Supporting Information

Synthesis of Unsymmetrical Benzotrichalcogenolphenes by N-Heterocyclic Carbene-Palladium-Catalyzed Intramolecular Direct C3-Arylation

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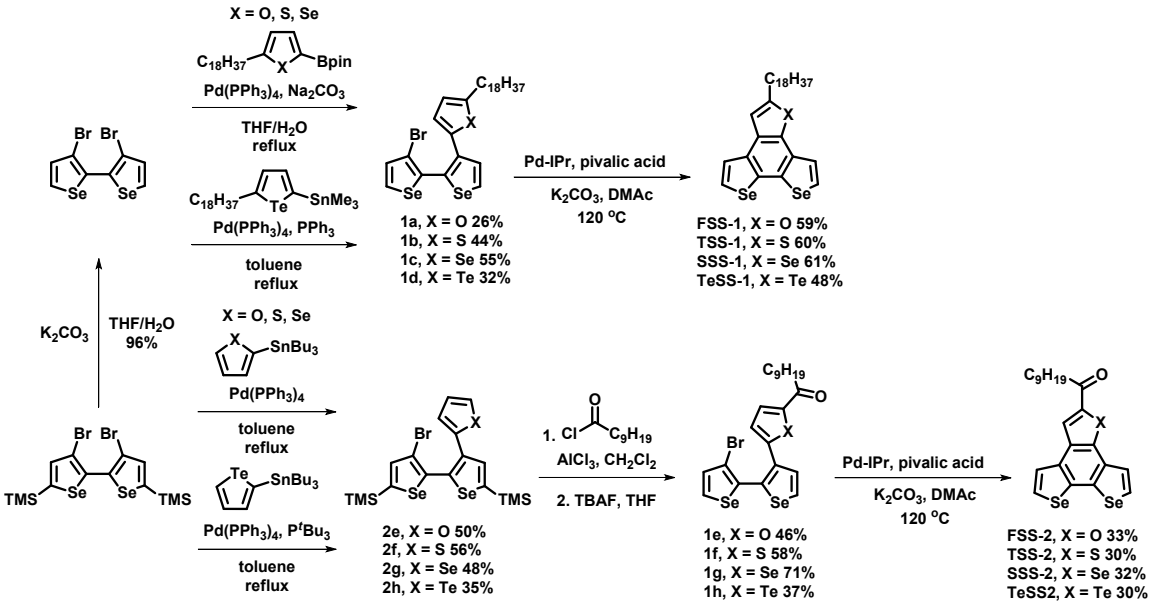
1. Synthetic procedures



Scheme S1. Synthetic route of **FSS-1**, **TSS-1**, **SSS-1**, **TeSS-1**, **FSS-2**, **TSS-2 and SSS-2**, **TeSS-2.**

Synthesis of 3-(5-octadecylfuranyl)-3'-bromo-2,2'-biselenophene (1a). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-furan (463 mg, 1.04 mmol), 3,3'-dibromo-2,2'-biselenophene (433 mg, 1.04 mmol), tetrakis(triphenylphosphine)palladium (60 mg, 5 mol%) and sodium carbonate (440 mg, 4.15 mmol) in THF/H_2O (29 mL /7 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1a** (184 mg, 26%, T_m = 37 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 7.0 Hz, 3H), 1.26–1.32 (m, 30H), 1.55–1.58 (m, 2H), 2.55 (t, J = 7.6 Hz, 2H), 5.92 (d, J = 3.2 Hz, 1H), 6.00 (d, J = 3.2 Hz, 1H), 7.30 (d, J = 6 Hz, 1H), 7.67 (d, J = 5.8 Hz, 1H), 8.03 (d, J = 5.8 Hz, 1H), 8.08 (d, J = 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 27.9, 28.1, 29.1, 29.4, 29.6, 29.65, 29.7, 31.9, 106.7, 108.3, 113.1, 129.5, 131.9, 132.2, 132.25, 133.2, 133.7, 137.5, 148.9, 155.7; HRMS (EI, [M^+], $C_{30}H_{43}OSe_2Br$): calcd, 658.0822; found, 658.0819.

Synthesis of 5-octadecybenzofurandiselenophene (FSS-1). A degassed solution

of **1a** (454 mg, 0.69 mmol), pivalic acid (21 mg, 0.21 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (22.3 mg, 5 mol%) and potassium carbonate (238 mg, 1.73 mmol) in DMAc (7 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **FSS-1** (235 mg, 59%, T_m = 58 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.26–1.40 (m, 28H), 1.42–1.43 (m, 2H), 1.78–1.83 (m, 2H), 2.87 (t, J = 7.6 Hz, 2H), 6.71 (s, 1H), 7.83 (d, J = 6 Hz, 1H), 7.97–8.04 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 28.0, 28.5, 29.2, 29.38, 29.4, 29.6, 29.7, 29.72, 31.9, 101.4, 122.2, 123.4, 125.5, 126.1, 127.7, 127.8, 132.2, 132.9, 134.1, 149.3, 158.0; HRMS (EI, [M^+], $C_{30}H_{42}OSe_2$): calcd, 578.1561; found, 578.1584.

Synthesis of 3-(5-octadecylthienyl)-3'-bromo-2,2'-biselenophene (1b). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-thiophene (222 mg, 0.48 mmol), 3,3'-dibromo-2,2'-biselenophene (200 mg, 0.48 mmol), tetrakis(triphenylphosphine)palladium (28 mg, 5 mol%) and sodium carbonate (203 mg, 1.92 mmol) in THF/H_2O (14 mL /3.5 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1b** (142 mg, 44%, T_m = 60 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 7.0 Hz, 3H), 1.26–1.34 (m, 30H), 1.58–1.64 (m, 2H), 2.73 (t, J = 7.4 Hz, 2H), 6.61 (d, J = 3.4 Hz, 1H), 6.82 (d, J = 3.4 Hz, 1H), 7.28 (d, J = 6 Hz, 1H), 7.54 (d, J = 5.6 Hz, 1H), 8.02 (d, J = 5.6 Hz, 1H), 8.08 (d, J = 6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 29.1, 29.37, 29.4, 29.6, 29.66, 29.68, 29.69, 29.7, 30.1. 31.5, 31.9, 113.8, 124.1, 125.9, 131.5, 131.6, 132.8, 133.3, 133.4, 136.1, 136.9, 137.2, 146.5; HRMS (FD, [M^+], $C_{30}H_{43}SSe_2Br$): calcd, 674.0594; found, 674.0601.

Synthesis of 5-octadecylbenzothiophenediselenophene (TSS-1). A degassed solution of **1b** (246 mg, 0.38 mmol), pivalic acid (12 mg, 0.11 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) 12 mg, 5

mol%) and potassium carbonate (131 mg, 0.95 mmol) in DMAc (1 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **TSS-1** (131 mg, 60%, T_m = 70 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.25–1.45 (m, 30H), 1.79–1.83 (m, 2H), 2.99 (t, J = 7.6 Hz, 2H), 7.41 (s, 1H), 7.81 (d, J = 6 Hz, 1H), 7.96 (d, J = 6 Hz, 1H), 8.02–8.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.38, 29.4, 29.6, 29.68, 29.7, 30.8, 31.5, 31.9, 119.6, 126.0, 126.4, 127.3, 128.1, 133.0, 133.2, 134.0, 134.4, 134.6, 135.6, 145.3; HRMS (EI, [M^+], $C_{30}H_{42}SSe_2$): calcd, 594.1338; found, 594.1333.

Synthesis of 3-(5-octadecylselenyl)-3'-bromo-2,2'-biselenophene (1c). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-selenophene (975 mg, 1.91 mmol), 3,3'-dibromo-2,2'-biselenophene (800 mg, 1.91 mmol), tetrakis(triphenylphosphine)palladium (111 mg, 5 mol%) and sodium carbonate (812 mg, 7.66 mmol) in THF/H_2O (55 mL /14 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (30 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1c** (760 mg, 55%, T_m = 56 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 7.0 Hz, 3H), 1.25–1.43 (m, 30H), 1.58–1.63 (m, 2H), 2.78 (t, J = 7.4 Hz, 2H), 6.79 (d, J = 3.8 Hz, 1H), 7.08 (d, J = 3.8 Hz, 1H), 7.30 (d, J = 6 Hz, 1H), 7.56 (d, J = 5.6 Hz, 1H), 8.05–8.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 29.1, 29.4, 29.6, 29.68, 29.71, 29.75, 32.0, 32.4, 32.8, 114.5, 126.1, 128.1, 131.1, 131.4, 133.1, 133.4, 137.0, 139.2, 141.3, 154.6; HRMS (FAB, [M^+], $C_{30}H_{43}BrSe_3$): calcd, 722.0044; found, 722.0049.

Synthesis of 5-octadecylbenzotriselenophene (SSS-1). A degassed solution of **1c** (200 mg, 0.28 mmol), pivalic acid (9 mg, 0.08 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (9 mg, 5 mol%) and potassium carbonate (96 mg, 0.70 mmol) in DMAc (1 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of

SSS-1 (109 mg, 61%, T_m = 69 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89 (t, J = 6.8 Hz, 3H), 1.26–1.46 (m, 30H), 1.76–1.83 (m, 2H), 3.03 (t, J = 7.4 Hz, 2H), 7.62 (s, 1H), 7.69 (d, J = 6 Hz, 1H), 7.95 (d, J = 6 Hz, 1H), 8.00 (d, J = 5.6 Hz, 1H), 8.03 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 29.1, 29.4, 29.44, 29.6, 29.68, 29.7, 29.74, 32.0, 32.3, 33.3, 123.0, 126.7, 127.3, 127.34, 128.0, 134.2, 135.2, 135.5, 135.8, 135.9, 136.5, 150.7; HRMS (FAB, [M^+], $C_{30}H_{42}Se_3$): calcd, 642.0782; found, 642.0786.

Synthesis of 3-(5-octadecyltellurophenyl)-3'-bromo-2,2'-biselenophene (1d). A degassed solution of 2-octadecyl-5-trimethylstannyltellurophene (427 mg, 0.72 mmol), 3,3'-dibromo-2,2'-biselenophene (300 mg, 0.72 mmol), tetrakis(triphenylphosphine)palladium (41 mg, 5 mol%) and triphenylphosphine (19 mg, 0.07 mmol) in toluene (7 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1d** (176 mg, 32%, T_m = 58 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.35 (m, 30H), 1.56–1.60 (m, 2H), 2.80 (t, J = 7.6 Hz, 2H), 7.21 (d, J = 4.0 Hz, 1H), 7.32 (d, J = 6 Hz, 1H), 7.57 (d, J = 4.0 Hz, 1H), 7.65 (d, J = 5.8 Hz, 1H), 8.04 (d, J = 5.8 Hz, 1H), 8.14 (d, J = 6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 29.2, 29.4, 29.42, 29.6, 29.66, 29.7, 29.73, 32.0, 34.2, 36.9, 115.8, 129.9, 130.9, 132.6, 133.3, 133.6, 134.4, 135.2, 136.4, 136.7, 143.0, 154.9; HRMS (EI, [M^+], $C_{30}H_{43}Se_2BrTe$): calcd, 771.9935; found, 771.9950.

Synthesis of 5-octadecylbenzotellurophenediselenophene (TeSS-1). A degassed solution of **1d** (163 mg, 0.24 mmol), pivalic acid (7.4 mg, 0.07 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (23 mg, 15 mol%) and potassium carbonate (83 mg, 0.60 mmol) in DMAc (1 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (10 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **TeSS-1** (80 mg, 48%, T_m = 63 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.25–1.37 (m, 28H), 1.41–1.47 (m, 2H), 1.69–1.77 (m, 2H), 3.01 (t, J = 7.4 Hz, 2H), 7.49 (d, J = 5.6 Hz, 1H), 7.97 (d, J = 5.6 Hz, 1H), 7.99–8.01 (m, 2H), 8.04 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.8, 29.2, 29.4, 29.5, 29.6, 29.7, 29.8, 32.0, 34.2,

37.3, 127.1, 127.4, 127.45, 127.8, 129.8, 131.5, 133.7, 137.0, 137.6, 140.6, 142.2, 147.3; HRMS (EI, [M^+], $C_{30}H_{42}Se_2Te$): calcd, 692.0674; found, 692.0696.

Synthesis of 3-furanyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (2e). A degassed solution of 2-tributylstannylfuran (953 mg, 2.67 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (1.5 g, 2.67 mmol), tetrakis(triphenylphosphine)palladium (154 mg, 5 mol%) in toluene (27 mL) was stirred for 17 h at 110 ^oC under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a liquid of **2e** (800 mg, 55%). ^1H NMR (400 MHz, $CDCl_3$): δ 0.33 (s, 9H), 0.36 (s, 9H), 6.08 (dd, J_1 = 3.4 Hz, J_2 = 0.6 Hz, 1H), 6.35 (dd, J_1 = 3.4 Hz, J_2 = 1.8 Hz, 1H), 7.37 (dd, J_1 = 1.8 Hz, J_2 = 0.6 Hz, 1H), 7.45 (s, 1H), 7.87 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ –0.02, 0.2, 107.6, 111.5, 113.5, 134.2, 136.0, 139.0, 139.3, 141.1, 141.8, 150.5, 150.7, 150.9; HRMS (EI, [M^+], $C_{18}H_{23}BrOSe_2Si_2$): calcd, 549.8801; found, 549.8798.

Synthesis of 3-(5-decanoylfuranyl)-3'-bromo-2,2'-biselenophene (1e). To an ice-cooled solution of **2e** (500 mg, 0.91 mmol) and decanoyl chloride (191 mg, 1.00 mmol) in dichloromethane (9 mL) was added aluminium chloride (146 mg, 1.09 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (9 mL). A 1 M solution of TBAF in THF (0.91 mL, 0.91 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give an oil of **1e** (236 mg, 46 %). ^1H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.27–1.37 (m, 12H), 1.63–1.69 (m, 2H), 2.64 (t, J = 7.6 Hz, 2H), 6.24 (d, J = 3.6 Hz, 1H), 7.11 (d, J = 3.6 Hz, 1H), 7.32 (d, J = 5.6 Hz, 1H), 7.77 (d, J = 5.6 Hz, 1H), 8.08 (d, J = 6 Hz, 1H), 8.15 (d, J = 6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.3, 29.3, 29.35, 29.4, 29.5, 31.9, 38.3, 109.8, 113.3, 118.2, 129.4, 132.1, 133.0, 133.03, 133.4, 136.4, 137.6, 151.3, 153.6, 189.9; HRMS (ESI, [M+H], $C_{22}H_{26}BrO_2Se_2$): calcd, 560.9441; found, 560.9448.

Synthesis of 5-decanoylbenzofurandiselenophene (FSS-2). A degassed solution of **1e** (143 mg, 0.26 mmol), pivalic acid (7.8 mg, 0.07 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (8.3 mg, 5 mol%) and potassium carbonate (88 mg, 0.64 mmol) in DMAc (1.5 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **FSS-2** (40 mg, 33%, T_m = 68 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.28–1.39 (m, 10H), 1.41–1.45 (m, 2H), 1.81–1.84 (m, 2H), 3.02 (t, J = 7.4 Hz, 2H), 7.83 (s, 1H), 7.91 (d, J = 5.6 Hz, 1H), 8.10–8.11 (m, 2H), 8.16 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.5, 29.3, 29.4, 29.5, 31.9, 38.9, 112.1, 120.7, 123.6, 125.4, 125.7, 128.8, 129.7, 132.7, 134.7, 139.7, 150.9, 151.2, 191.0; HRMS (FAB, [M^+], $C_{22}H_{24}O_2Se_2$): calcd, 480.0107; found, 480.0104.

Synthesis of 3-thienyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (2f). A degassed solution of 2-trimethylstannylthiophene (133 mg, 0.36 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (200 mg, 0.36 mmol), tetrakis(triphenylphosphine)palladium (21 mg, 5 mol%) in toluene (4 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **2f** (113 mg, 56%, T_m = 115 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.32 (s, 9H), 0.37 (s, 9H), 6.96 (dd, J_1 = 5.1 Hz, J_2 = 3.7 Hz, 1H), 7.03 (dd, J_1 = 3.7 Hz, J_2 = 1.2 Hz, 1H), 7.22 (dd, J_1 = 5.1 Hz, J_2 = 1.2 Hz, 1H), 7.42 (s, 1H). 7.71 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 0.04, 0.2, 114.2, 125.4, 126.1, 127.1, 137.3, 138.1, 138.9, 139.3, 139.8, 141.7, 150.0, 151.2; HRMS (EI, [M^+], $C_{18}H_{23}BrSSe_2Si_2$): calcd, 565.8573; found, 565.8572.

Synthesis of 3-(5-decanoylthienyl)-3'-bromo-2,2'-biselenophene (1f). To an ice-cooled solution of **2f** (429 mg, 0.76 mmol) and decanoyl chloride (159 mg, 0.83 mmol) in dichloromethane (8 mL) was added aluminium chloride (152 mg, 1.14 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was

dissolved in THF (8 mL). A 1 M solution of TBAF in THF (0.76 mL, 0.76 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give a solid of **1f** (252 mg, 58%, T_m = 53 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, J = 6.6 Hz, 3H), 1.26–1.34 (m, 12H), 1.67–1.72 (m, 2H), 2.81 (t, J = 7.6 Hz, 2H), 6.98 (d, J = 3.8 Hz, 1H), 7.29 (d, J = 5.8 Hz, 1H), 7.52 (d, J = 3.8 Hz, 1H), 7.60 (d, J = 5.8 Hz, 1H), 8.07 (d, J = 6 Hz, 1H), 8.14 (d, J = 6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.9, 29.3, 29.35, 29.4, 31.8, 39.1, 114.0, 126.7, 131.1, 131.9, 132.7, 133.5, 133.6, 135.6, 136.0, 137.3, 143.2, 146.5, 193.5; HRMS (EI, [M^+], $C_{22}H_{25}BrOSSe_2$): calcd, 575.9140; found, 575.9133.

Synthesis of 5-decanoylbenzothiophenediselenophene (TSS-2). A degassed solution of **1f** (252 mg, 0.44 mmol), pivalic acid (13 mg, 0.13 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (14 mg, 5 mol%) and potassium carbonate (151 mg, 1.09 mmol) in DMAc (2 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **TSS-2** (53 mg, 30%, T_m = 95 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.25–1.45 (m, 12H), 1.82–1.85 (m, 2H), 3.06 (t, J = 7.6 Hz, 1H), 7.89 (d, J = 5.6 Hz, 1H), 8.04 (d, J = 5.6 Hz, 1H), 8.12 (d, J = 5.6 Hz, 1H), 8.14 (d, J = 5.6 Hz, 1H), 8.31 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.8, 29.3, 29.4, 29.5, 31.9, 39.4, 126.0, 126.1, 127.3, 129.0, 129.1, 132.9, 133.8, 135.0, 136.7, 137.7, 138.9, 141.8, 194.6; HRMS (EI, [M^+], $C_{22}H_{24}OSSe_2$): calcd, 495.9878; found, 495.9879.

Synthesis of 3-selenyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (2g). A degassed solution of 2-trimethylstannylselenophene (1.01 g, 2.41 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (1.35 g, 2.41 mmol), tetrakis(triphenylphosphine)palladium (139 mg, 5 mol%) in toluene (24 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (30 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to

give a white solid of **2g** (707 mg, 48%, T_m = 120 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.33 (s, 9H), 0.39 (s, 9H), 7.21 (dd, J_1 = 5.7 Hz, J_2 = 3.9 Hz, 1H), 7.30 (dd, J_1 = 3.9 Hz, J_2 = 1.2 Hz, 1H), 7.44 (s, 1H), 7.74 (s, 1H), 7.92 (dd, J_1 = 5.7 Hz, J_2 = 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 0.004, 0.2, 114.8, 128.2, 129.3, 131.3, 137.8, 139.3, 139.4, 139.6, 141.4, 144.3, 149.8, 151.9; HRMS (EI, [M^+], $C_{18}H_{23}BrSe_3Si_2$): calcd, 613.8017; found, 613.8028.

Synthesis of 3-(5-decanoylselenyl)-3'-bromo-2,2'-biselenophene (1g). To an ice-cooled solution of **2g** (707 mg, 1.15 mmol) and decanoyl chloride (242 mg, 1.27 mmol) in dichloromethane (12 mL) was added aluminium chloride (230 mg, 1.72 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (12 mL). A 1 M solution of TBAF in THF (12 mL, 12 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give solid of **1g** (510 mg, 71%, T_m = 66 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.34 (m, 12H), 1.70–1.72 (m, 2H), 2.82 (t, J = 7.6 Hz, 2H), 7.31–7.33 (m, 2H), 7.63 (d, J = 5.6 Hz, 1H), 7.75 (d, J = 4.4 Hz, 1H), 8.11–8.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 25.1, 29.3, 29.4, 29.5, 31.9, 38.4, 114.9, 129.0, 130.5, 132.4, 133.7, 134.1, 134.4, 135.7, 137.1, 138.4, 150.6, 152.3, 194.7; HRMS (EI, [M^+], $C_{22}H_{25}OSe_3Br$): calcd, 623.8579; found, 623.8601.

Synthesis of 5-decanoylbenzotriselenophene (SSS-2). A degassed solution of **1g** (498 mg, 0.80 mmol), pivalic acid (25 mg, 0.24 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (26 mg, 5 mol%) and potassium carbonate (276 mg, 2.00 mmol) in DMAc (4 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **SSS-2** (140 mg, 32%, T_m = 110 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.4 Hz, 3H), 1.29–1.39 (m, 10H), 1.41–1.45 (m, 2H), 1.81–1.84 (m, 2H), 3.06 (t, J = 7.4 Hz, 2H), 7.78 (d, J = 5.6 Hz, 1H), 8.05 (d, J = 5.6 Hz, 1H), 8.09–8.13 (m, 2H), 8.56 (s,

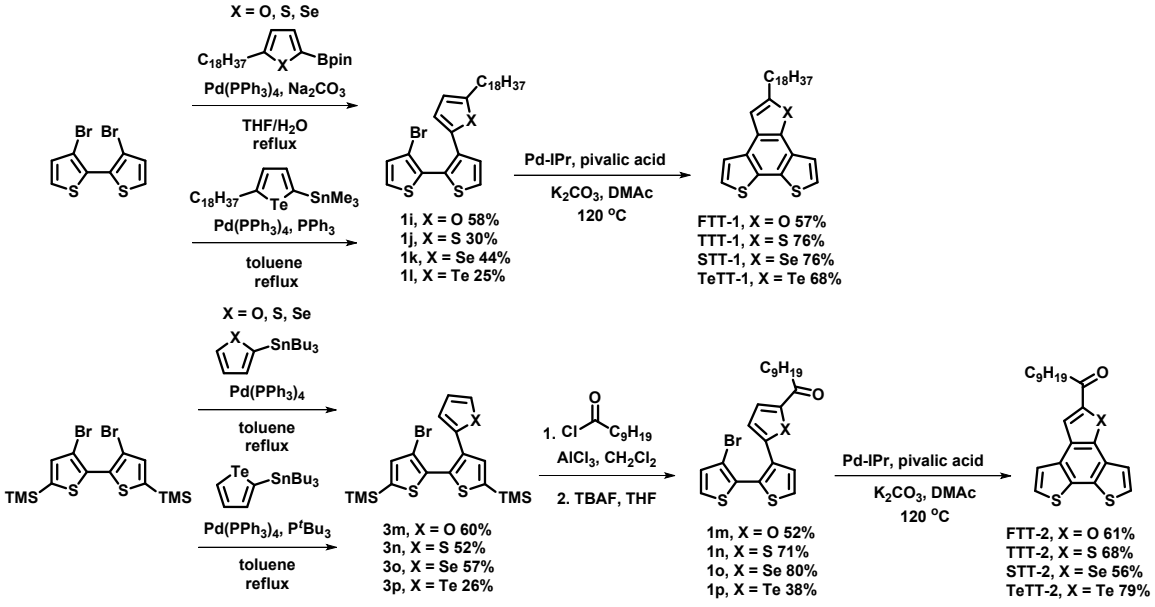
1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.9, 29.3, 29.4, 29.5, 29.52, 31.9, 38.7, 126.2, 127.4, 128.7, 128.8, 130.8, 135.5, 136.0, 136.6, 136.8, 138.4, 140.1, 146.9, 195.5; HRMS (EI, [M^+], $C_{22}H_{24}OSe_3$): calcd, 543.9323; found, 543.9323.

