Supporting Information for

General Synthesis of Dinaphtho[2,3-*b*:2′,3′-*f*]thieno[3,2-*b*]thiophene (DNTT) Derivatives

Kazuki Niimi, Myeong Jin Kang, Eigo Miyazaki, Itaru Osaka, Kazuo Takimiya

Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Higashi-Hiroshima 739-8527, Japan and Institute for Advanced Materials Research, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

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1. Experimental Details

General: All chemicals and solvents are of reagent grade unless otherwise indicated. 2-Methoxynaphthalene (**1a**) and 6-bromo-2-methoxynaphthalene (**6**) were purchased from TCI. Tetrahydrofuran (THF), triethylamine, *N*,*N*-dimethylformamide, (DMF), and dichloromethane were purified with standard distillation procedures prior to use. All reactions were carried out under nitrogen atmosphere unless otherwise mentioned. Melting points were uncorrected. Nuclear magnetic resonance spectra were obtained in deuterated chloroform with TMS as internal reference; chemical shifts (δ) are reported in parts per million. EI-MS spectra were obtained using an electron impact ionization procedure (70 eV). The molecular ion peaks of the chlorine, bromine, sulfur, or selenium containing compounds showed a typical isotopic pattern, and all the mass peaks are reported based on ^{32}S.

6-Decyl-2-methoxynaphthalene (1b)

To a solution of 6-bromo-2-methoxynaphthalene (**6**, 2.37 g, 10 mmol), Ni(dppp)Cl_2 (271 mg, 0.5 mmol) in THF (10 mL) was added at rt *n*-decylmagnesium bromide solution in THF, prepared from *n*-decylbromide (2.2 mL, 11 mmol) and Mg (292 mg, 12 mmol) in THF (2 mL), and the resulting mixture was refluxed for 19h. After cooling, the mixture was diluted with water (10 mL) and filtered to remove unreacted Mg and other resulting solids. The filtrate was extracted with ether (5 mL × 3), and the combined extracts were washed with brine (10 mL × 3), dried ($MgSO_4$), and evaporated in vacuo. The resulting solid was recrsytallized from hexane to give **1b** as a pale yellow solid (2.18g, 73%). Mp 48.6–49.3 ºC; ^1H NMR (270 MHz, $CDCl_3$) δ 0.87 (t, J = 6.7 Hz, 3H), 1.25–1.32 (m, 14H), 1.67 (quint,

J = 7.7 Hz, 2H), 2.72 (t, *J* = 7.2 Hz, 2H), 3.90 (s, 3H), 7.09–7.13 (m, 2H), 7.29 (dd, *J* = 8.2Hz, 1.6 Hz, 1H), 7.53 (brs, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.68 (d, *J* = 3.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$); δ 14.1, 22.7, 29.4, 29.6(× 3), 31.5, 31.9, 35.9, 55.2, 105.6, 118.5, 126.1, 126.0, 127.9, 128.9, 129.1, 132.9, 138.1, 157.0; EI-MS (70 eV) *m/z* = 298 (M^+); Anal. Calcd for $C_{21}H_{30}O$: C, 84.51; H, 10.13%. Found: C, 84.62; H, 10.41%.

7-Decyl-2-methoxynaphthalene (1d)

1-Decyne (1.2 g, 6.5 mmol), $PdCl_2(PPh_3)_2$ (0.12 g, 0.16 mmol), CuI (13 mg, 0.065 mmol), and triethylamine (14 mL, 9.8 mmol) were added successively to a deaerated solution of 7-methoxy-2-naphthyl trifluoromethanesulfonate[S1] (**7**, 1.0 g, 3.3 mmol) in and THF (20 mL). The resulting mixture was stirred for 4 h at rt, then diluted with water (30 mL), acidified with HCl aqueous solution (2 M), and extracted with dichloromethane (30 mL × 3). The combined extracts were washed with water (100 mL × 3) and dried ($MgSO_4$). Evaporation of the solvent gave a crude oily product, which was subjected to column chromatography on silica gel eluted with dichloromethane to give 7-decan-1-yl-2-methoxynaphthalene as pale yellow oil. 7-Decan-1-yl-2-methoxynaphthalene (2.8 mmol), 10% Pd/C (0.16 g), and THF (13 mL) were placed in a 50 mL round bottomed flask, and the vessel was carefully vacuumed and then purged with hydrogen gas several times. The mixture was stirred at rt, and the progress of hydrogenation was traced by TLC analysis. After the starting material disappeared on a TLC plate (usually it took more than 12 h), the catalyst was filtered off, and the filtrate was concentrated. Column chromatography of the residue on silica gel eluted with dichloromethane gave **1d** (0.80 g, 95%).

Mp 29.9–30.8 ºC; ^{1}H NMR (270 MHz, $CDCl_3$) 0.88 (t, *J* = 7.0 Hz, 3H), 1.27-1.171 (m, 16H), 2.74 (t, *J* = 7.7 Hz, 2H), 3.92 (s, 3H), 7.07 (dd, *J* = 9.7, 2.4 Hz, 1H), 7.09 (s, 1H), 7.19 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.51 (s, 1H), 7.68 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 9.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$); δ 14.4, 23.0, 29.6, 29.7, 29.9, 30.2(×2), 31.7, 32.3, 36.5, 55.6, 105.8, 118.1, 125.6, 125.7, 127.8 (×2), 129.4, 135.1, 141.4, 158.0; EI-MS (70 eV) *m/z* = 298 (M^+); Anal. Calcd for $C_{21}H_{30}O$: C, 84.51; H, 10.13%. Found: C, 84.48; H, 10.44%.

2-Methoxy-6-phenylnaphthalene (1c)

Tri-potassium phosphate n-hydrate (34 g, 0.16 mol) and phenylboronic acid (3.7 g, 30 mmol) were added to a solution **6** (6.1 g, 20 mmol) in DMF (350 mL). After bubbling for 30 min, the mixture was added $PdCl_2(PPh)_2$ (0.71 g, 1 mmol) in the shade and stirred for 4 h at 80 ºC. The mixture was added to saturated aqueous ammonium chloride solution (500 mL). The resulting precipitate was collected by filtration and was washed with water (100 mL ×3). Dryness of the solvent gave crude product, which was subjected to column chromatography on silica gel eluted with dichloromethane to give **1c** (3.4 g, 90%) as yellow crystals (from hexane). Mp 135.4–136.4 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.95 (s, 3H), 7.17 (s, 1H), 7.19 (dd, *J* = 7.9, 2.5 Hz, 1H), 7.38 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.45–7.49 (m, 2H), 7.72

(dd, J = 8.5, 1.8 Hz, 1H), 7.70–7.72 (m, 2H), 7.80 (d, J = 7.9 Hz, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.98 (d, J = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.5, 15.1, 23.0, 29.7(×2), 29.9(×2), 29.8, 31.7, 32.2, 36.4, 56.2, 104.8, 123.7, 125.4, 126.0, 126.6, 128.0, 128.6, 132.7, 140.6, 155.0; EI-MS, *m/z* = 234 (M^+); Anal. Calcd for $C_{17}H_{14}O$: C, 87.15; H, 6.02%. Found: C, 86.86; H, 5.94%.

2-Methoxy-7-phenylnaphthalene (1e)[S1]

A similar procedure as above using **7**[S1] as the substrate gave the title compound. 73% yield; yellow crystals from hexane. Mp 65.4–66.3 ºC (ref 62–64 ºC[S1]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.95 (s, 3H), 7.15 (dd, J = 8.9, 2.5 Hz, 1H), 7.38 (tt, J = 7.4, 1.2 Hz, 1H), 7.46–7.50 (m, 2H), 7.60 (dd, J = 8.5, 1.6 Hz, 1H), 7.70–7.72 (m, 2H), 7.76 (d, J = 8.9 Hz, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.95 (d, J = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 106.5, 119.1, 123.7, 125.1, 127.7, 127.8, 128.5(×2), 129.2, 129.5, 135.2, 139.5, 141.7, 158.4; EI-MS, *m/z* = 234 (M^+).

Typical procedure for the 3-methylthiolation via a selective lithiation on 2-methoxynaphthalenes

To a solution of 2-methoxynaphthalene (**1a**, 15.8 g, 100 mmol) in THF (100 mL) was added 1.67 M hexane solution of *n*-BuLi (66 mL, 110 mmol) at –78 ºC. After the mixture was stirred for 1 h at room temperature, dimethyldisulfide (11 mL, 120 mmol) was added to the solution at –78 ºC, and the resulting mixture was stirred for 20 h at room temperature. The mixture was poured into a saturated aqueous ammonium chloride solution (100 mL) and was extracted with ether (30 mL × 3). The combined ethereal extracts were washed with brine (50 mL × 3), dried ($MgSO_4$), and concentrated in vacuo. The residue was purified by recrystallization from hexane to give 3-methylthio-2-methoxynaphthalene (19.0 g, 93%) as a colorless solid. Analytical sample was obtained with recrystallization from Hexane.

2-Methoxy-3-methylthionaphthalene (2a)

93% isolated yield; colorless solid from hexane. Mp 86.9–87.8 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (s, 3H), 3.98 (s, 3H), 7.07 (s, 1H), 7.32 (ddd, J = 8.2, 8.2, 1.4 Hz, 1H), 7.37 (ddd, J = 8.2, 8.2, 1.4 Hz, 1H) 7.45 (s, 1H), 7.68 (d, J = 1.2 Hz, 1H), 7.70 (d, J = 1.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.8, 56.2, 105.0, 123.4, 124.4, 125.7, 126.7, 126.8, 129.6, 123.0, 132.4, 154.8; EI-MS (70 eV) *m/z* = 204 (M^+). Anal Calcd for $C_{12}H_{12}OS$: C, 70.55; H, 5.92%. Found: C, 70.32; H, 5.74%.

6-Decyl-2-methoxy-3-methylthionaphthalene (2b)

Quantitative yield; yellow oil (purified with column chromatography on silica gel eluted with dichloromethane-hexane (1:1, v/v, R_f = 0.35); ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.87 (t, J = 6.7 Hz, 3H), 1.25–1.32 (m, 14H), 1.67 (quint, J = 7.7 Hz, 2H), 2.72 (t, J = 7.2 Hz, 2H), 2.53 (s, 3H), 2.72 (t, J = 7.8 Hz, 2H), 3.98 (s, 3H), 7.05 (s, 1H), 7.23 (d, J = 6.8 Hz, 1H), 7.40 (s, 1H), 7.48 (s, 1H), 7.62 (d, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$); δ 14.1, 14.6, 22.7, 29.4, 29.6(× 3), 31.5, 31.9, 36.0, 55.8, 104.6, 122.9, 125.0, 126.3, 127.0, 129.4, 130.4, 138.7, 154.0; EI-MS (70 eV) *m/z* = 344 (M^+). Anal Calcd for $C_{22}H_{32}OS$: C, 76.69; H, 9.36%. Found: C, 76.83; H, 9.66%.

2-Methoxy-3-methylthio-6-phenylnaphthalene (2c)

Quantitative yield; yellow crystals from hexane. Mp 124–125.2 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 4.02 (s, 3H), 7.11 (s, 1H), 7.36 (tt, *J* = 7.4, 1.3 Hz, 1H), 7.45-7.50 (m, 2H), 7.53 (s, 1H), 7.66 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.69-7.72 (m, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 56.3, 104.8, 123.7, 124.8, 125.4, 127.3, 127.4, 127.6, 129.2, 129.9, 130.6, 131.6, 137.2, 141.6; EI-MS, *m/z* = 280 (M^+); Anal. Calcd for $C_{18}H_{16}OS$: C, 77.11; H, 5.75%. Found: C, 77.22; H, 5.75%.

7-Decyl-2-methoxy-3-methylthionaphthalene (2d)

93% yield; yellow crystals from hexane. Mp < 30 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.87 (t, *J* = 6.8 Hz, 3H), 1.24–1.69 (m, 16H), 2.53 (s, 3H), 2.72 (t, *J* = 7.8 Hz, 2H), 3.99 (s, 3H), 7.03 (s, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.44 (s, 1H), 7.48 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$); δ 14.5, 15.1, 23.0, 29.7(×2), 29.9(×2), 30.0, 31.7, 32.2, 36.4 56.2, 104.8, 123.7, 125.4, 126.0, 126.6, 128.0, 128.6, 132.7, 140.6, 155.0; EI-MS (70 eV) *m/z* = 344 (M^+). Anal Calcd for $C_{22}H_{32}OS$: C, 76.69; H, 9.36%. Found: C, 76.78; H, 9.64%.

2-Methoxy-3-methylthio-7-phenylnaphthalene (2e)

77% yield; yellow crystals from hexane. Mp 149–150 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 4.03 (s, 3H), 7.15 (s, 1H), 7.38 (tt, *J* = 7.4, 1.3 Hz, 1H), 7.46–7.49 (m, 2H), 7.47 (s, 1H), 7.61 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.70–7.72 (m, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 56.3, 105.4, 123.3, 124.2, 124.8, 127.3, 127.6(×3), 128.9, 129.2(×2), 130.2, 132.8, 141.6; EI-MS, *m/z* = 280 (M^+); Anal. Calcd for $C_{18}H_{16}OS$: C, 77.11; H, 5.75%. Found: C, 77.05; H, 5.64%.

Typical procedure for the selective demethylation on the methoxy group of 2-methoxy-3-methylthionaphthalenes

To a solution of 2-methoxy-3-methylthionaphthalene (**2a**, 10 g, 49 mmol) in dichloromethane (30 mL) was added dropwise a dichloromethane solution of BBr_3 (ca. 2 M 50 mL, 100 mmol) at –78 ºC. After the stirring was maintained for 19 h at room temperature, the mixture was added ice (approximately 30 g) at 0 ºC. The resulting mixture was extracted with dichloromethane (50 mL × 3). The combined organic layer was washed with brine (50 mL × 3), dried ($MgSO_4$) and concentrated in vacuo to give practically pure 3-methylthio-2-naphthol (9.2 g, quantitative yield) as a white solid.

3-Methylthio-2-naphthol (3a) [S2]

Quantitative yield. Mp 83.5–84.0 ºC (ref. 83–84 ºC[S2]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 6.60 (s, 1H), 7.30 (ddd, *J* = 8.2, 8.2, 1.4 Hz, 1H), 7.31 (s, 1H), 7.41 (ddd, *J* = 8.2, 8.2, 1.4 Hz, 1H), 7.67 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.71 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.99 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.3, 109.8, 124.4, 125.0, 127.0, 127.6, 127.9, 129.6, 134.4, 135.6, 153.2; IR (KBr) ν = 3348 cm^{-1} (OH); EIMS (70 eV) *m/z* = 190 (M^+).

6-Decyl-3-methylthio-2-naphthol (3b)

72% yield; white solid from hexane. Mp 65.5–66.0 ºC; ^{1}H NMR (270 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.7 Hz, 3H), 1.26–1.32 (m, 14H), 1.67 (quint, *J* = 7.7 Hz, 2H), 2.41 (s, 3H), 2.71 (t, *J* = 7.3 Hz, 2H), 6.57 (s, 1H), 7.28 (s, 1H), 7.28 (dd, *J* = 8.2 Hz, 1.6 Hz, 1H), 7.48 (brs, 1H), 7.61 (d, *J* = 8.6 Hz, 1H), 7.94 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 19.9, 22.7, 29.3, 29.6(× 3), 31.4, 31.9, 35.9, 109.1, 124.1, 125.7, 126.3, 128.7, 129.1, 133.5(× 2), 138.5, 152.1; IR (KBr) ν = 3402 cm^{-1} (OH); EIMS (70 eV) *m/z* = 330 (M^+); Anal. Calcd for $C_{21}H_{30}OS$: C, 76.31; H, 9.15%. Found: C, 76.34; H, 9.23%.

3-Methylthio-6-phenyl-2-naphthol (3c)

73% yield; yellow crystals from hexane. Mp 128.9–129.8 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 6.63 (s, 1H), 7.35 (s, 1H), 7.37 (tt, *J* = 7.4, 1.3 Hz, 1H), 7.45–7.50 (m, 2H), 7.72 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H) 7.68-7.72 (m, 2H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 109.4, 125.2, 125.5, 127.1, 127.3, 127.5, 127.6, 129.2, 129.5, 134.5 (×2), 137.0, 141.3, 153.1; IR (KBr) ν = 3402 cm^{-1} (OH); EI-MS, *m/z* = 266 (M^+); Anal. Calcd for $C_{17}H_{14}OS$: C, 76.66; H, 5.30%. Found: C, 76.50; H, 5.15%.

7-Decyl-3-methylthio-2-naphthol (3d)

85% yield; yellow crystals from hexane. Mp 64.4–65.4 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.24-1.72 (m, 16H), 2.40 (s, 3H), 2.72 (t, *J* = 7.7 Hz, 2H), 6.63 (s, 1H), 7.17 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.45 (s, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.97 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.4, 20.4, 23.0, 29.6, 29.7, 29.9 (×2), 31.6, 32.2, 36.5, 109.1, 123.4, 125.2, 125.9, 127.5, 127.8, 134.5, 135.8, 142.3, 153.2; IR (KBr) ν = 3402 cm^{-1} (OH); EI-MS, *m/z* = 330 (M^+); Anal. Calcd for $C_{21}H_{30}OS$: C, 76.31; H, 9.15%. Found: C, 76.62; H, 9.38%.

3-Methylthio-7-phenyl-2-naphthol (3e)

94% yield; yellow crystals from hexane; Mp 149–150 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 6.64 (s, 1H), 7.38–7.40 (m, 2H), 7.48 (tt, *J* = 7.6, 1.8 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.70–7.72 (m, 2H), 7.80 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.88 (s, 1H), 8.02 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 109.8, 124.1, 124.7, 127.7, 127.9, 128.5, 129.2(×2), 134.1, 135.7, 140.1, 141.3, 153.4; IR (KBr) ν = 3497 cm^{-1} (OH); EI-MS, *m/z* = 266 (M^+); Anal. Calcd for $C_{17}H_{14}OS$: C, 76.66; H, 5.30%. Found: C, 76.97; H, 5.14%.

Typical procedure for the synthesis of 3-methylthio-2-naphthyl trifluoromethanesulfonate

To a deaerated solution of 3-methylthio-2-naphthol (**3a**, 7.4 g, 39 mmol) and pyridine (10.0 mL, 124 mmol) in dichloromethane (100 mL) was added trifluoromethanesulfonic anhydride (7.5 mL, 45 mmol) at 0 ºC. After stirring for 15 h at room temperature, the mixture was diluted with water (10 mL) and hydrochloric acid (4 M, 50 mL). The resulting mixture was extracted with dichloromethane (30 mL × 3). The combined organic layers were washed with brine (50 mL × 3), dried ($MgSO_4$), and concentrated in vacuo to give practically pure 3-methylthio-2-(trifluoromethanesulfonyloxy)naphthalene (13.0 g, quantitative yield) as a yellow solid.

3-Methylthio-2-naphthyl trifluoromethanesulfonate (4a)

Quantitative yield; yellow solid from hexane. Mp 56.5–57.0 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.59 (s, 3H), 7.49 (ddd, *J* = 8.2, 8.2, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.2, 8.2, 1.4 Hz, 1H), 7.69 (s, 1H), 7.72 (s, 1H), 7.78 (d, *J* = 5.2 Hz, 1H), 7.80 (d, *J* = 5.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 15.8, 118.8 (q, *J* = 319 Hz), 119.5, 126.7, 126.7, 126.8, 126.9, 127.8, 128.0, 131.1, 132.8, 145.4; IR (KBr) ν = 1414, 1219 cm^{-1} (-O-SO_2-); EIMS (70 eV) *m/z* = 322 (M^+); Anal Calcd for $C_{12}H_9F_3O_3S_2$: C, 44.72; H, 2.81%. Found C, 44.57; H, 2.60%.

6-Decyl-3-methylthio-2-naphthyl trifluoromethanesulfonate (4b)

Quantitative yield; yellow solid from hexane. Mp 42.0–42.9 ºC; ^{1}H NMR (270 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.7 Hz, 3H), 1.26–1.32 (m, 14H), 1.68 (quint, *J* = 7.7 Hz, 2H), 2.59 (s, 3H), 2.76 (t, *J* = 7.3 Hz, 2H), 7.36 (dd, *J* = 8.7 Hz, 1.8 Hz, 1H), 7.57 (brs, 1H), 7.63 (s, 1H), 7.68 (s, 1H), 7.72 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 15.8, 22.7, 29.3(× 2), 29.5, 29.6(× 2), 31.2, 31.9, 36.1, 118.7 (q, *J* = 319 Hz), 119.2, 125.2, 126.3, 127.7, 128.4, 129.4, 130.7, 133.0, 142.7, 144.8; IR (KBr) ν = 1423, 1211 cm^{-1} (-O-SO_2-); EIMS (70 eV) *m/z* = 462 (M^+); Anal Calcd for $C_{22}H_{29}F_3O_3S_2$: C, 57.12; H, 6.32%. Found C, 56.91; H, 6.15%.

3-Methylthio-6-phenyl-2-naphthyl trifluoromethanesulfonate (4c)

Quantitative yield; yellow crystals from hexane. Mp 79.4–80.3 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (s, 3H), 7.42 (tt, *J* = 7.4, 1.3 Hz, 1H), 7.43–7.52 (m, 2H), 7.68–7.71 (m, 2H), 7.74 (s, 1H), 7.75 (s, 1H), 7.77 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 1.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 16.0, 119.0 (q, *J* = 321 Hz), 119.6, 124.9, 126.8, 127.1, 127.8, 128.2, 128.7, 129.3, 130.5, 131.9, 133.4, 140.7, 140.9, 145.6; IR (KBr) ν = 1429, 1225 cm^{-1} (O-SO_2-); EI-MS, *m/z* = 398 (M^+); Anal. Calcd for $C_{18}H_{13}O_3S_2F_3$: C, 54.26; H, 3.29%. Found: C, 54.17; H, 3.01%.

7-Decyl-3-methylthio-2-naphthyl trifluoromethanesulfonate (4d)

94% yield; yellow crystals from hexane. Mp 149–150 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 6.64 (s, 1H), 7.38–7.40 (m, 2H), 7.48 (tt, *J* = 7.6, 1.8 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.70–7.72 (m, 2H), 7.80 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.88 (s, 1H), 8.02 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 14.4, 16.4, 23.0, 29.6, 29.7, 29.8, 29.9, 30.0, 31.5, 32.2, 36.3, 119.0 (q, *J* = 320 Hz), 119.3, 126.6, 127.0, 127.5, 129.7, 129.9, 131.6, 131.8, 142.1, 125.9; IR (KBr) ν = 1427, 1213 cm^{-1} (-O-SO_2-); EI-MS, *m/z* = 266 (M^+); Anal. Calcd for $C_{17}H_{14}OS$: C, 76.66; H, 5.30%. Found: C, 76.97; H, 5.14%.

3-Methylthio-7-phenyl-2-naphthyl trifluoromethanesulfonate (4e)

Quantitative yield; yellow crystals from hexane. Mp 87.8–88.7 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (s, 3H), 7.41 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.45-7.52 (m, 2H), 7.68–7.71 (m, 2H), 7.72 (s, 1H), 7.79 (s, 1H), 7.82 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 8.00 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 16.0, 119.0 (q, *J* = 321 Hz), 120.0, 125.9, 126.8, 127.6, 127.7, 127.8, 128.2, 129.3, 131.3, 131.7, 132.3, 139.8, 140.5, 146.0; IR (KBr) ν = 1425, 1209 cm^{-1} (O-SO_2-); EI-MS, *m/z* = 398 (M^+); Anal. Calcd for $C_{18}H_{13}O_3S_2F_3$: C, 54.26; H, 3.29%. Found: C, 54.42; H, 3.08%.

Typical procedure for the Stille cross-coupling reaction between

***trans*-1,2-bis(tributylstannyl)ethene and 3-methylthio-2-naphthyl trifluoromethanesulfonate**

To a deaerated solution of 3-methylthio-2-naphthyl trifluoromethanesulfonate (**4a**, 3.2 g, 10 mmol) and *trans*-1,2-bis(tributylstannyl)ethene (3.0 g, 5.0 mmol) in DMF (40 mL) was added $Pd(PPh_3)_4$ (322 mg, 3.0 mmol, 3 mol%). The mixture was heated at 100 ºC for 18 h in dark and then diluted with water. Then the mixture was extracted with chloroform. The combined extracts were washed with brine, dried ($MgSO_4$), and concentrated in vacuo. The residue was passed through a silica gel pad with dichloromethane as eluent to give *trans*-1,2-bis(3-methylthionaphthalen-2-yl)ethene (1.8 g, quantitative yield) as a yellow solid.

