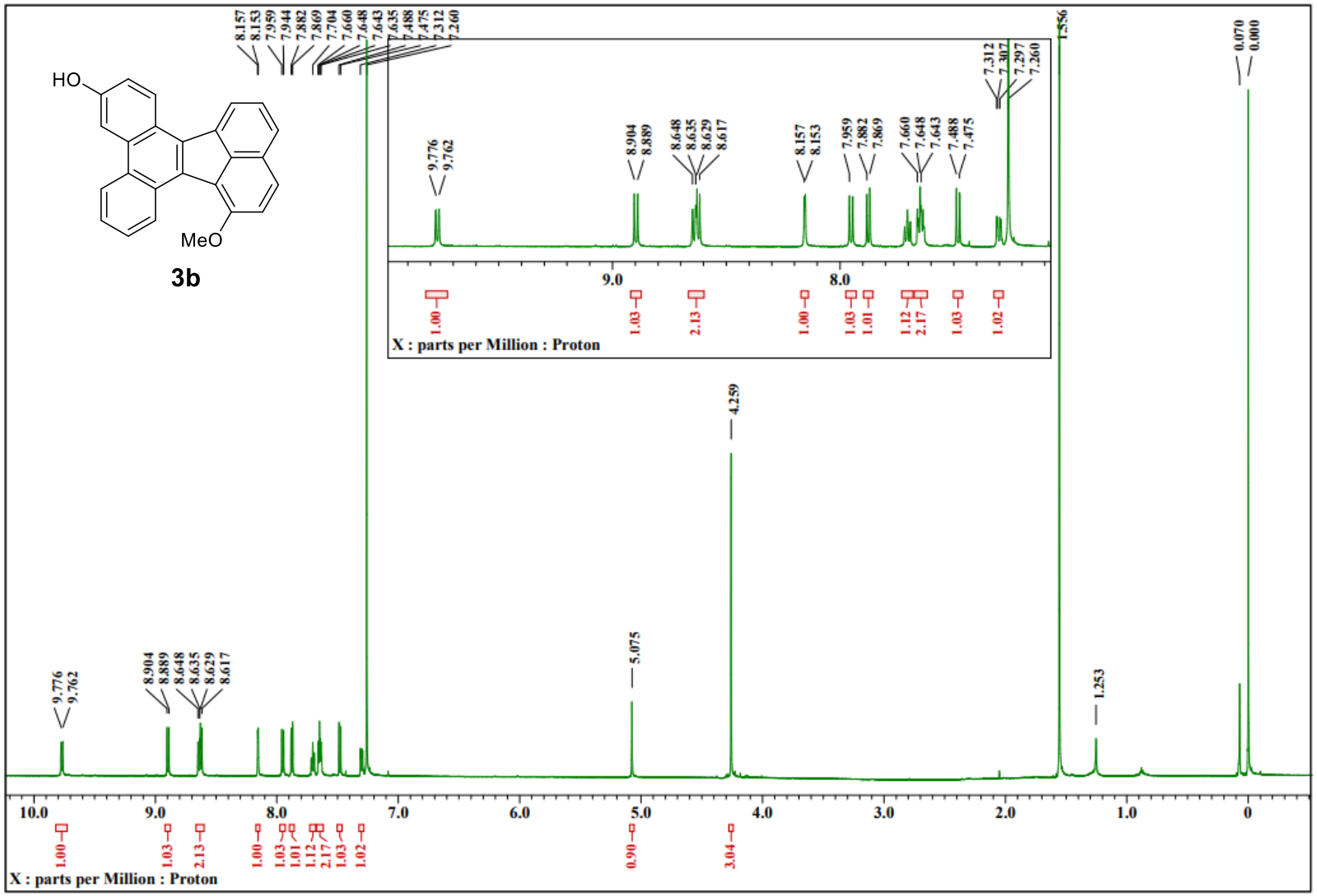
6: ^{1}H NMR, DMSO-d6, 600 MHz



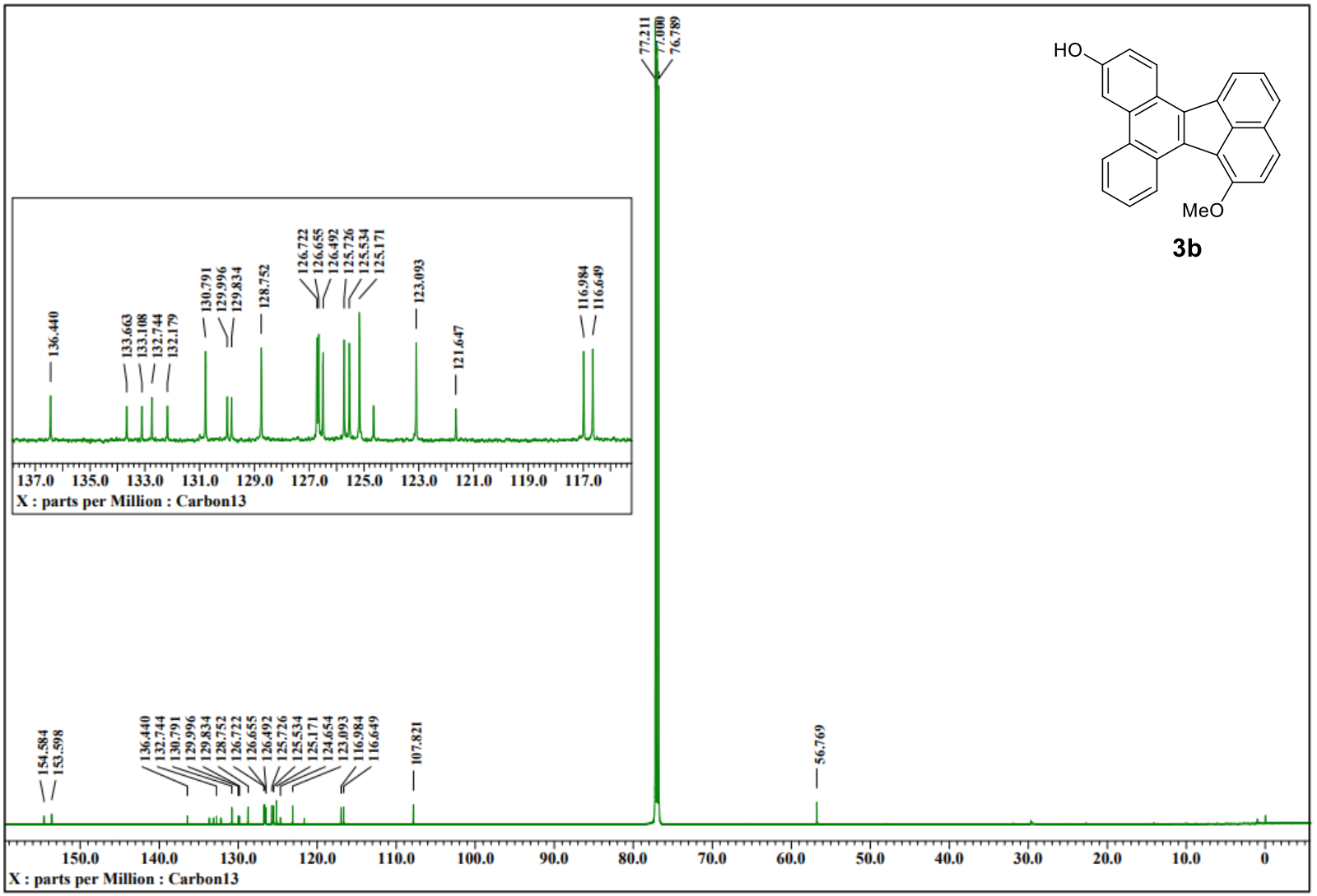