Synthesis of 3-tellurophenyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (2h). A degassed solution of 2-tributylstannyltellurophene (1.25 g, 2.67 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-biselenophene (1.5 g, 2.67 mmol), tri-*tert*-butylphosphine (108 mg, 0.53 mmol), tetrakis(triphenylphosphine)palladium (154 mg, 5 mol%) in toluene (27 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (30 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **2h** (611 mg, 35%, T_m = 98 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.34 (s, 3H), 0.37 (s, 9H), 7.47 (s, 1H), 7.71 (dd, J_1 = 6.8 Hz, J_2 = 4.0 Hz, 1H), 7.81–7.83 (m, 2H), 8.85 (dd, J_1 = 6.8 Hz, J_2 = 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 0.1, 0.2, 116.2, 127.9, 135.8, 136.5, 136.8, 138.9, 139.6, 140.7, 140.8, 143.6, 149.2, 153.5; HRMS (FD, [M^+], $C_{18}H_{23}Si_2Se_2BrTe$): calcd, 663.7909; found, 663.7899.

Synthesis of 3-(5-decanoyltellurophenyl)-3'-bromo-2,2'-biselenophene (1h). To an ice-cooled solution of **2h** (143 mg, 0.22 mmol) and decanoyl chloride (45 mg, 0.24 mmol) in dichloromethane (2 mL) was added aluminium chloride (35 mg, 0.26 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (2 mL). A 1 M solution of TBAF in THF (0.22 mL, 0.22 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give a solid of **1h** (53 mg, 37%, T_m = 107 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, J = 6.8 Hz, 3H), 1.25–1.33 (m, 12H), 1.67–1.71 (m, 2H), 2.84 (t, J = 7.4 Hz, 1H), 7.36 (d, J = 6 Hz, 1H), 7.71 (d, J = 6 Hz, 1H), 7.96 (d, J = 4.6 Hz, 1H), 8.11 (d, J = 5.8 Hz, 1H), 8.20 (d, J = 5.8 Hz, 1H), 8.25 (d, J = 4.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 25.3, 29.3, 29.5, 29.7, 31.9, 37.5, 116.3, 129.1, 131.8, 134.1, 135.2, 135.5, 136.7, 136.9, 140.8, 142.7, 149.5, 152.1, 197.8; HRMS (EI, [M^+],

$C_{22}H_{25}OSe_2BrTe$): calcd, 673.8476; found, 673.8475.

Synthesis of 5-decanoylbenzotellurophenediselenophene (TeSS-2). A degassed solution of **1h** (102 mg, 0.15 mmol), pivalic acid (4.6 mg, 0.05 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (30 mg, 30 mol%) and potassium carbonate (53 mg, 0.38 mmol) in DMAc (1 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **TeSS-2** (27 mg, 30%, T_m = 90 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.29–1.41 (m, 10H), 1.43–1.45 (m, 2H), 1.80–1.84 (m, 2H), 3.09 (t, J = 7.4 Hz, 2H), 7.59 (d, J = 5.6 Hz, 1H), 8.06–8.10 (m, 3H), 9.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 25.1, 29.3, 29.4, 29.48, 29.5, 31.9, 37.6, 126.7, 128.5, 128.6, 129.9, 133.5, 137.6, 139.1, 139.2, 140.7, 142.4, 145.8, 198.2; HRMS (EI, [M^+], $C_{22}H_{24}OSe_2Te$): calcd, 593.9214; found, 593.9226.



Scheme S2. Synthetic route of **FTT-1**, **TTT-1**, **STT-1**, **TeTT-1**, **FTT-2**, **TTT-2** and **STT-2**, **TeTT-2**.

Synthesis of 3-(5-octadecylfuranyl)-3'-bromo-2,2'-bithiophene (1i). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-furan (403 mg, 0.90 mmol), 3,3'-dibromo-2,2'-bithiophene (292 mg, 0.90 mmol), tetrakis(triphenylphosphine)palladium (52 mg, 5 mol%) and sodium carbonate (382

mg, 3.60 mmol) in THF/H_2O (25 mL /6 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a liquid of **1i** (297 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.28 (m, 30H), 1.55–1.59 (m, 2H), 2.56 (t, J = 7.6 Hz, 2H), 5.92 (m, 2H), 7.07 (d, J = 5.6 Hz, 1H), 7.38–7.41 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 27.9, 28.0, 29.2, 29.4, 29.6, 29.7, 29.71, 31.9, 106.7, 107.7, 113.2, 124.4, 126.2, 127.0, 127.4, 130.5, 130.8, 132.6, 147.9, 155.8; HRMS (EI, [M^+], $C_{30}H_{43}OS_2Br$): calcd, 562.1933; found, 562.1942.

Synthesis of 5-octadecylbenzofurandithiophene (FTT-1). A degassed solution of **1i** (261 mg, 0.46 mmol), pivalic acid (71 mg, 0.69 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (15 mg, 5 mol%) and potassium carbonate (256 mg, 1.85 mmol) in DMAc (5 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **FTT-1** (127 mg, 57%, T_m = 71 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.42 (m, 28H), 1.43–1.44 (m, 2H), 1.80–1.84 (m, 2H), 2.89 (t, J = 7.6 Hz, 2H), 6.74 (s, 1H), 7.45 (d, J = 5.2 Hz, 1H), 7.48 (d, J = 5.6 Hz, 1H), 7.58 (d, J = 5.2 Hz, 1H), 7.71 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 28.0, 28.5, 29.2, 29.37, 29.39, 29.6, 29.7, 31.9, 101.3, 119.8, 120.1, 122.5, 124.0, 124.4, 124.6, 128.6, 129.8, 130.5, 147.6, 158.0; HRMS (ESI, [M^+], $C_{30}H_{42}OS_2$): calcd, 482.2672; found, 482.2664.

Synthesis of 3-(5-octadecylthienyl)-3'-bromo-2,2'-bithiophene (1j). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-thiophene (300 mg, 0.64 mmol), 3,3'-dibromo-2,2'-bithiophene (210 mg, 0.64 mmol), tetrakis(triphenylphosphine)palladium (37 mg, 5 mol%) and sodium carbonate (275 mg, 2.59 mmol) in THF/H_2O (19 mL /5 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1j** (113 mg, 30%, T_m

= 57 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.6 Hz, 3H), 1.26 (m, 30H), 1.59–1.63 (m, 2H), 2.71 (t, J = 7.6 Hz, 2H), 6.61 (d, J = 3.6 Hz, 1H), 6.78 (d, J = 3.6 Hz, 1H), 7.07 (d, J = 5.6 Hz, 1H), 7.28 (d, J = 5.2 Hz, 1H), 7.40–7.42 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.35, 29.37, 29.6, 29.65, 29.68, 29.7, 30.0, 31.5, 31.9, 114.0, 124.1, 125.1, 126.8, 127.9, 128.0, 130.4, 130.7, 134.9, 135.8, 146.2, HRMS (EI, [M^+], $C_{30}H_{43}BrS_3$): calcd, 578.1710; found, 578.1714.

Synthesis of 5-octadecylbenzotrithiophene (TTT-1). A degassed solution of **1j** (162 mg, 0.28 mmol), pivalic acid (43 mg, 0.42 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (9 mg, 5 mol%) and potassium carbonate (154 mg, 1.11 mmol) in DMAc (5 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **TTT-1** (106 mg, 76%, T_m = 65 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89 (t, J = 6.8 Hz, 3H), 1.26–1.38 (m, 30H), 1.42–1.46 (m, 2H), 1.80–1.84 (m, 2H), 3.01 (t, J = 7.4 Hz, 2H), 7.42 (s, 1H), 7.46–7.49 (m, 2H), 7.55 (d, J = 5.6 Hz, 1H), 7.69 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.37, 29.4, 29.6, 29.67, 29.7, 30.8, 31.5, 31.9, 119.4, 122.3, 122.7, 124.0, 124.7, 129.7, 130.8, 131.0, 131.5, 132.3, 132.8, 145.4; HRMS (EI, [M^+], $C_{30}H_{42}S_3$): calcd, 498.2449; found, 498.2455.

Synthesis of 3-(5-octadecylselenyl)-3'-bromo-2,2'-bithiophene (1k). A degassed solution of 5-octadecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-selenophene (1.10 g, 2.16 mmol), 3,3'-dibromo-2,2'-bithiophene (700 mg, 2.16 mmol), tetrakis(triphenylphosphine)palladium (125 mg, 5 mol%) and sodium carbonate (915 mg, 8.63 mmol) in THF/H_2O (62 mL /15 mL) was stirred for 17 h at 80 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (30 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1k** (600 mg, 44%, T_m = 48 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (t, J = 6.6 Hz, 3H), 1.28 (m, 30H), 1.59–1.66 (m, 2H), 2.79 (t, J = 7.6 Hz, 2H), 6.80 (d, J = 3.6 Hz, 1H), 7.07–7.10 (m, 2H), 7.30 (d, J = 5.6 Hz, 1H), 7.39 (d, J = 5.2 Hz, 1H), 7.45 (d, J = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.36, 29.4, 29.6, 29.65, 29.68, 29.7, 31.9, 32.4, 32.7, 114.7, 125.2, 126.1, 126.7, 127.3, 127.5, 128.4, 130.1, 130.7, 138.1, 139.9, 154.2;

HRMS (EI, [M^+], $C_{30}H_{43}BrS_2Se$): calcd, 626.1155; found, 626.1158.

Synthesis of 5-octadecylbenzoselenophenedithiophene (STT-1). A degassed solution of **1k** (500 mg, 0.80 mmol), pivalic acid (24 mg, 0.24 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (26 mg, 5 mol%) and potassium carbonate (276 mg, 1.99 mmol) in DMAc (3.5 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **STT-1** (330 mg, 76%, T_m = 71 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89 (t, J = 6.8 Hz, 3H), 1.26–1.38 (m, 28H), 1.43–1.47 (m, 2H), 1.78–1.82 (m, 2H) 3.05 (t, J = 7.6 Hz, 2H), 7.44–7.48 (m, 3H), 7.63 (s, 1H), 7.68 (d, J = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.4, 29.44, 29.6, 29.7, 29.73, 32.0, 32.4, 33.3, 122.7, 123.0, 123.5, 124.0, 124.8, 129.6, 131.1, 133.3, 133.8, 134.0, 134.8, 150.8; HRMS (EI, [M^+], $C_{30}H_{42}S_2Se$): calcd, 546.1893; found, 546.1891.

Synthesis of 3-(5-octadecyltellurophenyl)-3'-bromo-2,2'-bithiophene (1l). A degassed solution of 2-octadecyl-5-trimethylstannyltellurophene (551 mg, 0.93 mmol), 3,3'-dibromo-2,2'-bithiophene (300 mg, 0.93 mmol), tetrakis(triphenylphosphine)palladium (53 mg, 5 mol%) and triphenylphosphine (24 mg, 0.09 mmol) in toluene (9 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **1l** (155 mg, 25%, T_m = 50 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.34 (m, 30H), 1.56–1.59 (m, 2H), 2.79 (t, J = 7.4 Hz, 2H), 7.11 (d, J = 5.6 Hz, 1H), 7.21 (d, J = 4.4 Hz, 1H), 7.36–7.39 (m, 2H), 7.51 (d, J = 5.6 Hz, 1H), 7.56 (d, J = 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 29.1, 29.4, 29.5, 29.6, 29.7, 31.9, 34.2, 36.8, 115.9, 125.1, 126.3, 126.4, 129.3, 129.5, 131.0, 133.3, 134.6, 135.0, 142.0, 154.4; HRMS (EI, [M^+], $C_{30}H_{43}S_2BrTe$): calcd, 676.1046; found, 676.1057.

Synthesis of 5-octadecylbenzotellurophenedithiophene (TeTT-1). A degassed solution of **1l** (132 mg, 0.20 mmol), pivalic acid (6 mg, 0.06 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (19 mg, 15 mol%) and potassium carbonate (68 mg, 0.49 mmol) in DMAc (1 mL) was stirred for

17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (10 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **TeTT-1** (79 mg, 68%, T_m = 56 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.36 (m, 28H), 1.44–1.46 (m, 2H), 1.72–1.74 (m, 2H), 3.02 (t, J = 7.6 Hz, 2H), 7.27 (d, J = 5.2 Hz, 1H), 7.42 (d, J = 5.6 Hz, 1H), 7.45 (d, J = 5.2 Hz, 1H), 7.71 (d, J = 5.6 Hz, 1H), 8.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.8, 29.2, 29.4, 29.5, 29.6, 29.7, 29.8, 32.0, 34.2, 37.3, 123.6, 123.9, 124.7, 125.4, 125.7, 129.0, 131.1, 132.0, 135.9, 138.9, 140.5, 147.6; HRMS (EI, [M^+], $C_{30}H_{42}S_2Te$): calcd, 596.1785; found, 596.1800.

Synthesis of 3-furanyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (3m). A degassed solution of 2-tributylstannylfuran (406 mg, 1.14 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (532mg, 1.14 mmol), tetrakis(triphenylphosphine)palladium (66 mg, 5 mol%) in toluene (11 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a liquid of **3m** (310 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.35 (s, 9H), 0.37 (s, 9H), 6.00 (dd, J_1 = 3.4 Hz, J_2 = 0.6 Hz, 1H), 6.34 (dd, J_1 = 3.4 Hz, J_2 = 1.8 Hz, 1H), 7.16 (s, 1H), 7.36 (dd, J_1 = 1.8 Hz, J_2 = 0.6 Hz, 1H), 7.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ –0.4, –0.2, 106.8, 111.5, 113.5, 131.4, 132.8, 133.1, 135.5, 136.9, 141.1, 142.6, 143.1, 149.8; HRMS (EI, [M^+], $C_{22}H_{25}BrO_2S_2$): calcd, 464.0479; found, 464.0468.

Synthesis of 3-(5-decanoylfuranyl)-3'-bromo-2,2'-bithiophene (1m). To an ice-cooled solution of **3m** (310 mg, 0.68 mmol) and decanoyl chloride (142 mg, 0.74 mmol) in dichloromethane (7 mL) was added aluminium chloride (136 mg, 1.02 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (7 mL). A 1 M solution of TBAF in THF (0.68 mL, 0.68 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced

pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give a oil of **1m** (164 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.25–1.33 (m, 12H), 1.61–1.66 (m, 2H), 2.65 (t, J = 7.6 Hz), 6.18 (d, J = 3.6 Hz, 1H), 7.10–7.12 (m, 2H), 7.45 (d, J = 5.6 Hz, 1H), 7.48 (d, J = 5.4 Hz, 1H), 7.51 (d, J = 5.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.6, 24.3, 29.27, 29.32, 29.40, 29.44, 31.9, 38.3, 109.3, 113.5, 118.1, 126.6, 127.7, 127.9, 129.1, 129.8, 130.8, 130.9, 151.4, 152.6, 189.8; HRMS (EI, [M^+], $C_{22}H_{25}BrO_2S_2$): calcd, 464.0479; found, 464.0468.

Synthesis of 5-decanoylbenzofurandithiophene (FTT-2). A degassed solution of **1m** (147 mg, 0.32 mmol), pivalic acid (48 mg, 0.47 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (10 mg, 5 mol%) and potassium carbonate (174 mg, 1.26 mmol) in DMAc (5 mL) was stirred for 17 h at 120 ^{o}C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **FTT-2** (74 mg, 61%, T_m = 57 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.25–1.39 (m, 10H), 1.41–1.47 (m, 2H), 1.81–1.85 (m, 2H), 3.04 (t, J = 7.4 Hz, 2H), 7.53, (d, J = 5.2 Hz, 1H), 7.58, (d J = 5.6 Hz, 1H), 7.67, (d, J = 5.2 Hz, 1H), 7.85 (d, J = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.5, 29.3, 29.4, 29.5, 31.9, 38.9, 112.2, 119.1, 120.5, 122.4, 123.8, 125.2, 126.0, 130.1, 131.0, 134.8, 149.7, 151.6, 190.9; HRMS (EI, [M^+], $C_{22}H_{24}O_2S_2$): calcd, 384.1218; found, 384.1215.

Synthesis of 3-thienyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (3n). A degassed solution of 2-trimethylstannylthiophene (858 mg, 2.30 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (1.08 g, 2.31 mmol), tetrakis(triphenylphosphine)palladium (133 mg, 5 mol%) in toluene (23 mL) was stirred for 17 h at 110 ^{o}C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (30 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **3n** (565 mg, 52%, T_m = 104 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.34 (s, 9H), 0.38 (s, 9H), 6.95 (dd, J_1 = 5.2 Hz, J_2 = 3.7, 1H), 6.99 (dd, J_1 = 3.7, J_2 = 1.5 Hz, 1H), 7.14 (s, 1H), 7.19 (dd, J_1 = 5.2, J_2 = 1.5, 1H), 7.39 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ –0.3, –0.2, 114.2, 125.1, 125.2, 127.1, 132.1, 134.9, 135.4, 135.9,

136.9, 137.8, 142.4, 143.7; HRMS (EI, [M^+], $C_{18}H_{23}BrS_3Si_2$): calcd, 469.9684; found, 469.9678.

Synthesis of 3-(5-decanoylthienyl)-3'-bromo-2,2'-bithiophene (1n). To an ice-cooled solution of **3n** (350 mg, 0.74 mmol) and decanoyl chloride (156 mg, 0.82 mmol) in dichloromethane (8 mL) was added aluminium chloride (148 mg, 1.5 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (8 mL). A 1 M solution of TBAF in THF (0.74 mL, 0.74 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give a solid of **1n** (252 mg, 71%, T_m = 49 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 7.0 Hz, 3H), 1.26–1.36 (m, 12H), 1.69–1.72 (m, 2H), 2.81 (t, J = 7.4, 2H), 6.94 (d, J = 4.0 Hz, 1H), 7.08 (d, J = 5.4 Hz, 1H), 7.34 (d, J = 5.6 Hz, 1H), 7.44 (d, J = 5.4 Hz, 1H), 7.46 (d, J = 5.6 Hz, 1H), 7.53 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.6, 24.9, 29.2, 29.3, 29.4, 31.8, 39.1, 114.2, 126.1, 127.6, 128.0, 128.5, 128.9, 129.3, 131.0, 131.9, 134.5, 143.3, 145.3, 193.5; HRMS (EI, [M^+], $C_{22}H_{25}BrOS_3$): calcd, 480.0251; found, 480.0246.

Synthesis of 5-decanoylbenzotrithiophene (TTT-2). A degassed solution of **1n** (463 mg, 0.96 mmol), pivalic acid (29 mg, 0.29 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (31 mg, 5 mol%) and potassium carbonate (332 mg, 2.41 mmol) in DMAc (4 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **TTT-2** (262 mg, 68%, T_m = 77 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 5.8 Hz, 3H), 1.29–1.37 (m, 10H,), 1.41–1.45 (m, 2H), 1.80–1.85 (m, 2H), 3.07 (t, J = 7.6 Hz, 2H), 7.53–7.56 (m, 2H), 7.64 (d, J = 5.2 Hz, 1H), 7.76 (d, J = 5.2 Hz, 1H), 8.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.8, 29.3, 29.4, 29.5, 31.9, 39.4, 122.4, 122.6, 125.2, 125.4, 127.0, 131.0, 131.5, 132.1, 133.1, 133.4, 136.1, 142.0, 194.4; HRMS (EI, [M^+], $C_{22}H_{24}OS_3$): calcd, 400.0989; found, 400.0997.

Synthesis of 3-selenyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (3o). A degassed solution of 2-tributylstannylselenophene (942 mg, 2.24 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (1.05 g, 2.24 mmol), tetrakis(triphenylphosphine)palladium (130 mg, 5 mol%) in toluene (22 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (30 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a white solid of **3o** (662 mg, 57%, T_m = 114 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.34 (s, 9H), 0.37 (s, 9H), 7.15 (s, 1H), 7.20 (dd, J_1 = 5.8 Hz, J_2 = 3.9 Hz, 1H), 7.27 (dd, J_1 = 3.9 Hz, J_2 = 0.8 Hz, 1H), 7.40 (s, 1H), 7.88 (dd, J_1 = 5.8 Hz, J_2 = 0.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ –0.3, –0.2, 114.9, 127.4, 129.4, 130.9, 131.8, 134.5, 135.0, 136.9, 138.3, 142.3, 143.0, 144.3; HRMS (EI, [M^+], $C_{18}H_{23}BrS_2SeSi_2$): calcd, 517.9128; found, 517.9126.

Synthesis of 3-(5-decanoylselenyl)-3'-bromo-2,2'-bithiophene (1o). To an ice-cooled solution of **3o** (440 mg, 0.85 mmol) and decanoyl chloride (178 mg, 0.93 mmol) in dichloromethane (8.5 mL) was added aluminium chloride (170 mg, 1.27 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (8.5 mL). A 1 M solution of TBAF in THF (0.85 mL, 0.85 mmol) was added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give solid of **1o** (360 mg, 80%, T_m = 58 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, J = 6.6 Hz, 3H), 1.26–1.31 (m, 12H), 1.68–1.71 (m, 2H), 2.82 (t, J = 7.4 Hz, 2H), 7.10 (d, J = 5.2 Hz, 1H), 7.30 (d, J = 4.0 Hz, 1H), 7.35 (d, J = 5.4 Hz, 1H), 7.44 (d, J = 5.4 Hz, 1H), 7.48 (d, J = 5.2 Hz, 1H), 7.75 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 25.0, 29.3, 29.4, 29.42, 31.8, 38.4, 115.0, 127.3, 127.4, 128.5, 128.7, 128.9, 129.2, 131.1, 134.1, 137.2, 150.5, 151.0, 194.7; HRMS (EI, [M^+], $C_{22}H_{25}BrOS_2Se$): calcd, 527.9695; found, 527.9695.