***trans*-1,2-Bis(3-methylthionaphthalen-2-yl)ethene (5a)** [S3]

Quantitative yield; yellow solid from chloroform. Mp 197.5–198.0 ºC (ref 195.0–196.0 ºC[S3]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 6H), 7.43 (ddd, *J* = 7.4, 7.4, 1.7 Hz, 2H), 7.46 (ddd, *J* = 7.6, 7.6, 1.7 Hz, 2H), 7.64 (s, 2H), 7.66 (s, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.0 Hz, 2H), 8.10 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 124.1, 125.2, 125.6, 126.45, 126.54, 127.9, 128.5, 131.5, 133.4, 134.9, 135.9; EI-MS (70 eV) *m/z* = 372 (M^+).

***trans*-1,2-Bis(6-decyl-3-methylthionaphthalen-2-yl)ethene (5b)** [S4]

Quantitative yield; yellow solid from hexane. Mp 116.8–117.7 ºC (ref 116.8–117.7 ºC[S4]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.4 Hz, 6H), 1.29–1.70 (m, 32H), 2.58 (s, 6H), 2.75 (t, *J* = 8.4 Hz, 4H), 7.29 (dd, *J* = 8.8, 1.6 Hz, 2H), 7.52 (s, 2H), 7.59 (s, 2H), 7.64 (s, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 8.06 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.4, 16.8, 23.0, 24.2, 29.6, 29.8, 29.9, 30.0, 31.7, 32.2, 36.5, 124.3, 125.2, 125.3 127.6, 128.0, 128.4, 130.3, 133.9, 134.5, 136.0 141.6; EI-MS *m/z* = 652 (M^+).

***trans*-1,2-Bis(3-methylthio-6-phenylnaphthalen-2-yl)ethane (5c)**

57% yield; yellow crystals from hexane. Mp 191.5–192.4 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (s, 6H), 7.40 (tt, *J* = 7.2, 1.6 Hz, 2H), 7.48–7.53 (m, 4H), 7.71 (s, 2H), 7.72 (s, 2H), 7.73–7.76 (m, 4H), 7.76 (d, *J* = 8.7 Hz, 2H), 7.94 (d, *J* = 8.7 Hz, 2H), 7.97 (s, 2H), 8.14 (s, 2H); EI-MS, *m/z* = 524 (M^+); Anal. Calcd for $C_{34}H_{25}S_2$: C, 82.40; H, 5.38%. Found: C, 82.22; H, 5.29%.

***trans*-1,2-Bis(7-decyl-3-methylthionaphthalen-2-yl)ethene (5d)**

Quantitative yield; yellow crystals from hexane. Mp 87.8–88.7 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (s, 3H), 7.41 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.45–7.52 (m, 2H), 7.68–7.71 (m, 2H), 7.72 (s, 1H), 7.79 (s, 1H), 7.82 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 8.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.2, 120.0, 125.9, 126.9, 127.7, 127.8, 128.1, 129.4, 131.3, 131.8, 132.2, 139.9, 140.5, 146.1; EI-MS, *m/z* = 398 (M^+); Anal. Calcd for $C_{18}H_{13}O_3S_2F_3$: C, 54.26; H, 3.29%. Found: C, 54.42; H, 3.08%.

***trans*-1,2-Bis(3-methylthio-7-phenylnaphthalen-2-yl)ethane (5e)**

63% yield; yellow crystals from hexane. Mp 87.8–88.7 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 6H), 7.40 (tt, *J* = 7.4, 1.2 Hz, 2H), 7.48–7.52 (m, 4H), 7.68 (s, 2H), 7.73–7.76 (m, 4H), 7.72 (s, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 2H), 8.08 (s, 2H), 8.17 (s, 2H); EI-MS, *m/z* = 524 (M^+); Anal. Calcd for $C_{34}H_{25}S_2$: C, 82.40; H, 5.38%. Found: C, 82.38; H, 5.22%.

Typical procedure for the synthesis of DNTT derivatives

A solution of *trans*-1,2-bis(3-methylthionaphthalen-2-yl)ethene (**5a**, 0.2235 g, 0.60 mmol) and iodine (4.87 g, 19.2 mmol) in chloroform (15 mL) was refluxed for 21 h. After cooling to room temperature, saturated aqueous sodium hydrogen sulfite solution (20 mL) was added, and the resulting precipitate was collected by filtration and was washed with water and chloroform. The crude product was purified by vacuum sublimation (source temperature: 220 ºC under ~10^{-3} Pa) to give analytical sample of DNTT as a yellow solid (0.173 g, 85%).

Dinaphtho[2,3-*b*:2',3'-*f*]thieno[3,2-*b*]thiophene

85% yield; yellow crystals. Mp >300 ºC (ref >300 ºC[S3]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.57 (m, 4H), 7.96–7.98 (m, 2H), 8.05–8.07 (m, 2H), 8.40 (s, 2H), 8.45 (s, 2H); EI-MS (70 eV) *m/z* = 340 (M^+).

2,9-Didecyldinaphtho[2,3-*b*:2',3'-*f*]thieno[3,2-*b*]thiophene (2,9-C_{10}-DNTT)

81% yield; yellow solid from chlorobenzene. Mp > 300 ºC (ref >300 ºC[S4]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* =8.4 Hz, 6H), 1.21–1.74 (m, 32H), 2.80 (t, *J* = 7.6 Hz, 4H), 7.40 (dd, *J* = 8.8, 1.9 Hz, 2H), 7.71 (s, 2H), 7.95 (d, *J* = 8.8 Hz, 2H), 8.32 (s, 2H), 8.34 (s, 2H); EI-MS (70 eV) *m/z* = 620 (M^+).

2,9-Diphenyldinaphtho[2,3-*b*:2'.3'-*f*]thieno[3,2-*b*]thiophene (2,9-DPhDNTT)

89% yield; yellow crystals from chlorobenzene. Mp > 300 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) no peak owing to poor solubility; EI-MS, *m/z* = 492 (M^+); Anal. Calcd for $C_{34}H_{20}S_2$: C, 82.89; H, 4.09%. Found: C, 82.73; H 3.75%.

3,10-Didecyldinaphtho[2,3-*b*:2´,3´-*f*]thieno[3,2-*b*]thiophene (3,10-C_{10}-DNTT)

71% yield; yellow crystals from chlorobenzene. Mp 187–188 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.9 Hz, 6H), 1.24–1.79 (m, 32H), 2.82 (t, *J* = 7.7 Hz, 4H), 7.38 (dd, *J* = 8.5, 1.6 Hz, 2H), 7.79 (s, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 8.29 (s, 2H), 8.36 (s, 2H); EI-MS, *m/z* = 620 (M^+); Anal. Calcd for $C_{42}H_{52}S_2$: C, 81.46; H, 8.43%. Found: C, 81.13; H, 8.43%.

3,10-Diphenyldinaphtho[2,3-*b*:2'.3'-*f*]thieno[3,2-*b*]thiophene (3,10-DPhDNTT)

85% yield; yellow crystals from chlorobenzene. Mp > 300 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) no peak owing to poor solubility; EI-MS, *m/z* = 492 (M^+); Anal. Calcd for $C_{34}H_{20}S_2$: C, 82.89; H, 4.09%. Found: C, 82.80; H 3.78%.

2. FET characteristics of C10- and DPh-DNTTs-based devices

OFETs were fabricated in a "top-contact" configuration on a heavily doped n^+-Si (100) wafer with a 200 nm thermally grown SiO_2 (C_i = 17.3 nF cm^{-2}). The substrate surfaces were treated with octyltrichlorosilane (OTS) or octadecylsilane (ODTS) as reported previously.[S4] A thin film of DNTT derivatives as the active layer was vacuum-deposited on the Si/SiO_2 substrates maintained at various temperatures (T_{sub}) at a rate of 1 Å s^{-1} under a pressure of ~10^{-3} Pa. On top of the organic thin film, gold films (80 nm) as drain and source electrodes were deposited through a shadow mask. For a typical device, the drain-source channel length (L) and width (W) are 50 μm and 1.5 mm, respectively. Characteristics of the OFET devices were measured at room temperature under ambient conditions with a Keithley 4200 semiconducting parameter analyzer. Field-effect mobility (μ_{FET}) was calculated in the saturation (V_d = –60 V) of the I_d using the following equation,

$$I_d = C_i \mu_{FET} (W/2L) (V_g - V_{th})^2$$

where C_i is the capacitance of the SiO_2 insulator, and V_g and V_{th} are the gate and threshold voltages, respectively. Current on/off ratio (I_{on}/I_{off}) was determined from the I_d at V_g = 0 V (I_{off}) and V_g = –60 V (I_{on}). The μ_{FET} data reported are typical values from more than six different devices.

Table S1. Characteristics of FETs based on new DNTT derivatives.

SAM	Material	T_{sub} / ºC	μ_{FET}[a] / cm^2 V^{-1} s^{-1}	I_{on}/I_{off}	V_{th} / V
OTS[b]	3,10-C_{10}-DNTT	rt	3.71	1×10^7	–7.7
	2,9-DPh-DNTT	100	1.44	3×10^8	–8.8
	3,10-DPh-DNTT	100	2.27	2×10^8	–18
ODTS[b]	3,10-C_{10}-DNTT	100	8.02	1×10^9	–15
	2,9-DPh-DNTT	100	3.43	6×10^8	–9.4
	3,10-DPh-DNTT	100	3.81	5×10^8	–21

[a] data from more than 6 devices. [b] OTS: octyltrichlorosilane, ODTS: octadecyltrichlorosilane.

3. References

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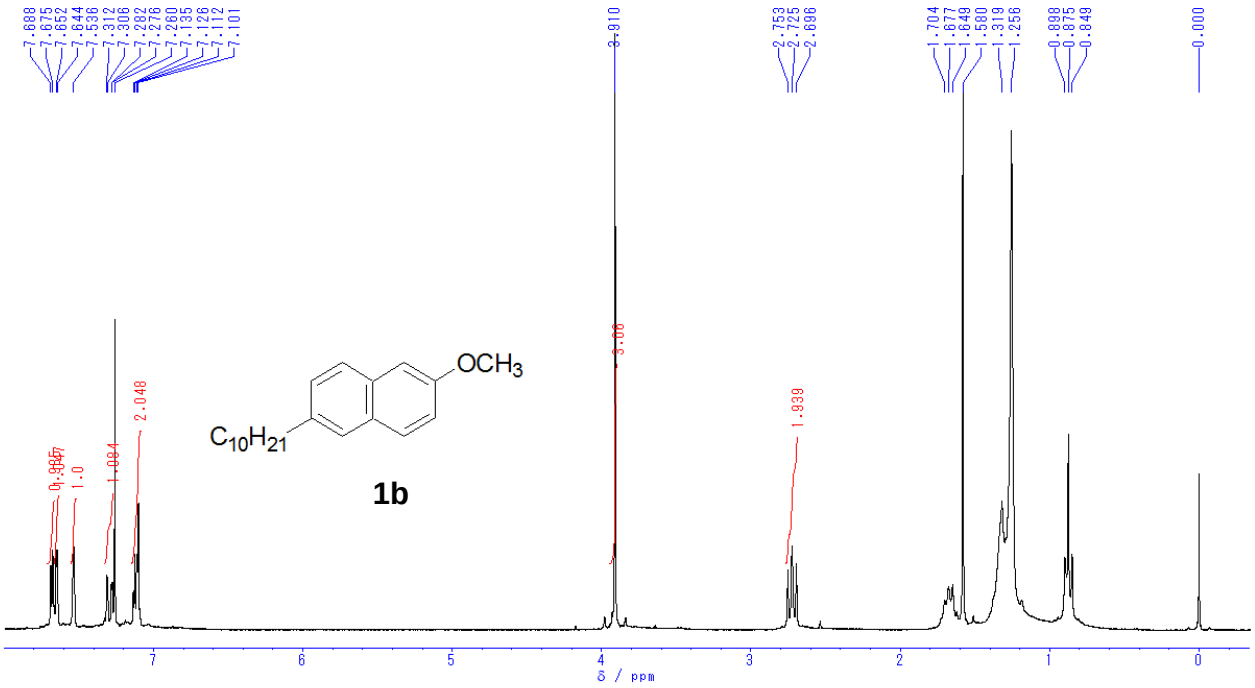
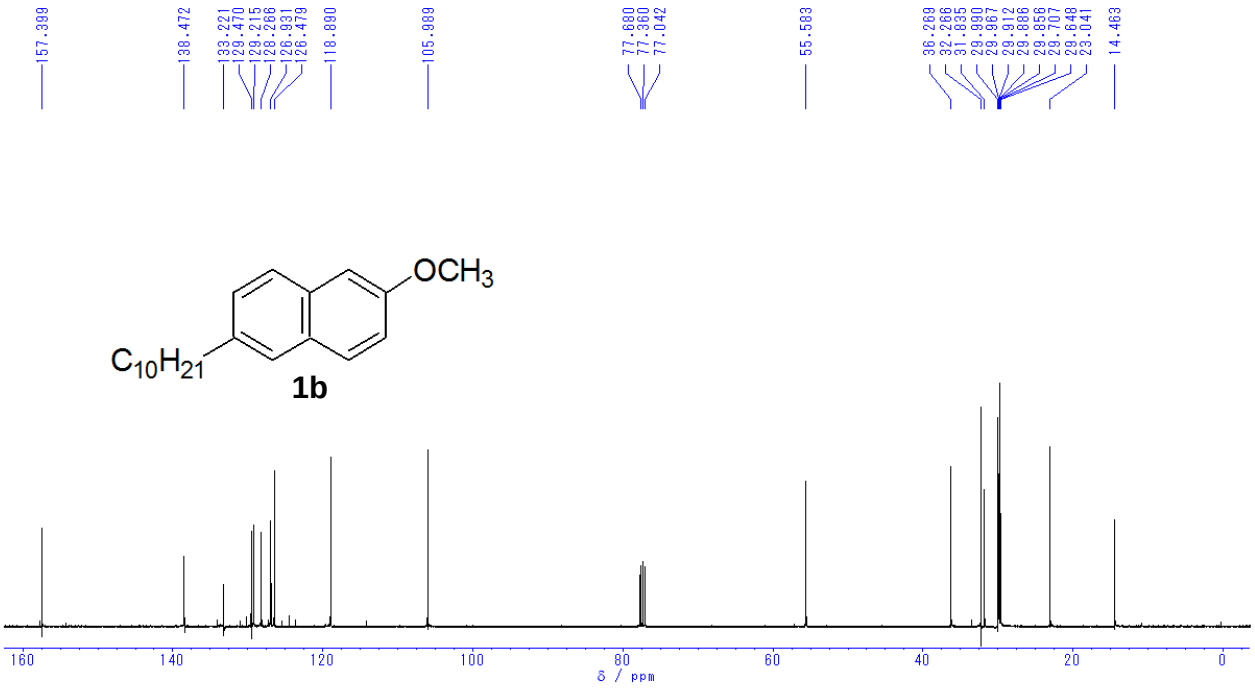
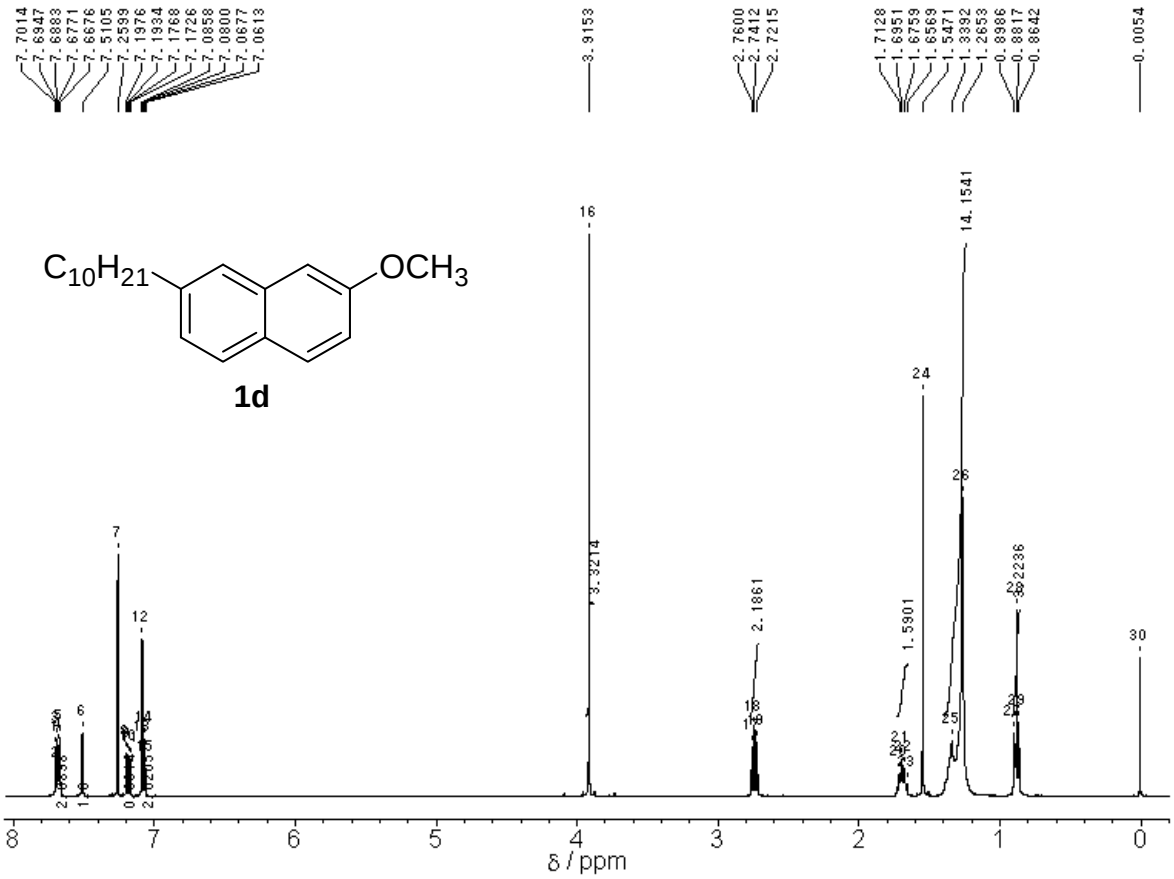
4. NMR spectra