6: ^{13}C NMR, DMSO-d6, 151 MHz



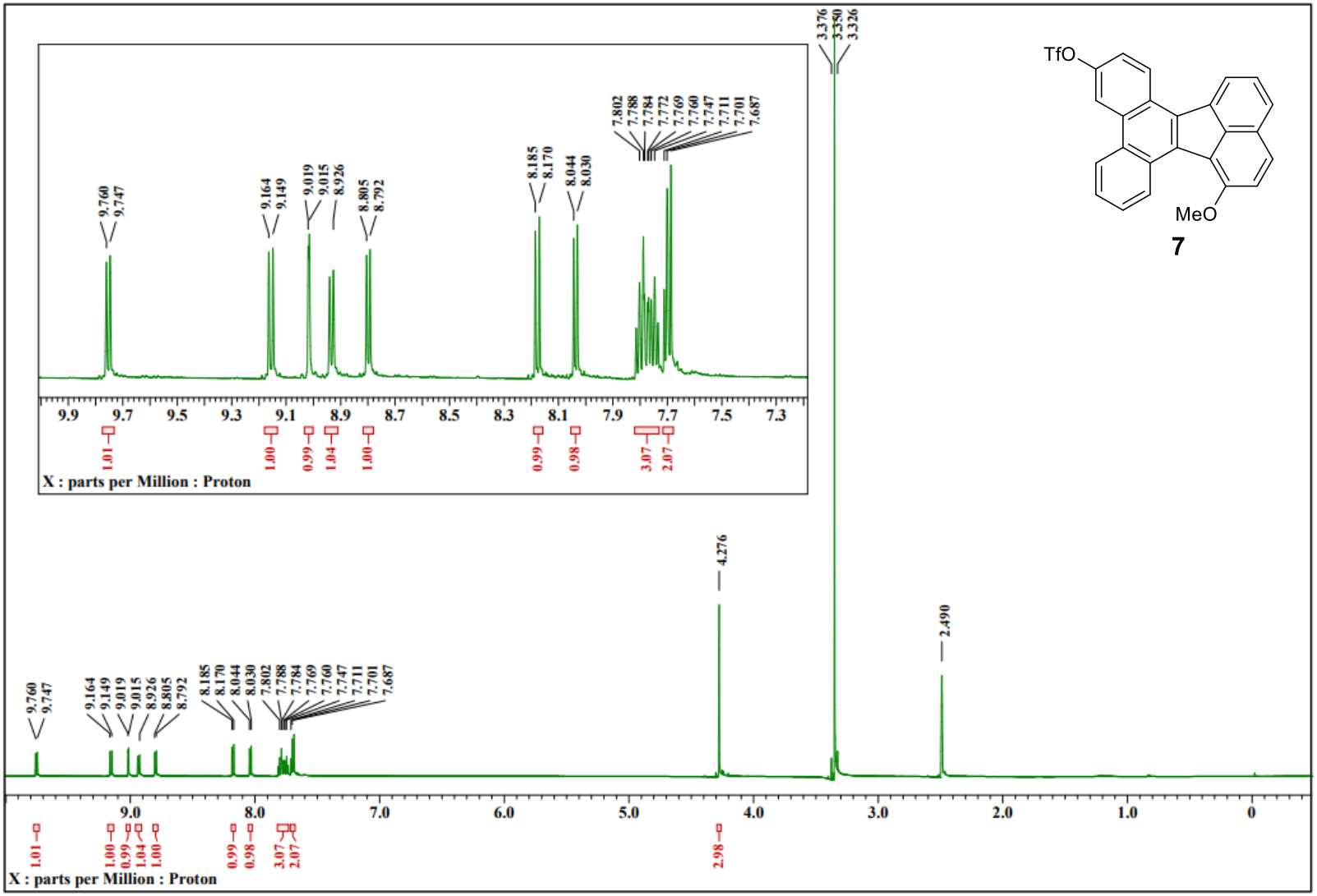
3b: ^{1}H NMR, $CDCl_3$, 600 MHz



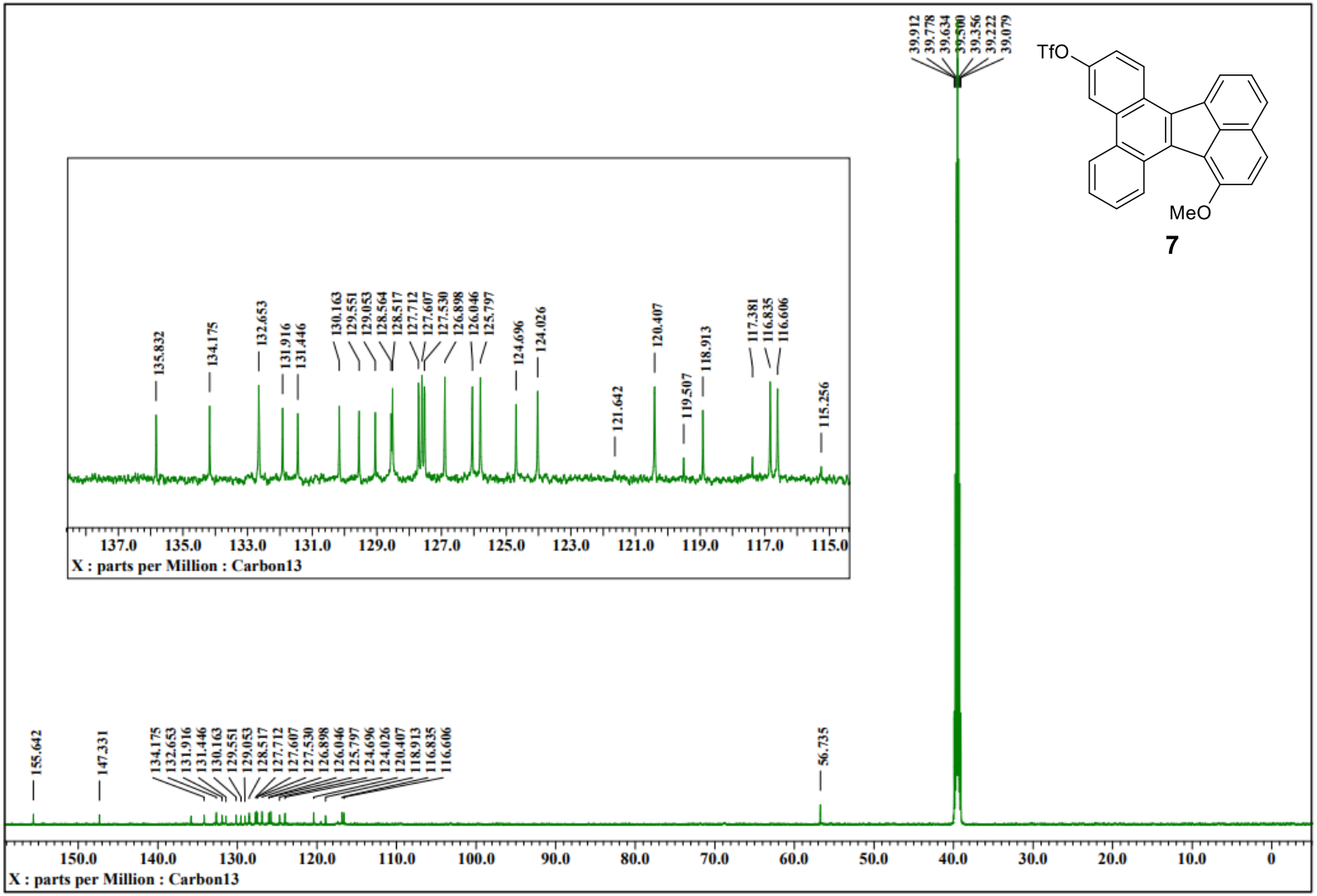