Synthesis of 5-decanoylbenzoselenophenedithiophene (STT-2). A degassed solution of **1o** (335 mg, 0.63 mmol), pivalic acid (19 mg, 0.19 mmol), [1,3-bis(2,6-

diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (21 mg, 5 mol%) and potassium carbonate (219 mg, 1.58 mmol) in DMAc (3 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **STT-2** (160 mg, 56%, T_m = 86 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.4 Hz, 3H), 1.28–1.37 (m, 10H), 1.41–1.45 (m, 2H), 1.79–1.85 (m, 2H), 3.08 (t, J = 7.6 Hz, 2H), 7.53–7.57 (m, 3H), 7.78 (d, J = 5.2 Hz, 1H), 8.58 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 24.9, 29.3, 29.4, 29.5, 31.9, 38.7, 122.6, 123.9, 125.2, 125.4, 130.5, 131.8, 133.0, 133.7, 134.4, 134.8, 138.7, 147.3, 195.4; HRMS (EI, [M^+], $C_{22}H_{24}OS_2Se_2$): calcd, 448.0434; found, 448.0441

Synthesis of 3-tellurophenyl-3'-bromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (3p). A degassed solution of 2-tributylstannyltellurophene (1.46 g, 3.12 mmol), 3,3'-dibromo-5,5'-bistrimethylsilyl-2,2'-bithiophene (1.46 g, 3.11 mmol), tri-*tert*-butylphosphine (126 mg, 0.62 mmol), tetrakis(triphenylphosphine)palladium (180 mg, 5 mol%) in toluene (31 mL) was stirred for 17 h at 110 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (20 mL × 3) and water (30 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a solid of **3p** (454 mg, 26%, T_m = 97 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.35 (s, 9H), 0.37 (s, 9H), 7.19 (s, 1H), 7.48 (s, 1H), 7.71 (dd, J_1 = 6.8 Hz, J_2 = 4.0 Hz, 1H), 7.81–7.82 (m, 1H), 8.80–8.82 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ –0.2, –0.1, 116.2, 127.3, 131.7, 133.2, 134.4, 135.1, 136.9, 137.2, 139.1, 141.8, 142.4, 145.6; HRMS (EI, [M^+], $C_{18}H_{23}Si_2S_2BrTe$): calcd, 567.9020; found, 567.9008.

Synthesis of 3-(5-decanoyltellurophenyl)-3'-bromo-2,2'-bithiophene (1p). To an ice-cooled solution of **3p** (124 mg, 0.22 mmol) and decanoyl chloride (46 mg, 0.24 mmol) in dichloromethane (2 mL) was added aluminium chloride (32 mg, 0.24 mmol). The reaction mixture was stirred for 1 h in room temperature and extracted with dichloromethane (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was dissolved in THF (2 mL). A 1 M solution of TBAF in THF (0.22 mL, 0.22 mmol) was

added to the above mixture dropwise at room temperature. After stirring for 30 min, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EA/hexane = 1/30) to give a solid of **1p** (48 mg, 38%, T_m = 101 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, J = 7.0 Hz, 3H), 1.25–1.36 (m, 12H), 1.67–1.71 (m, 2H), 2.84 (t, J = 7.4 Hz, 2H), 7.14 (d, J = 5.6 Hz, 1H), 7.42–7.45 (m, 2H), 7.56 (d, J = 5.6 Hz, 1H), 7.94 (d, J = 4.6 Hz, 1H), 8.25 (d, J = 4.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 25.3, 29.3, 29.5, 29.7, 31.9, 37.5, 116.3, 125.8, 127.0, 128.3, 128.7, 130.2, 131.5, 136.2, 140.8, 141.6, 148.0, 152.0, 197.7; HRMS (EI, [M^+], $C_{22}H_{25}OS_2BrTe$): calcd, 577.9587; found, 577.9591.

Synthesis of 5-decanoylbenzotellurophenedithiophene (TeTT-2). A degassed solution of **1p** (137 mg, 0.24 mmol), pivalic acid (7.2 mg, 0.07 mmol), [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]chloro[3-phenylallyl]palladium(II) (23 mg, 15 mol%) and potassium carbonate (82 mg, 0.59 mmol) in DMAc (1 mL) was stirred for 17 h at 120 °C under N_2 atmosphere. After cooling to room temperature, the solution was extracted with ether (10 mL × 3) and water (20 mL). The combined organic layer was dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane) to give a yellow solid of **TeTT-2** (93 mg, 79%, T_m = 87 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 3H), 1.26–1.39 (m, 10H), 1.41–1.45 (m, 2H), 1.80–1.84 (m, 2H), 3.09 (t, J = 7.4 Hz, 2H), 7.35 (d, J = 5.6 Hz, 1H), 7.49–7.51 (m, 2H), 7.79 (d, J = 5.2 Hz, 1H), 9.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.7, 25.1, 29.3, 29.5, 29.51, 29.53, 31.9, 37.5, 123.1, 124.9, 125.2, 126.1, 131.9, 132.0, 132.3, 137.2, 138.5, 138.7, 140.7, 146.1, 198.0; HRMS (EI, [M^+], $C_{22}H_{24}OS_2Te$): calcd, 498.0325; found, 498.0333.

2. Optical properties

Absorption spectra were taken on a HP8453 UV-vis spectrophotometer. Each molecule was dissolved in chloroform into $1*10^{-5}$ M solution.

Table S1. Optical and electron chemical properties of **FTT-1**, **TTT-1**, **STT-1**, and **TeTT-1**

	FTT-1	TTT-1	STT-1	TeTT-1

λ_{max} (nm)	255, 304, 317, 339, 355	268, 277, 302, 313, 343	272, 283, 304, 315	295, 321
E_g^{opt} (eV)	3.38	3.55	3.49	3.42
HOMO (eV)	−5.69	−5.90	−5.89	−5.39
LUMO (eV)	−2.31	−2.35	−2.40	−1.97

Table S2. Optical and electron chemical properties of **FSS-1**, **TSS-1**, **SSS-1**, and **TeSS-1**

	FSS-1	**TSS-1**	**SSS-1**	**TeSS-1**
λ_{max} (nm)	257, 304, 317, 339, 355	274, 281, 311, 323, 337, 354	279, 287, 312, 325, 340, 356	300, 332, 361
E_g^{opt} (eV)	3.38	3.43	3.38	3.34
HOMO (eV)	−5.63	−5.68	−5.62	−5.38
LUMO (eV)	−2.38	−2.25	−2.24	−2.04

Table S3. Optical and electron chemical properties of **FTT-2**, **TTT-2**, **STT-2**, and **TeTT-2**

	FTT-2	**TTT-2**	**STT-2**	**TeTT-2**
λ_{max} (nm)	294, 339	289, 300, 341	297, 305, 351	301, 307, 362
E_g^{opt} (eV)	3.36	3.26	3.20	2.81
HOMO (eV)	−5.94	−5.89	−5.88	−5.51
LUMO (eV)	−2.58	−2.63	−2.68	−2.70

Table S4. Optical and electron chemical properties of **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2**

	FSS-2	**TSS-2**	**SSS-2**	**TeSS-2**
λ_{max} (nm)	289, 302, 351	297, 309, 352	314, 356	312, 367
E_g^{opt} (eV)	3.26	3.20	3.15	2.79
HOMO (eV)	−5.89	−5.84	−5.81	−5.43

LUMO (eV)	−2.63	−2.64	−2.66	−2.64

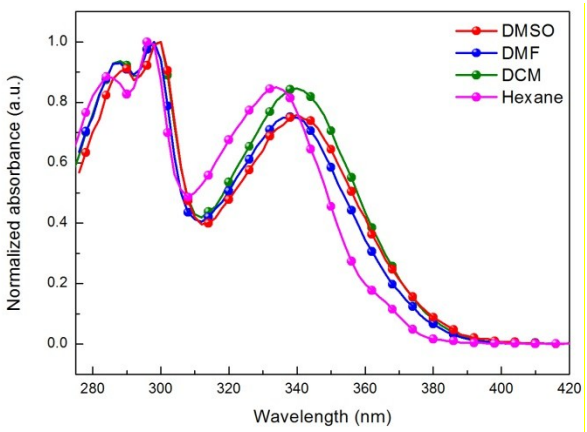


Figure S1. Absorption spectra of **TTT-2** in different solvents (DMSO, DMF, DCM and hexane).

Table S5. Optical properties of **TTT-2** in DMSO, DMF, DCM and hexane.

TTT-2	DMSO	DMF	DCM	Hexane
λ_{max} (nm)	290, 300, 340	288, 298, 338	288, 296, 338	284, 296, 334

Relative polarity to water: DMSO (0.444) > DMF (0.386) > DCM (0.309) > hexane (0.009)

3. Electrochemical properties

Electrochemical cyclic voltammetry was conducted on a CH instruments electrochemical analyzer. A carbon glass was used as the working electrode, Pt wire was used as the counter electrode, and Ag/Ag+ electrode (0.01 M $AgNO_3$, 0.1 M TBAP in acetonitrile) was used as the reference electrode in a solution of dichloromethane with 0.1 M $TBAPF_6$ (tetrabutylammonium hexafluorophosophate) at 100 mV/s. CV curves were calibrated using ferrocence as the standard, $E_{(ferrocene)}{}^{onset} = 0.40$ V. The HOMO energy levels were obtained from the equation HOMO = $-(E_{ox}{}^{onset} - E_{(ferrocene)}{}^{onset} + 4.8)$ eV.

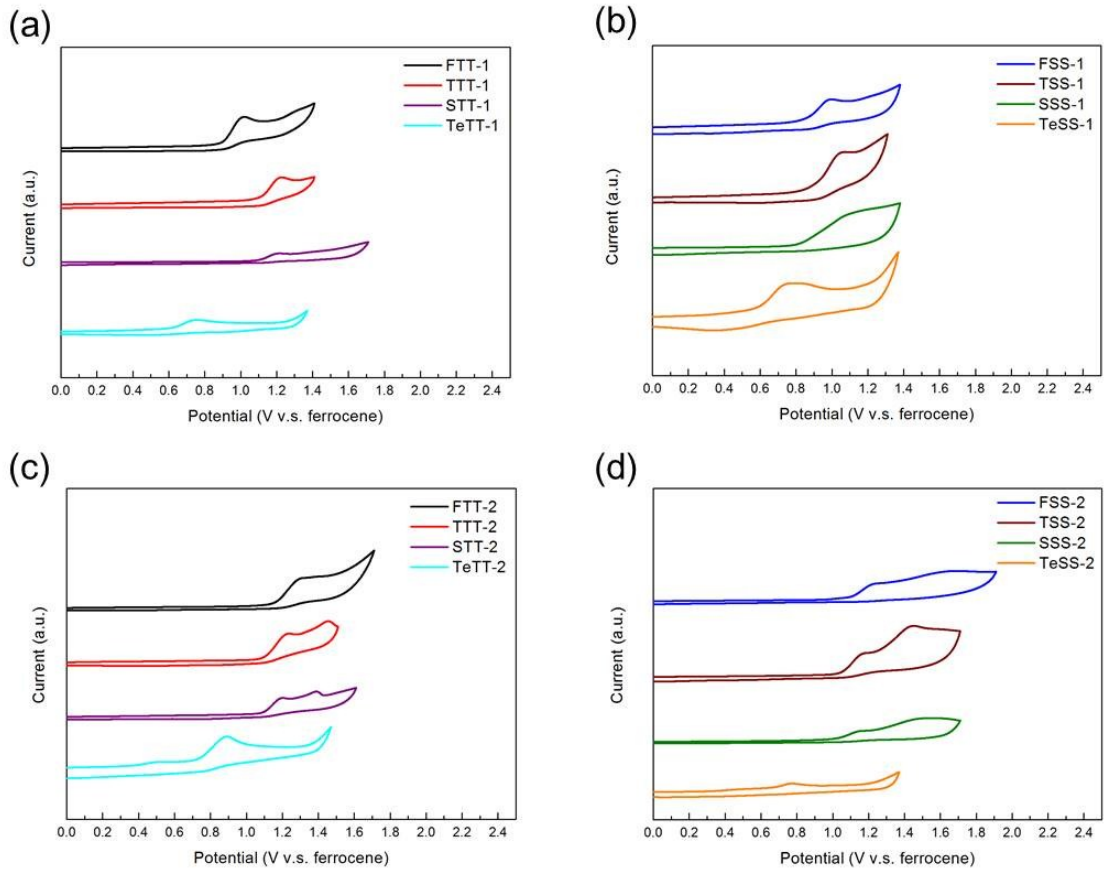
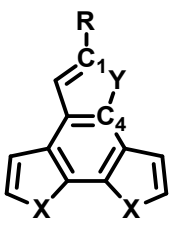


Figure S2. Cyclic voltammograms of (a) **FTT-1**, **TTT-1**, **STT-1**, **TeTT-1**, (b) **FSS-1**, **TSS-1**, **SSS-1**, **TeSS-1**, (c) **FTT-2**, **TTT-2**, **STT-2**, **TeTT-2**, (d) **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2.**

4. Theoretical calculations

DFT calculations were carried out with the Gaussian09 suite employing the cam-B3LYP density function in combination with the LanL2DZ(d,p) basis set for the chalcogens and the 6-31G(d) basis set for the remaining atoms. Tight SCF/convergence criteria and ultrafine integration grid were implemented in geometry optimization. Frequency analysis was employed to confirm the minimum characteristics of each stationary point. Natural-orbital-bond (NBO) analysis was performed at the same level of theory as geometry optimization.



X = S, Se
Y = O, S, Se or Te
R = $C_{18}H_{37}$ or COC_9H_{19}

Table S6. Selected second-order perturbation estimates of donor-acceptor interactions in the NBO analysis for uBTCs, calculated at the cam-B3LYP/LanL2DZ(d,p):6-31G(d) level of theory.

	Y	Acceptor	Interaction energy
FTT-1	O	C_1=C_2 C_3=C_4	36.06 33.79
TTT-1	S	C_1=C_2 C_3=C_4	28.52 26.16
STT-1	Se	C_1=C_2 C_3=C_4	22.56 20.58
TeTT-1	Te	C_1=C_2 C_3=C_4	16.28 14.54
FTT-2	O	C_1=C_2 C_3=C_4	36.4 38.22
TTT-2	S	C_1=C_2 C_3=C_4	29.83 30.49
STT-2	Se	C_1=C_2 C_3=C_4	24.2 24.03
TeTT-2	Te	C_1=C_2 C_3=C_4	18.13 17.08
FSS-1	O	C_1=C_2 C_3=C_4	36.03 33.49
TSS-1	S	C_1=C_2 C_3=C_4	28.44 25.84
SSS-1	Se	C_1=C_2 C_3=C_4	22.51 20.3
TeSS-1	Te	C_1=C_2 C_3=C_4	16.22 14.39
FSS-2	O	C_1=C_2 C_3=C_4	36.43 37.8
TSS-2	S	C_1=C_2 C_3=C_4	29.72 30.09
SSS-2	Se	C_1=C_2 C_3=C_4	24.12 23.68
TeSS-2	Te	C_1=C_2 C_3=C_4	18.08 16.81

Table S7. Calculated bond length and bond angle of BTCs at the cam-b3lyp/gencep level of theory

	C_1-Y bond length (Å)	C_4-Y bond length (Å)	∠C_1-Y-C_4 (°)
FTT-1	1.38	1.36	106.74
TTT-1	1.76	1.75	91.34

STT-1	1.90	1.89	87.23
TeTT-1	2.09	2.08	82.14
FTT-2	1.37	1.35	106.57
TTT-2	1.75	1.74	90.56
STT-2	1.89	1.88	86.38
TeTT-2	2.07	2.08	81.10
FSS-1	1.38	1.36	106.73
TSS-1	1.76	1.75	91.32
SSS-1	1.90	1.89	87.22
TeSS-1	2.09	2.08	82.12
FSS-2	1.37	1.35	106.56
TSS-2	1.75	1.74	90.54
SSS-2	1.89	1.88	86.36
TeSS-2	2.07	2.08	81.08

The frontier molecular orbitals of **FSS-1**, **TSS-1**, **SSS-1** and **TeSS-1** are shown in Figure S2. Octadecyl side chains are simplified to propyl group to shorten the calculation time. Although there are some deviations, the trend of the HOMO/LUMO values correlates well with the experimental data. Similarly, decanoyl groups are simplified to propanoyl group in **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2** (Figure S3). Again, the trend of the HOMO/LUMO values in this series correlates well with the experimental data. The calculated band gaps of **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2** are narrower than those of **FSS-1**, **TSS-1**, **SSS-1** and **TeSS-1** due to the electron-withdrawing effect of the carbonyl groups. The electron densities of HOMO orbitals of **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2** are similar to the C18-counterparts; however, the electron densities of LUMO orbitals are extended to the propanoyl groups, which may result in the ICT band observed in UV absorption. The HOMO/LUMO of the bithiophene-based series show similar phenomena (Figure S4 and S5).

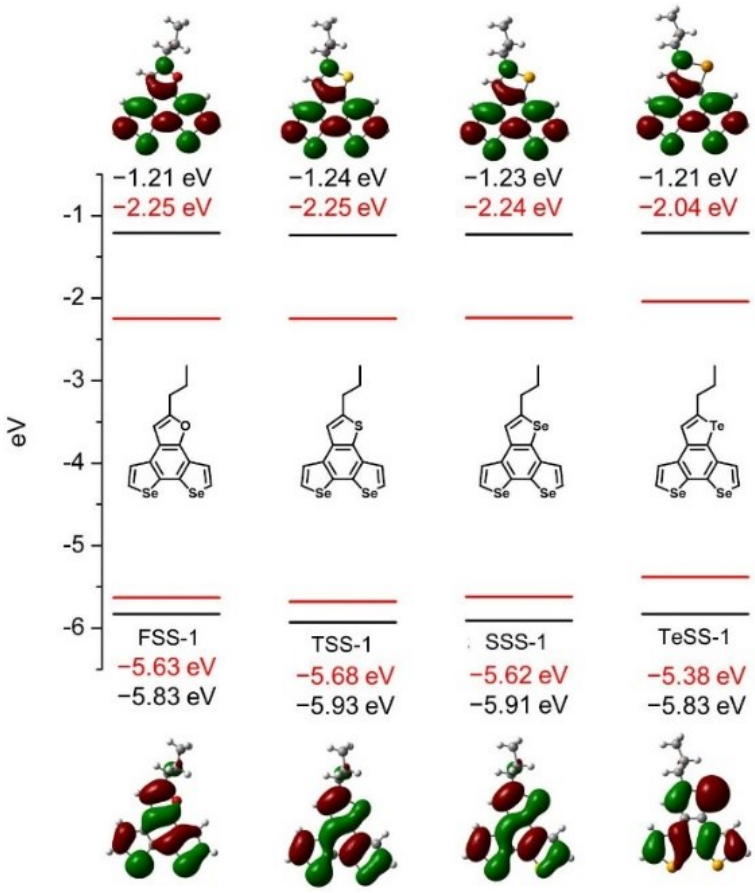


Figure S3. Frontier molecular orbitals of **FSS-1**, **TSS-1**, **SSS-1** and **TeSS-1**; experimental and theoretical HOMO/LUMO values are represented by red and black lines, respectively.

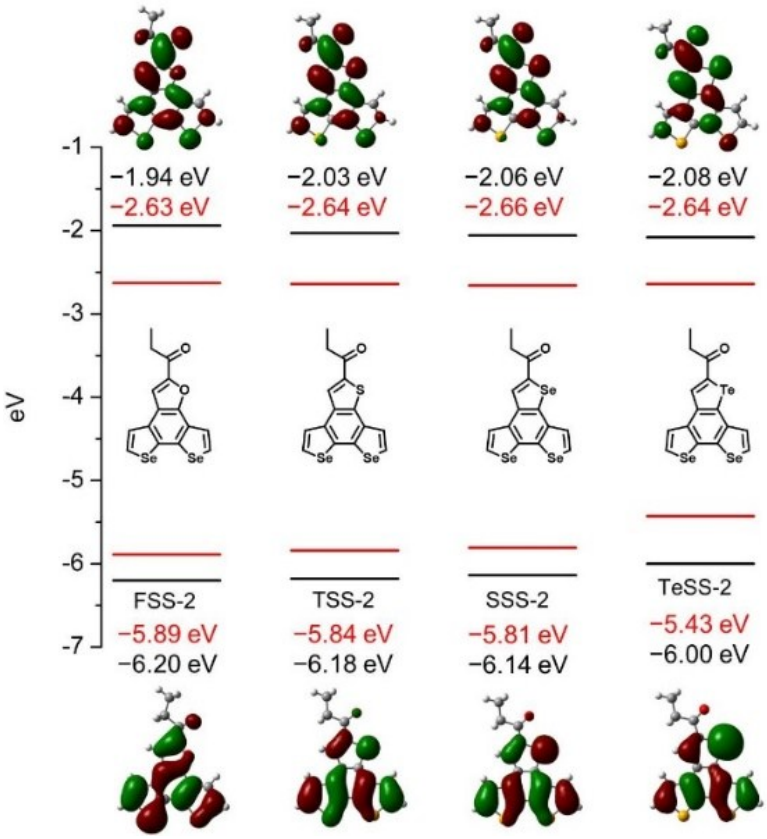


Figure S4. Frontier molecular orbitals of **FSS-2**, **TSS-2**, **SSS-2** and **TeSS-2**; experimental and theoretical HOMO/LUMO values are represented by red and black lines, respectively.

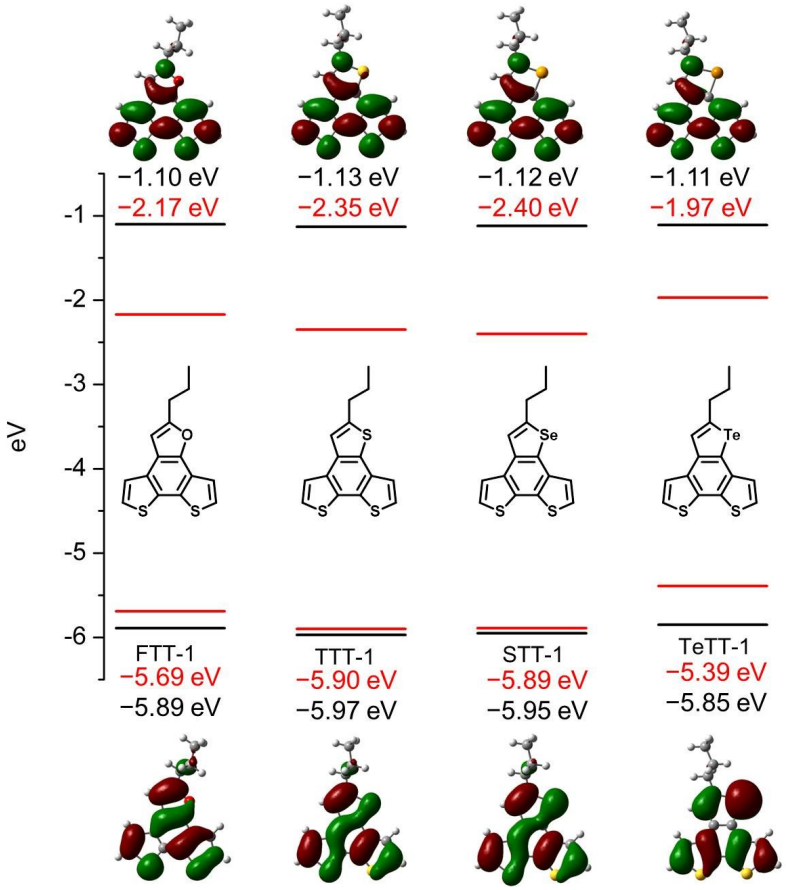


Figure S5. Frontier molecular orbitals of **FTT-1**, **TTT-1**, **STT-1** and **TeTT-1** calculated at the MPW1PW91/LanL2DZ(d,p):6-31G(d) level of theory; experimental and theoretical HOMO/LUMO values are represented by red and black lines, respectively.