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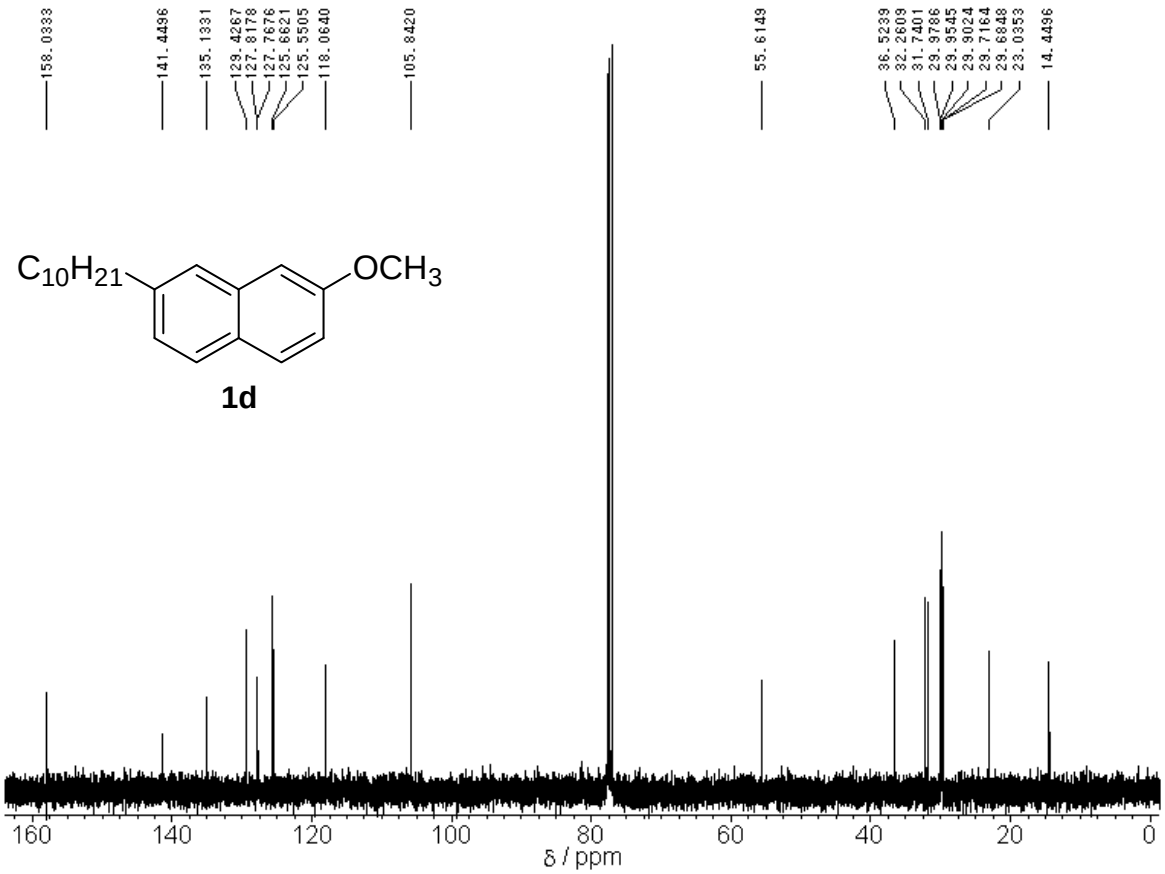
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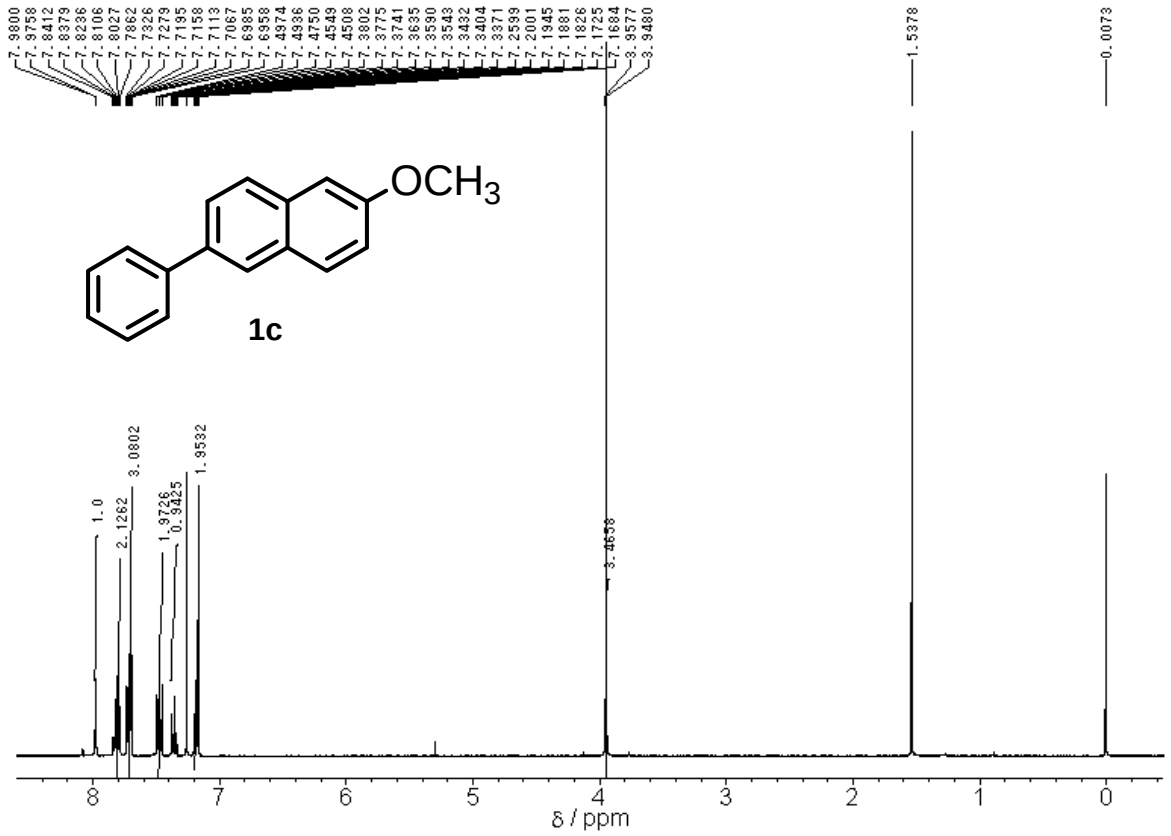
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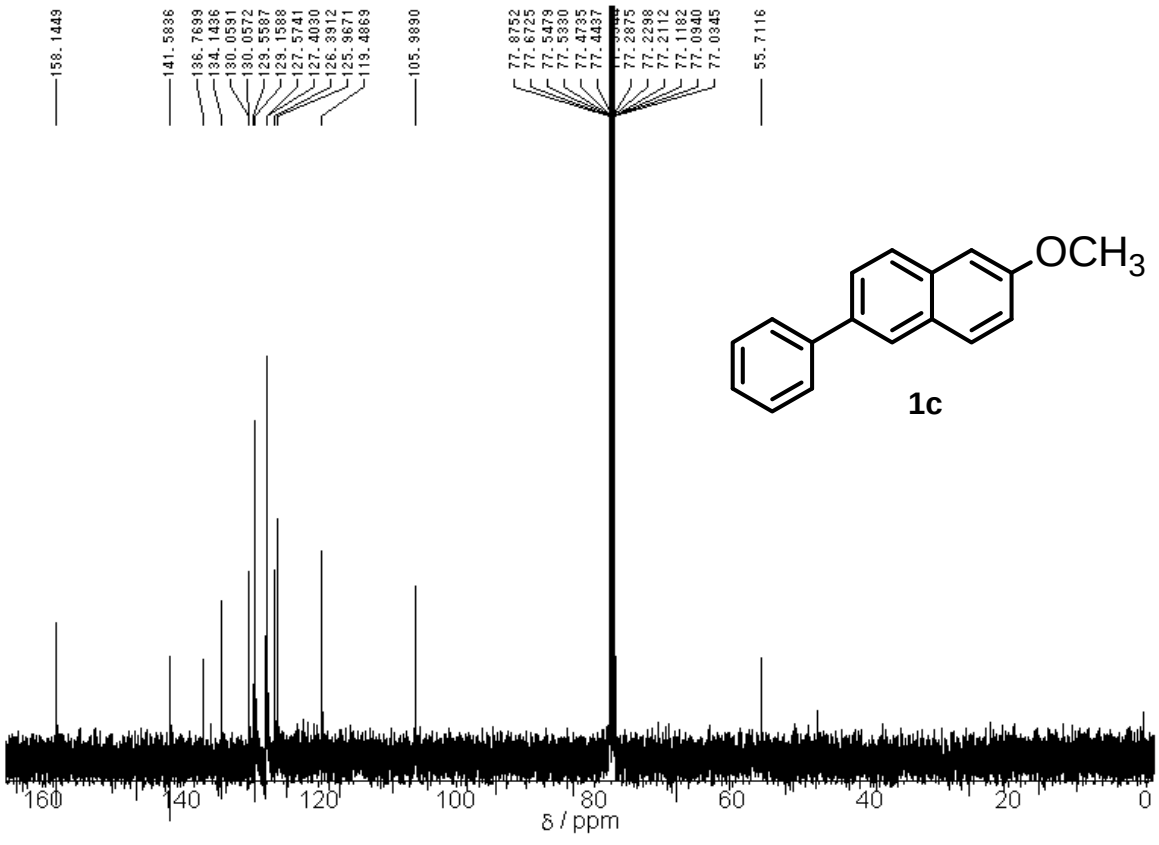
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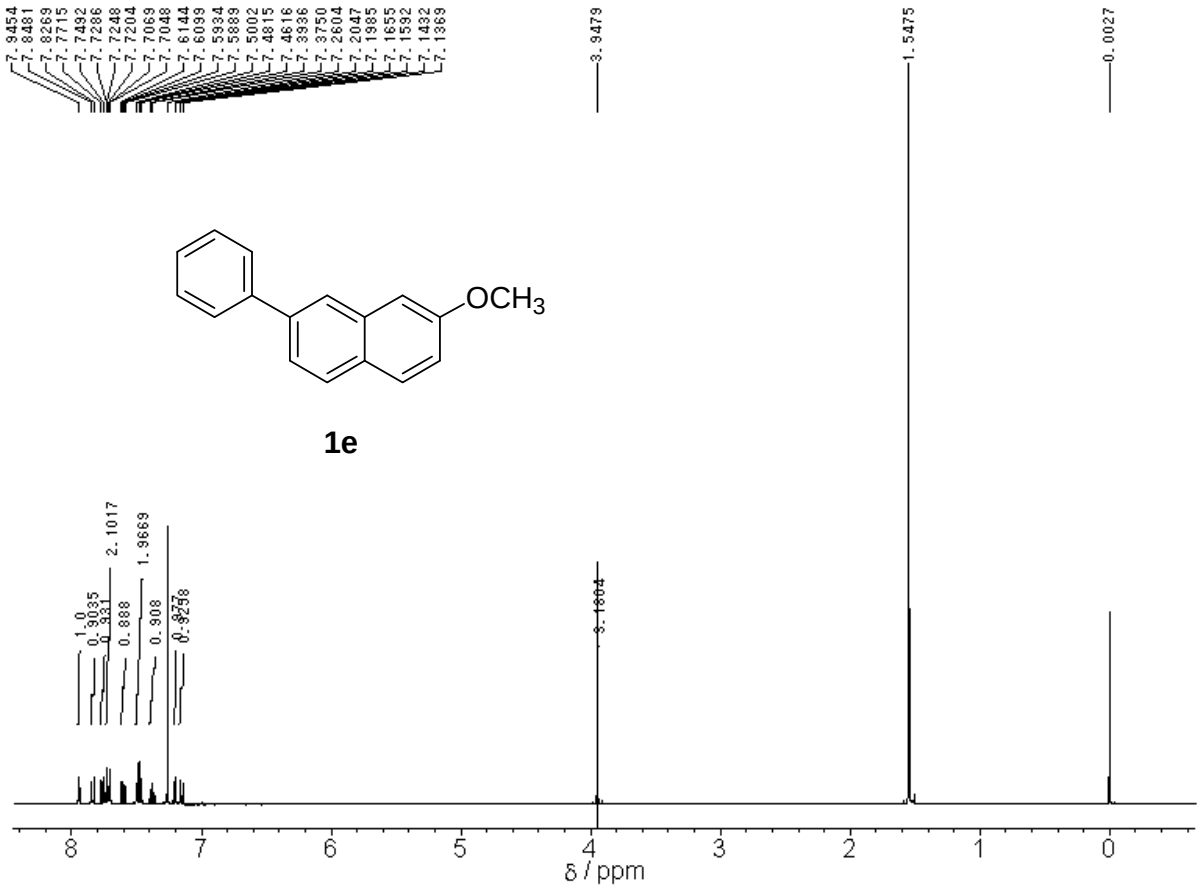
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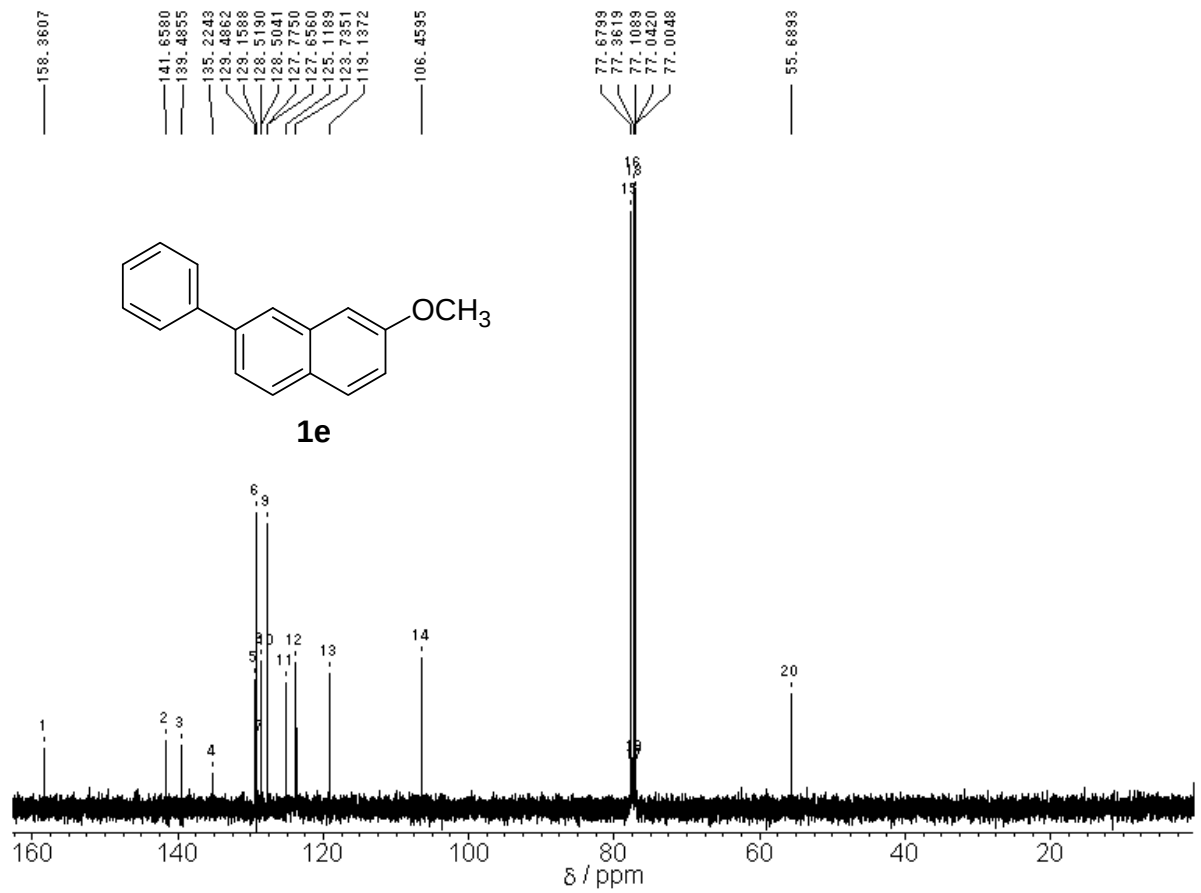
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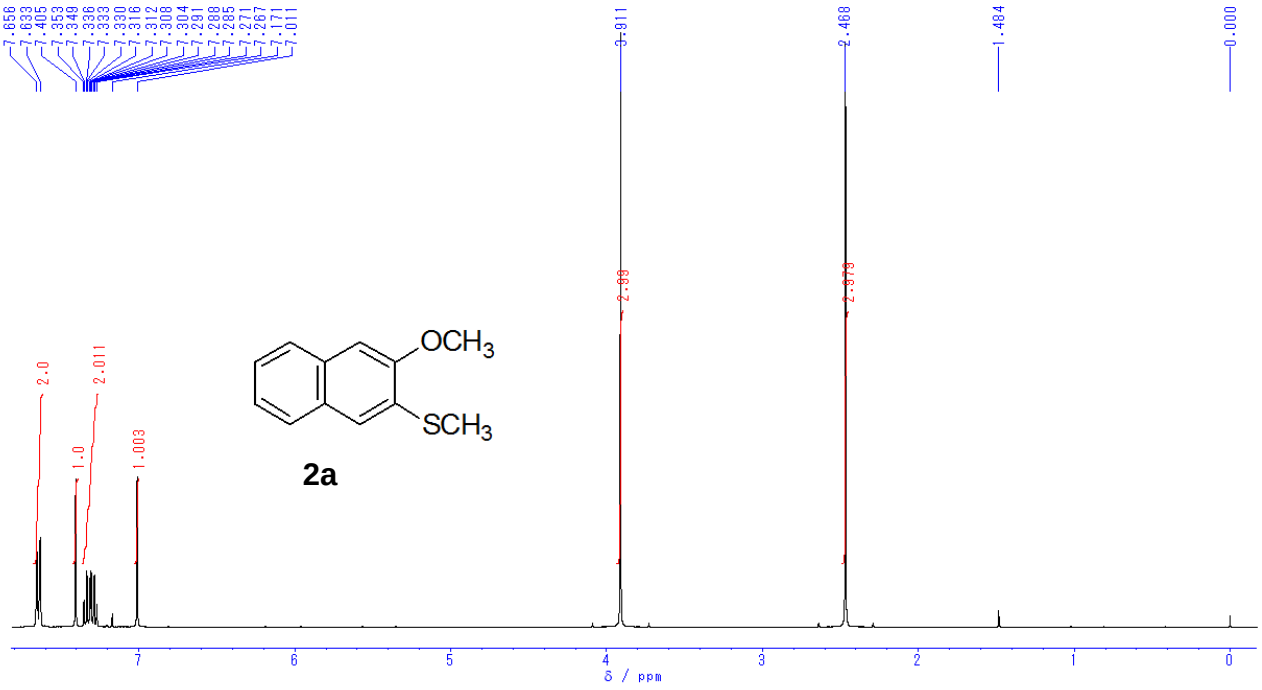
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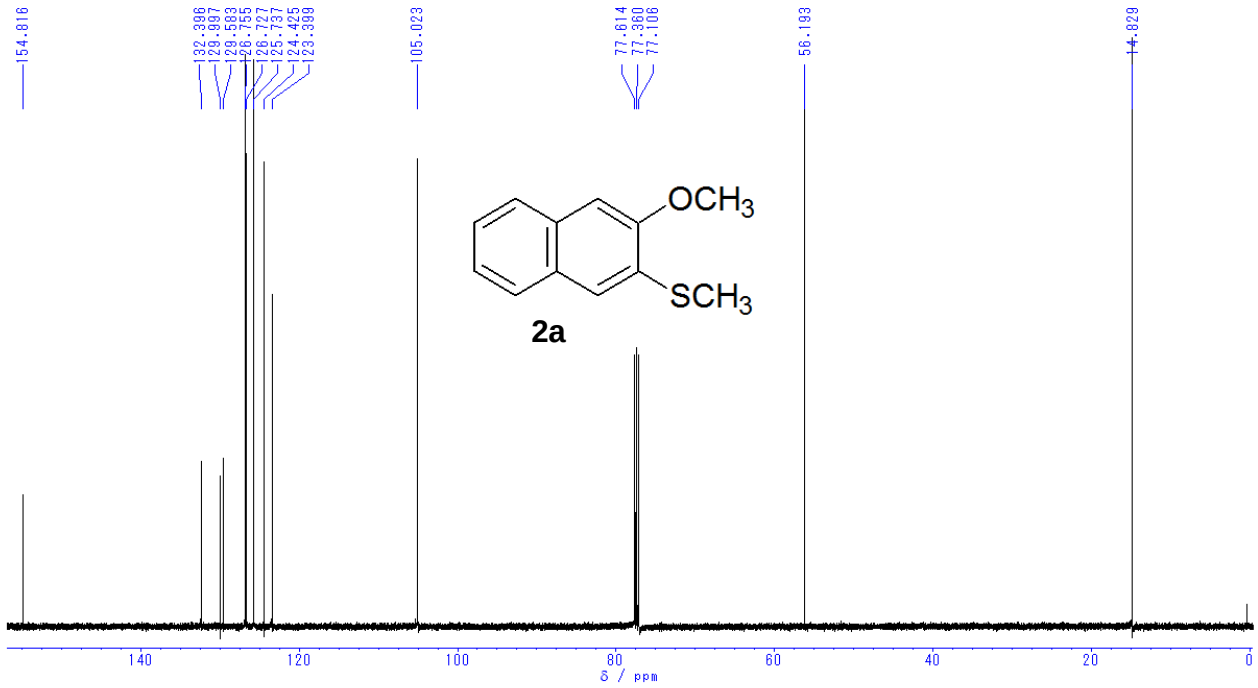
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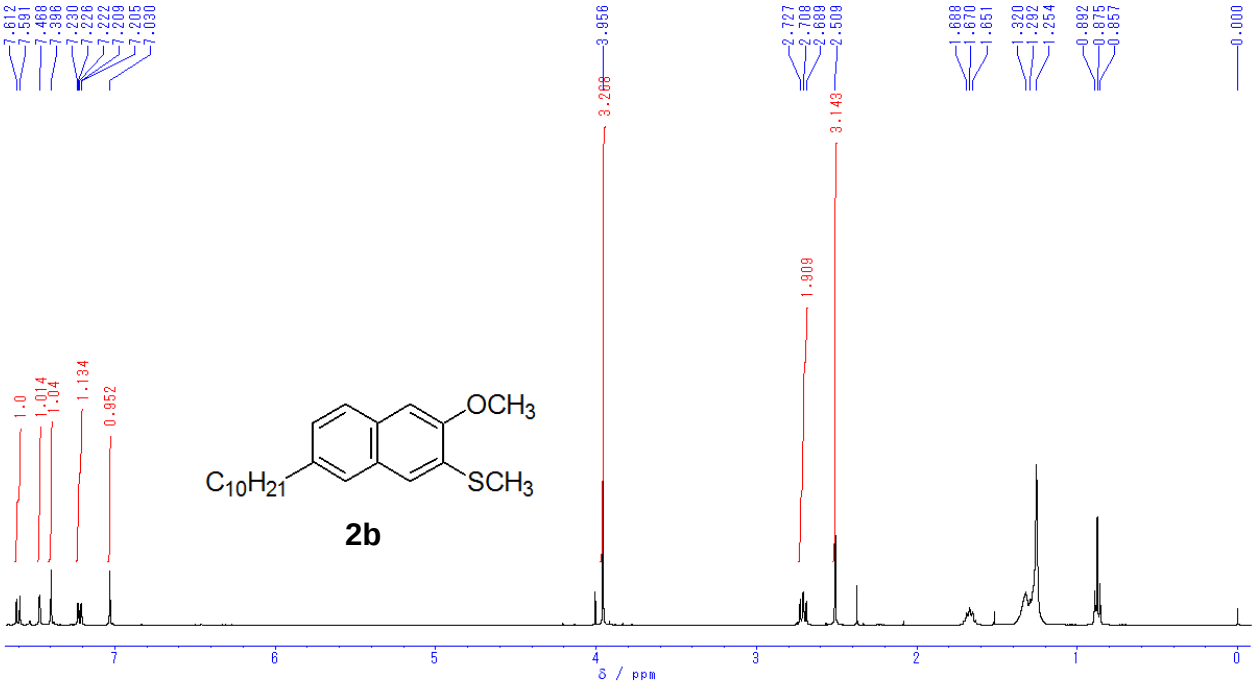
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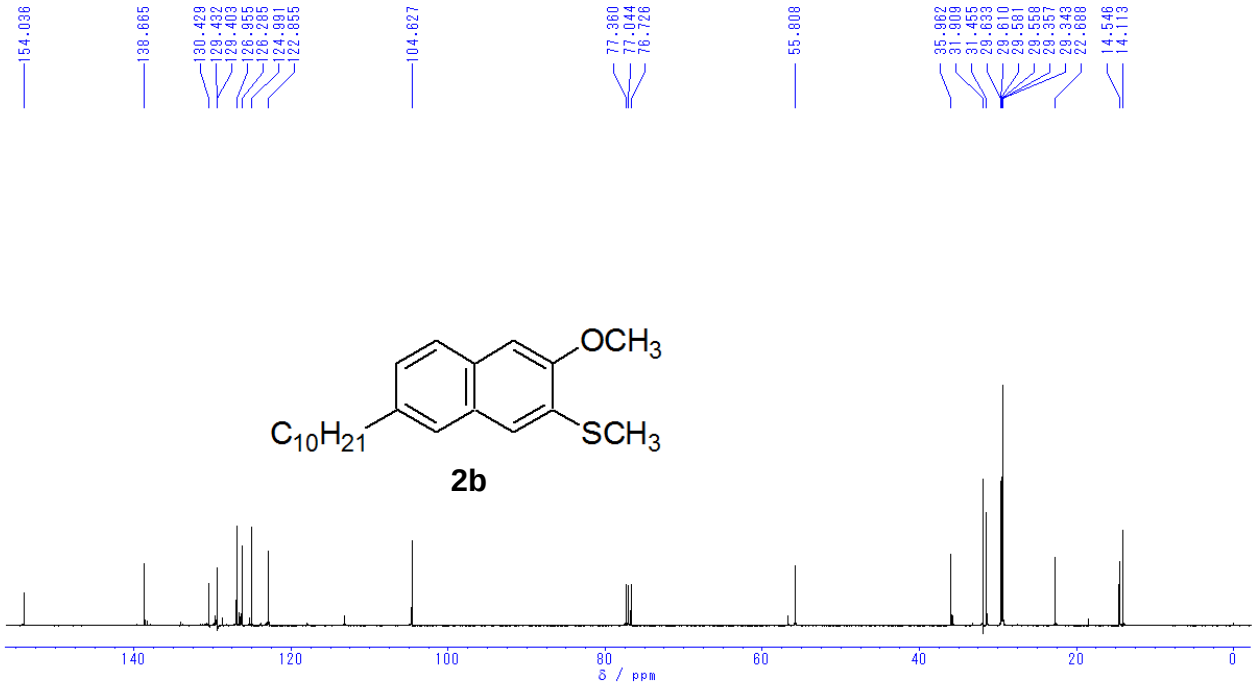
C10H21
SCH3