3b: ^{13}C NMR, $CDCl_3$, 151 MHz



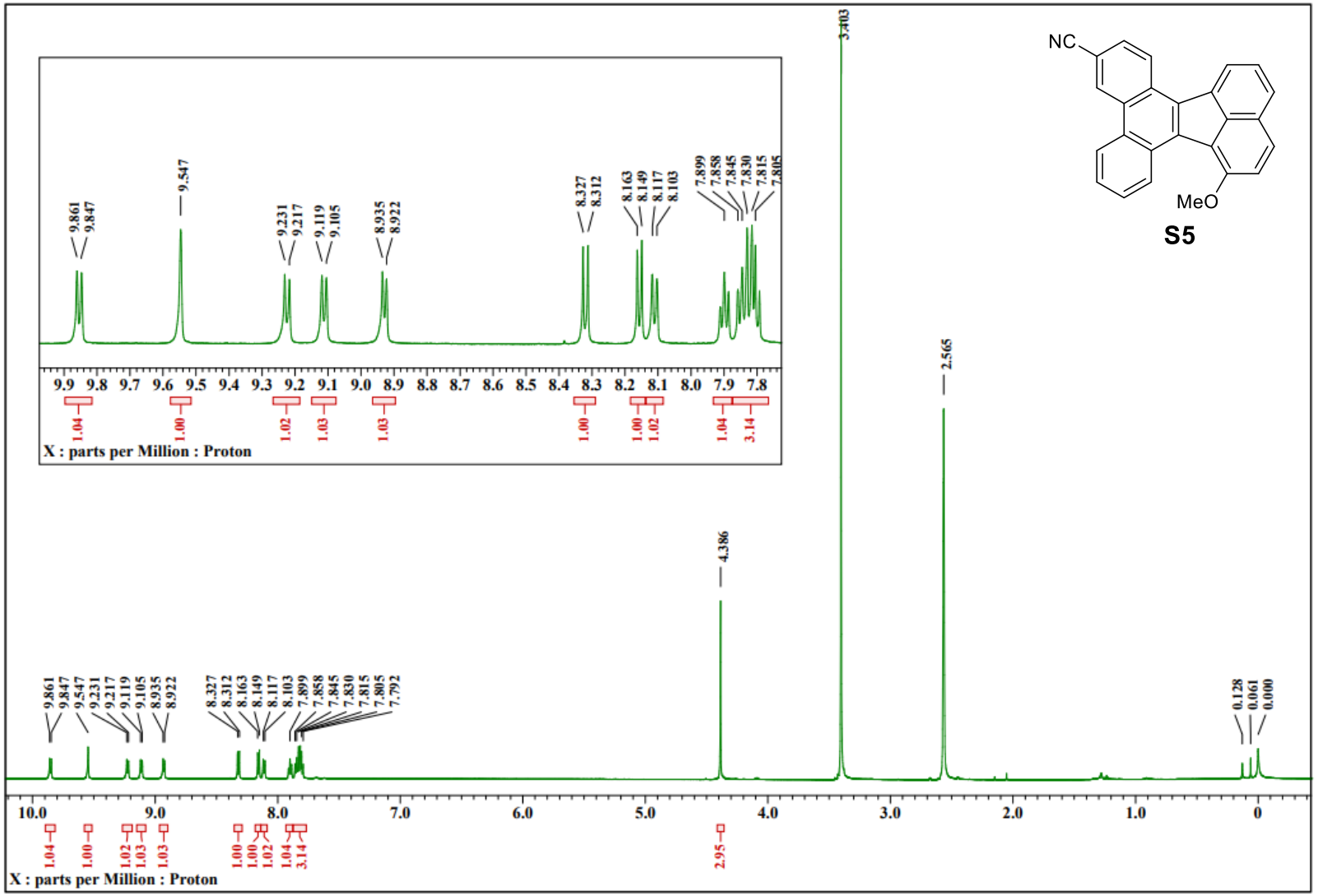
7: ^{1}H NMR, DMSO-d6, 600 MHz