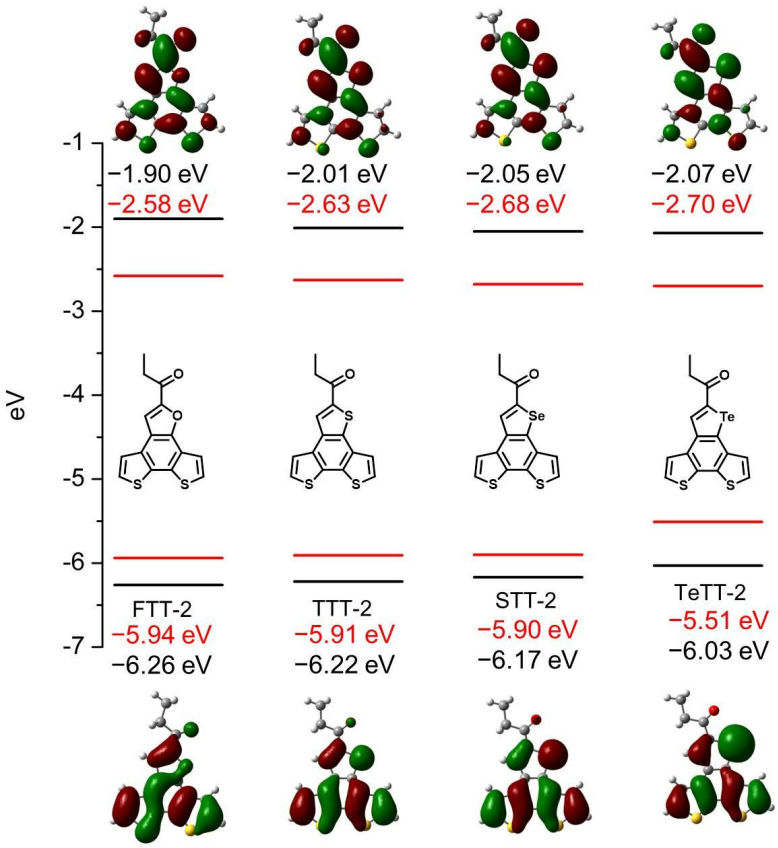


Figure S6. Frontier molecular orbitals of **FTT-2**, **TTT-2**, **STT-2** and **TeTT-2** calculated at the MPW1PW91/LanL2DZ(d,p):6-31G(d) level of theory; experimental and theoretical HOMO/LUMO values are represented by red and black lines, respectively.

5. Single crystal data and ORTEP view

Table S8. Actual bond length and bond angle of BTCs calculated from single-crystal data.

	C_1-Y bond length (Å)	C_4-Y bond length (Å)	$\angle C_1$-Y-C_4 (°)
STT-2	1.88	1.87	86.2
FSS-2	1.37	1.38	105.8
TSS-2	1.74	1.73	91.0
SSS-2	1.89	1.88	86.9

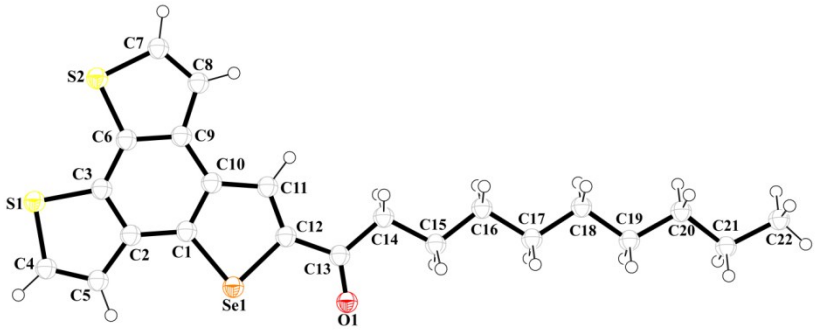


Figure S7. ORTEP view of **STT-2** (Here, $C_{12} = C_1$ and $C_1 = C_4$). CCDC No.- 1543182

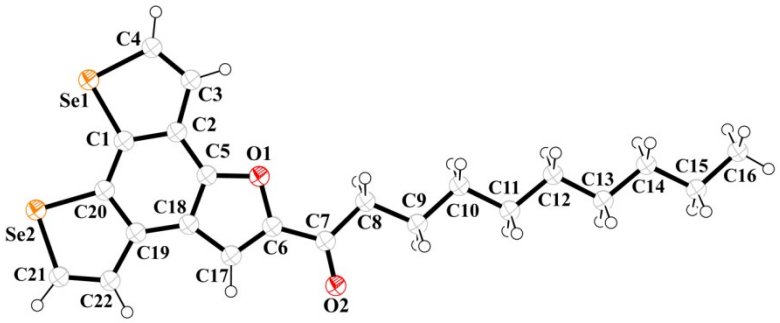


Figure S8. ORTEP view of **FSS-2** (Here, $C_6 = C_1$ and $C_5 = C_4$). CCDC No.- 1543180

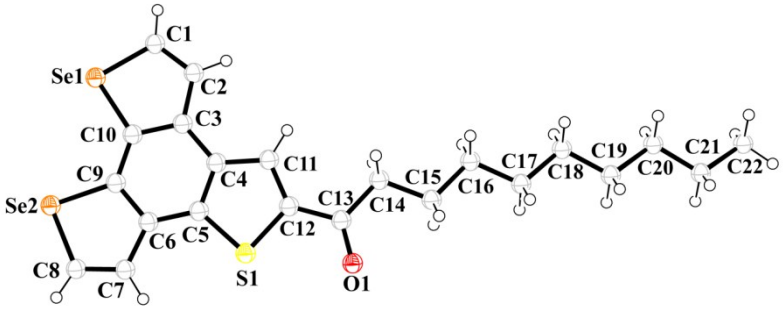


Figure S9. ORTEP view of **TSS-2** (Here, $C_{12} = C_1$ and $C_5 = C_4$). CCDC No.- 1543179

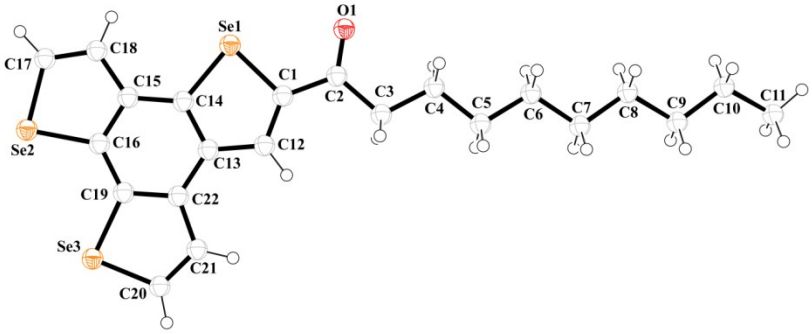
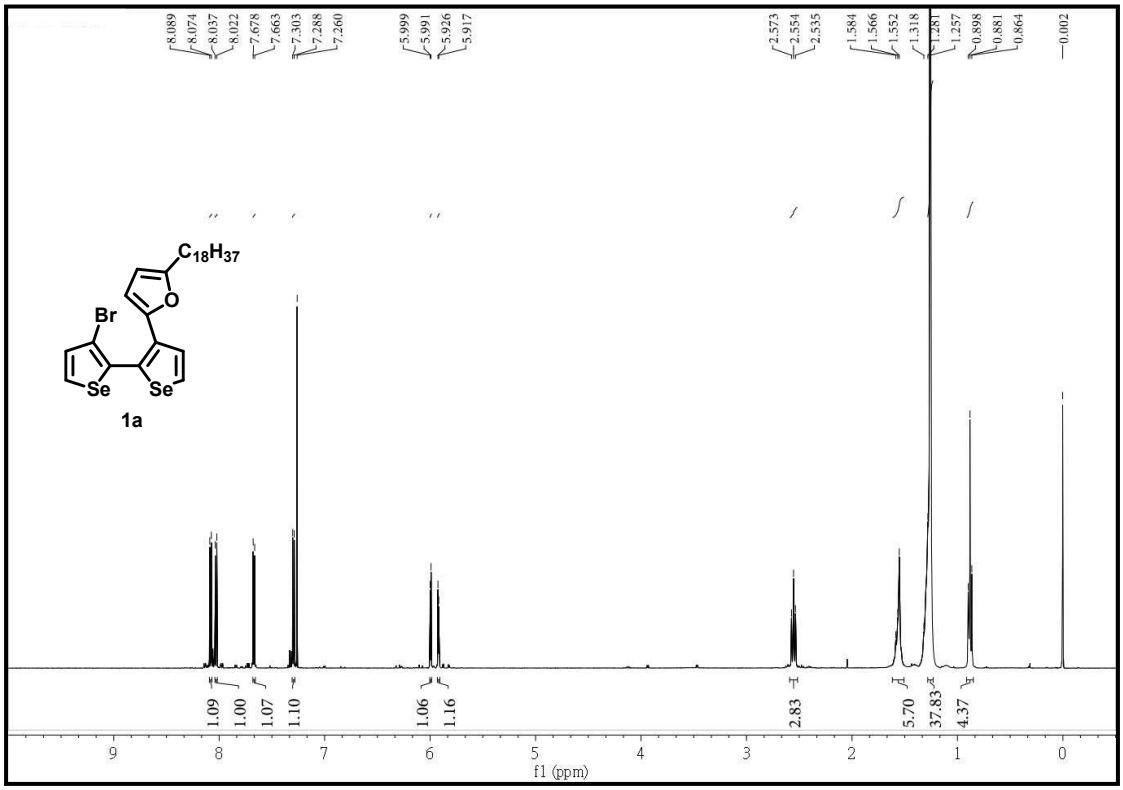
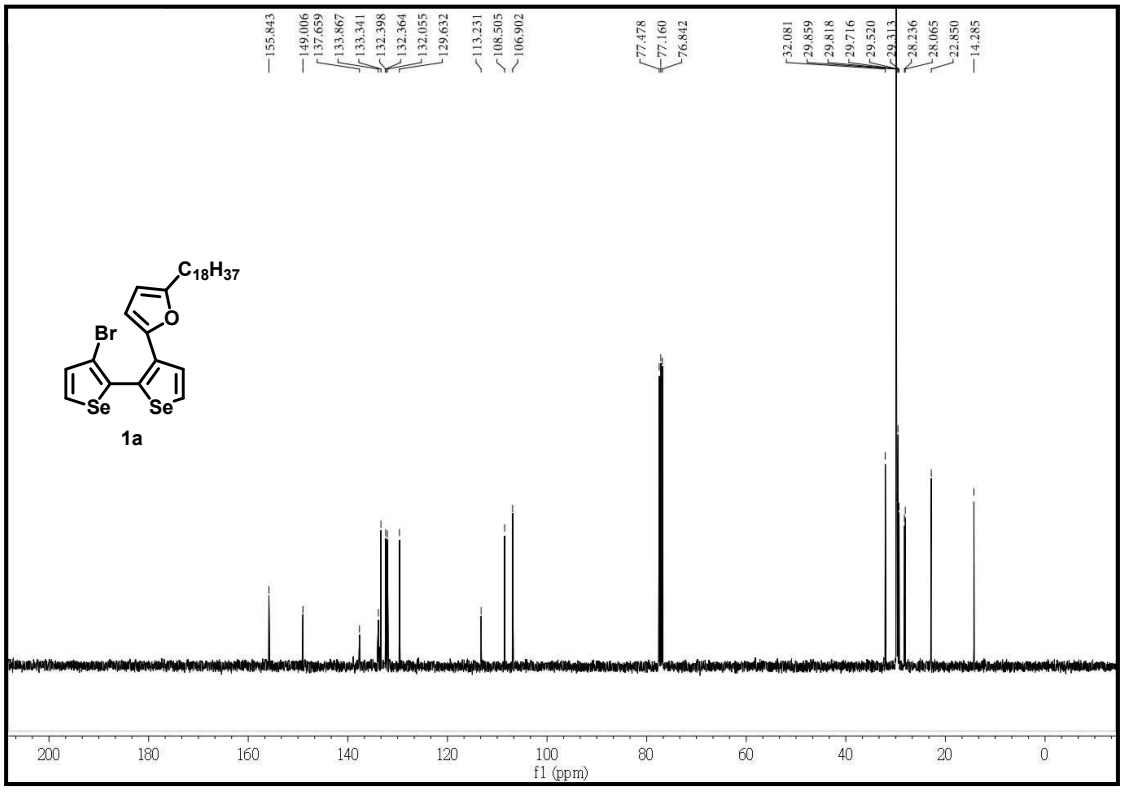
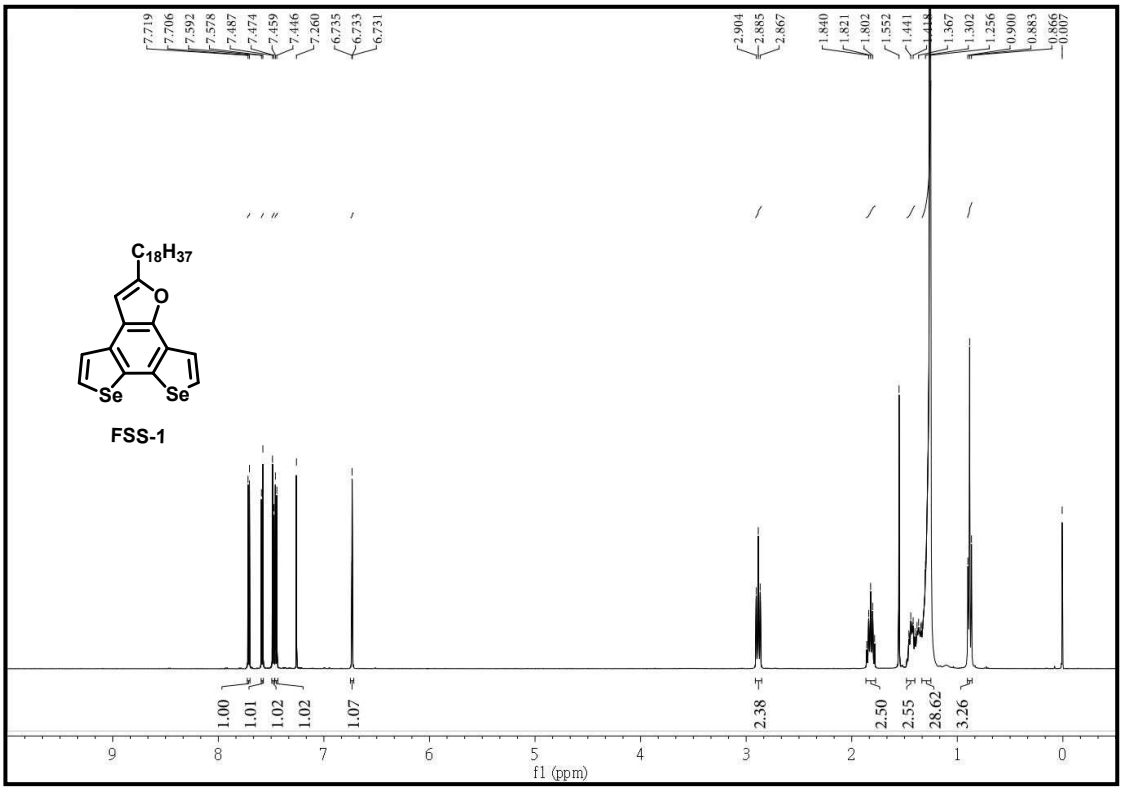