2b
δ / ppm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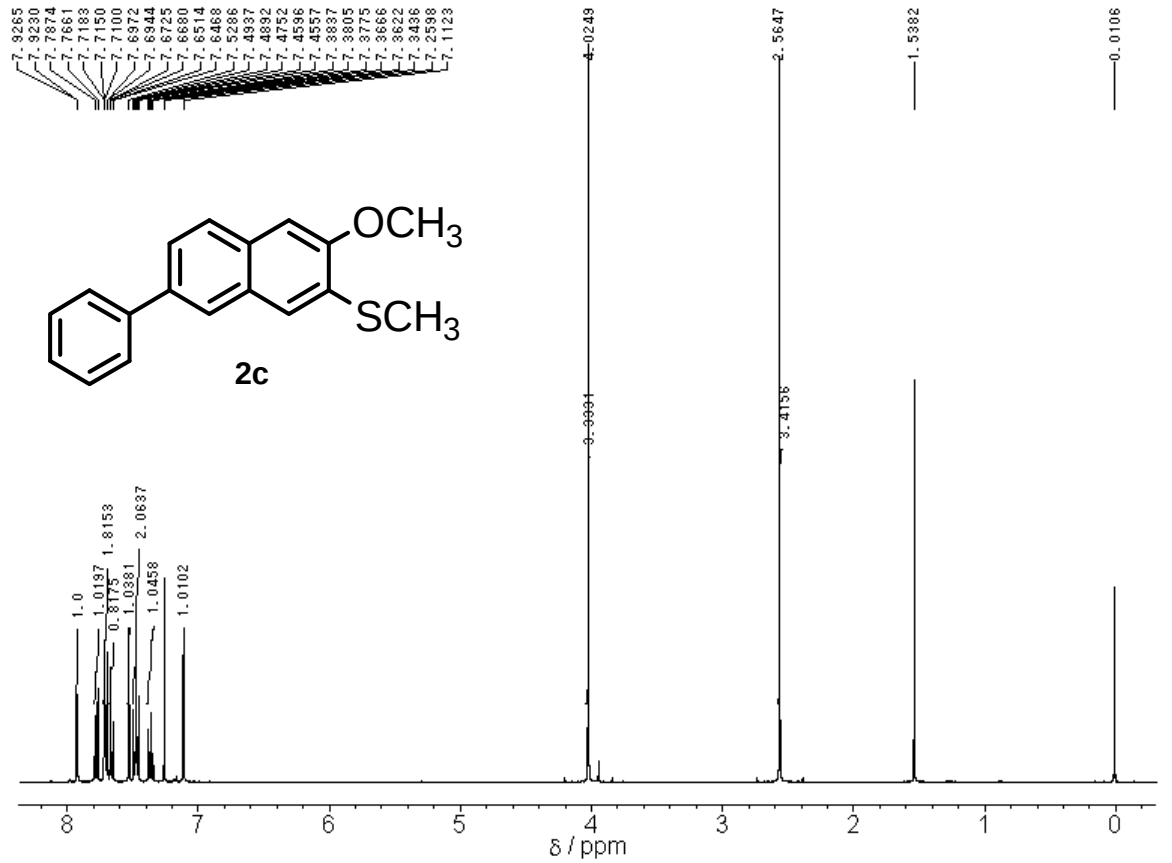
138.665
130.429
129.432
129.403
126.955
126.285
124.991
122.855
104.627
77.360
77.044
76.726
55.808
35.962
31.909
31.455
29.633
29.610
29.581
29.558
29.357
29.343
22.688
14.546
14.113
OCH3
C10H21
SCH3
2b
δ / ppm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7.9230
7.7874
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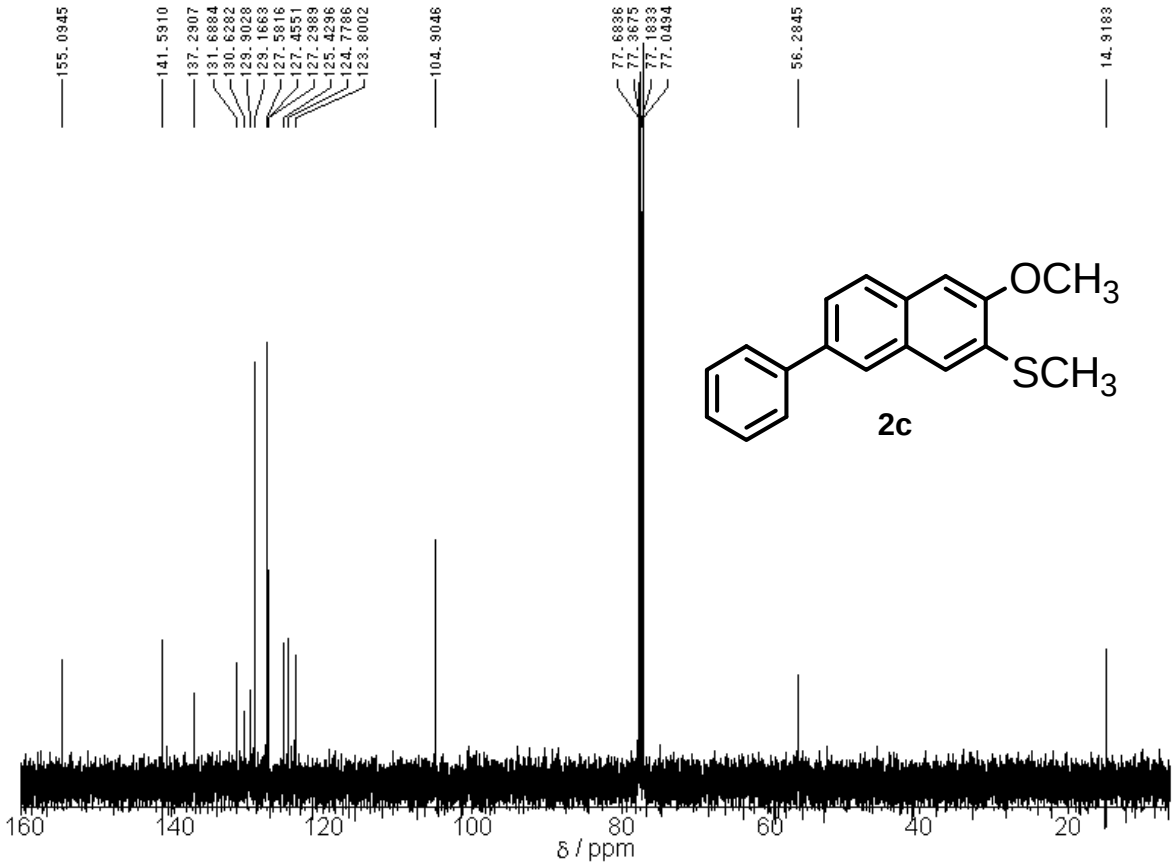
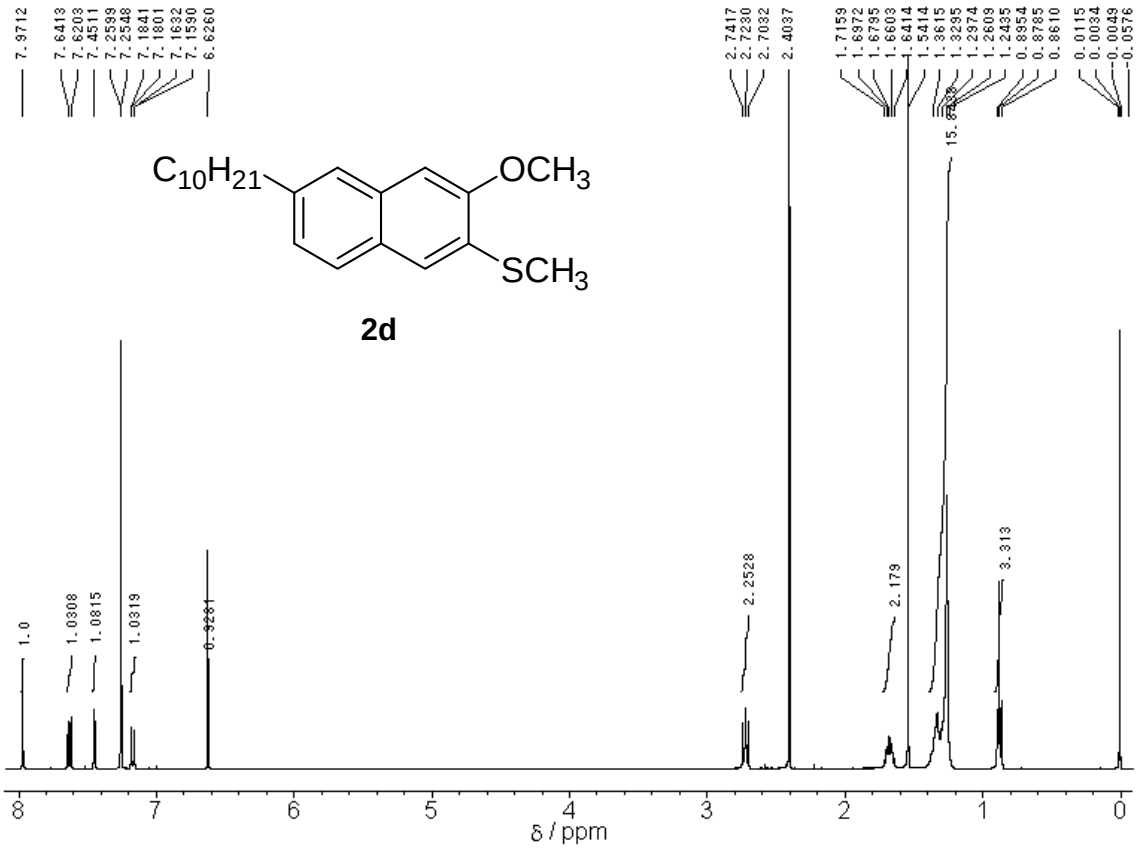
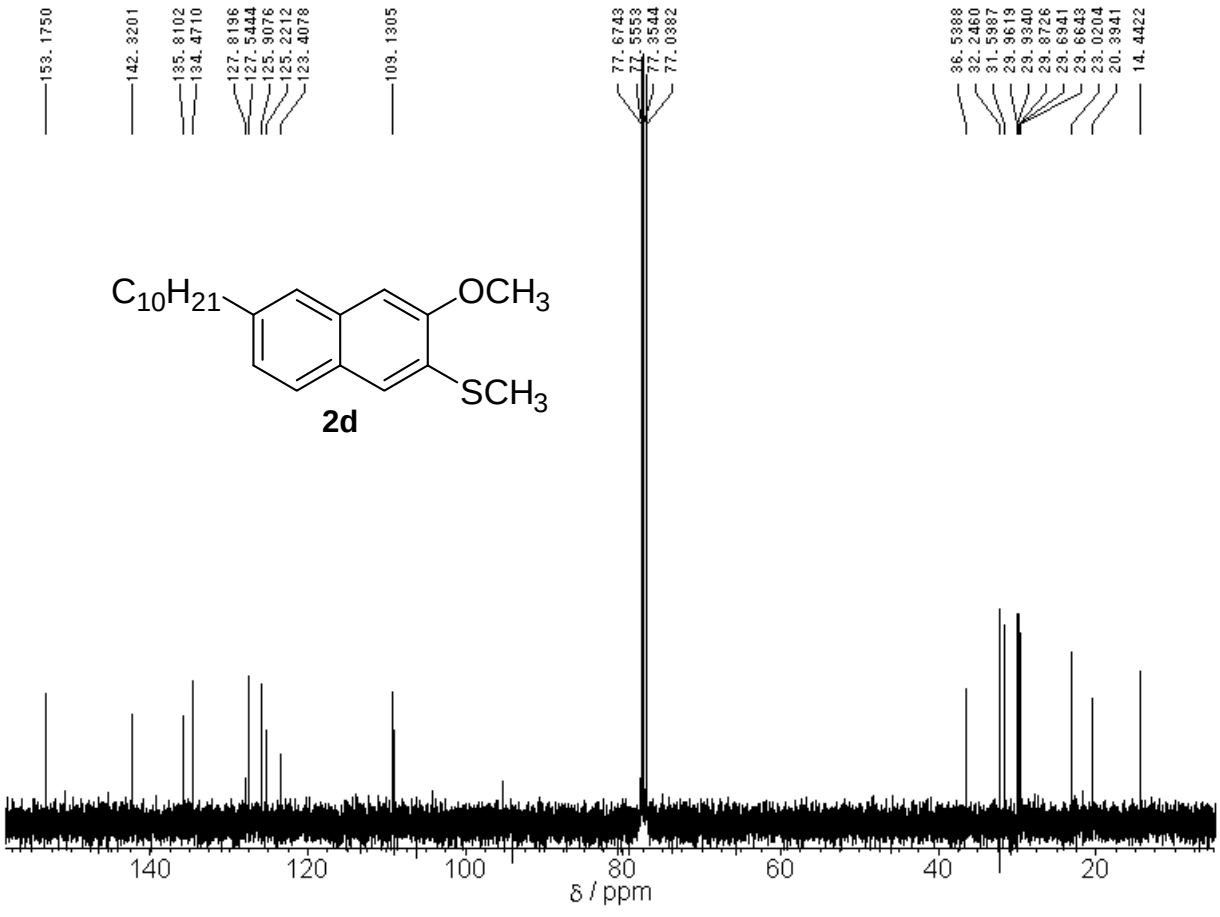
7.7183
7.7150
7.7100
7.6972
7.6944
7.6725
7.6680
7.6514
7.6468
7.5286
7.4937
7.4892
7.4752
7.4596
7.4557
7.3837
7.3805
7.3775
7.3666
7.3622
7.3436
7.2598
7.1123
4.0249
2.5647
1.5382
0.0106
3.0331
3.4156
1.0
1.0197
1.8153
0.8175
1.0381
2.0637
1.0458
1.0102
OCH3
SCH3
2c
8
7
6
5
4
3
2
1
0
δ / ppm