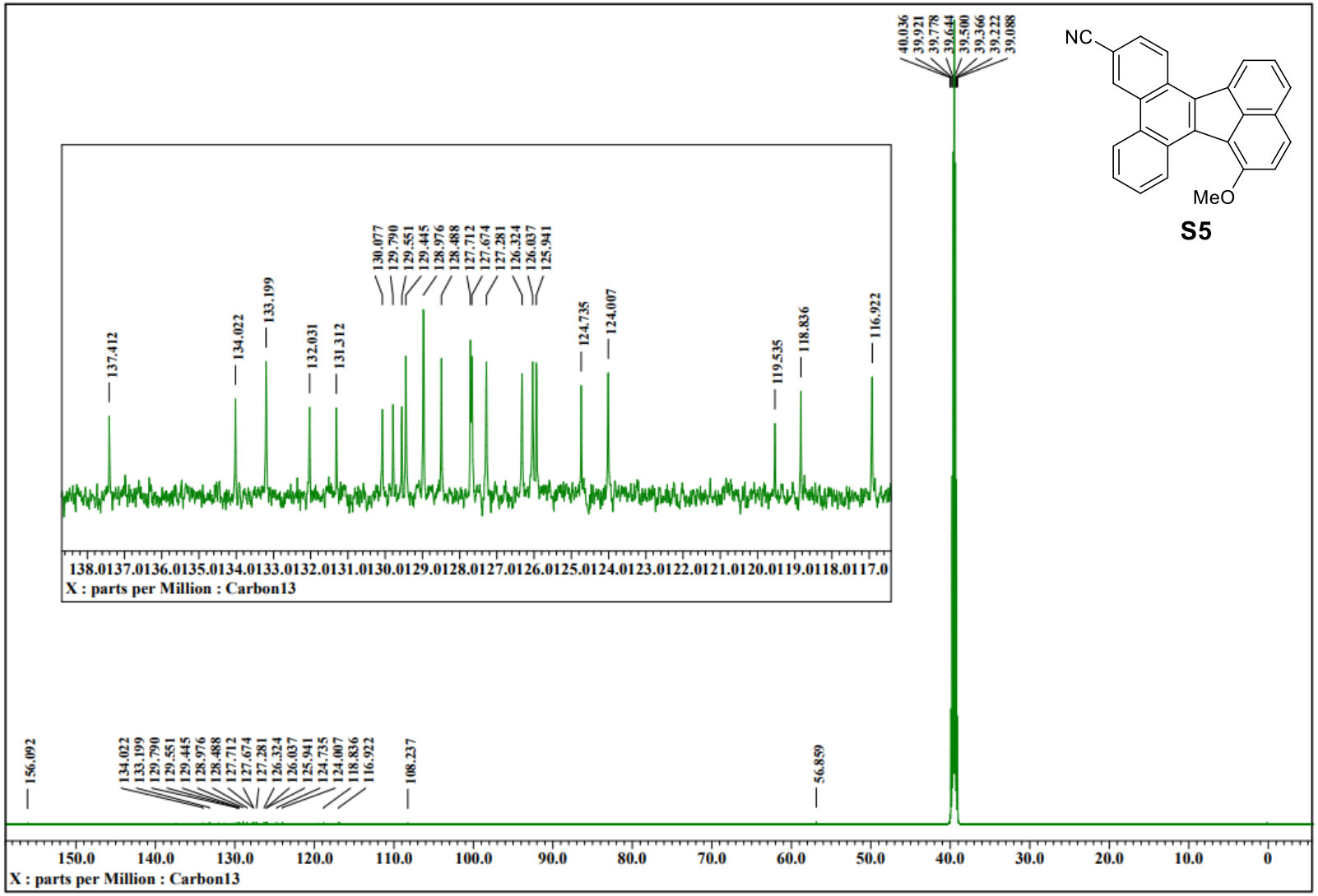
7: ^{13}C NMR, DMSO-d6, 151 MHz



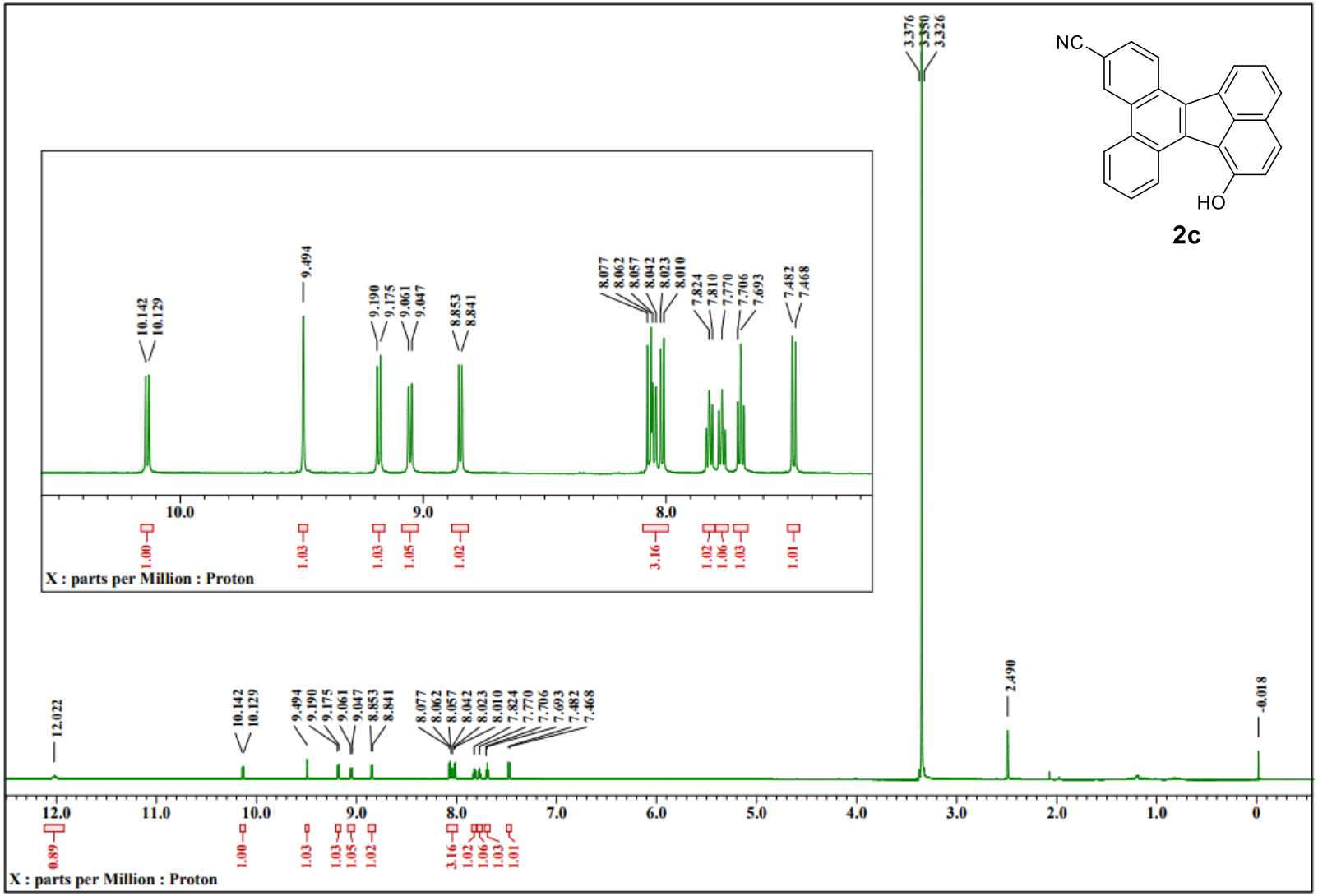