Figure S10. ORTEP view of **SSS-2** (Here $C_{14} = C_4$). CCDC No.- 1543181

6. ^{1}H and ^{13}C NMR spectra



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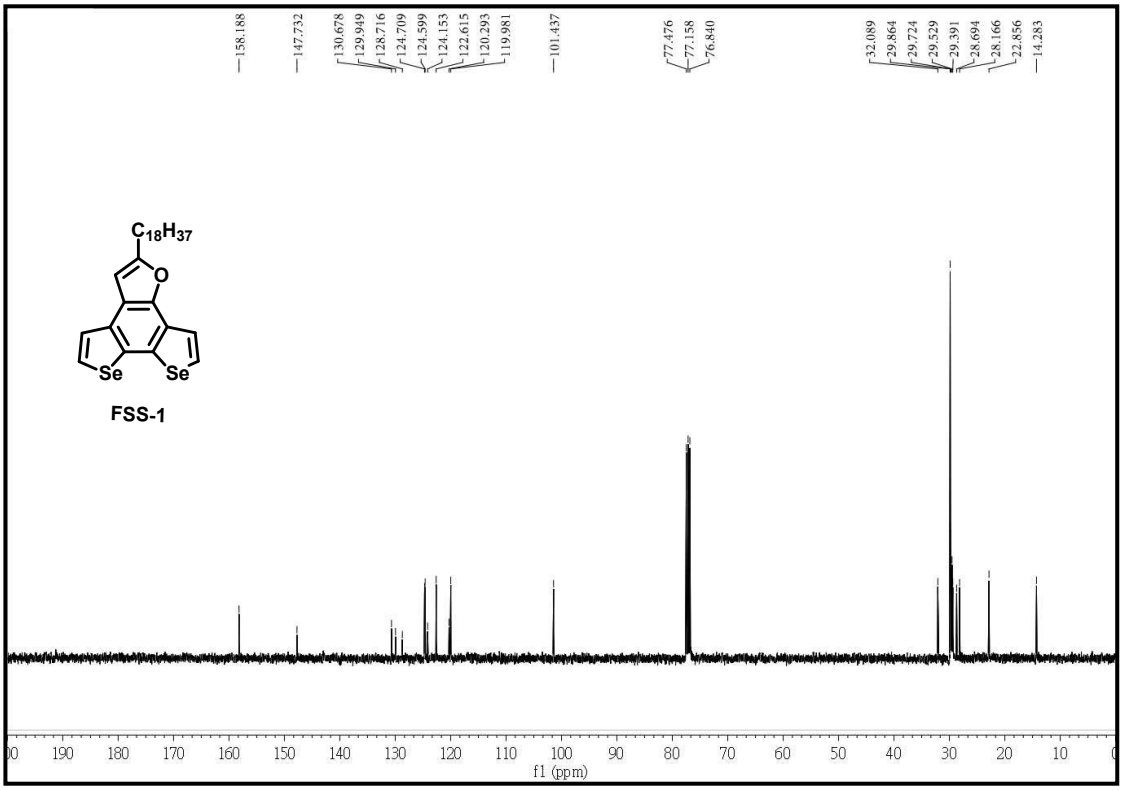
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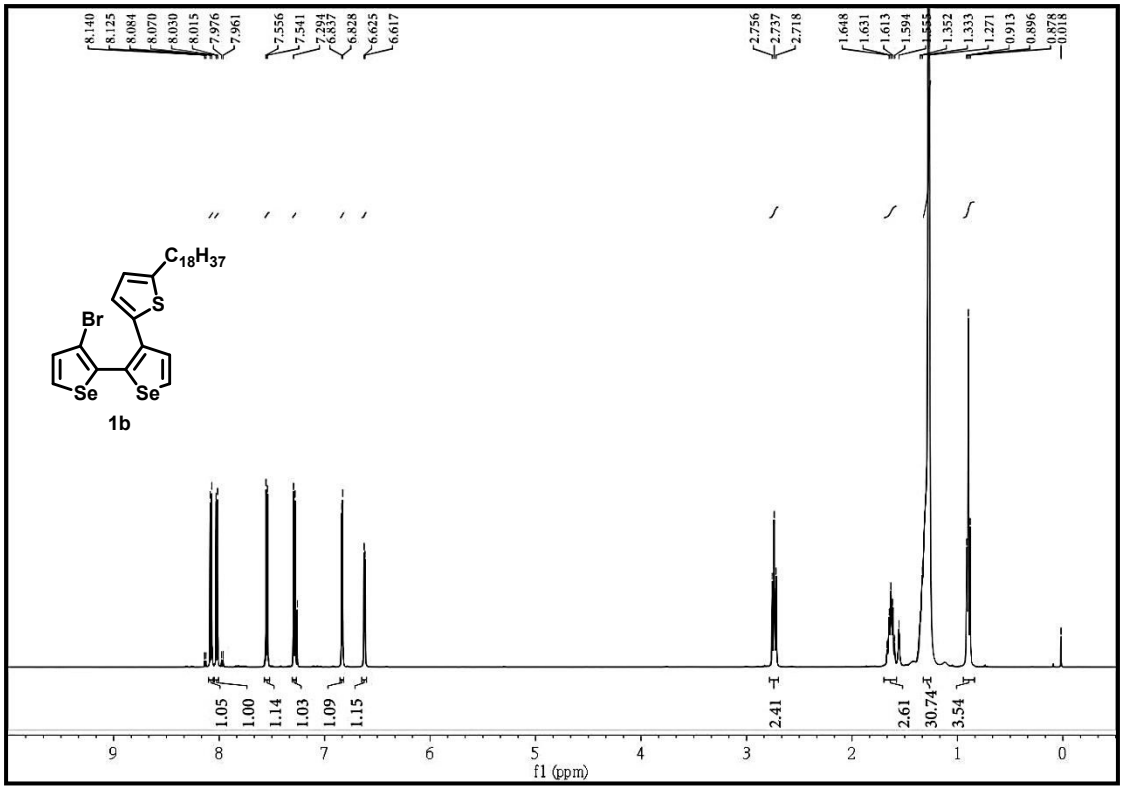
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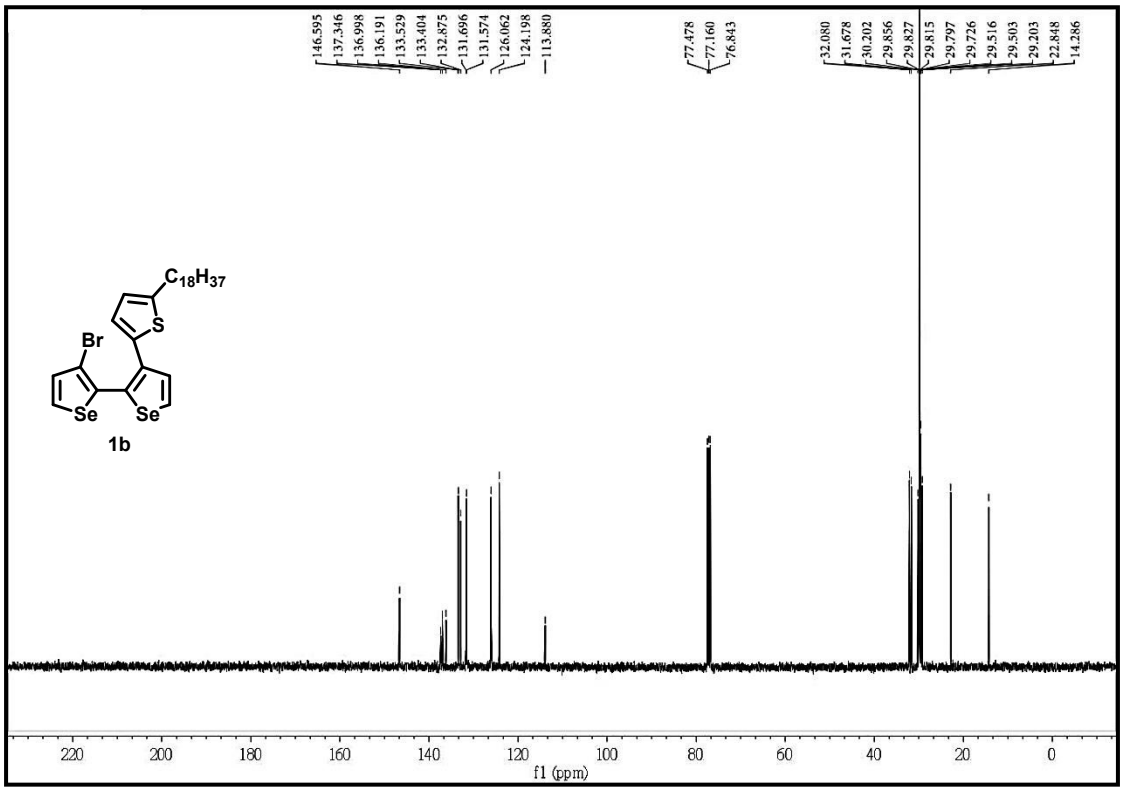
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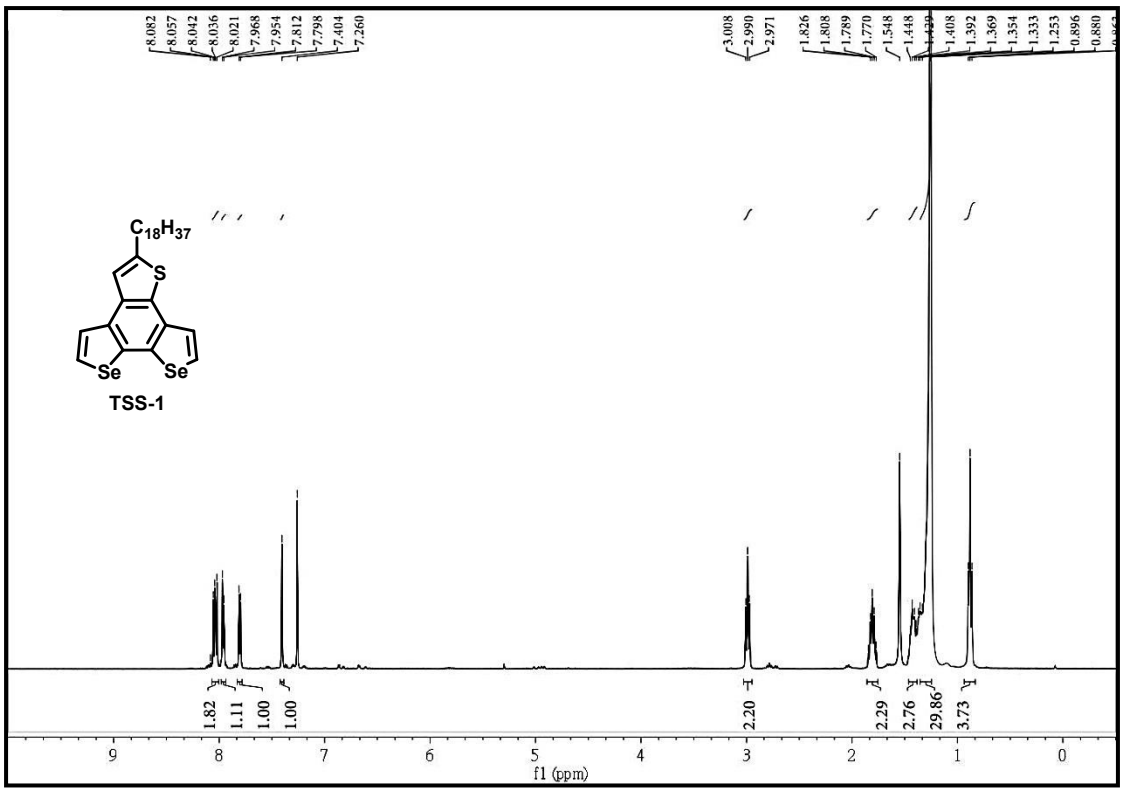
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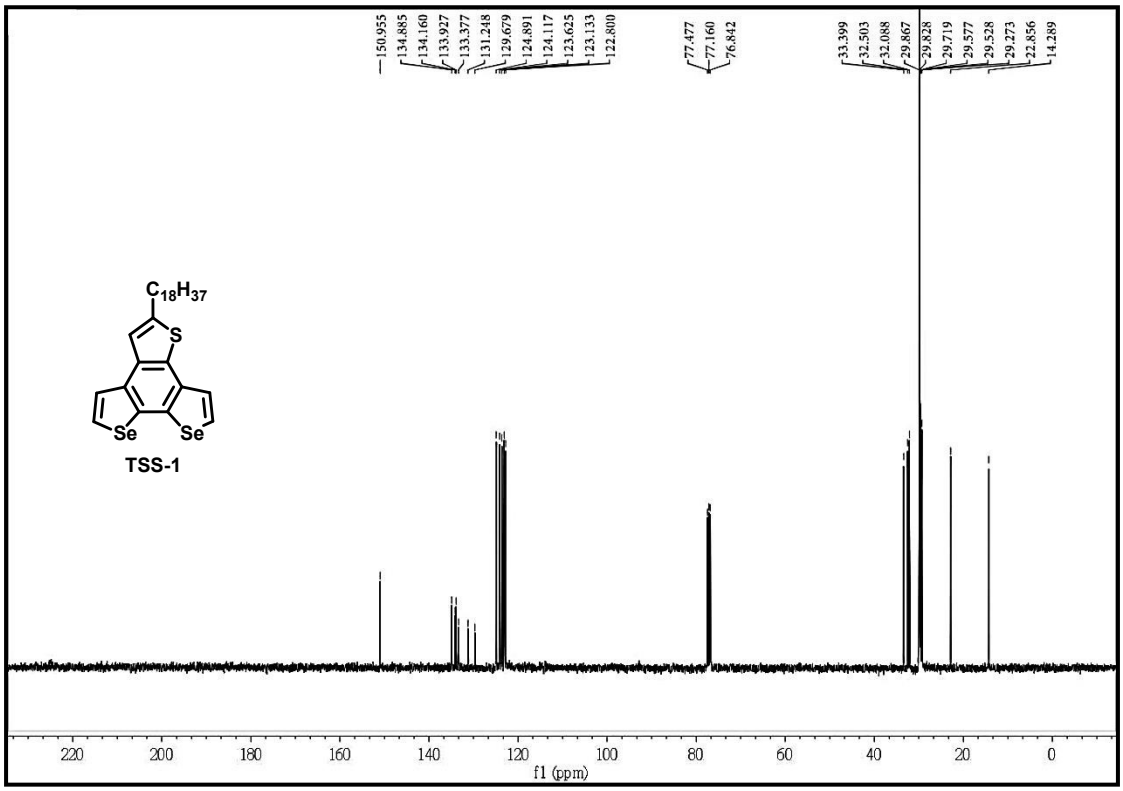
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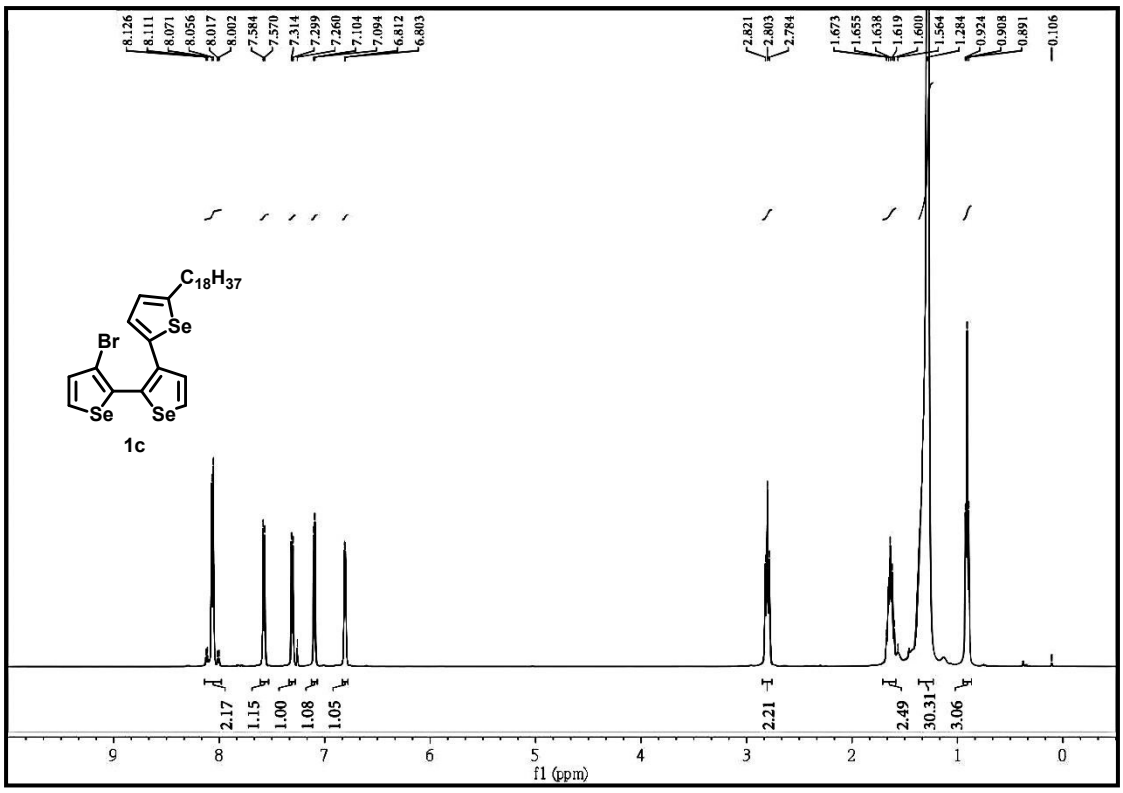
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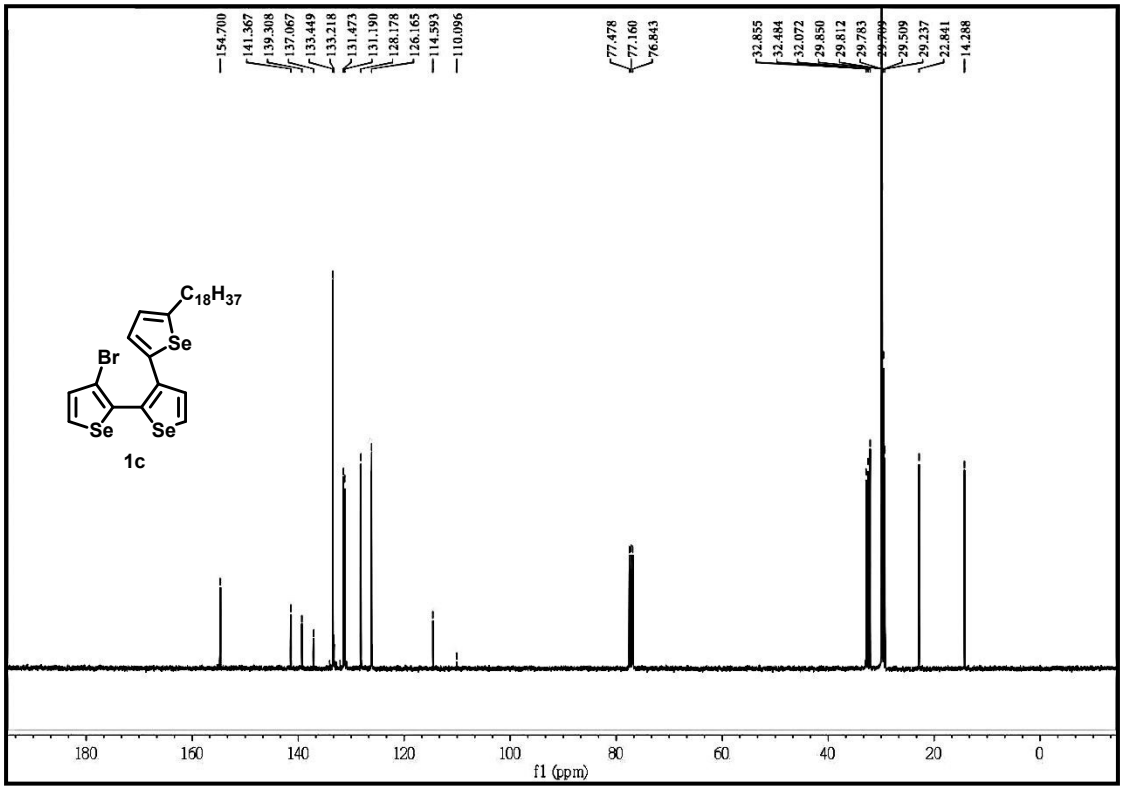
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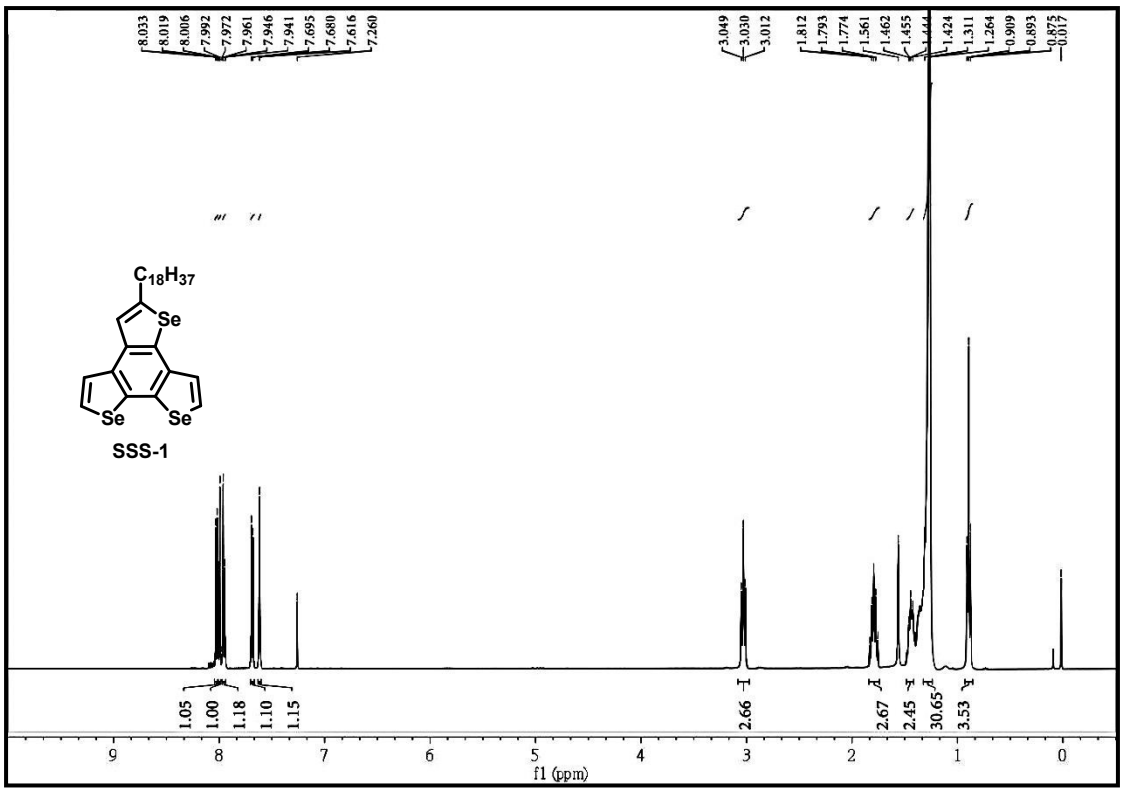
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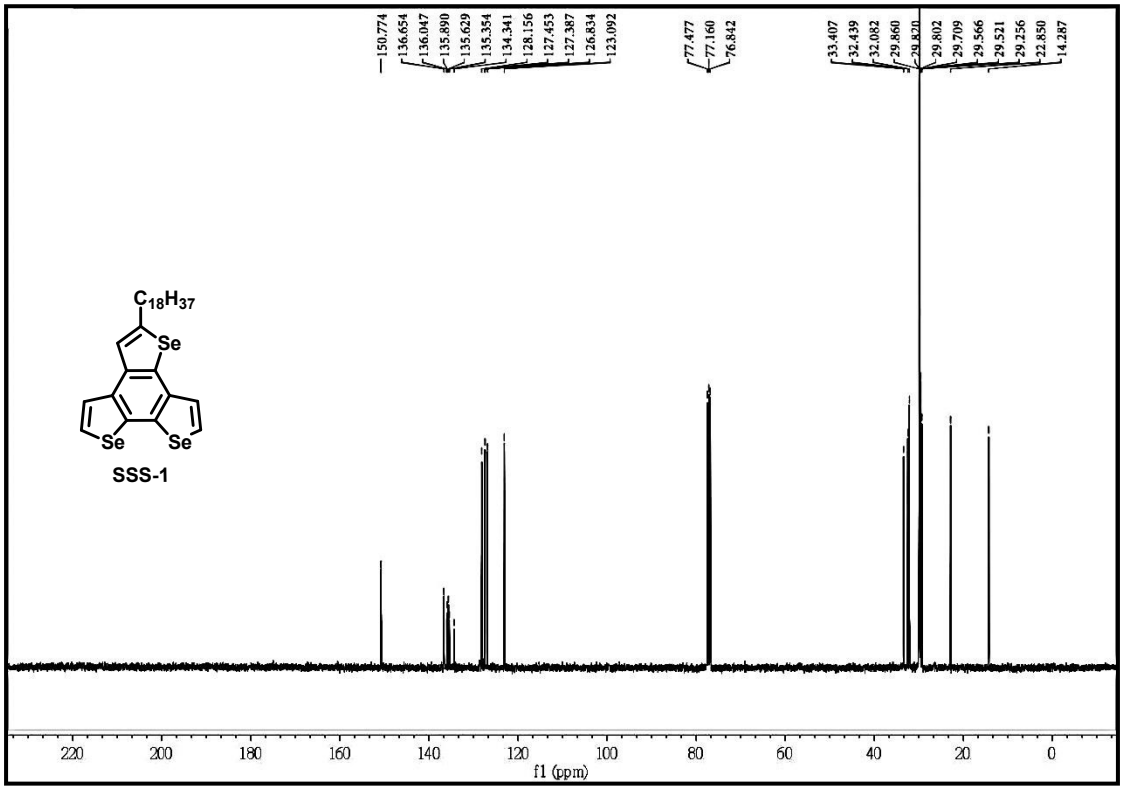
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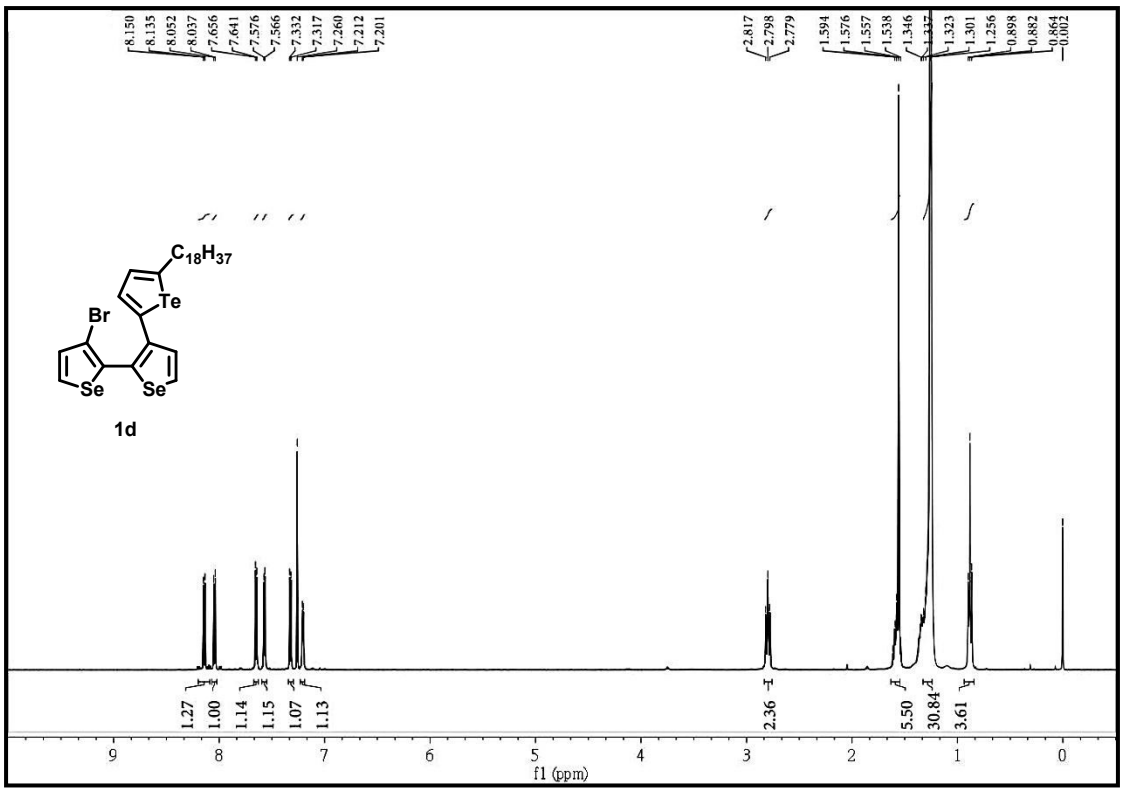
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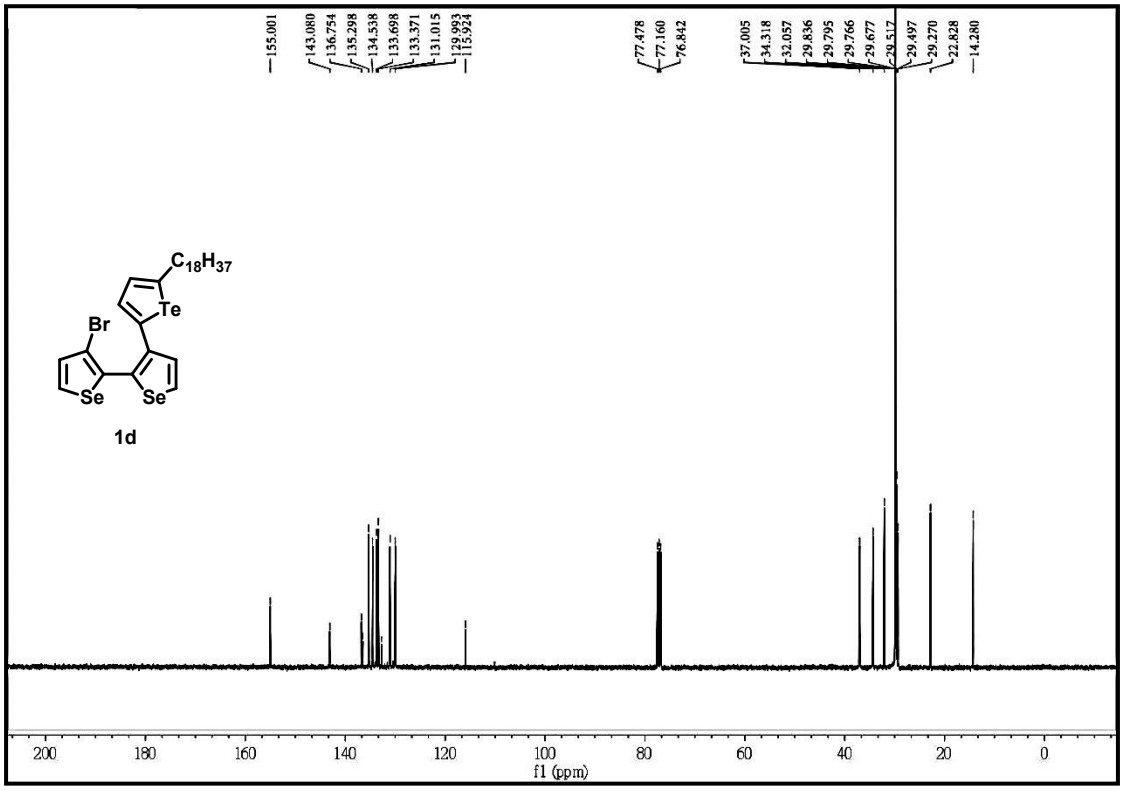
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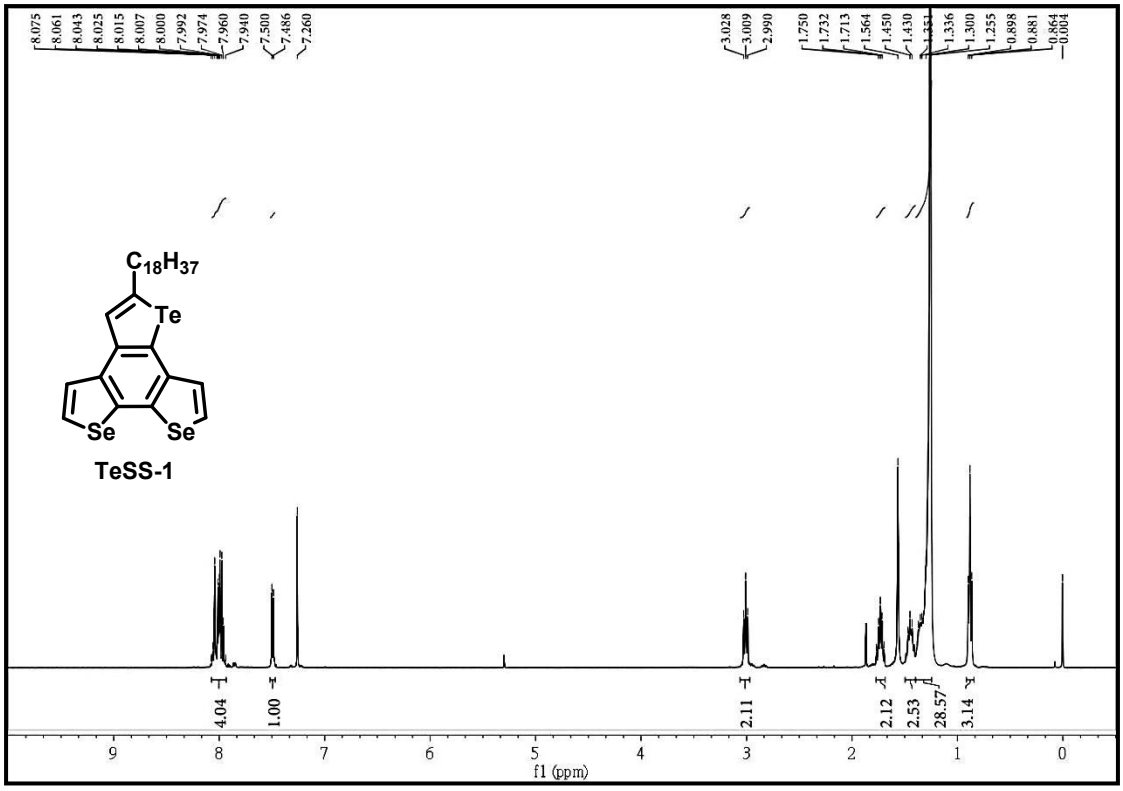
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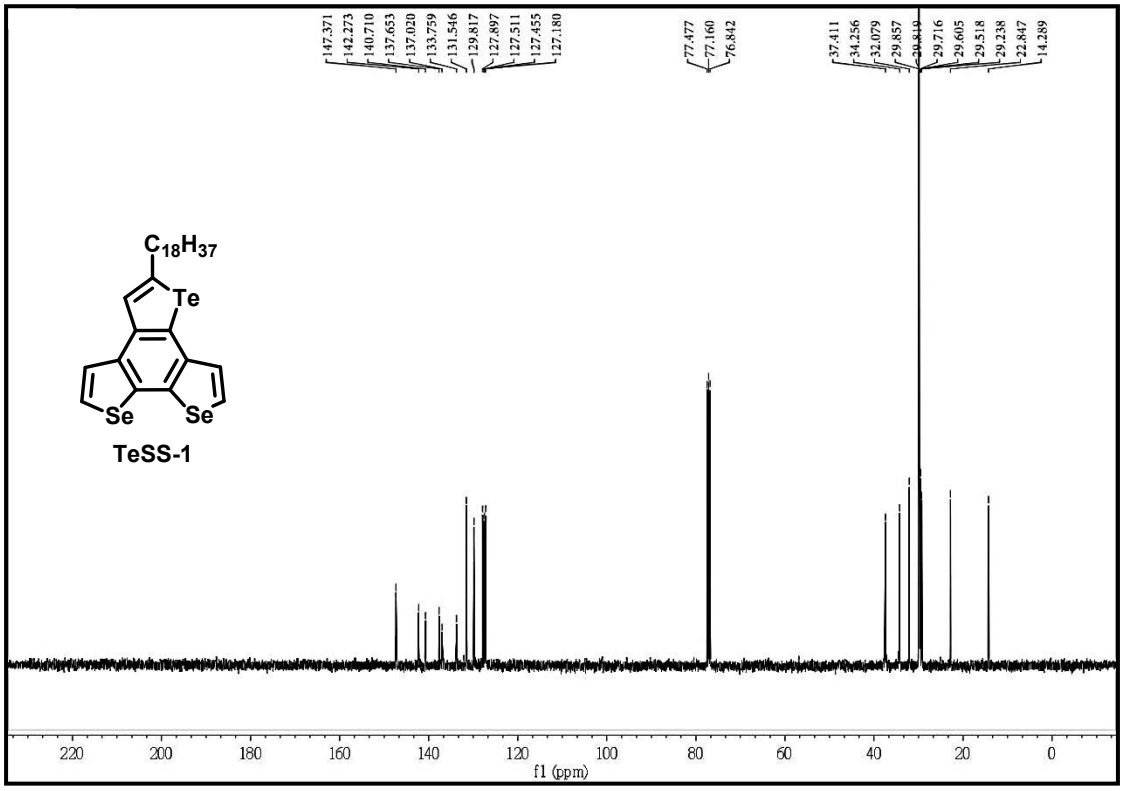
1.430
1.331
1.336
1.300
1.255
0.898
0.881
0.864
0.004
C18H37
Te
Se
Se
TeSS-1
4.04
1.00
2.11
2.12
2.53
28.57
3.14
f1 (ppm)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133.759
131.546
129.817
127.897
127.511
127.455
127.180
77.477
77.160
76.842
37.411
34.256
32.079
29.857
29.819
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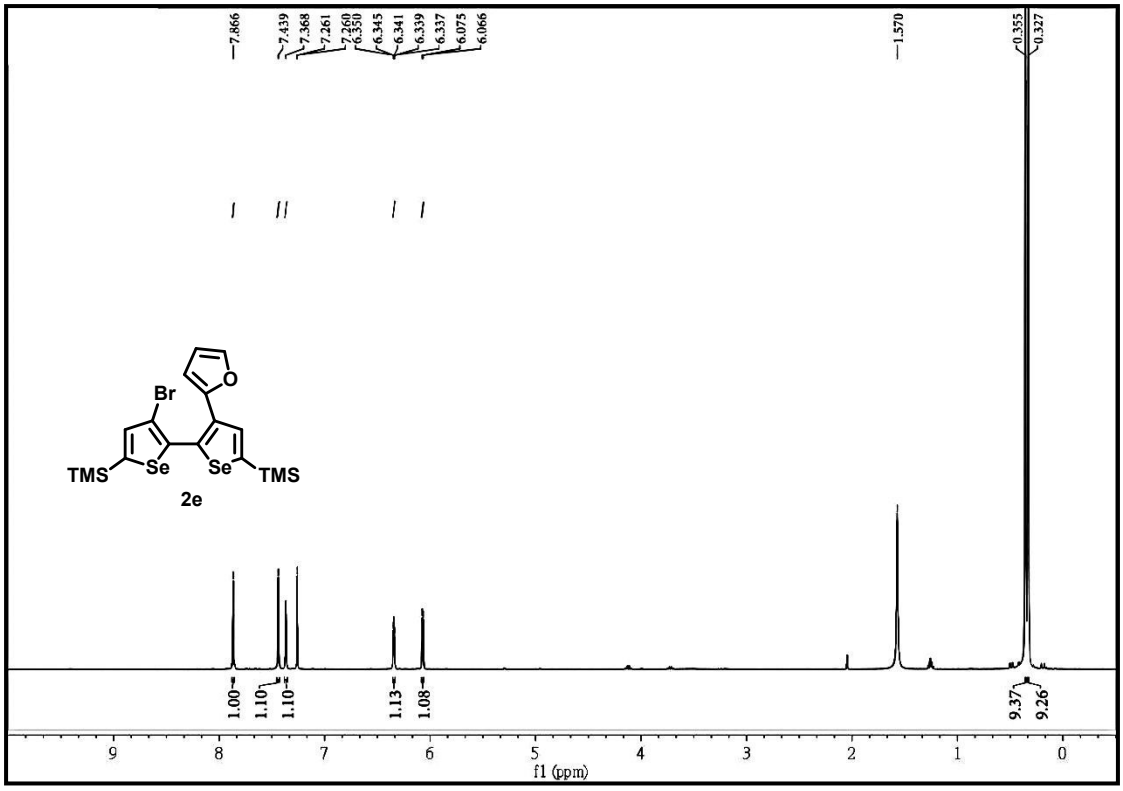
29.605
29.518
29.238
22.847
14.289
C18H37
Te
Se
Se
TeSS-1
f1 (ppm)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7.368
7.261
7.260
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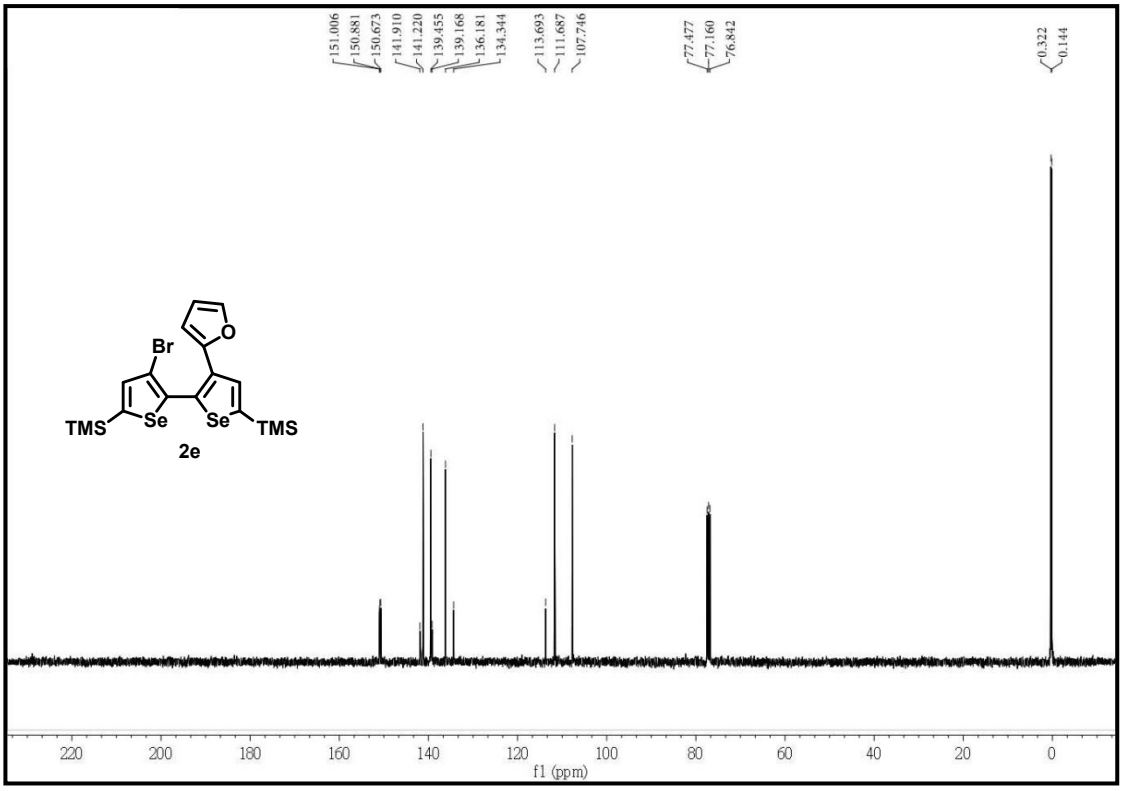
6.345
6.341
6.339
6.337