155.0945
141.5910
137.2907
131.6884
130.6282
129.9028
129.1663
127.5816
127.4551
127.2989
125.4296
124.7786
123.8002
104.9046
77.6836
77.3675
77.1833
77.0494
56.2845
14.9183
OCH3
SCH3
2c
160
140
120
100
80
60
40
20
δ / ppm



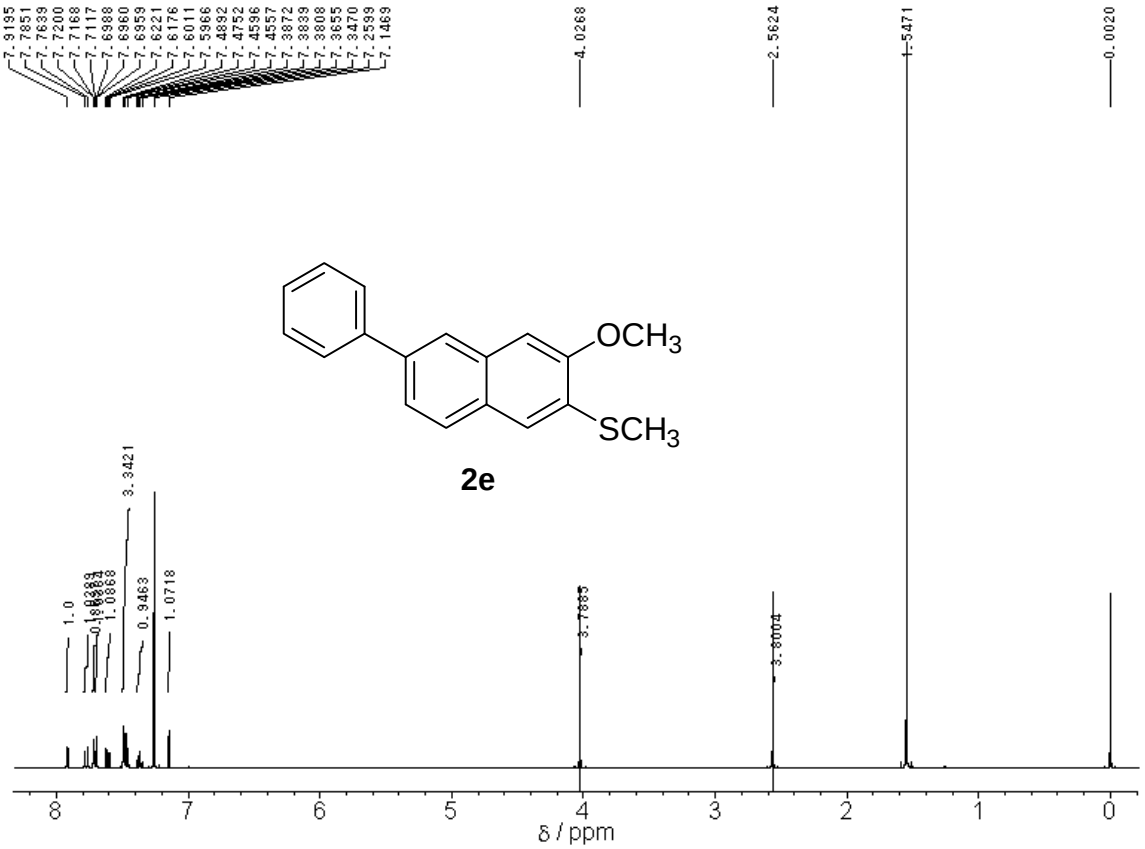
$C_{10}H_{21}$ OCH_3 SCH_3

2d

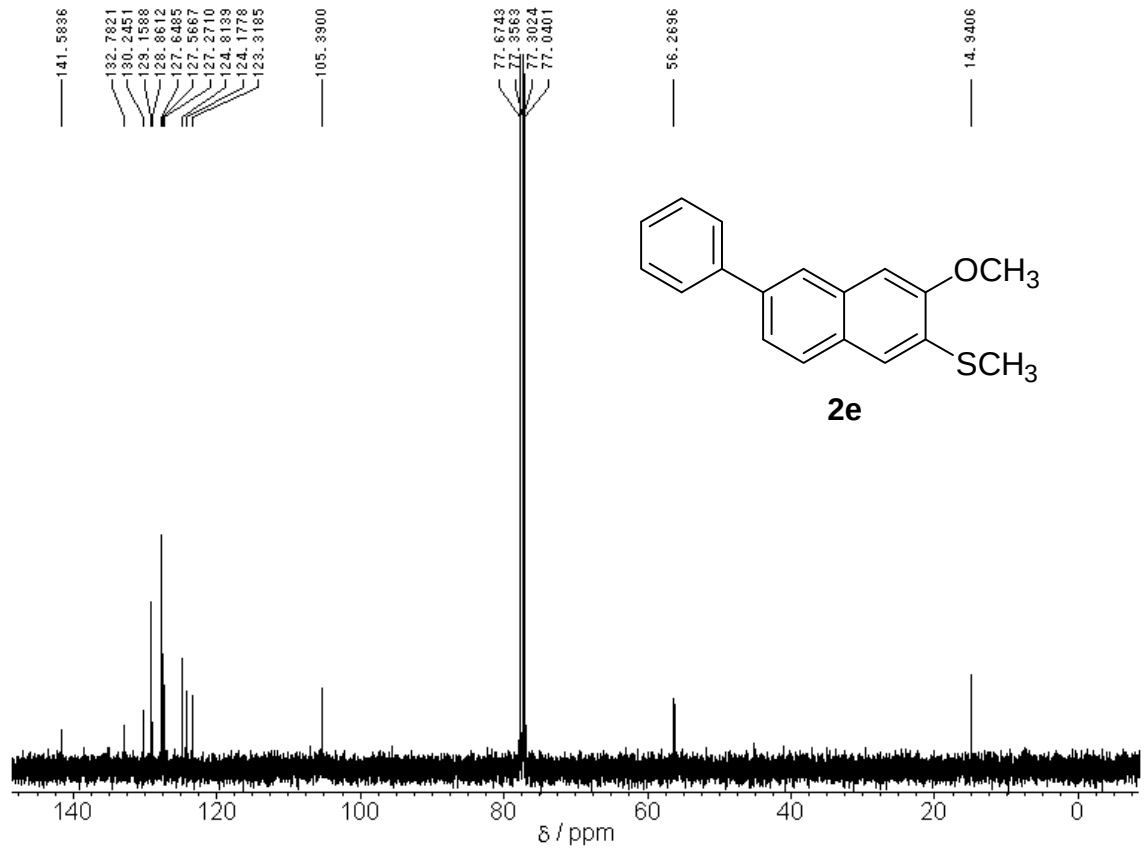


$C_{10}H_{21}$ OCH_3 SCH_3

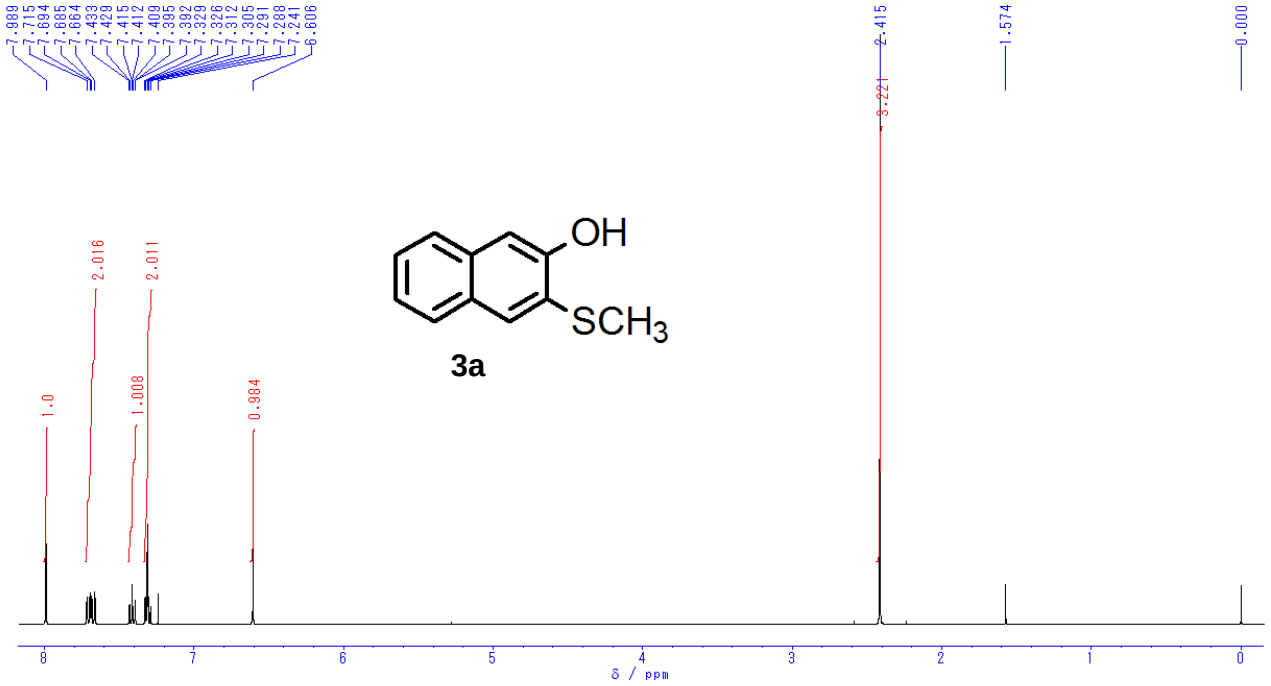
2d

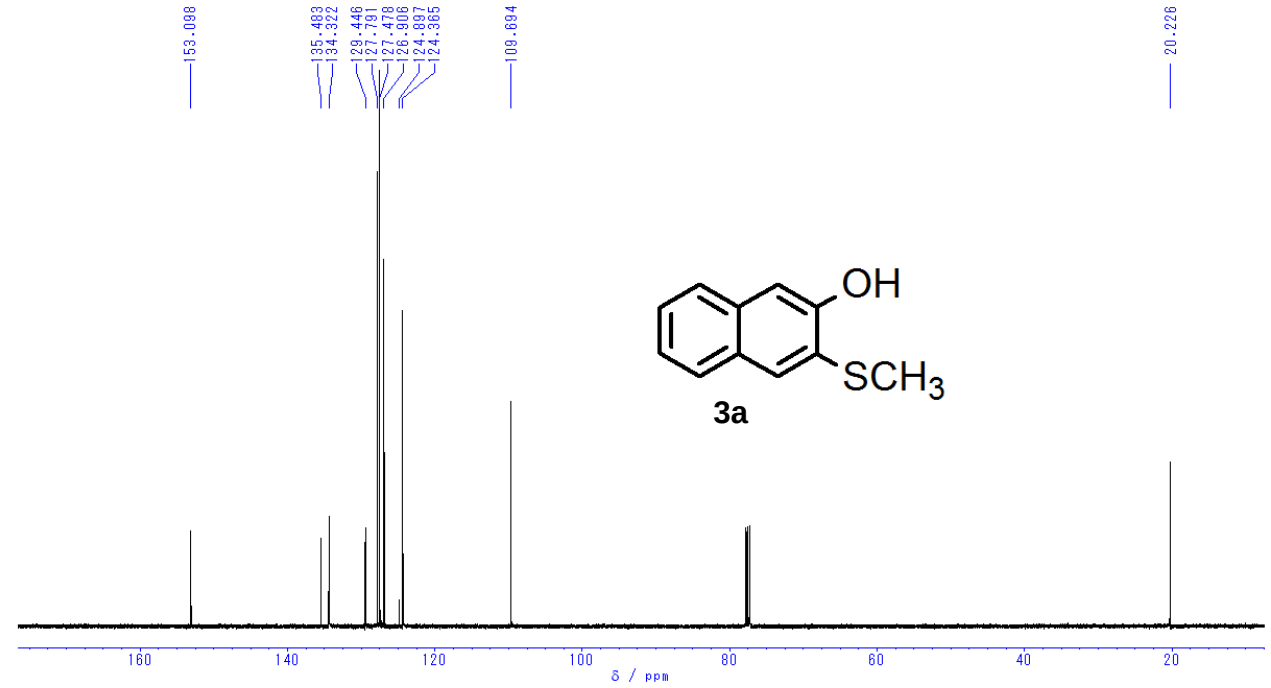


2e



2e


7.909
7.715
7.694
7.685
7.664
7.433
7.429
7.415
7.412
7.409
7.395
7.392
7.329
7.326
7.312
7.305
7.291
7.288
7.241
6.606
2.415
1.574
0.000
3.221
2.016
2.011
1.008
0.984
1.0
OH
SCH3
3a
8
7
6
5
4
3
2
1
0
δ / ppm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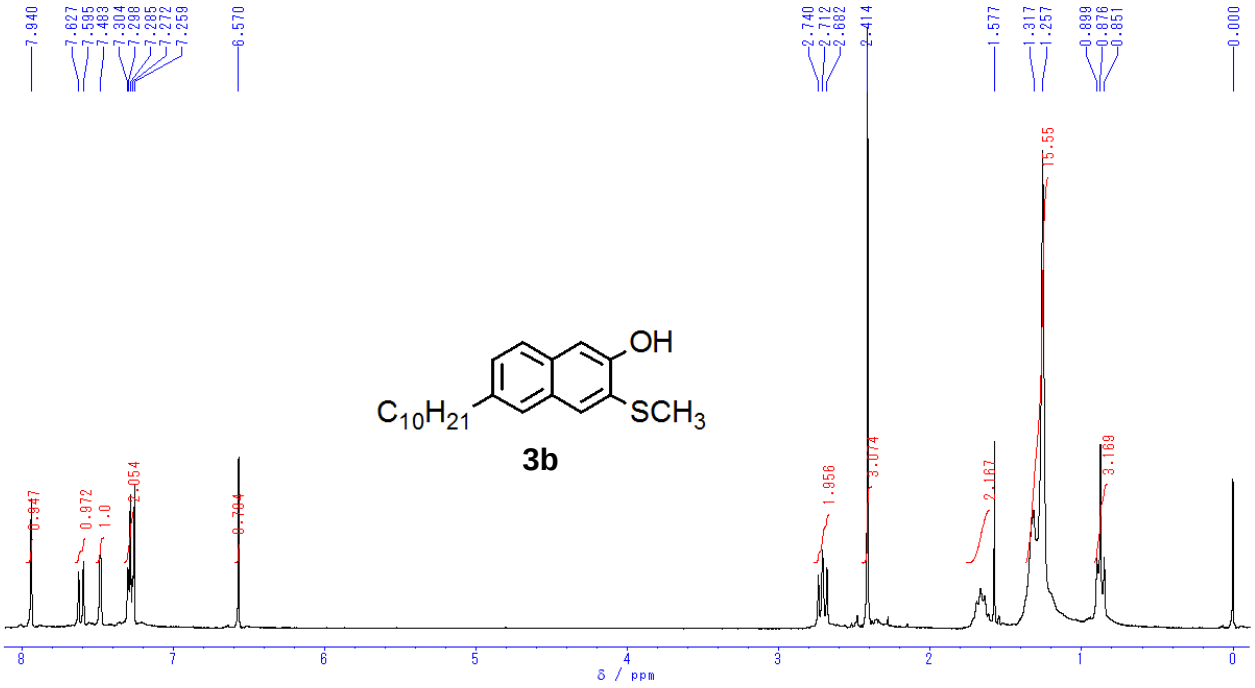
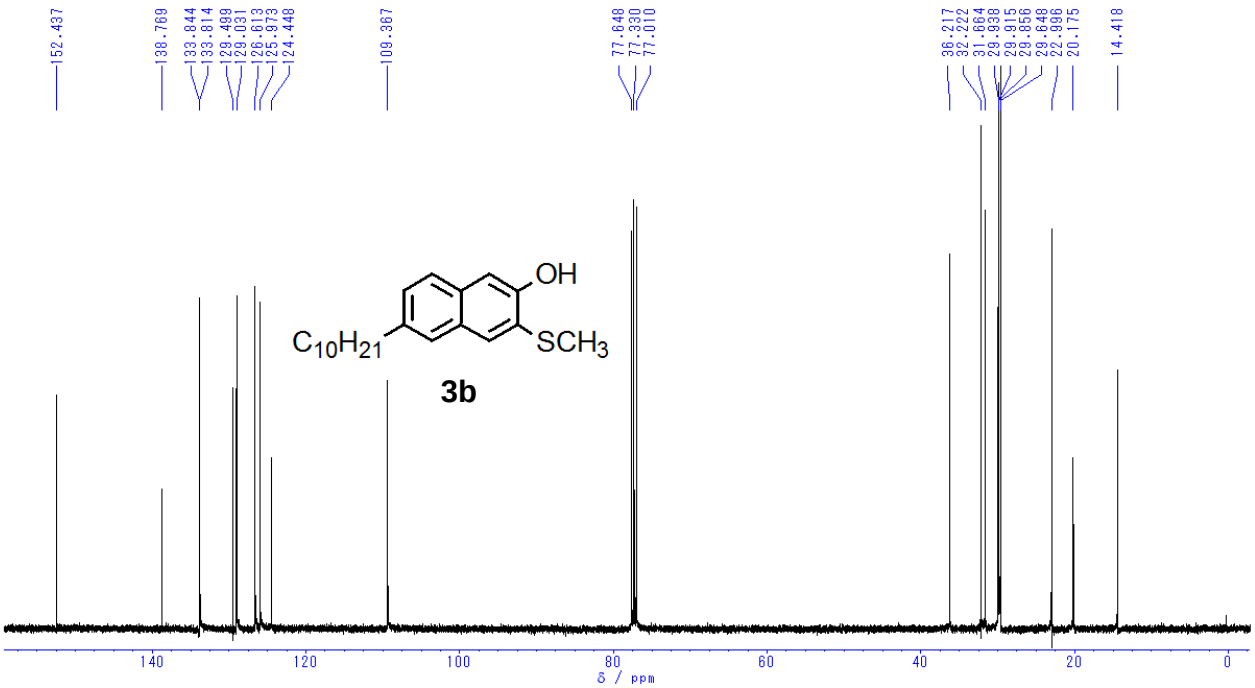
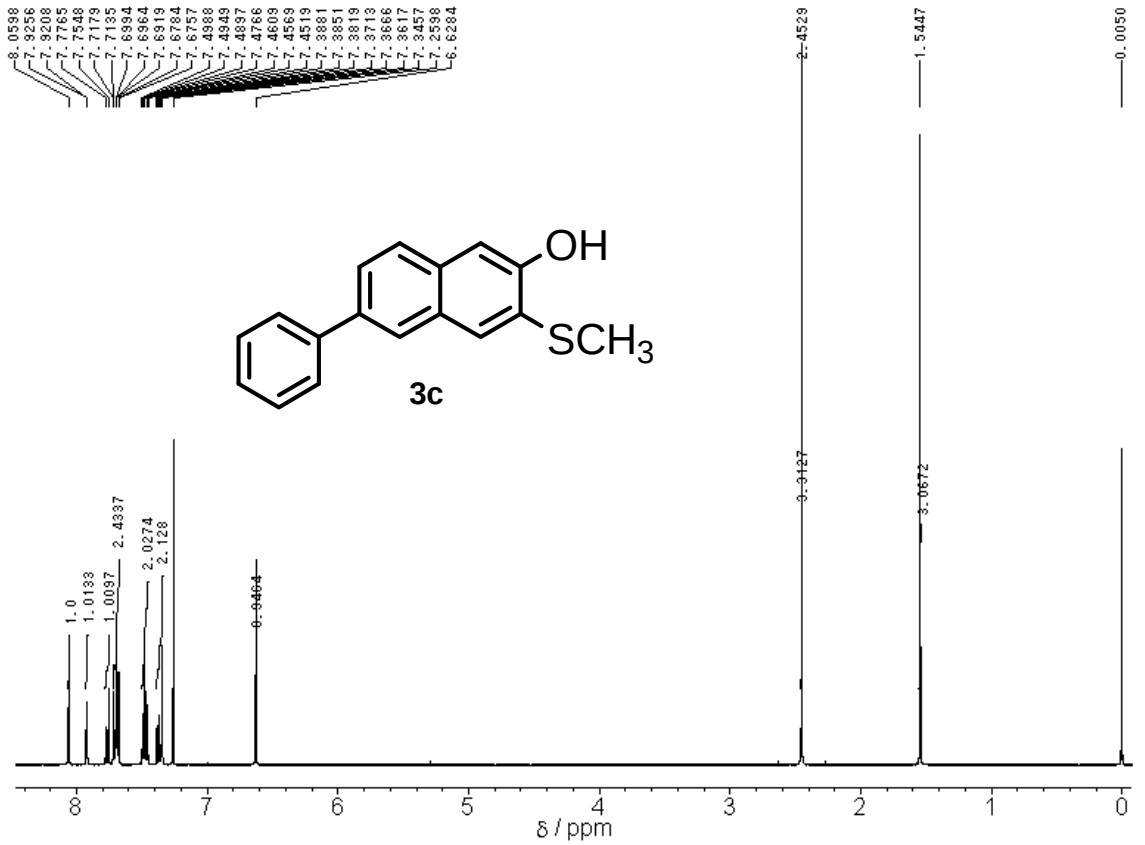
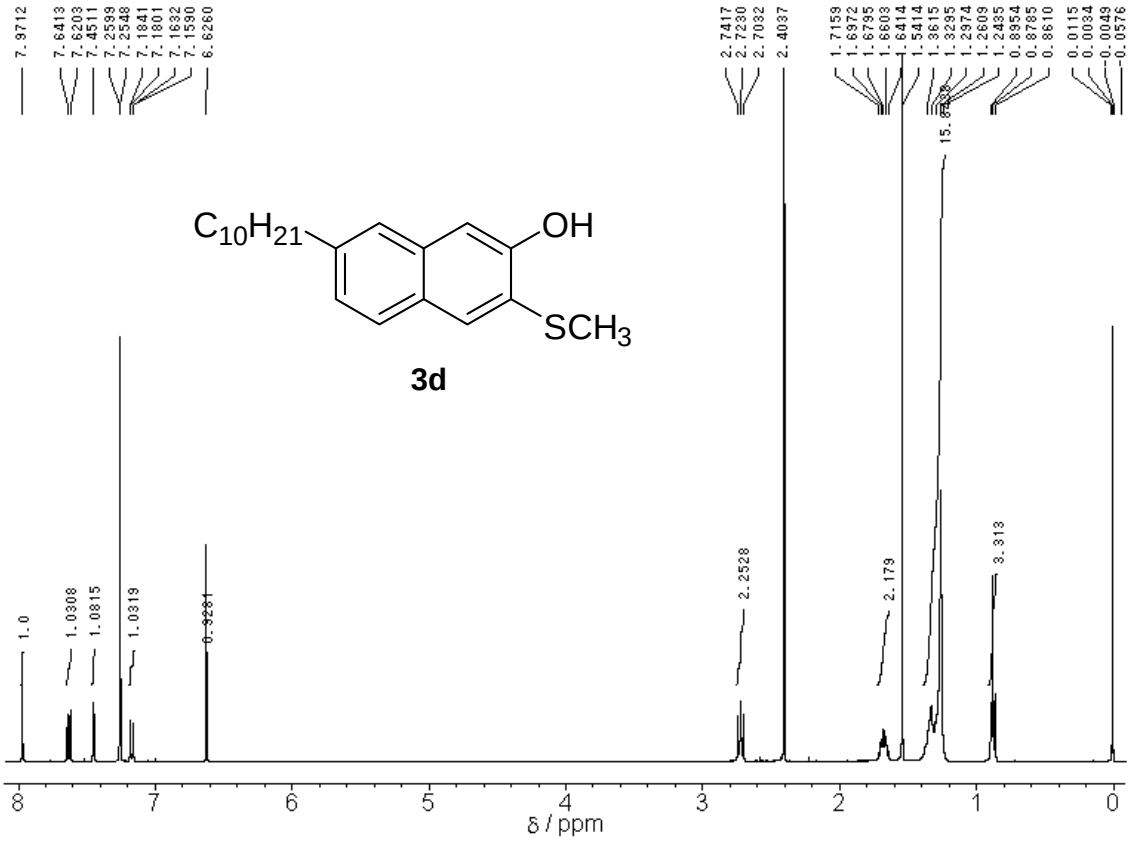
135.483
134.322
129.446
127.791
127.478
126.906
124.897
124.365
109.694
20.226
OH
SCH3
3a
160
140
120
100
80
60
40
20
δ / ppm

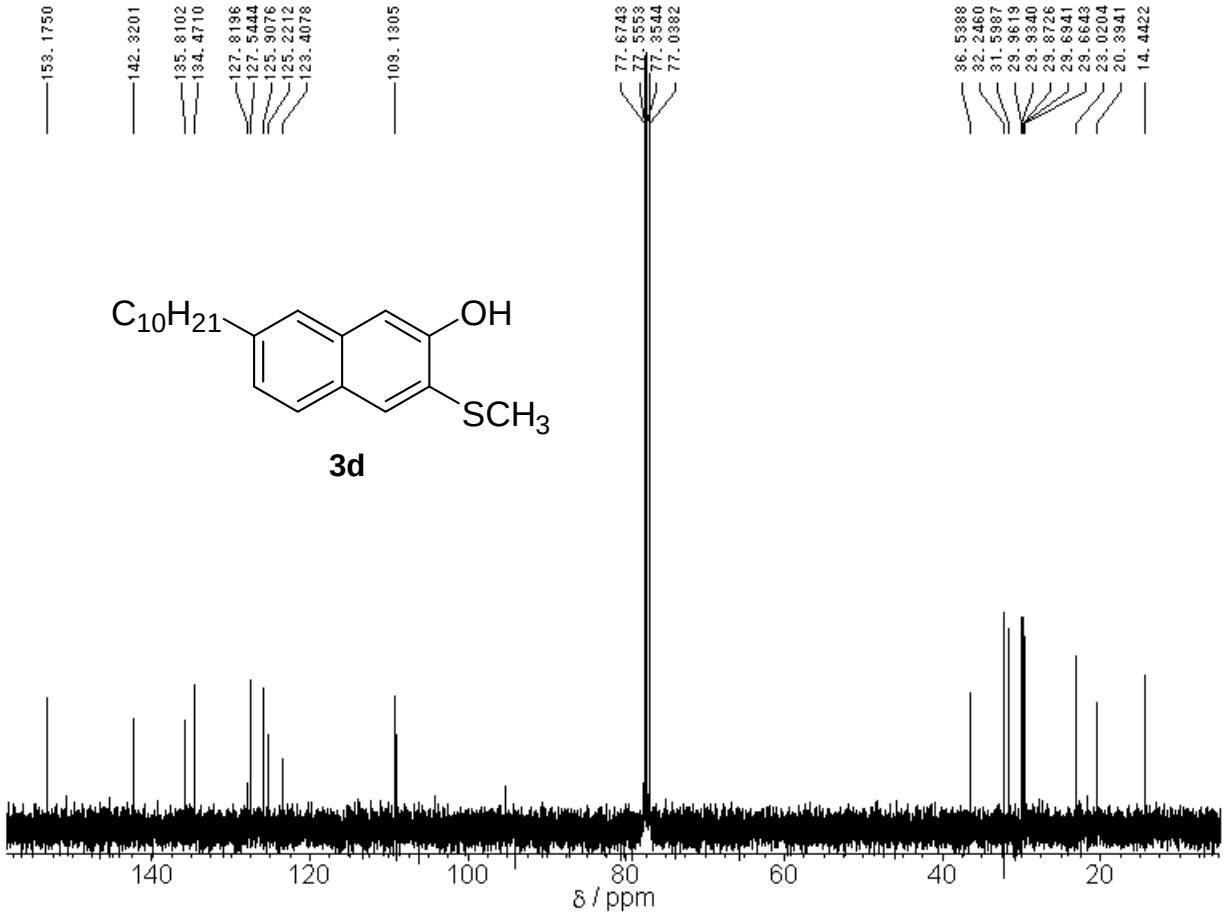

7.940
7.627
7.595
7.483
7.304
7.298
7.285
7.272
7.259
6.570
2.740
2.712
2.682
2.414
1.577
1.317
1.257
0.899
0.876
0.851
0.000
15.55
3.169
3.074
1.956
2.187
0.947
0.972
1.0
2.054
0.784
OH
SCH3
C10H21
3b
δ / ppm

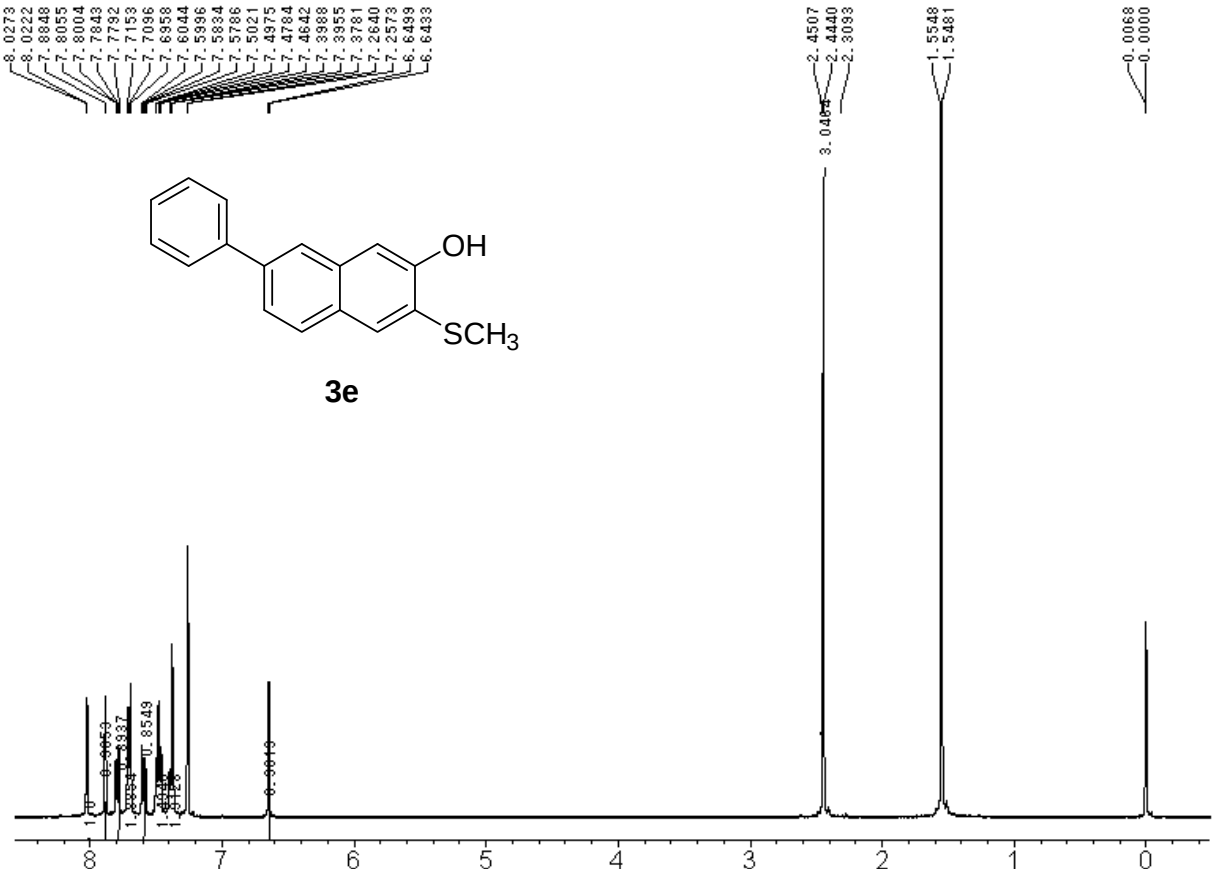

152.437
138.769
133.844
133.814
129.499
129.031
126.613
125.973
124.448
109.367
77.648
77.330
77.010
36.217
32.222
31.664
29.938
29.915
29.856
29.648
22.986
20.175
14.418
OH
SCH3
C10H21
3b
δ / ppm


OH
SCH3
3c
δ / ppm

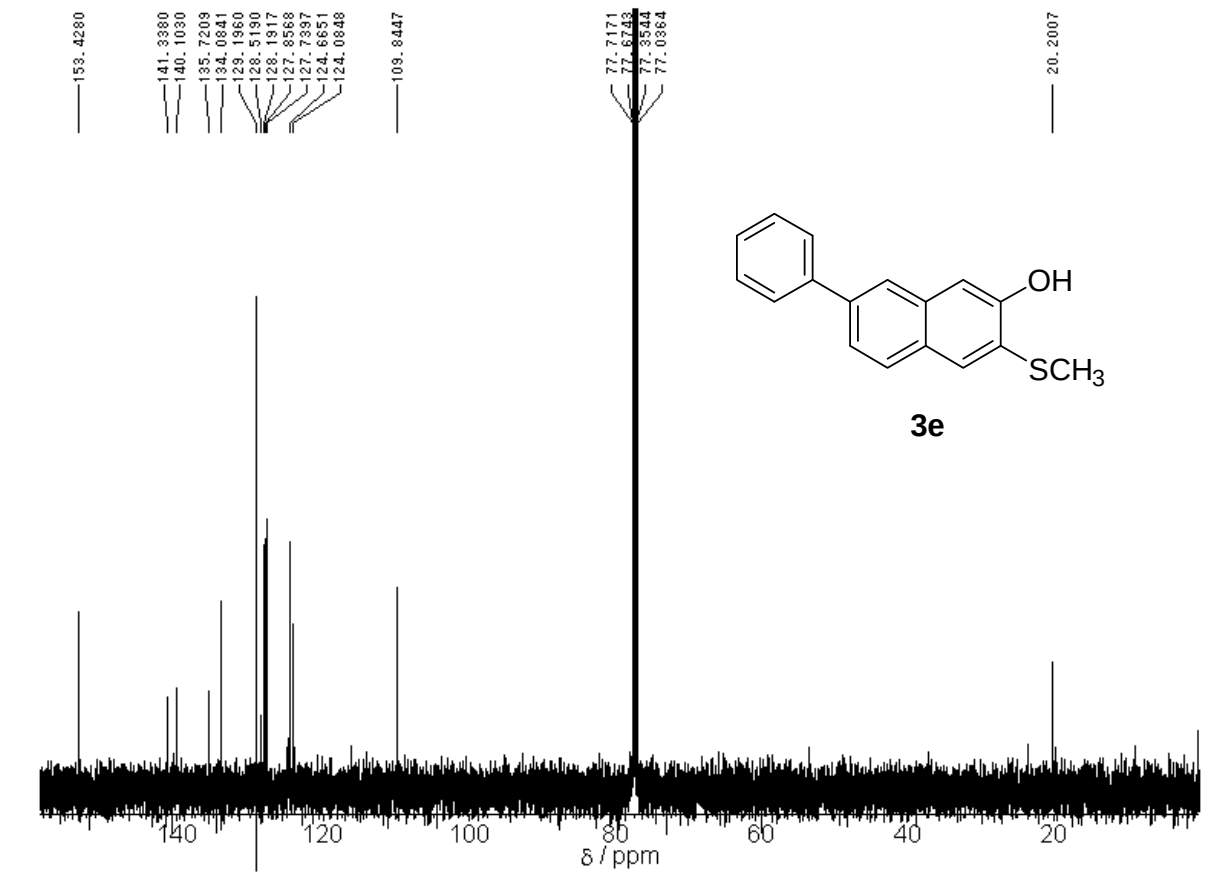

OH
SCH3
3c
δ / ppm


7.9712
7.6413
7.6203
7.4511
7.2599
7.2548
7.1841
7.1801
7.1632
7.1590
6.6260
2.7417
2.7230
2.7032
2.4037
1.7159
1.6972
1.6795
1.6603
1.6414
1.5414
1.3615
1.3295
1.2974
1.2609
1.2435
0.8954
0.8785
0.8610
0.0115
0.0034
0.0049
-0.0576
15.6469
1.0
1.0308
1.0815
1.0319
6.3281
2.2528
2.179
3.313
C10H21
OH
SCH3
3d
8
7
6
5
4
3
2
1
0
δ / ppm