S5: ^{1}H NMR, DMSO-d6, 600 MHz



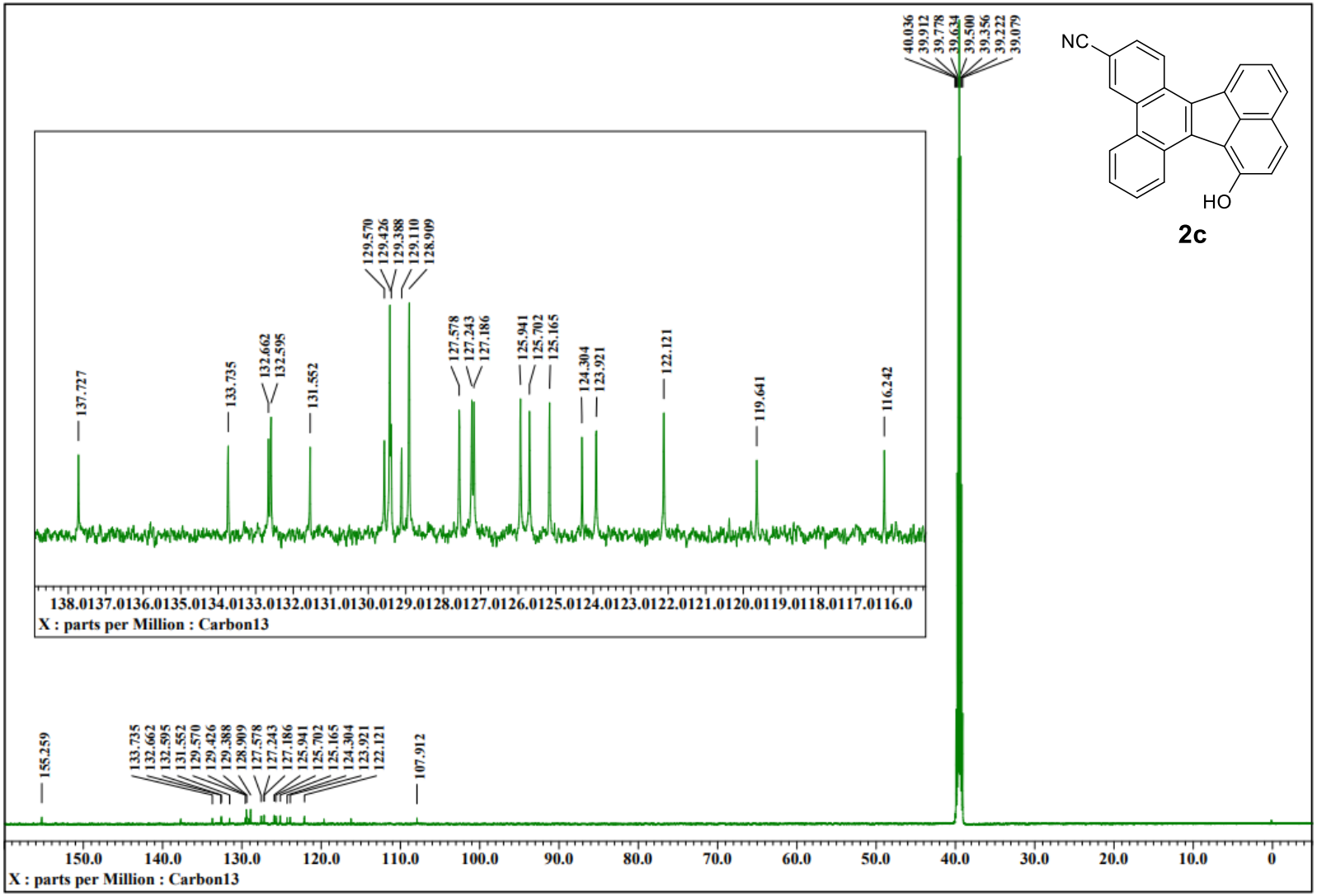
S5: ^{13}C NMR, DMSO-d6, 151 MHz



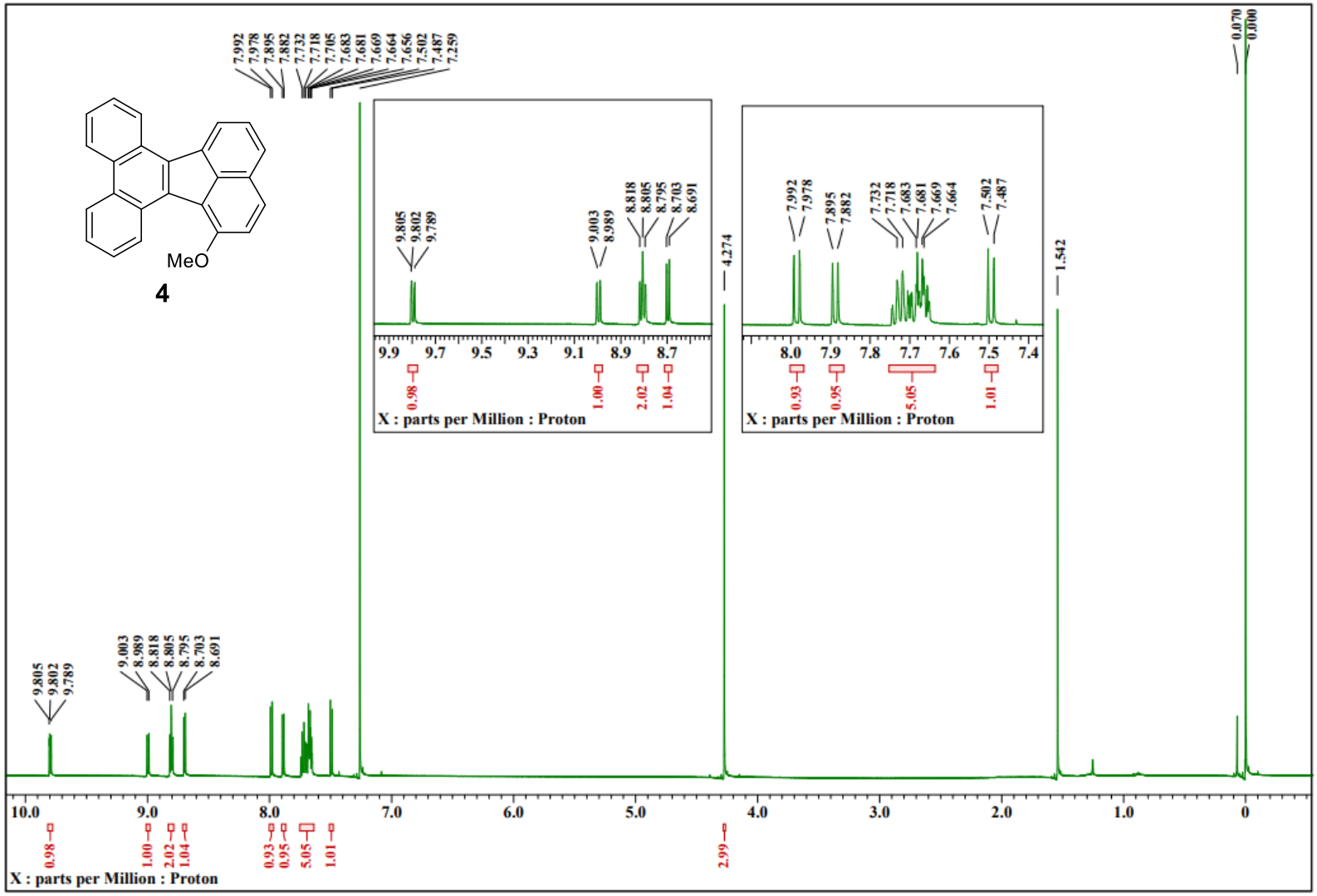