6.075
6.066
1.570
0.355
0.327
Br
O
TMS
Se
Se
TMS
2e
1.00
1.10
1.10
1.13
1.08
9.37
9.26
f1 (ppm)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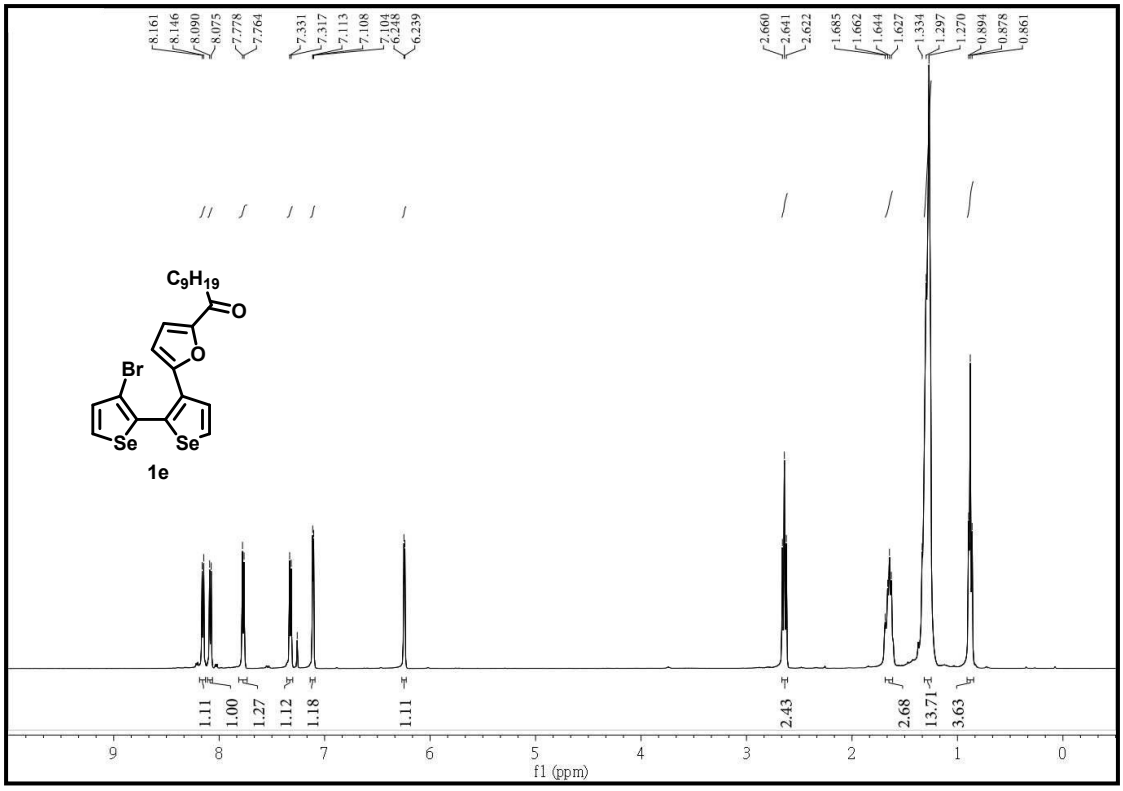
141.220
139.455
139.168
136.181
134.344
113.693
111.687
107.746
77.477
77.160
76.842
0.322
0.144
Br
O
TMS
Se
Se
TMS
2e
f1 (ppm)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8.090
8.075
7.778
7.764
7.331
7.317
7.113
7.108
7.104
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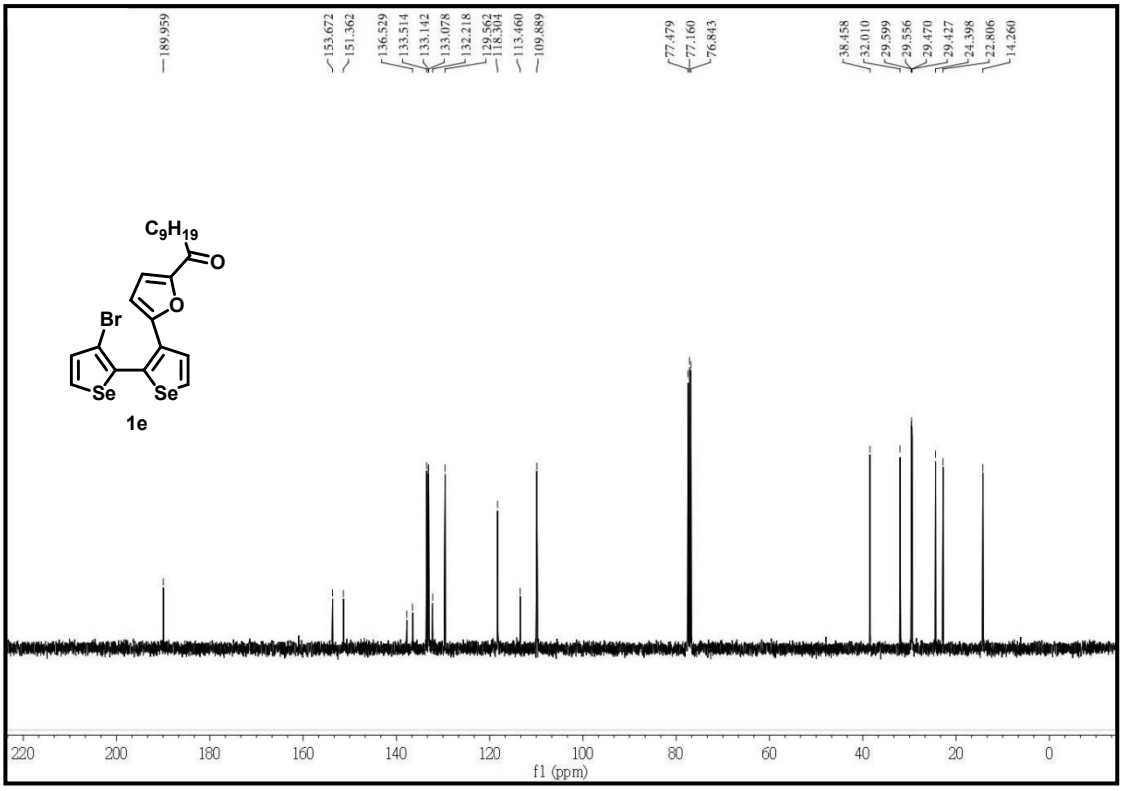
6.239
2.660
2.641
2.622
1.685
1.662
1.644
1.627
1.334
1.297
1.270
0.894
0.878
0.861
C9H19
O
O
Br
Se
Se
1e
1.11
1.00
1.27
1.12
1.18
1.11
2.43
2.68
13.71
3.63
f1 (ppm)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133.142
133.078
132.218
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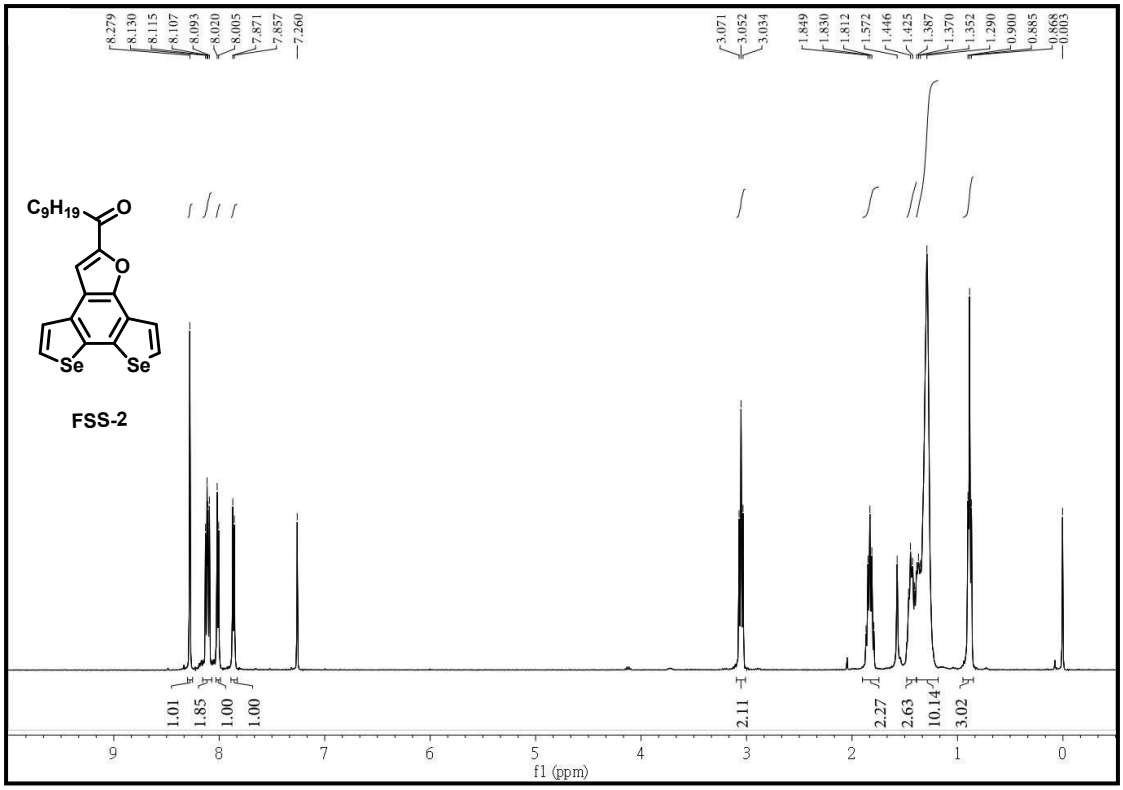
118.304
113.460
109.889
77.479
77.160
76.843
38.458
32.010
29.599
29.556
29.470
29.427
24.398
22.806
14.260
C9H19
O
O
Br
Se
Se
1e
f1 (ppm)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8.130
8.115
8.107
8.093
8.020
8.005
7.871
7.857
7.260
3.071
3.052
3.034
1.849
1.830
1.812
1.572
1.446
1.425
1.387
1.370
1.352
1.290
0.900
0.885
0.868
0.005
C9H19
O
O
Se
Se
FSS-2
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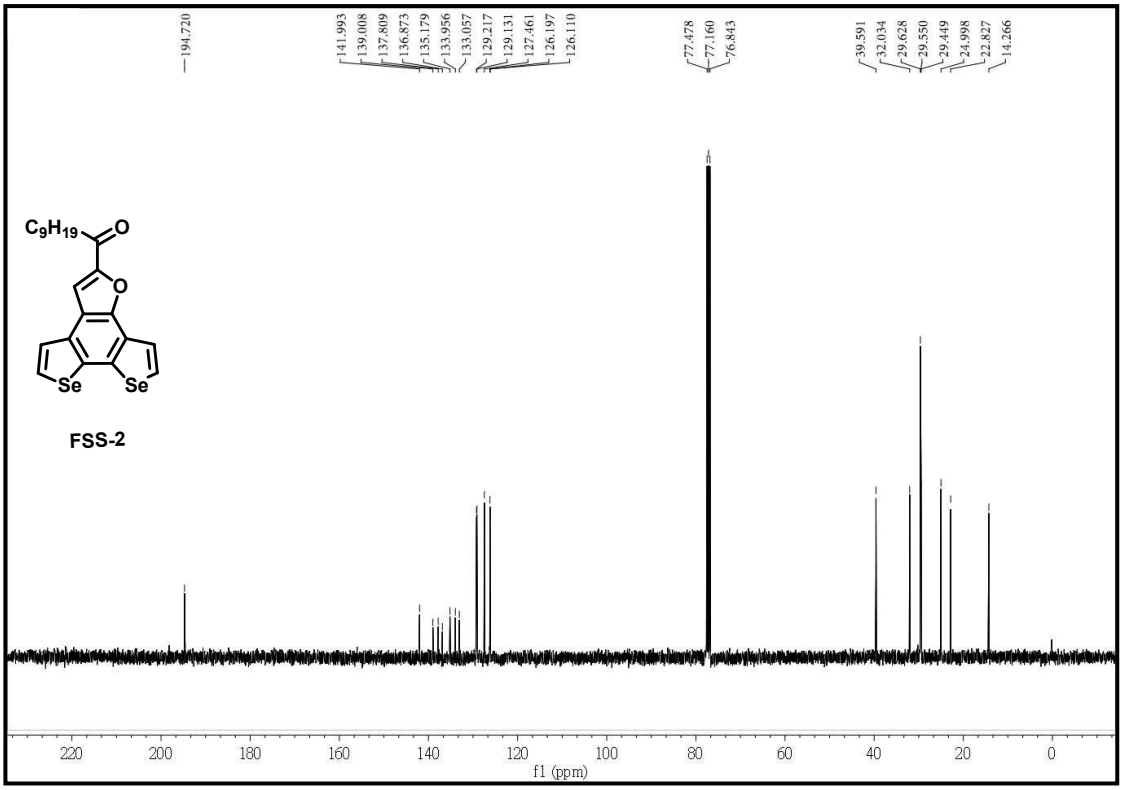
1.85
1.00
1.00
2.11
2.27
2.63
10.14
3.02
f1 (ppm)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135.179
133.956
133.057
129.217
129.131
127.461
126.197
126.110
77.478
77.160
76.843
39.591
32.034
29.628
29.550
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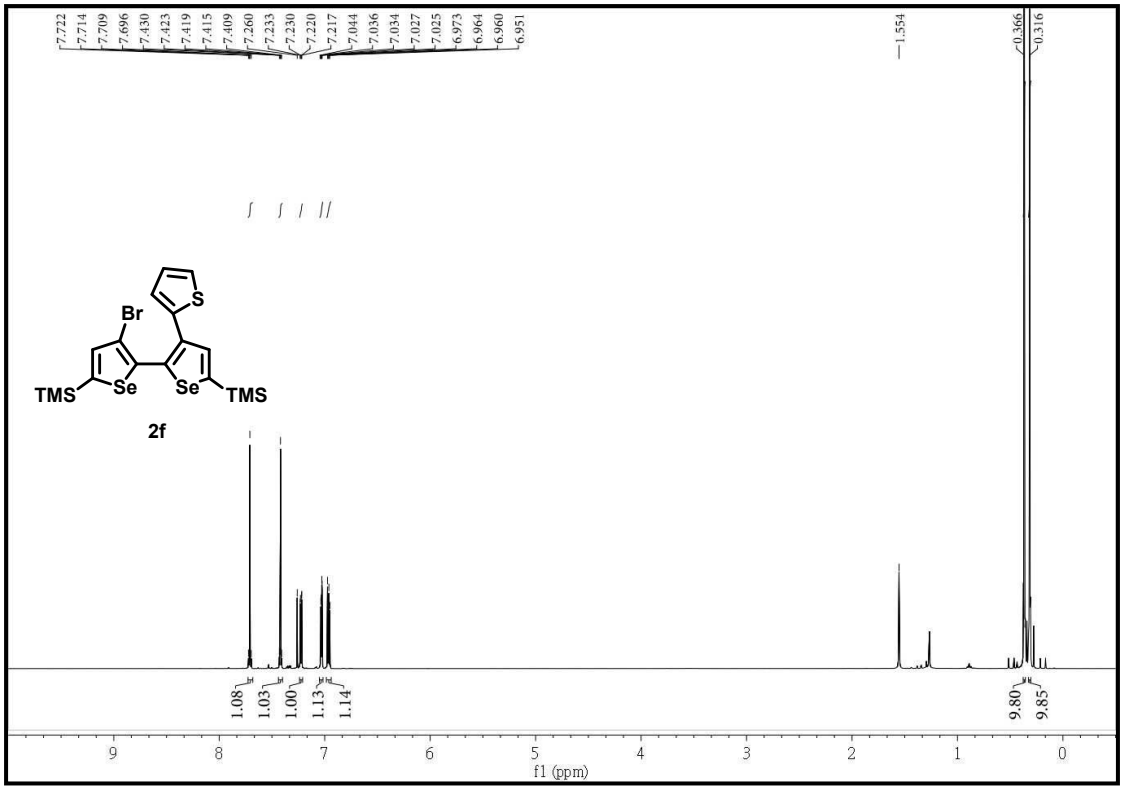
24.998
22.827
14.266
C9H19
O
O
Se
Se
FSS-2
f1 (ppm)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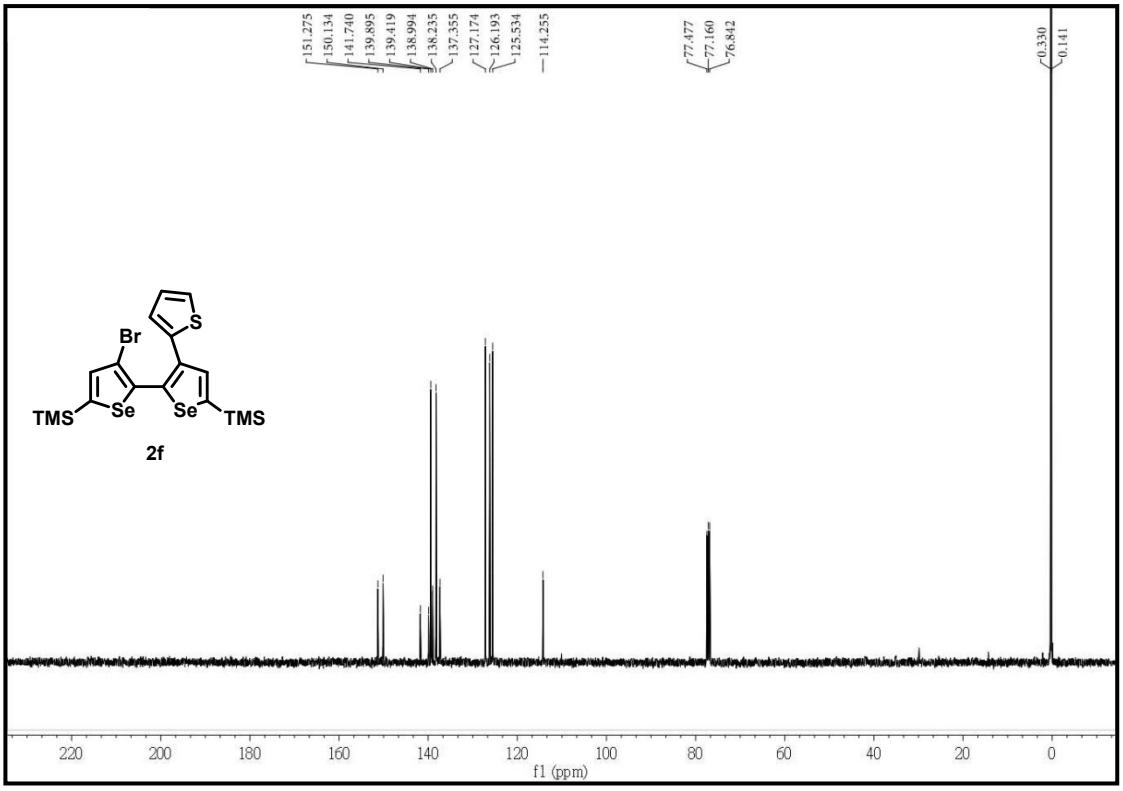
7.714
7.709
7.696
7.430
7.423
7.419
7.415
7.409
7.260
7.233
7.230
7.220
7.217
7.044
7.036
7.034
7.027
7.025
6.973
6.964
6.960
6.951
1.554
0.366
0.316
Br
S
TMS
Se
Se
TMS
2f
1.08
1.03
1.00
1.13
1.14
9.80