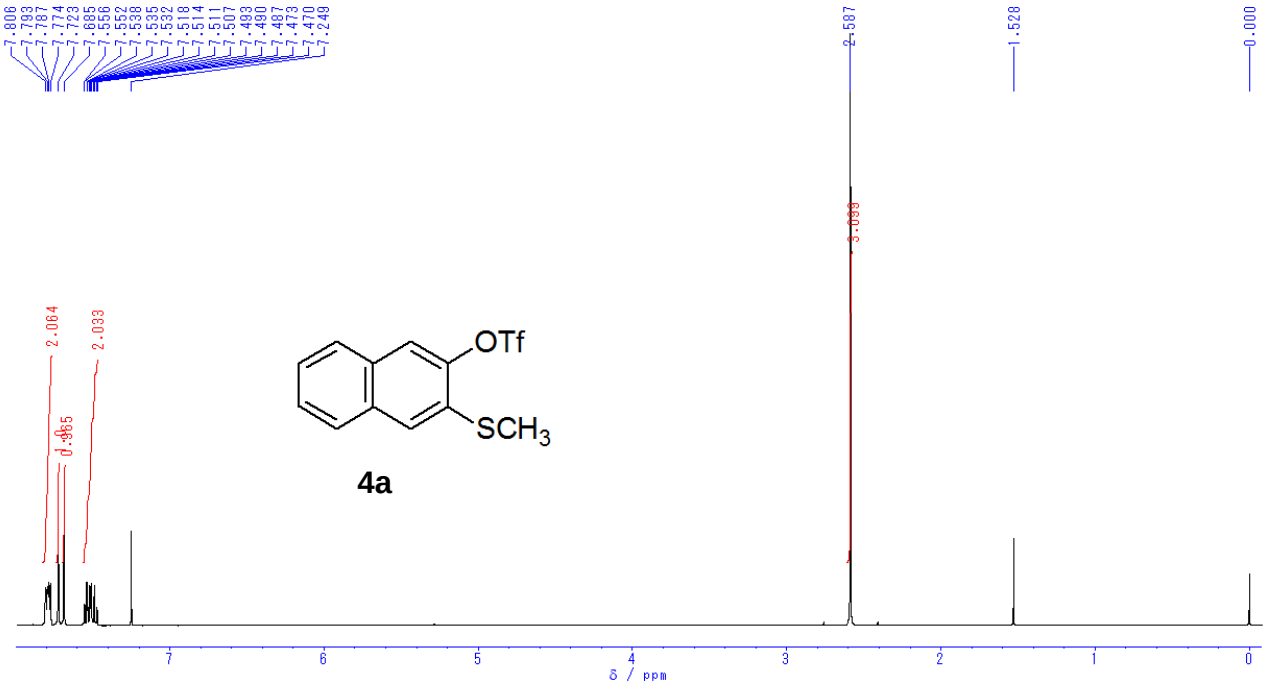

153.1750
142.3201
135.8102
134.4710
127.8196
127.5444
125.9076
125.2212
123.4078
109.1305
77.6743
77.5553
77.3544
77.0382
36.5388
32.2460
31.5987
29.9619
29.9340
29.8726
29.6941
29.6643
23.0204
20.3941
14.4422
C10H21
OH
SCH3
3d
140
120
100
80
60
40
20
δ / ppm

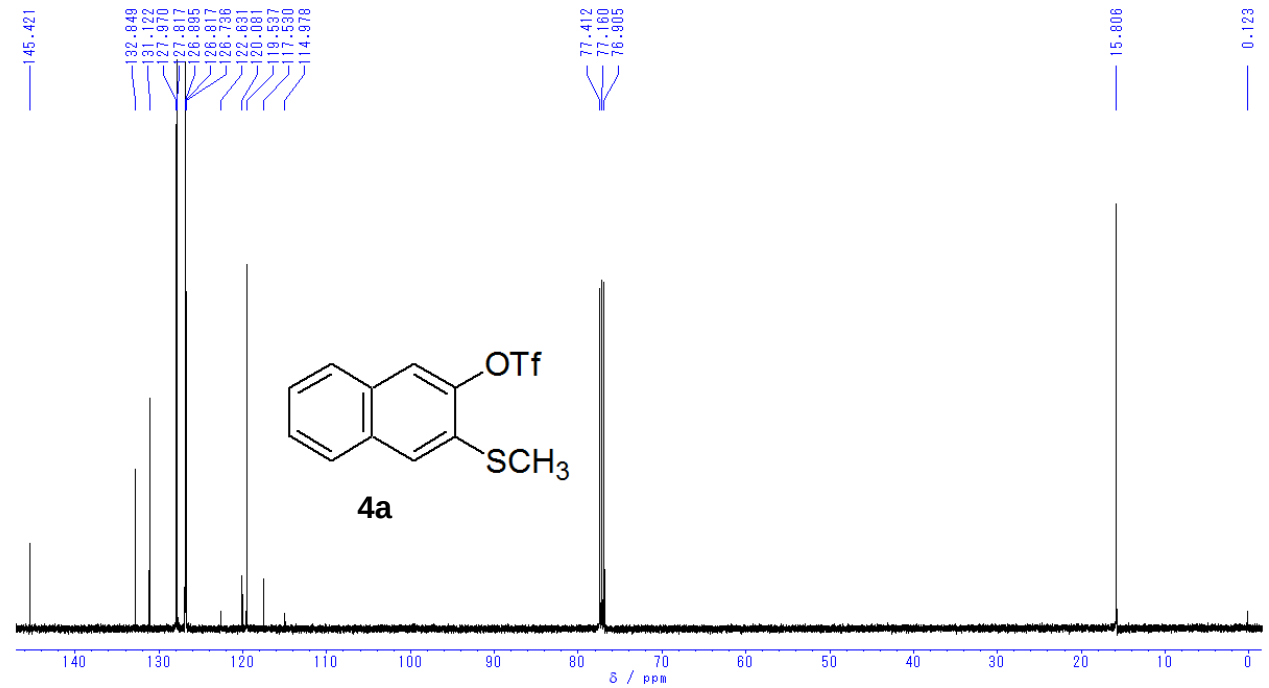


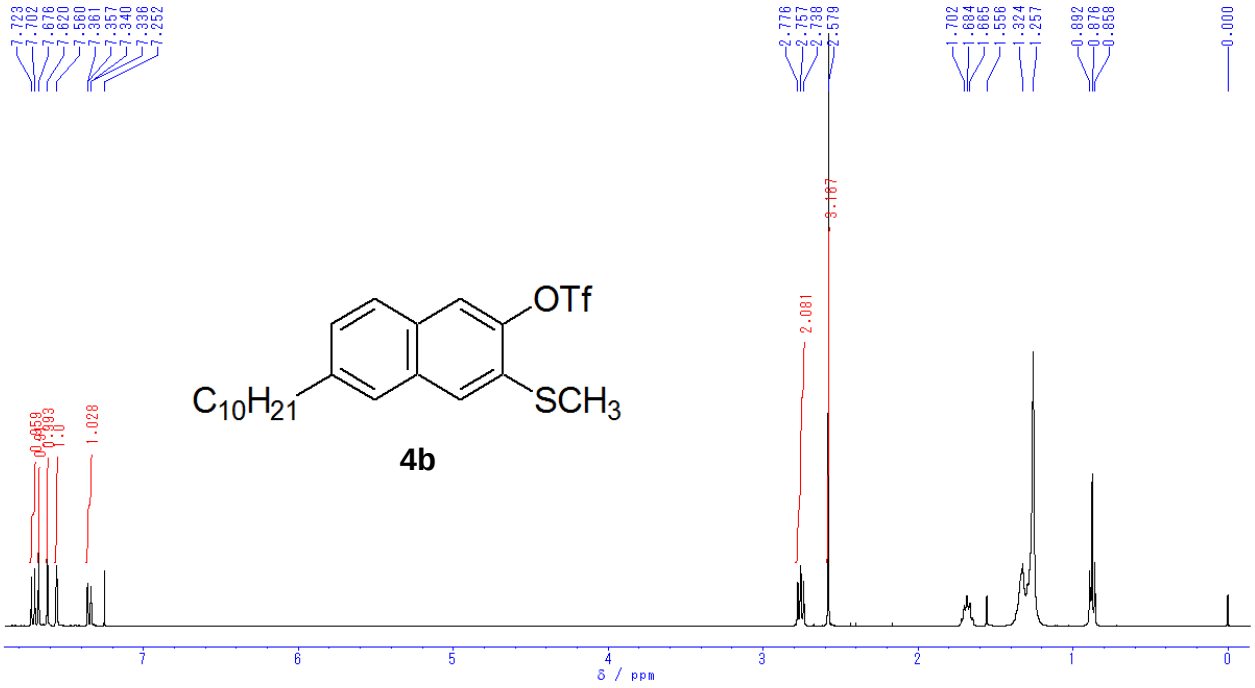
3e

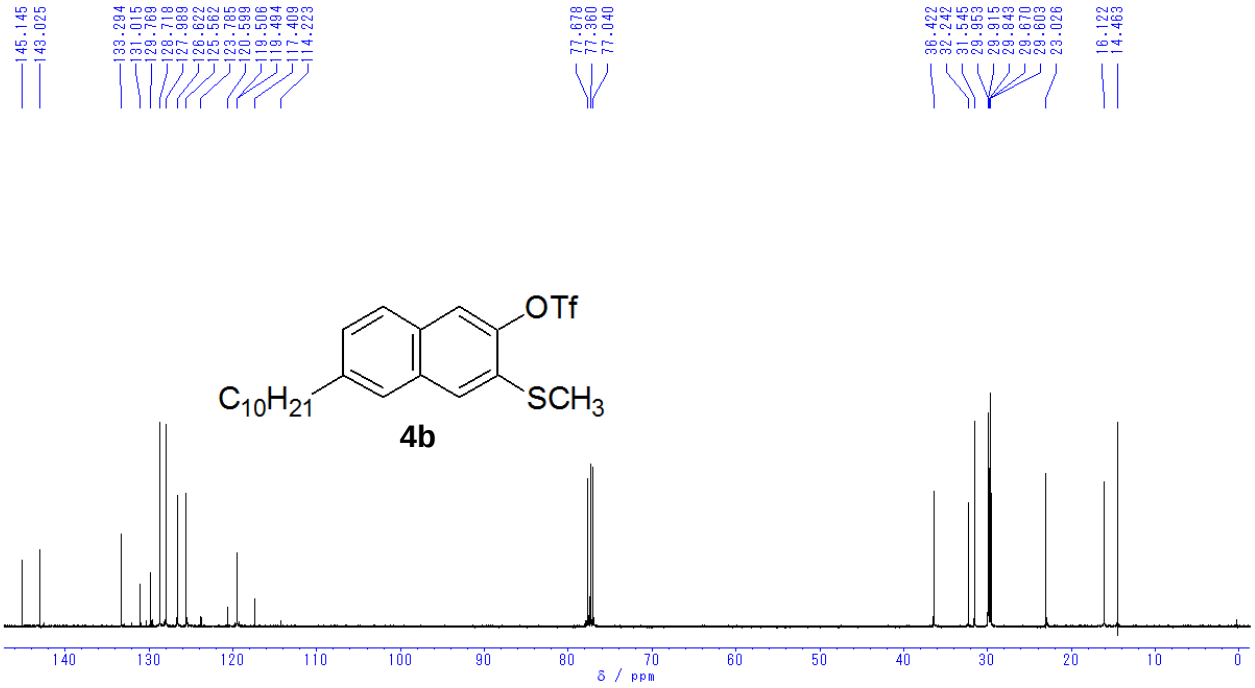


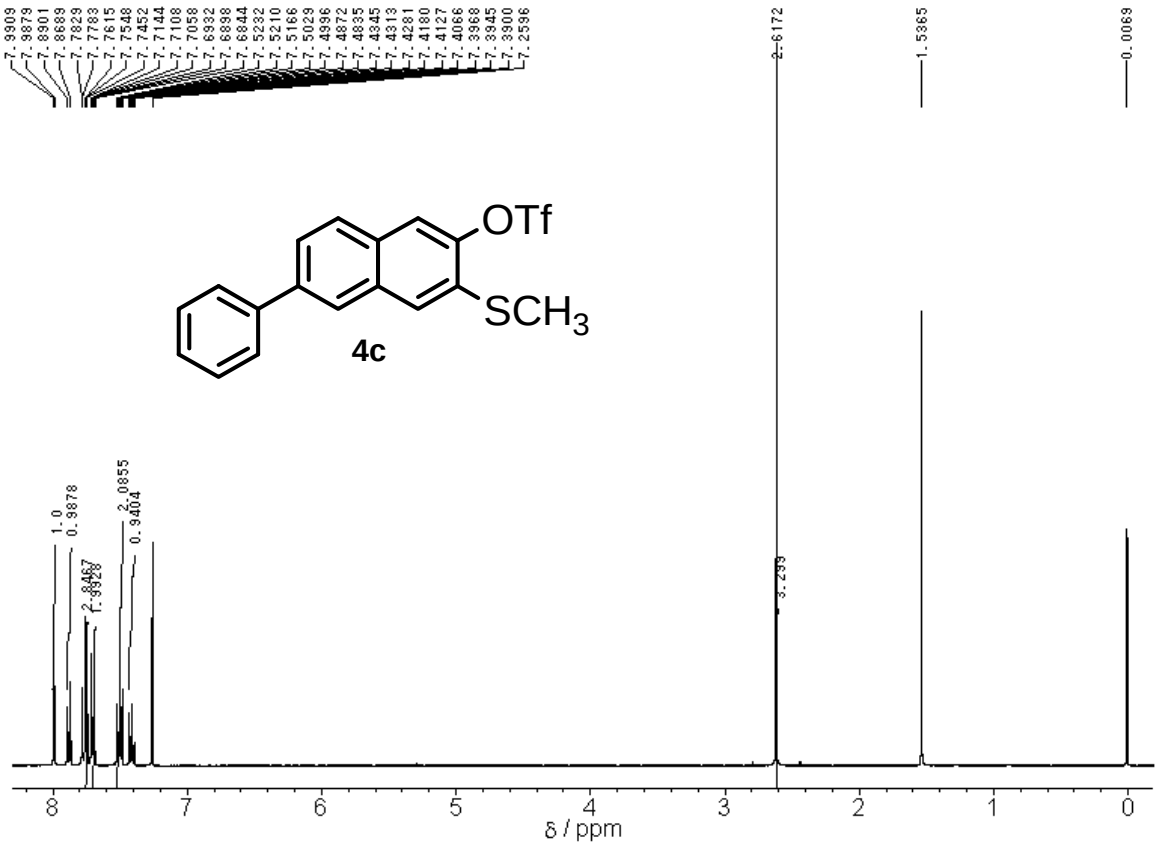
3e

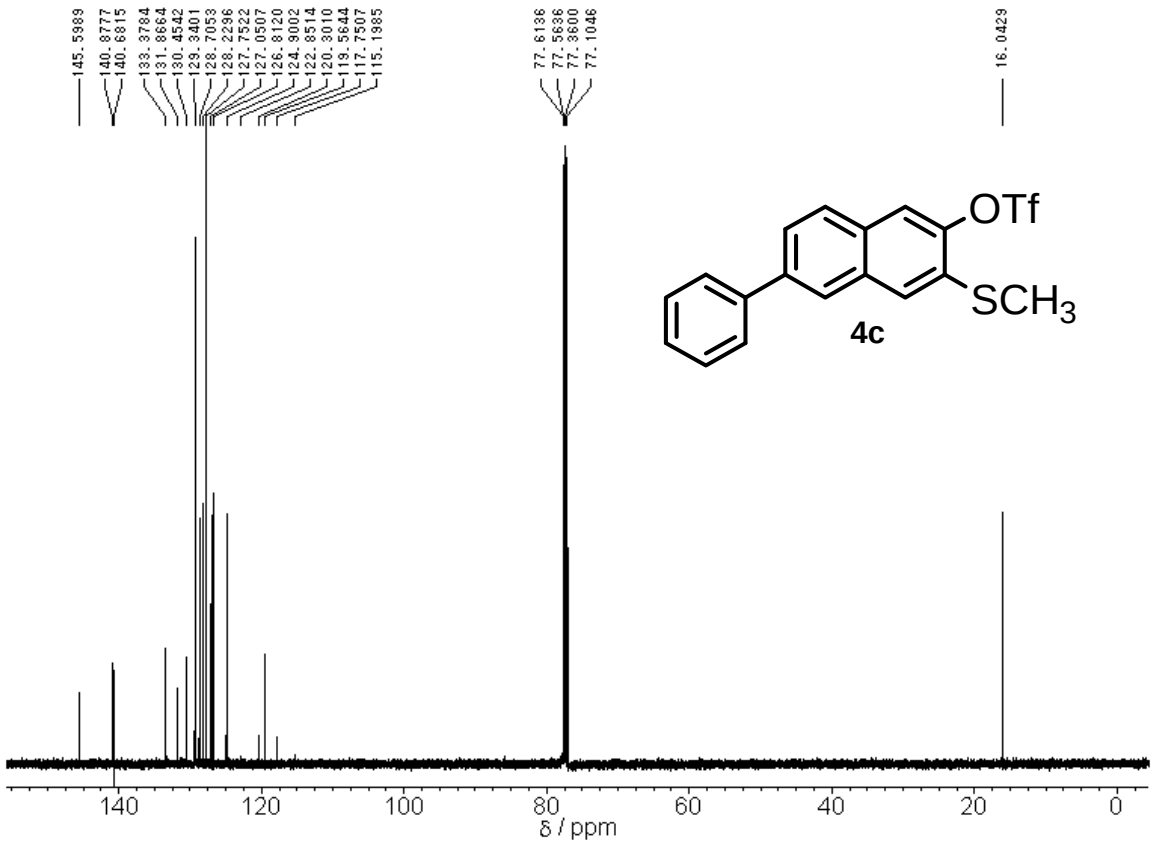

7.806
7.793
7.787
7.774
7.723
7.685
7.556
7.552
7.538
7.535
7.532
7.518
7.514
7.511
7.507
7.493
7.490
7.487
7.473
7.470
7.249
2.587
1.528
0.000
3.000
2.064
2.033
0.965
OTf
SCH3
4a
7
6
5
4
3
2
1
0
δ / ppm

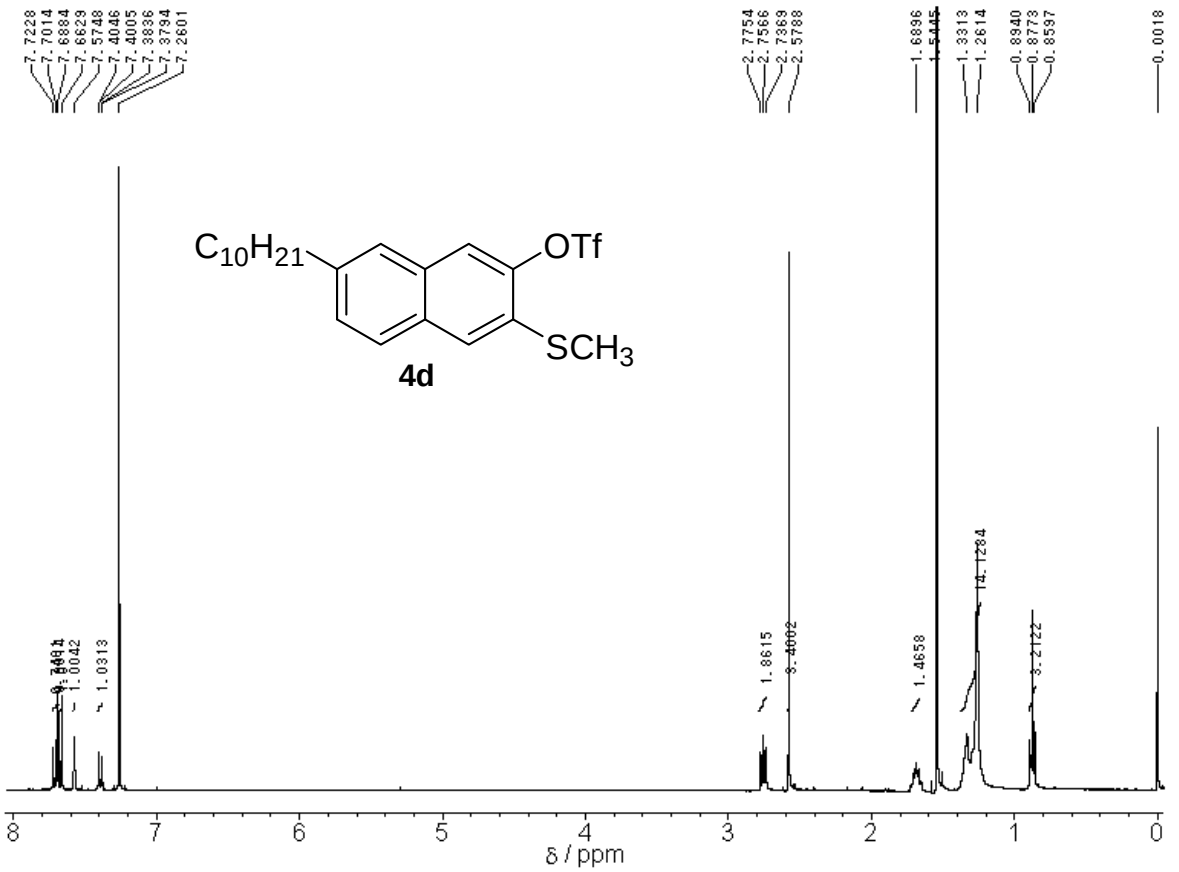

145.421
132.849
131.122
127.970
127.817
126.895
126.817
126.736
122.631
120.081
119.537
117.530
114.978
77.412
77.160
76.905
15.806
0.123
OTf
SCH3
4a
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ / ppm


7.723
7.702
7.676
7.620
7.560
7.361
7.357
7.340
7.336
7.252
2.776
2.757
2.738
2.579
1.702
1.684
1.665
1.556
1.324
1.257
0.892
0.876
0.858
0.000
3.167
2.081
1.028
OTf
C10H21
SCH3
4b
δ / ppm


145.145
143.025
133.294
131.015
129.769
128.718
127.989
126.622
125.562
123.785
120.599
119.506
119.494
117.409
114.223
77.678
77.360
77.040
36.422
32.242
31.545
29.953
29.915
29.843
29.670
29.603
23.026
16.122
14.463
OTf
C10H21
SCH3
4b
δ / ppm