2c: ^{1}H NMR, DMSO-d6, 600 MHz



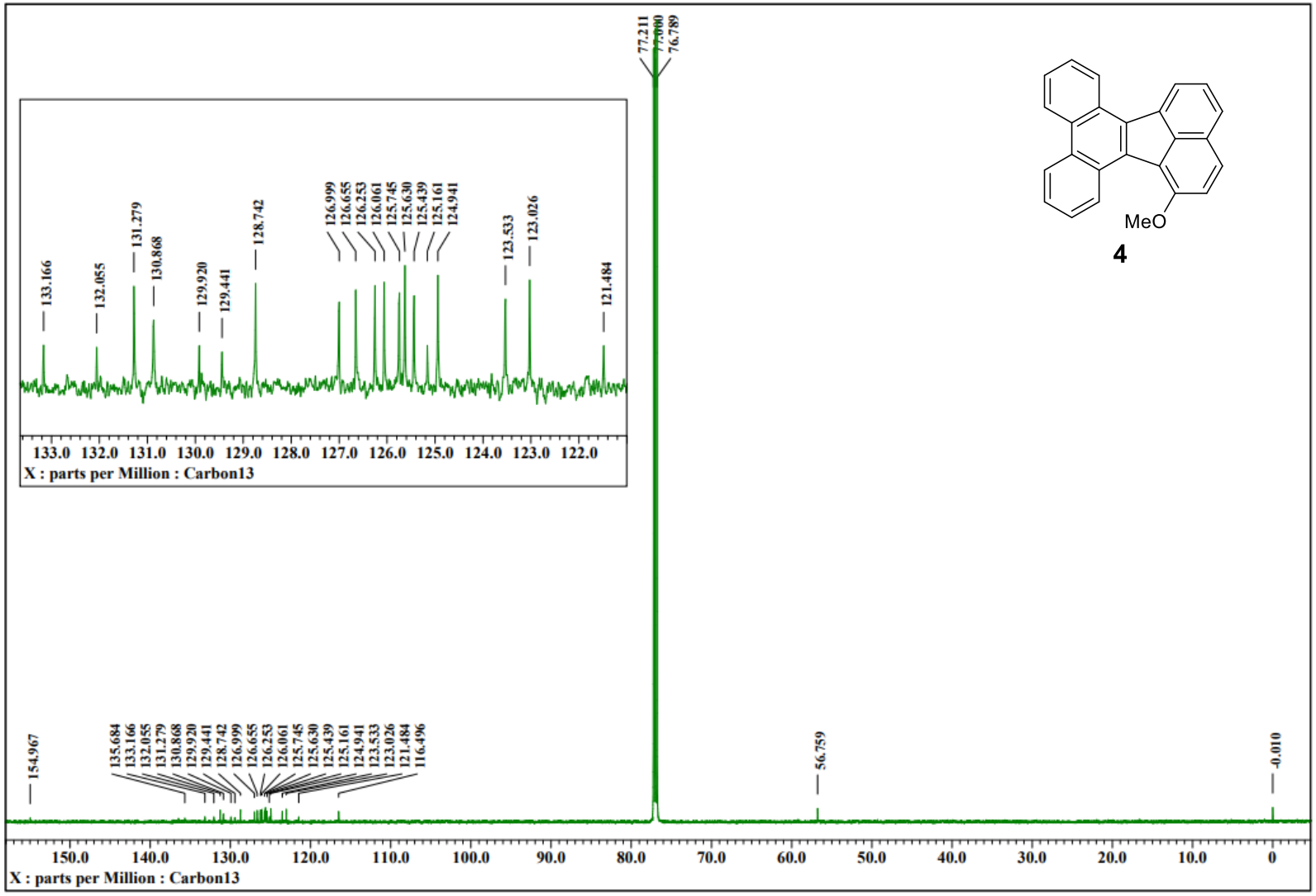
2c: ^{13}C NMR, DMSO-d6, 151 MHz



4: ^{1}H NMR, $CDCl_3$, 600 MHz



4: ^{13}C NMR, $CDCl_3$, 151 MHz



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3. J. Kruszewski and T. M. Krygowski, *Tetrahedron Lett.*, 1972, **13**, 3839–3842.
4. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.