9.85
f1 (ppm)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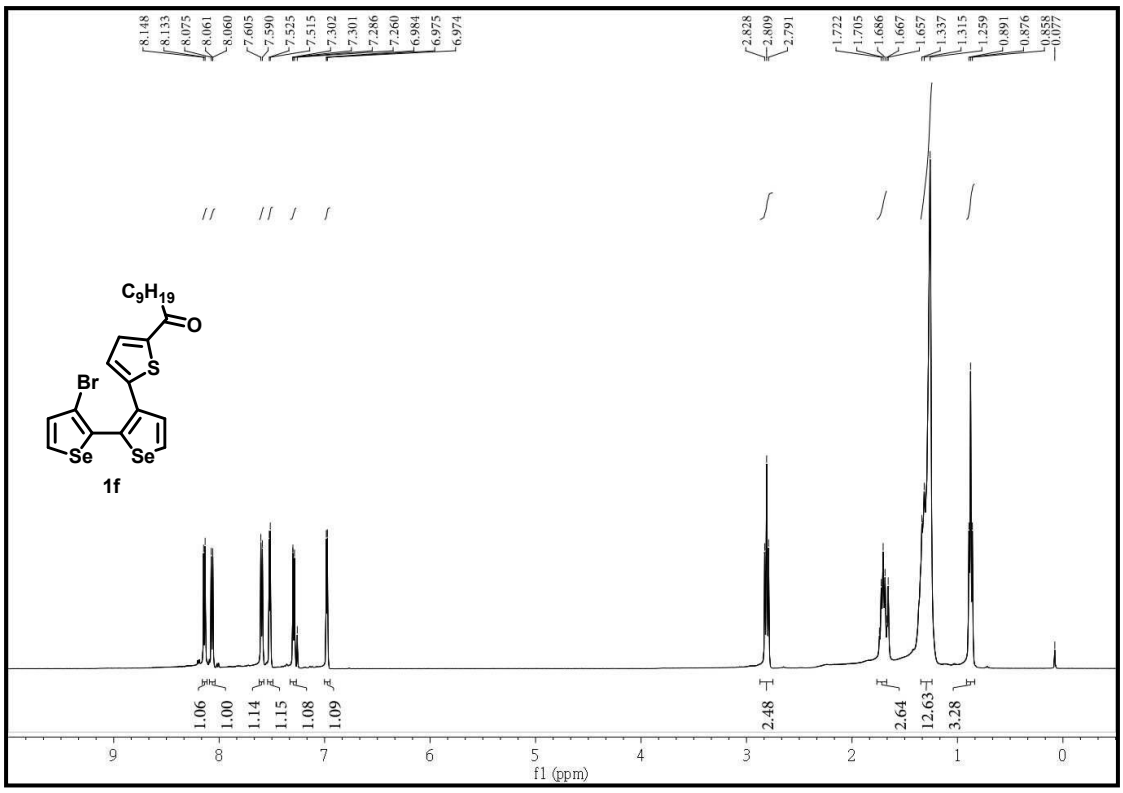
150.134
141.740
139.895
139.419
138.994
138.235
137.355
127.174
126.193
125.534
114.255
77.477
77.160
76.842
0.330
0.141
Br
S
TMS
Se
Se
TMS
2f
f1 (ppm)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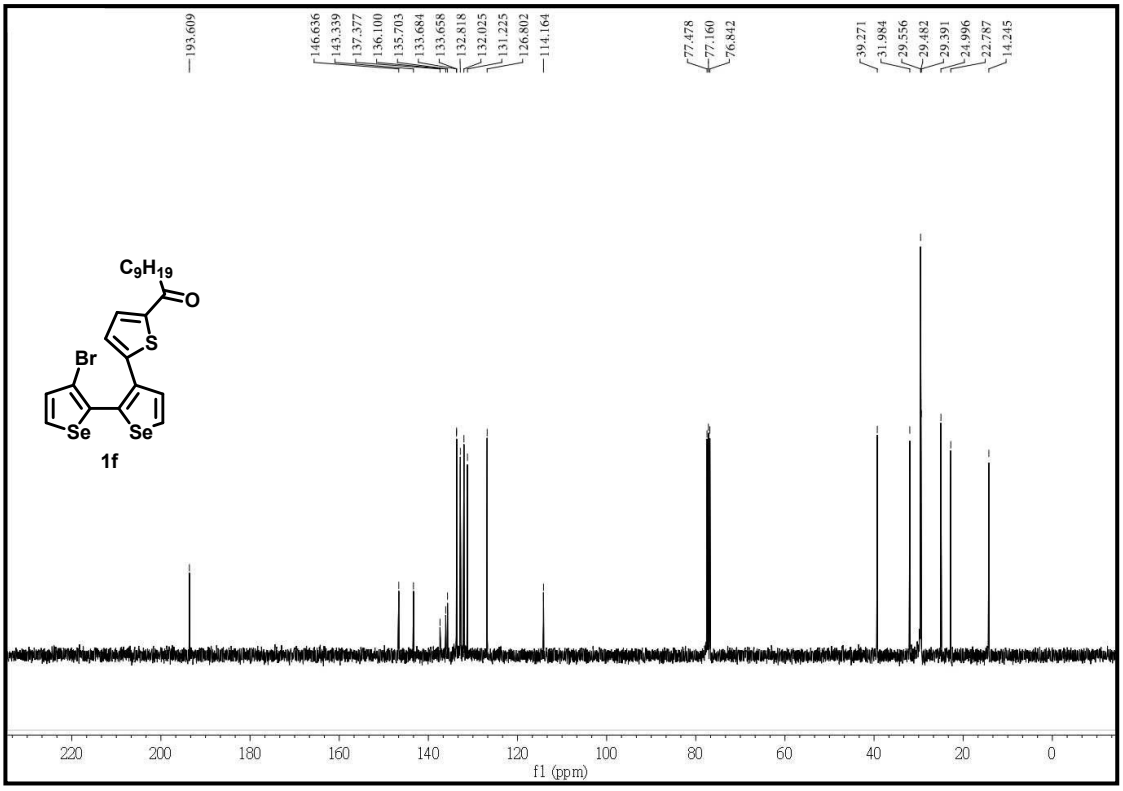
8.133
8.075
8.061
8.060
7.605
7.590
7.525
7.515
7.302
7.301
7.286
7.260
6.984
6.975
6.974
2.828
2.809
2.791
1.722
1.705
1.686
1.667
1.657
1.337
1.315
1.259
0.891
0.876
0.858
0.077
C9H19
O
S
Br
Se
Se
1f
1.06
1.00
1.14
1.15
1.08
1.09
2.48
2.64
12.63
3.28
f1 (ppm)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143.339
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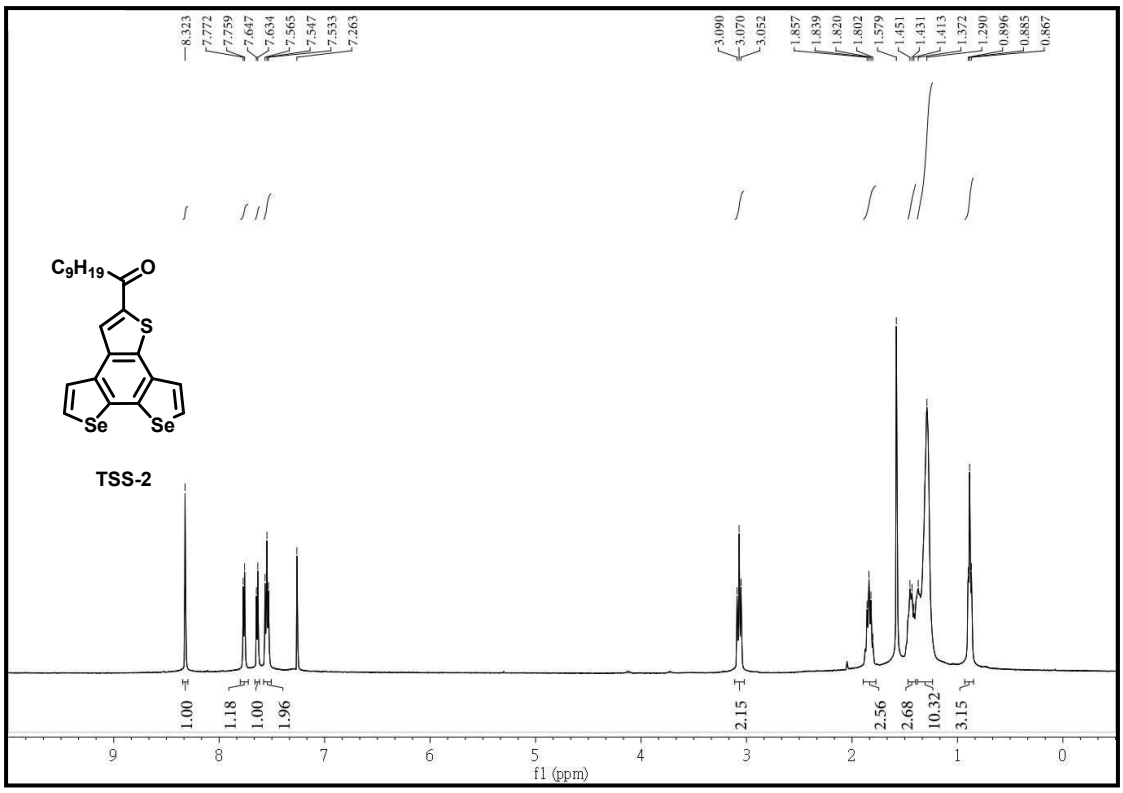
133.658
132.818
132.025
131.225
126.802
114.164
77.478
77.160
76.842
39.271
31.984
29.556
29.482
29.391
24.996
22.787
14.245
C9H19
O
S
Br
Se
Se
1f
f1 (ppm)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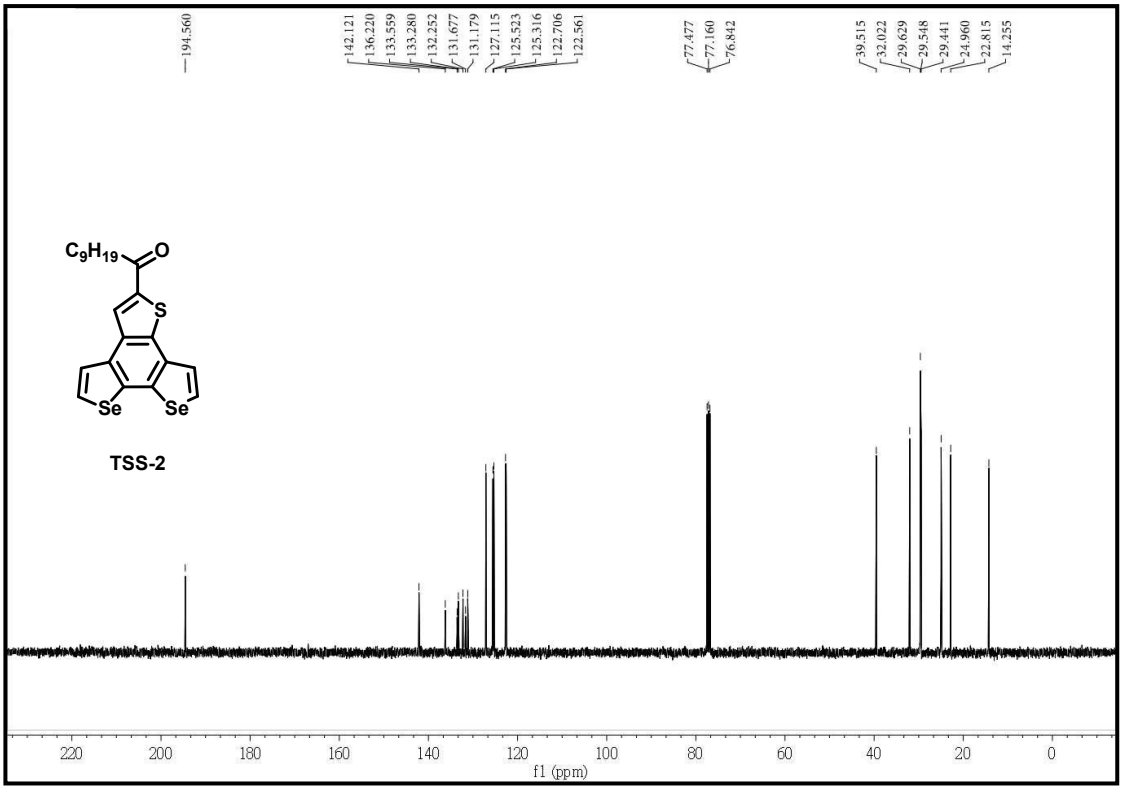
7.647
7.634
7.565
7.547
7.533
7.263
3.090
3.070
3.052
1.857
1.839
1.820
1.802
1.579
1.451
1.431
1.413
1.372
1.290
0.896
0.885
0.867
C9H19
O
S
Se
Se
TSS-2
1.00
1.18
1.00
1.96
2.15
2.56
2.68
10.32
3.15
f1 (ppm)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132.252
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131.179
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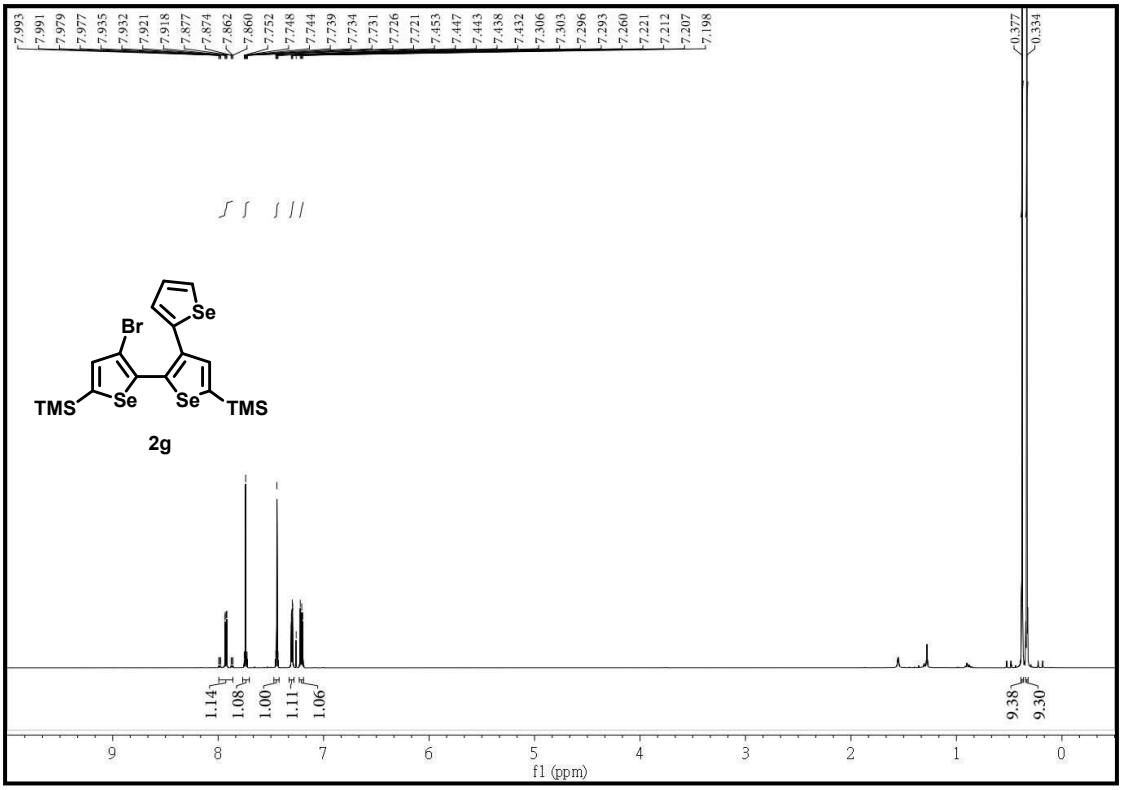
125.523
125.316
122.706
122.561
77.477
77.160
76.842
39.515
32.022
29.629
29.548
29.441
24.960
22.815
14.255
C9H19
O
S
Se
Se
TSS-2
f1 (ppm)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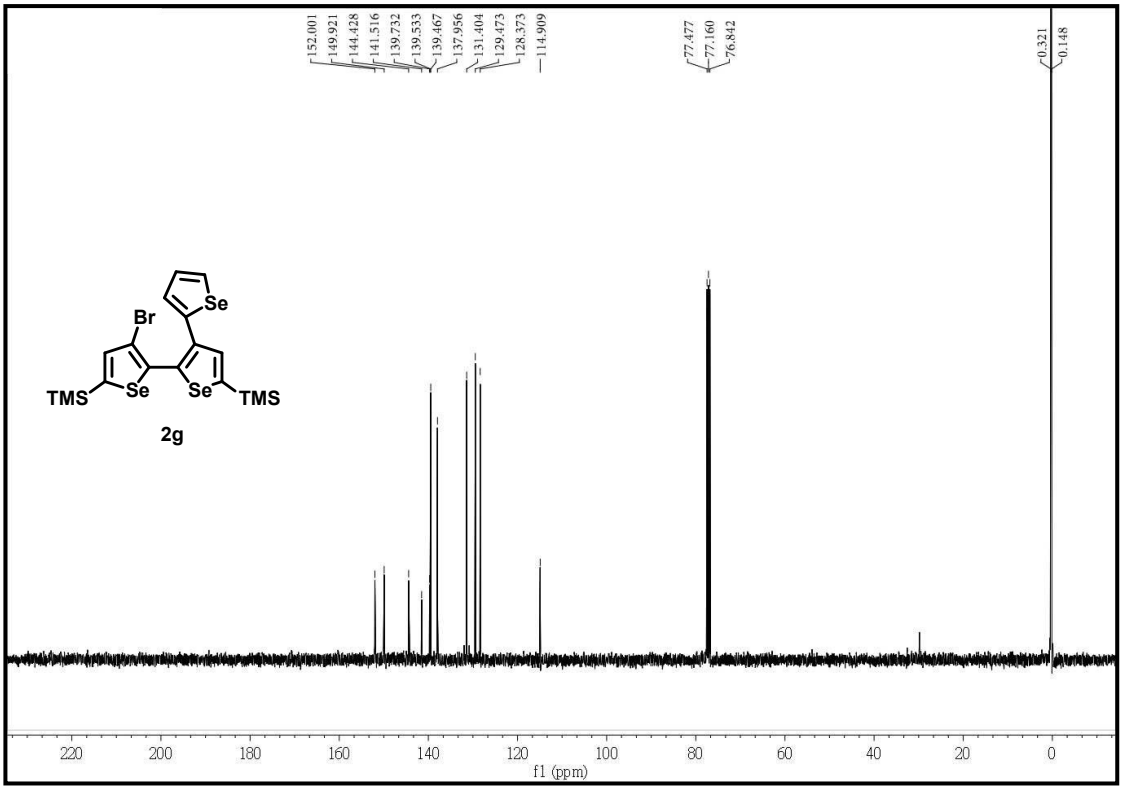
7.991
7.979
7.977
7.935
7.932
7.921
7.918
7.877
7.874
7.862
7.860
7.752
7.748
7.744
7.739
7.734
7.731
7.726
7.721
7.453
7.447
7.443
7.438
7.432
7.306
7.303
7.296
7.293
7.260
7.221
7.212
7.207
7.198
0.377
0.334
Br
Se
TMS
Se
Se
TMS
2g
1.14
1.08
1.00
1.11
1.06
9.38
9.30