OTf
SCH3
4c
δ / ppm


OTf
SCH3
4c
δ / ppm


7.7228
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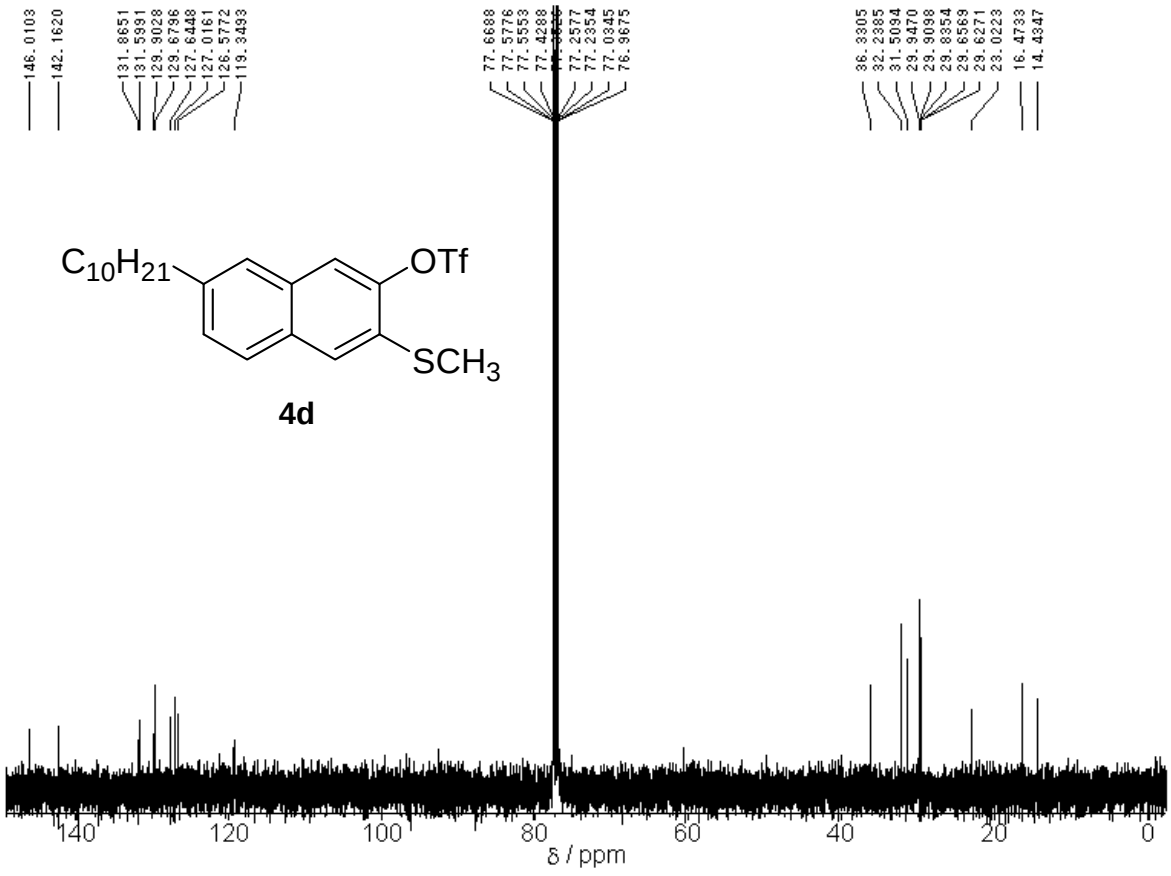
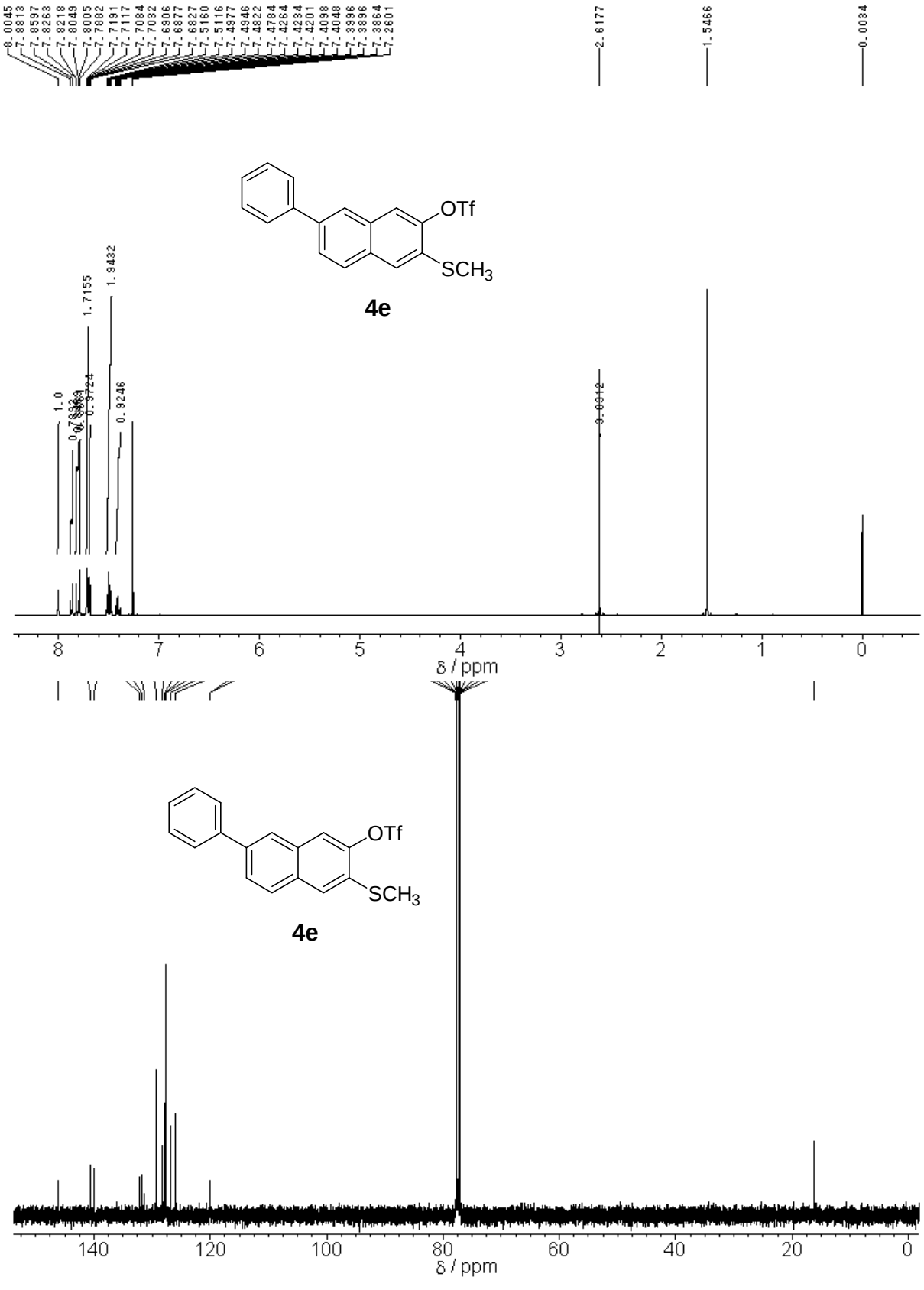
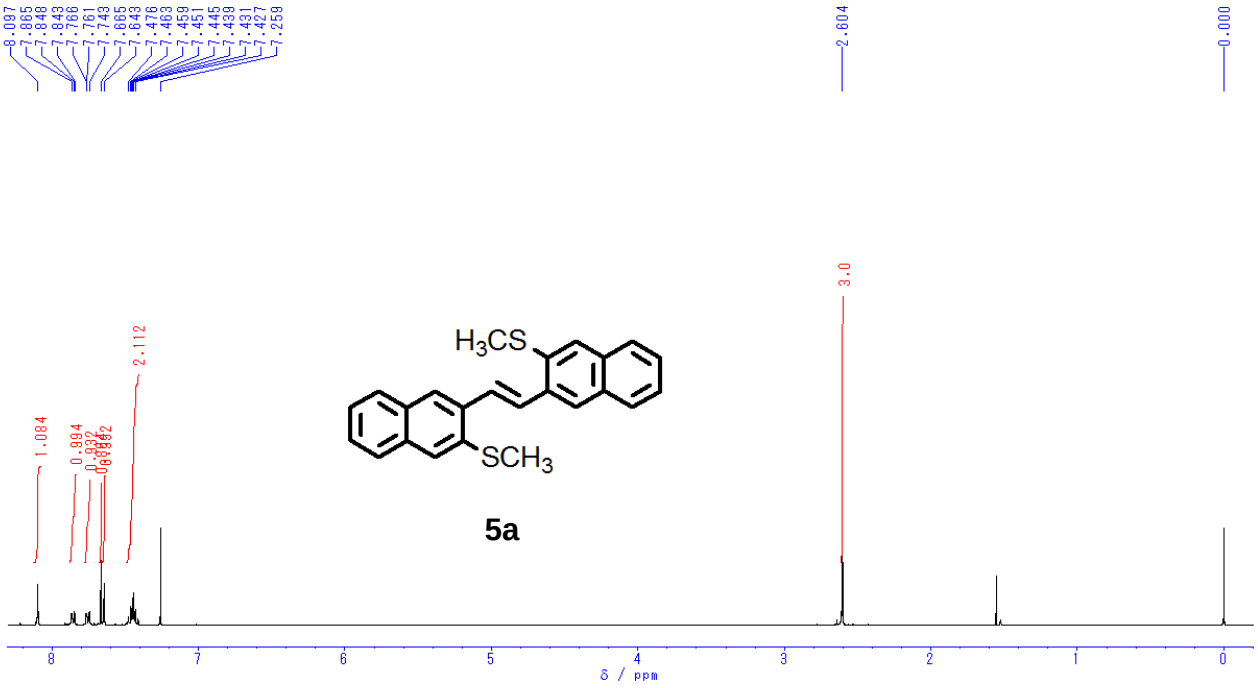
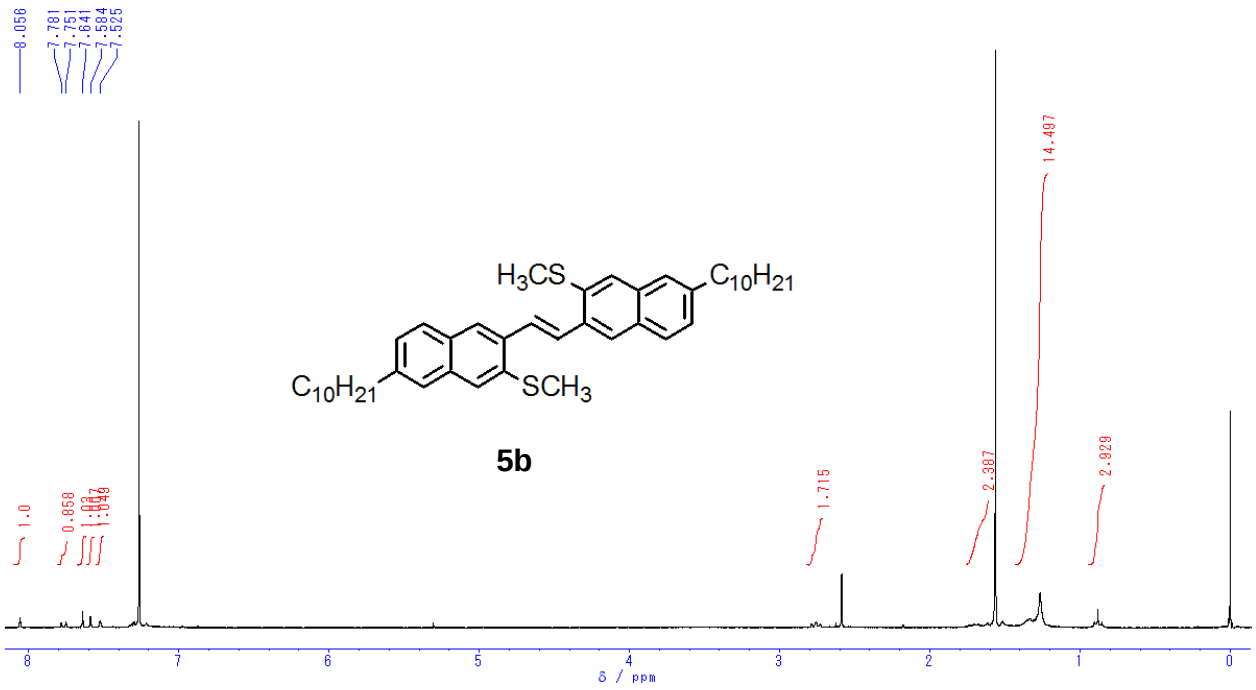
7.6884
7.6629
7.5748
7.4046
7.4005
7.3836
7.3794
7.2601
2.7754
2.7566
2.7369
2.5788
1.6896
1.3313
1.2614
0.8940
0.8773
0.8597
0.0018
1.0042
1.0313
1.8615
3.4002
1.4658
14.1284
3.2122
C10H21
OTf
SCH3
4d
8
7
6
5
4
3
2
1
0
δ / ppm


146.0103
142.1620
131.8651
131.5991
129.9028
129.6796
127.6448
127.0161
126.5772
119.3493
77.6688
77.5776
77.5553
77.4288
77.2577
77.2354
77.0345
76.9675
36.3305
32.2385
31.5094
29.9470
29.9098
29.8354
29.6569
29.6271
23.0223
16.4733
14.4347
C10H21
OTf
SCH3
4d
140
120
100
80
60
40
20
0
δ / ppm

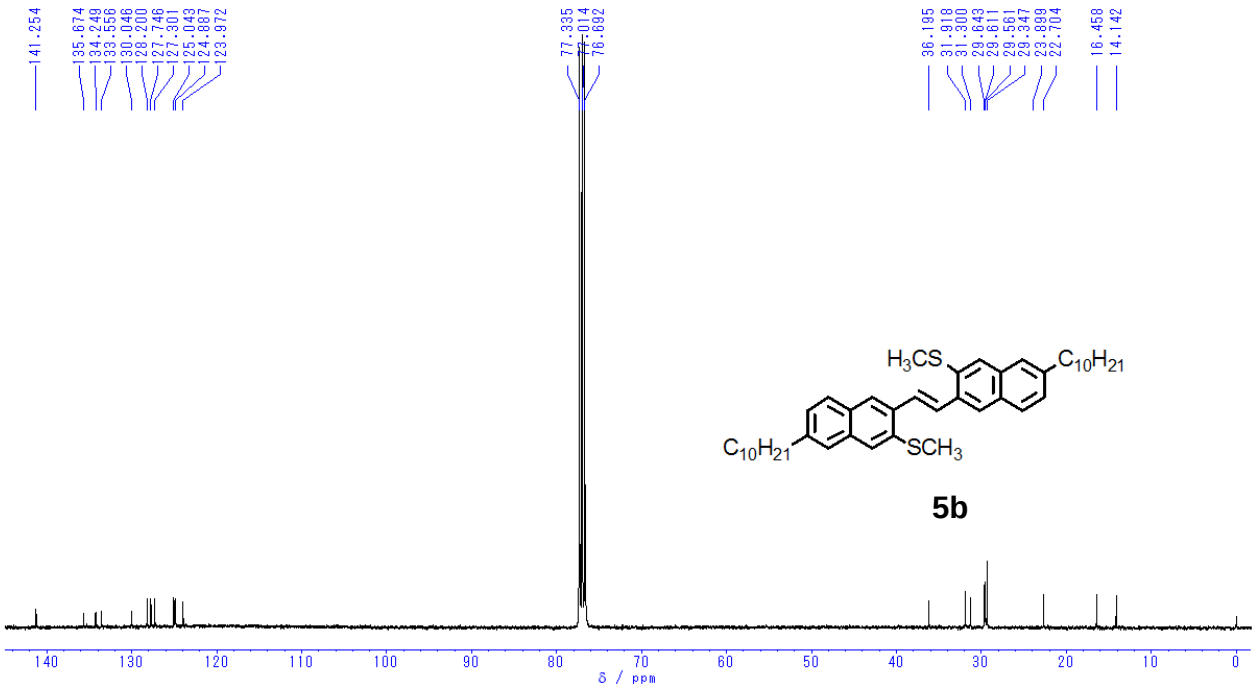

8.0045
7.8813
7.8597
7.8263
7.8218
7.8049
7.8005
7.7882
7.7191
7.7117
7.7084
7.7032
7.6906
7.6877
7.6827
7.5160
7.5116
7.4977
7.4946
7.4822
7.4784
7.4264
7.4234
7.4201
7.4098
7.4048
7.3996
7.3896
7.3864
7.2601
2.6177
1.5466
0.0034
OTf
SCH3
4e
1.0
1.7155
1.9432
0.9246
0.0012
8
7
6
5
4
3
2
1
0
δ / ppm
OTf
SCH3
4e
140
120
100
80
60
40
20
0
δ / ppm


8.097
7.865
7.848
7.843
7.766
7.761
7.743
7.665
7.643
7.476
7.463
7.459
7.451
7.445
7.439
7.431
7.427
7.259
2.604
0.000
3.0
2.112
1.084
0.994
0.932
H3CS
SCH3
5a
8
7
6
5
4
3
2
1
0
δ / ppm


8.058
7.781
7.751
7.641
7.584
7.525
14.497
2.387
2.929
1.715
1.0
0.858
δ / ppm

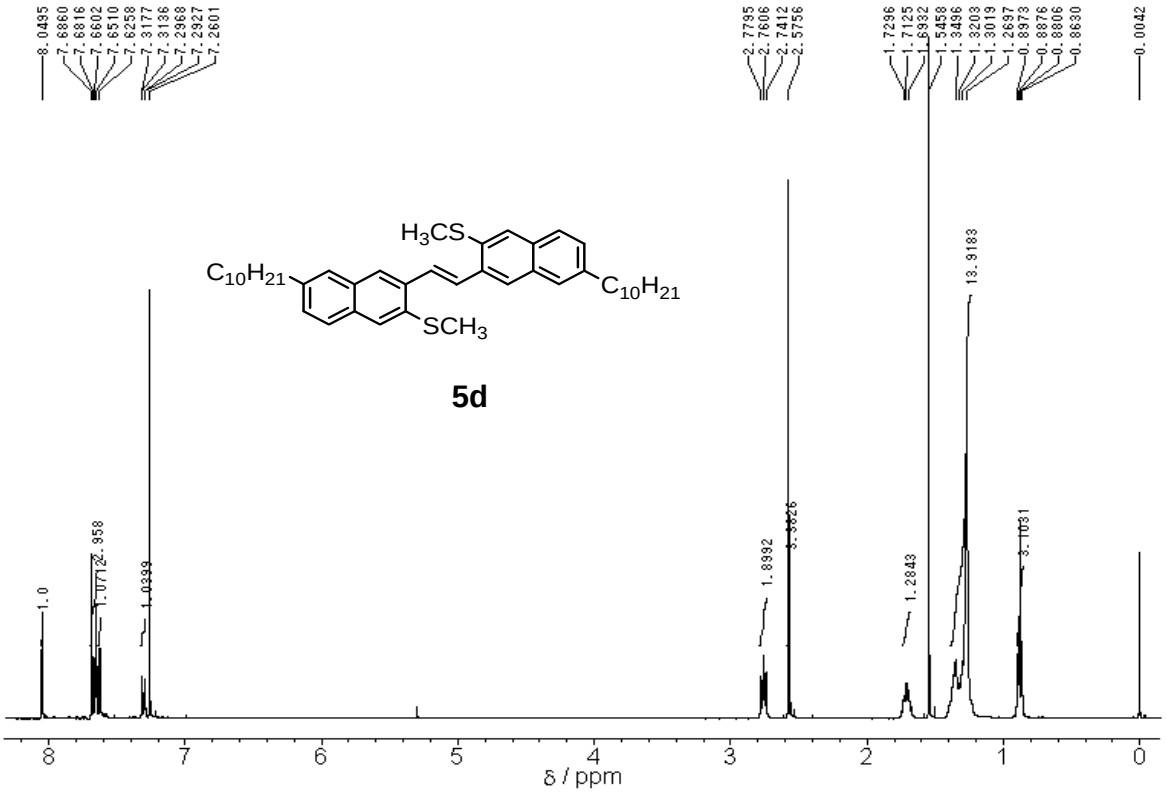
H3CS
C10H21
C10H21
SCH3

5b

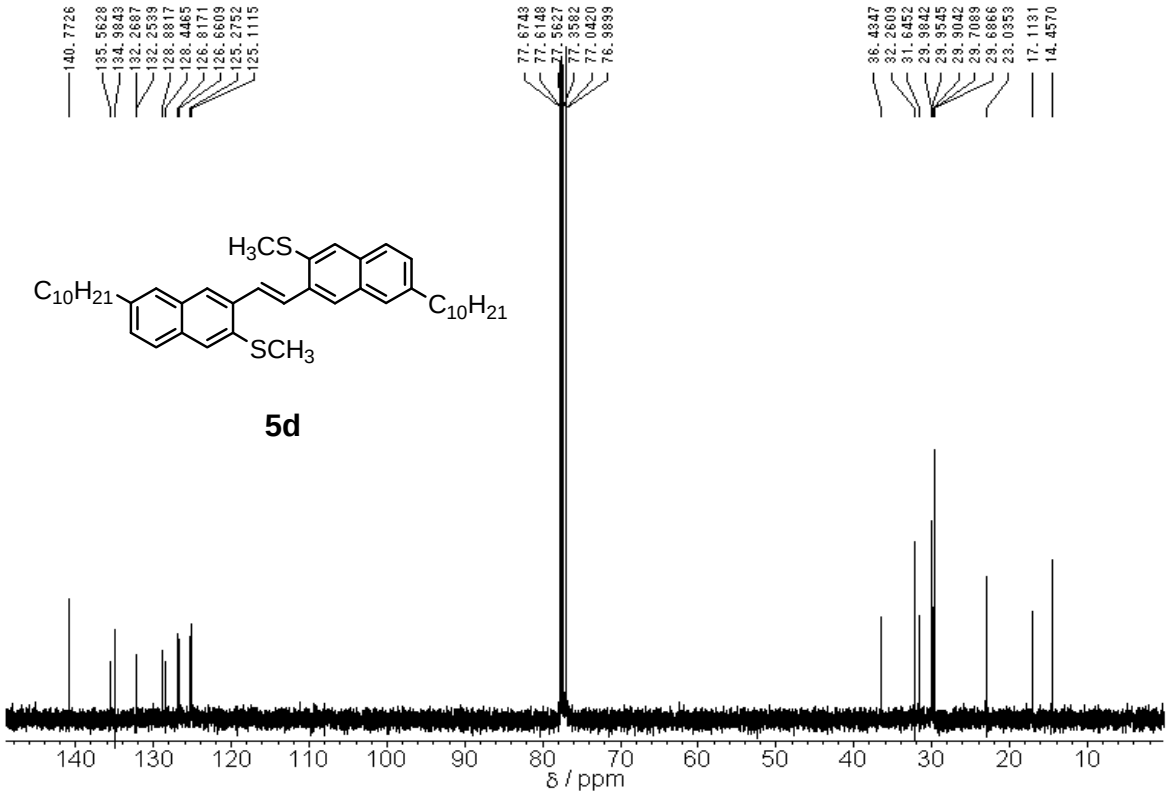

141.254
135.674
134.249
133.556
130.046
128.200
127.746
127.301
125.043
124.887
123.972
77.335
77.014
76.692
36.195
31.918
31.300
29.643
29.611
29.561
29.347
23.899
22.704
16.458
14.142
δ / ppm

H3CS
C10H21
C10H21
SCH3

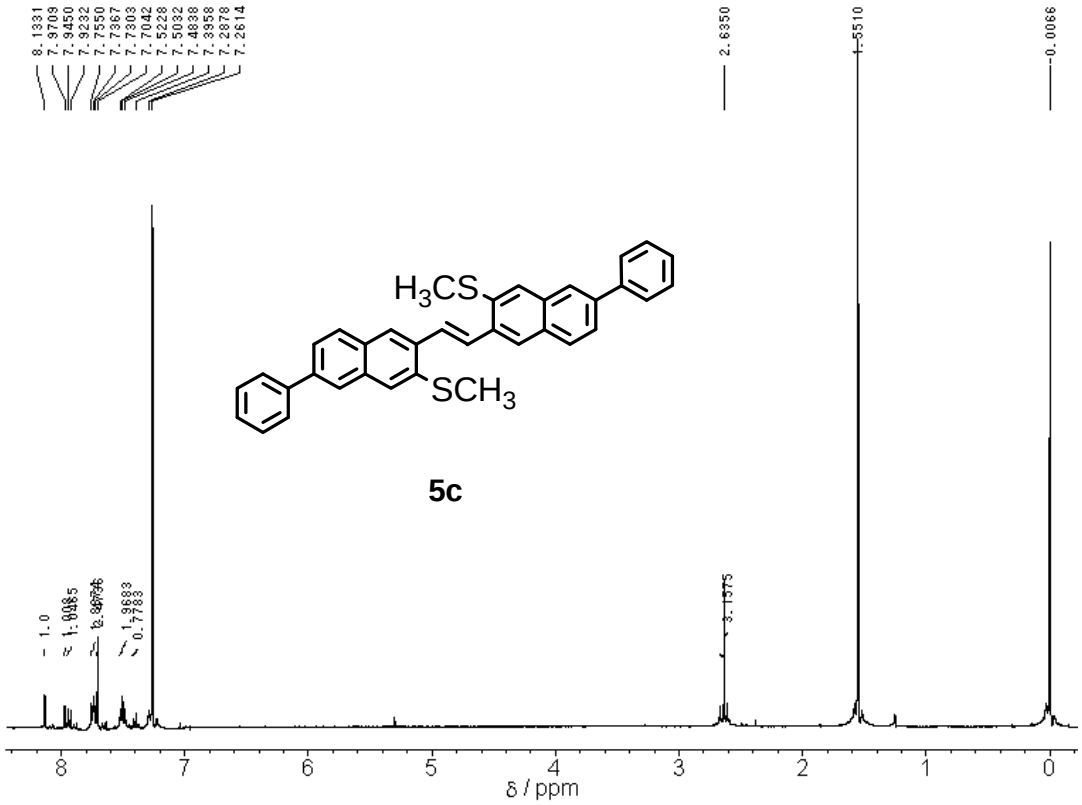
5b


8.0495
7.6860
7.6816
7.6602
7.6510
7.6258
7.3177
7.3136
7.2968
7.2927
7.2601
2.7735
2.7606
2.7412
2.5756
1.7296
1.7125
1.6932
1.5458
1.3486
1.3203
1.3019
1.2697
0.8973
0.8876
0.8806
0.8630
0.0042
1.0
2.958
1.0712
1.0339
1.8992
3.9826
1.2843
13.9183
3.1031
8
7
6
5
4
3
2
1
0
δ / ppm
H_3CS
$C_{10}H_{21}$
$C_{10}H_{21}$
SCH_3

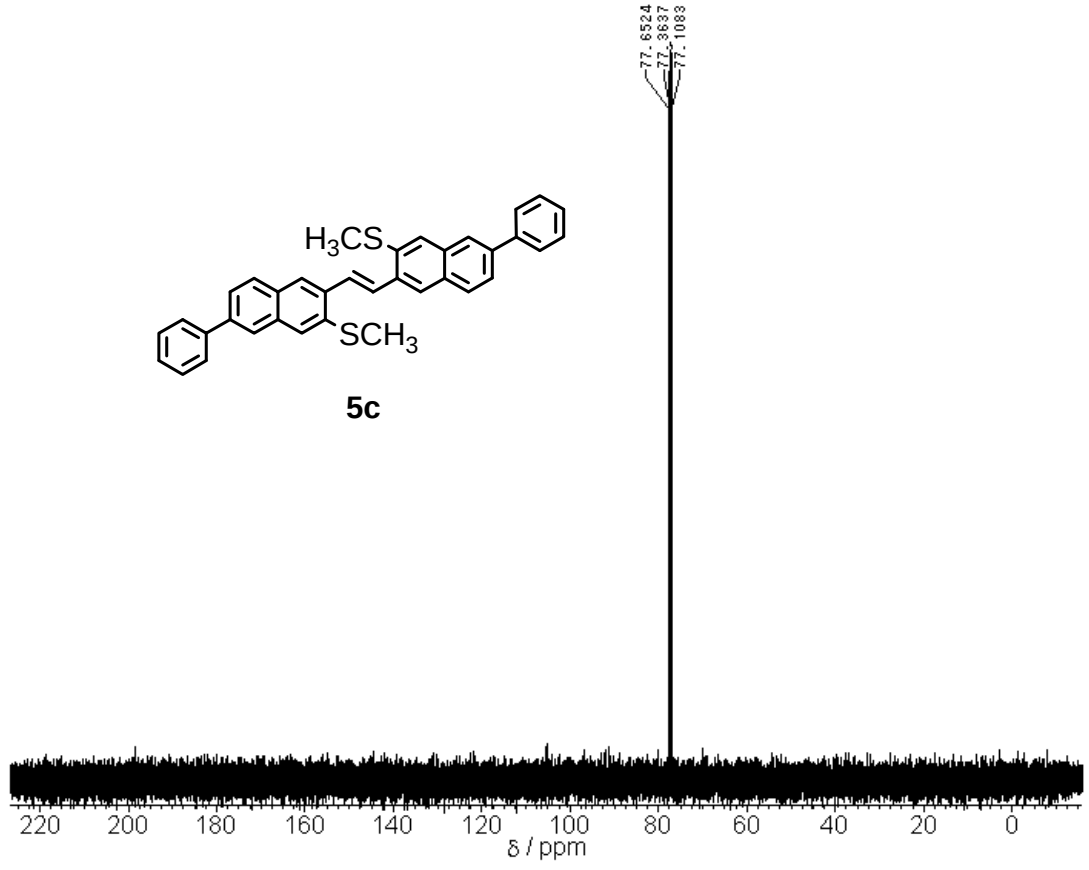
5d


140.7726
135.5628
134.9843
132.2687
132.2539
128.8817
128.4465
126.8171
126.6609
125.2752
125.1115
77.6743
77.6148
77.5627
77.3582
77.0420
76.3899
36.4347
32.2609
31.6452
29.9842
29.9545
29.9042
29.7089
29.6866
23.0353
17.1131
14.4570
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ / ppm
H_3CS
$C_{10}H_{21}$
$C_{10}H_{21}$
SCH_3

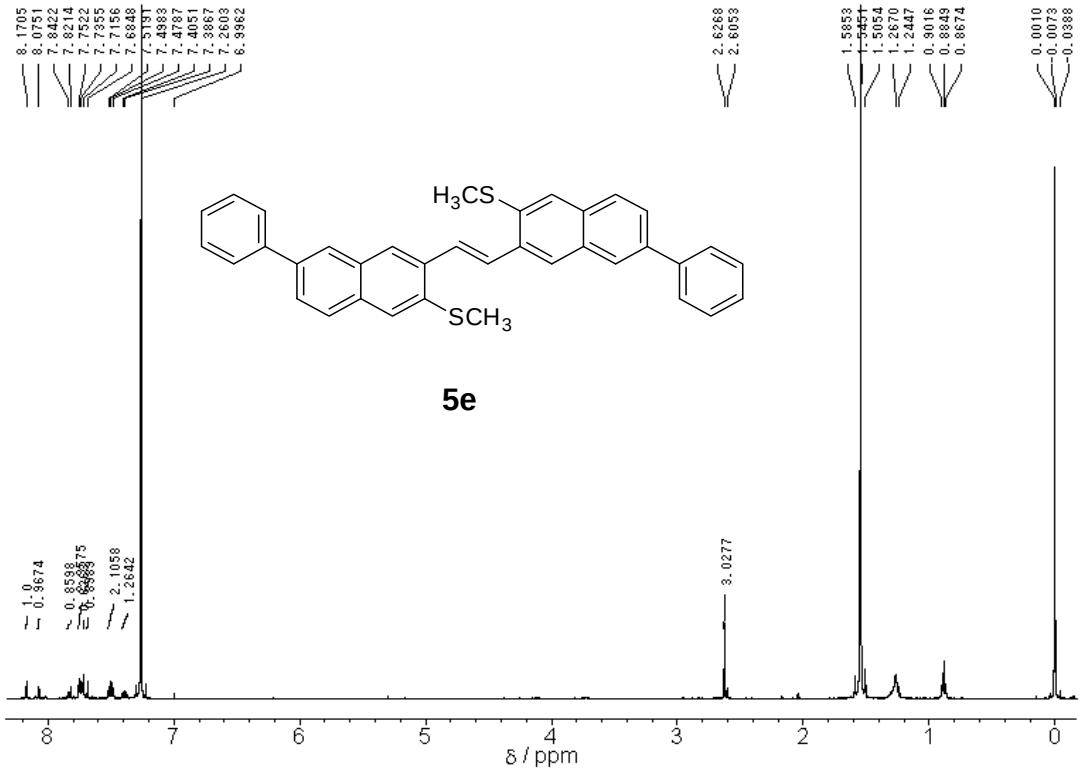
5d


8.1331
7.9709
7.9450
7.9232
7.7550
7.7367
7.7303
7.7042
7.5228
7.5032
7.4838
7.3958
7.2878
7.2614
2.6350
1.5510
0.0066
H3CS
SCH3
δ / ppm

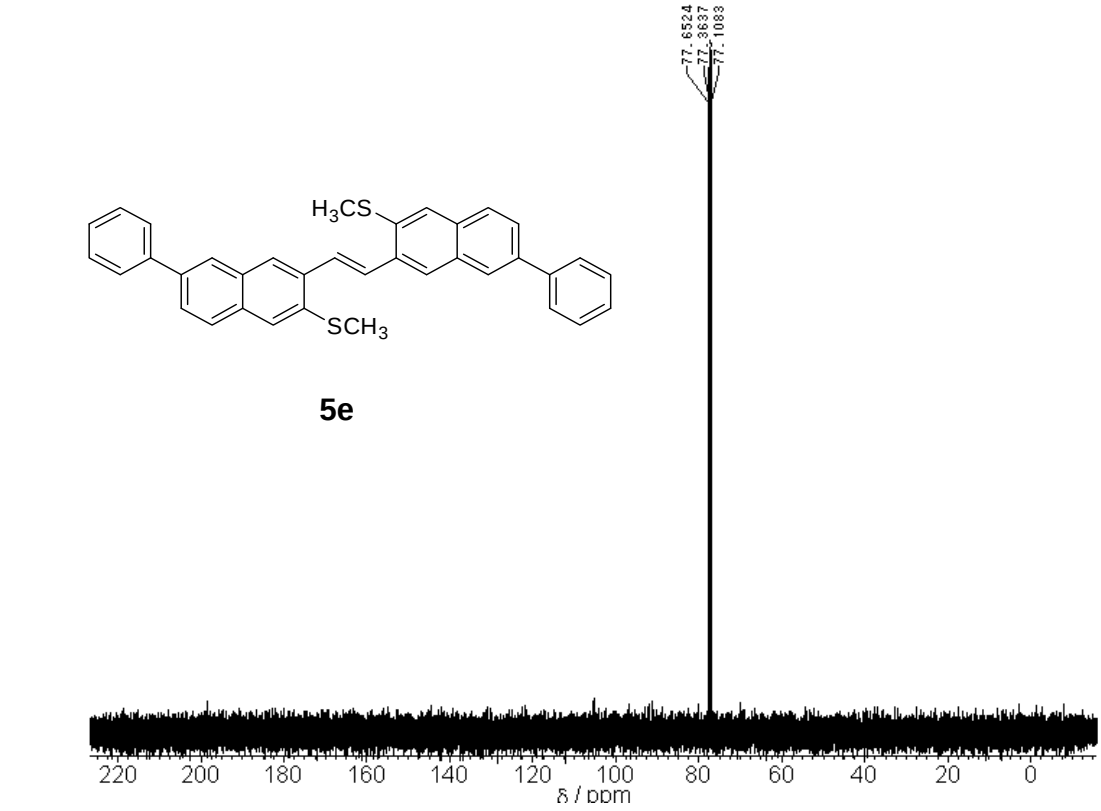
5c


77.6524
77.3637
77.1083
H3CS
SCH3
δ / ppm

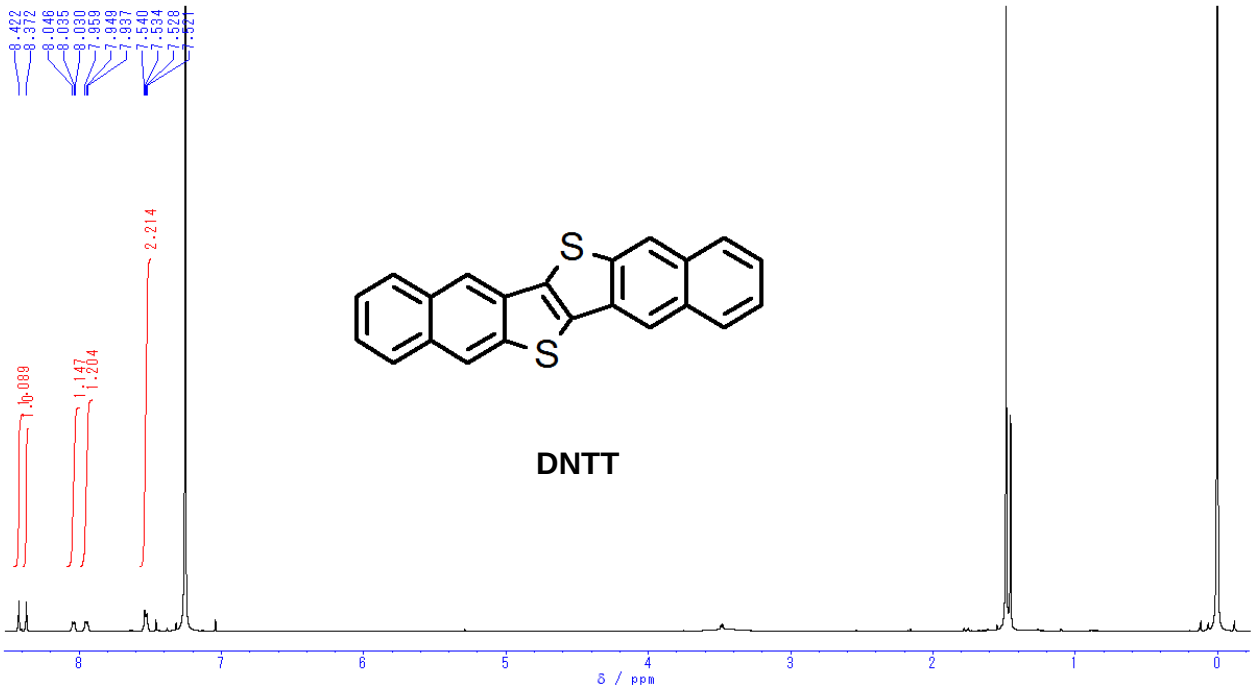
5c

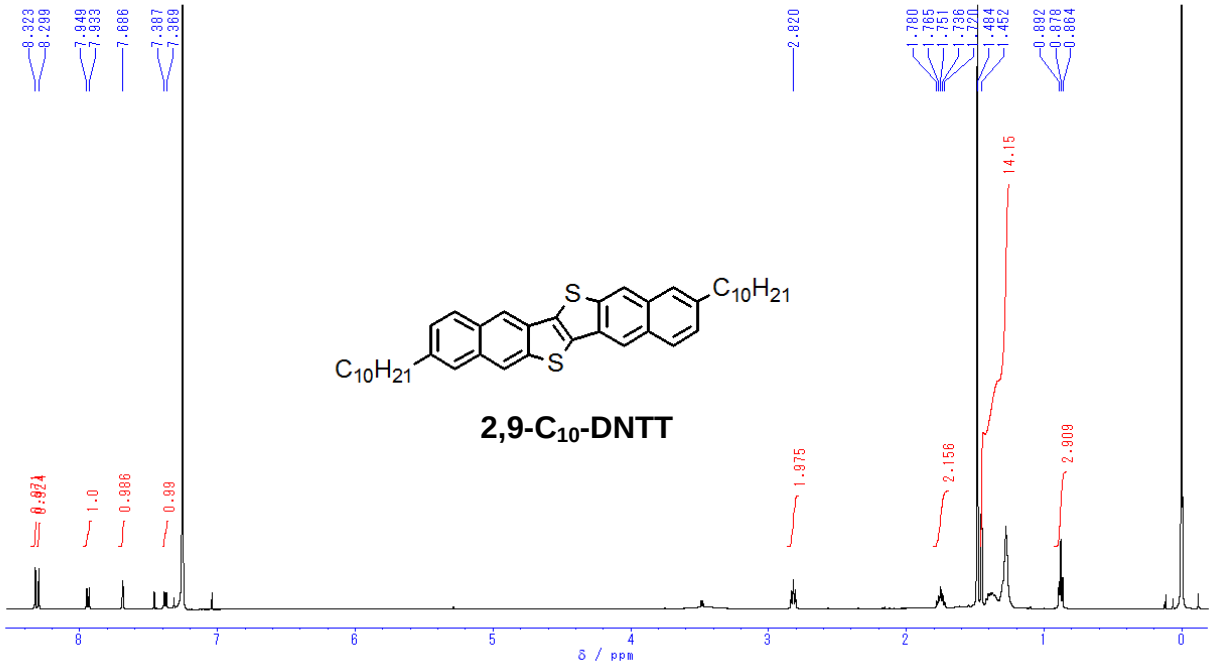

8.1705
8.0751
7.8422
7.8214
7.7522
7.7355
7.7156
7.6848
7.5191
7.4983
7.4787
7.4051
7.3867
7.2603
6.9962
2.6268
2.6053
1.5853
1.5451
1.5054
1.2670
1.2447
0.9016
0.8849
0.8674
0.0010
0.0073
-0.0388
1.0
0.9674
0.8538
2.1058
1.2642
3.0277
H3CS
SCH3
8
7
6
5
4
3
2
1
0
δ / ppm

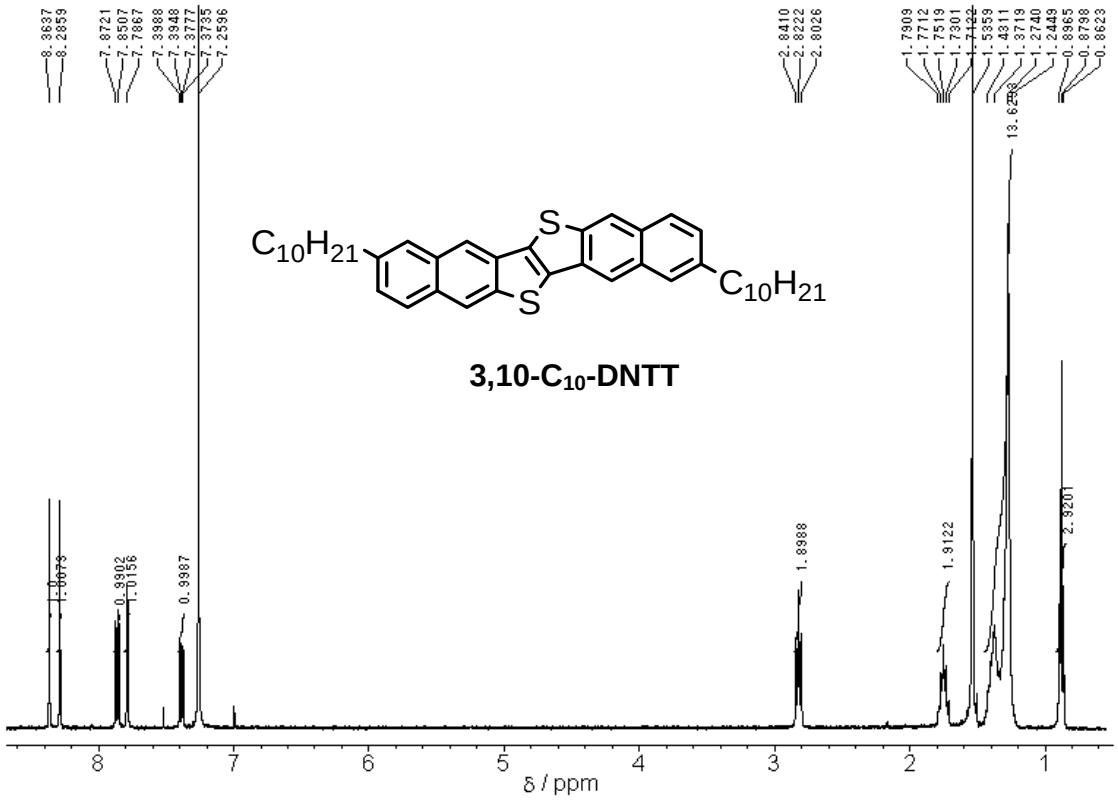
5e


77.6524
77.3637
77.1083
H3CS
SCH3
220
200
180
160
140
120
100
80
60
40
20
0
δ / ppm

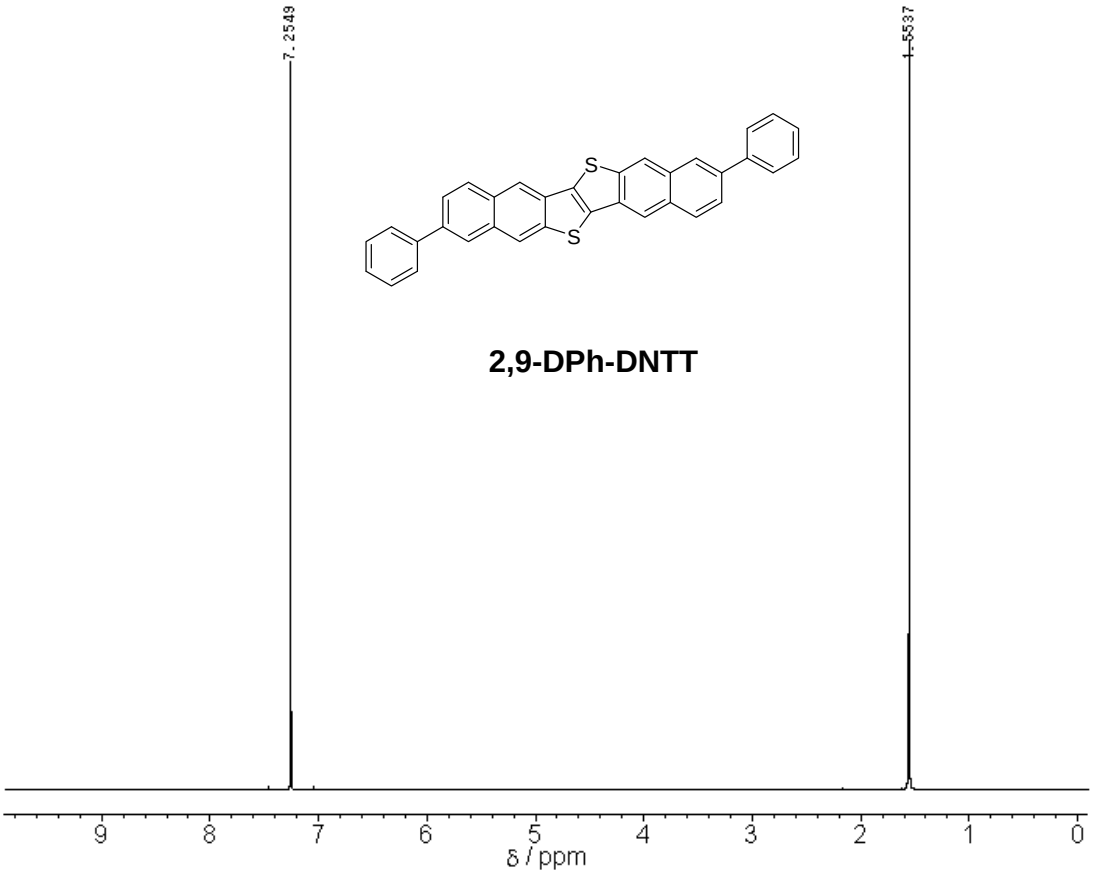
5e


8.422
8.372
8.046
8.035
8.030
7.959
7.949
7.937
7.540
7.534
7.528
7.521
2.214
1.089
1.147
1.204
S
S
DNTT
8
7
6
5
4
3
2
1
0
δ / ppm

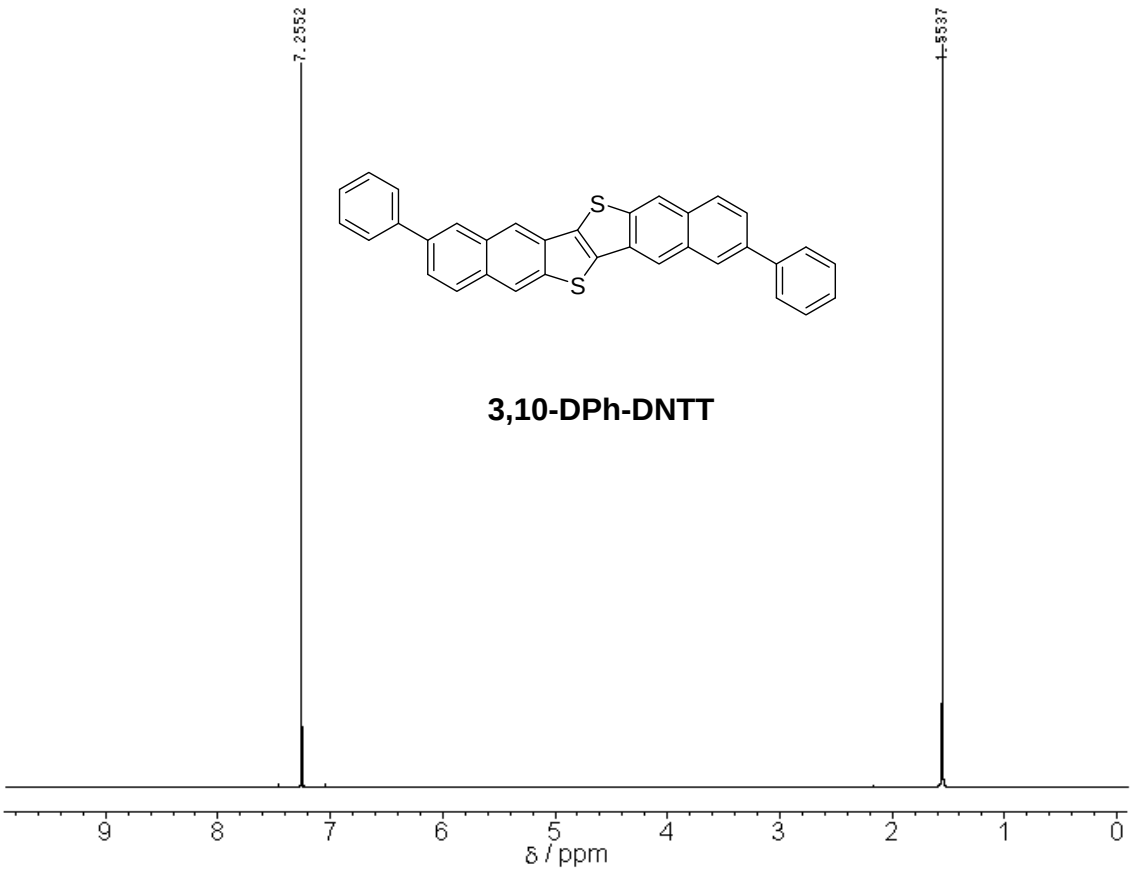

8.323
8.299
7.949
7.933
7.686
7.387
7.369
2.820
1.780
1.765
1.751
1.736
1.720
1.484
1.452
0.892
0.878
0.864
14.15
2.156
2.009
1.975
1.0
0.986
0.99
S
S
C10H21
C10H21
2,9-C10-DNTT
8
7
6
5
4
3
2
1
0
δ / ppm



3,10-C_{10}-DNTT



2,9-DPh-DNTT



3,10-DPh-DNTT