f1 (ppm)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141.516
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139.467
137.956
131.404
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128.373
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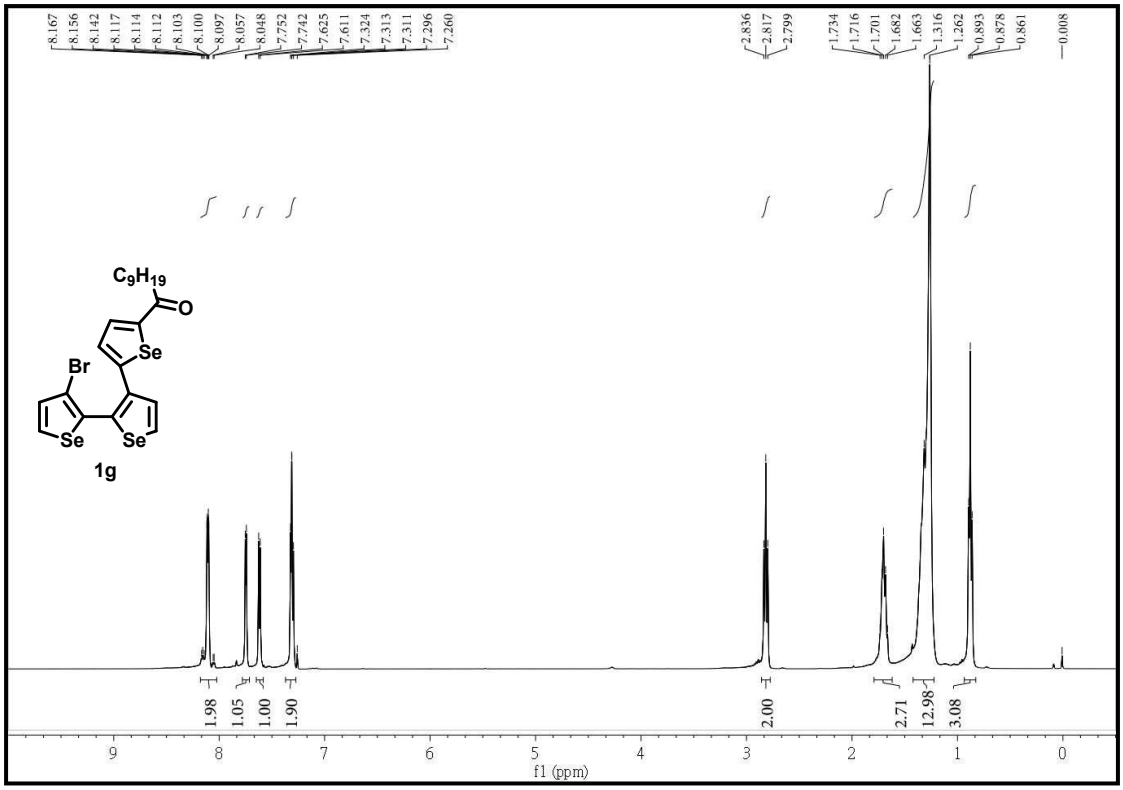
77.160
76.842
0.321
0.148
Br
Se
TMS
Se
Se
TMS
2g
f1 (ppm)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8.100
8.097
8.057
8.048
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7.742
7.625
7.611
7.324
7.313
7.311
7.296
7.260
2.836
2.817
2.799
1.734
1.716
1.701
1.682
1.663
1.316
1.262
0.893
0.878
0.861
0.008
C9H19
O
Se
Br
Se
Se
1g
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1.00
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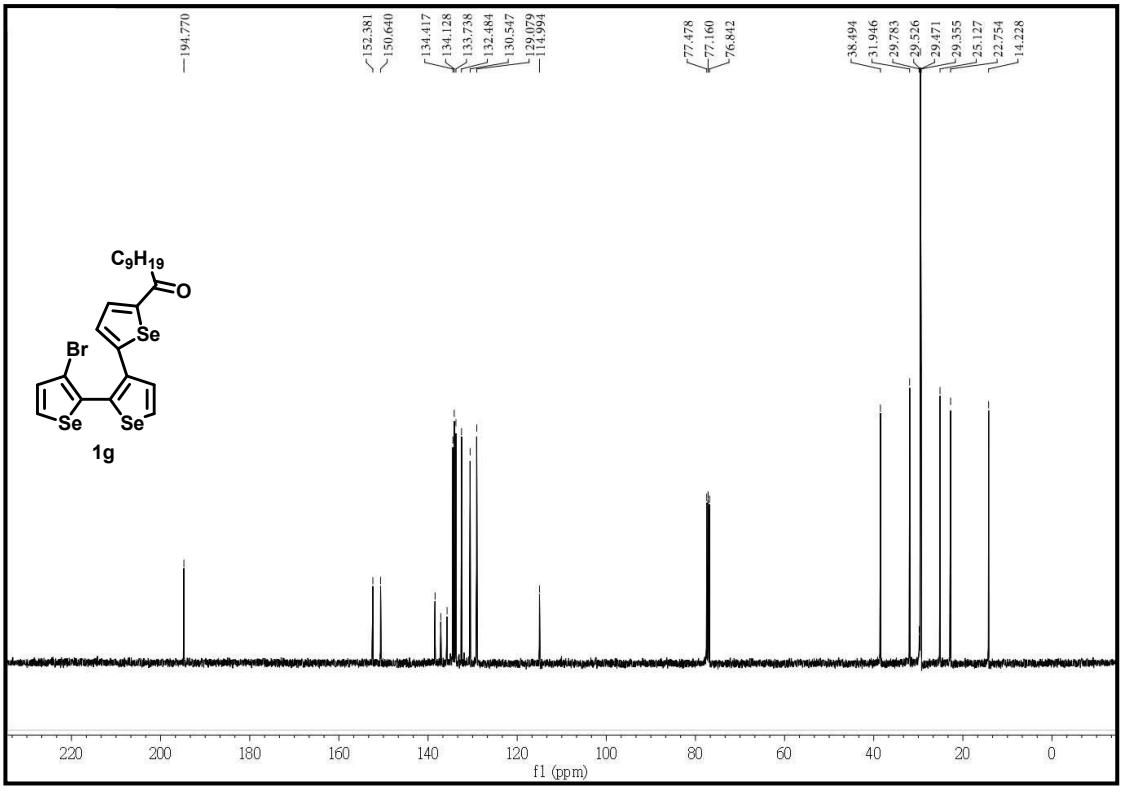
2.00
2.71
12.98
3.08
f1 (ppm)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130.547
129.079
114.994
77.478
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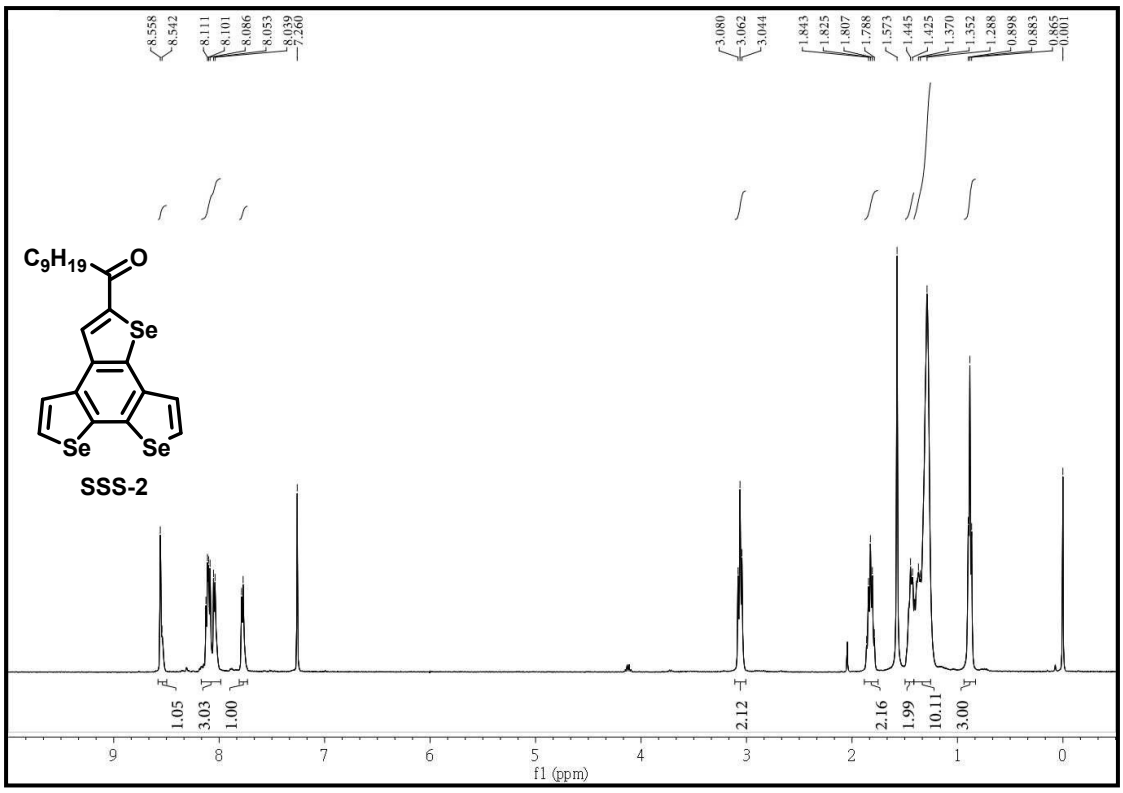
38.494
31.946
29.783
29.526
29.471
29.355
25.127
22.754
14.228
C9H19
O
Se
Br
Se
Se
1g
f1 (ppm)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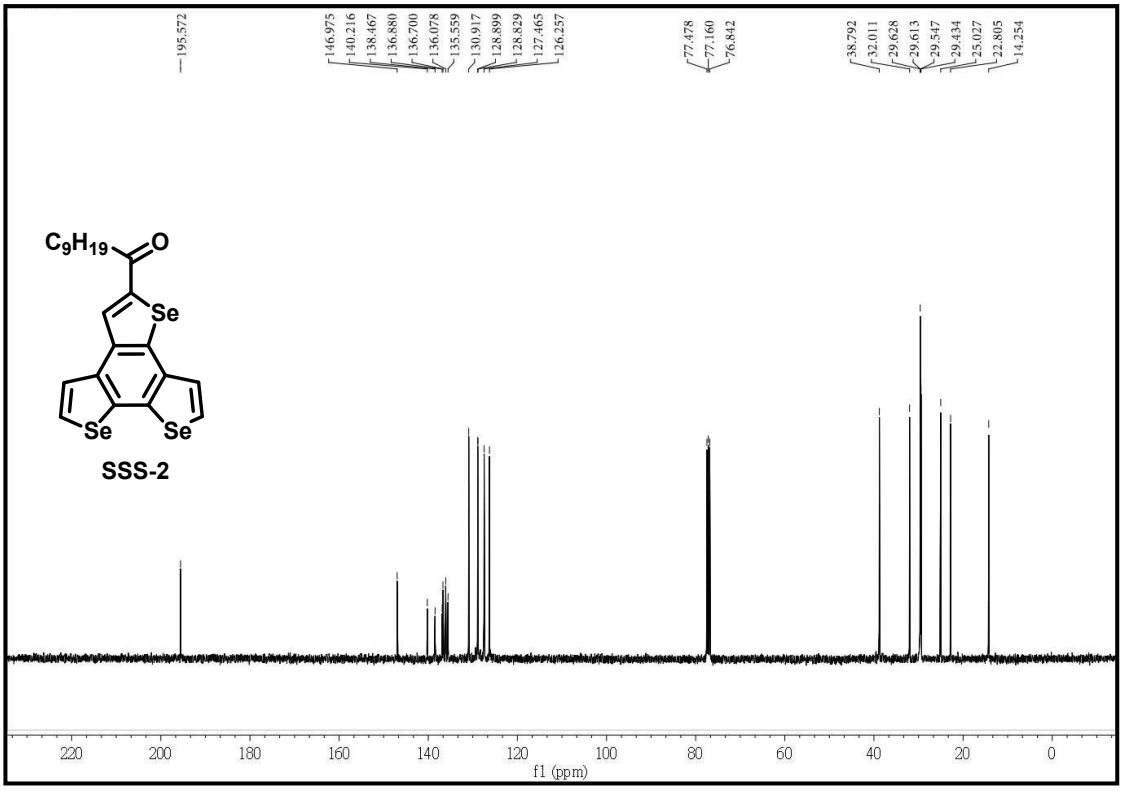
8.039
7.260
3.080
3.062
3.044
1.843
1.825
1.807
1.788
1.573
1.445
1.425
1.370
1.352
1.288
0.898
0.883
0.865
0.001
C9H19
O
Se
Se
Se
SSS-2
1.05
3.03
1.00
2.12
2.16
1.99
10.11
3.00
f1 (ppm)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135.559
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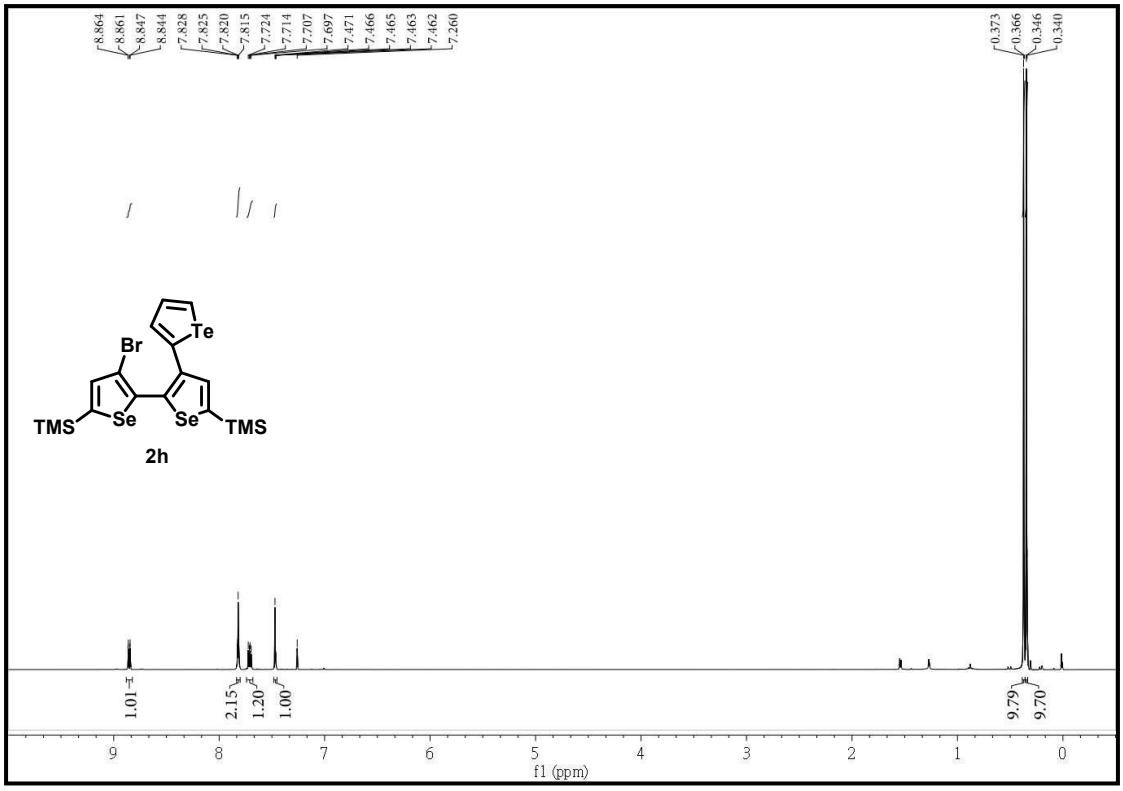
128.829
127.465
126.257
77.478
77.160
76.842
38.792
32.011
29.628
29.613
29.547
29.434
25.027
22.805
14.254
C9H19
O
Se
Se
Se
SSS-2
f1 (ppm)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7.815
7.724
7.714
7.707
7.697
7.471
7.466
7.465
7.463
7.462
7.260
0.373
0.366
0.346
0.340
Br
Te
TMS
Se
Se
TMS
2h
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2.15
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1.00
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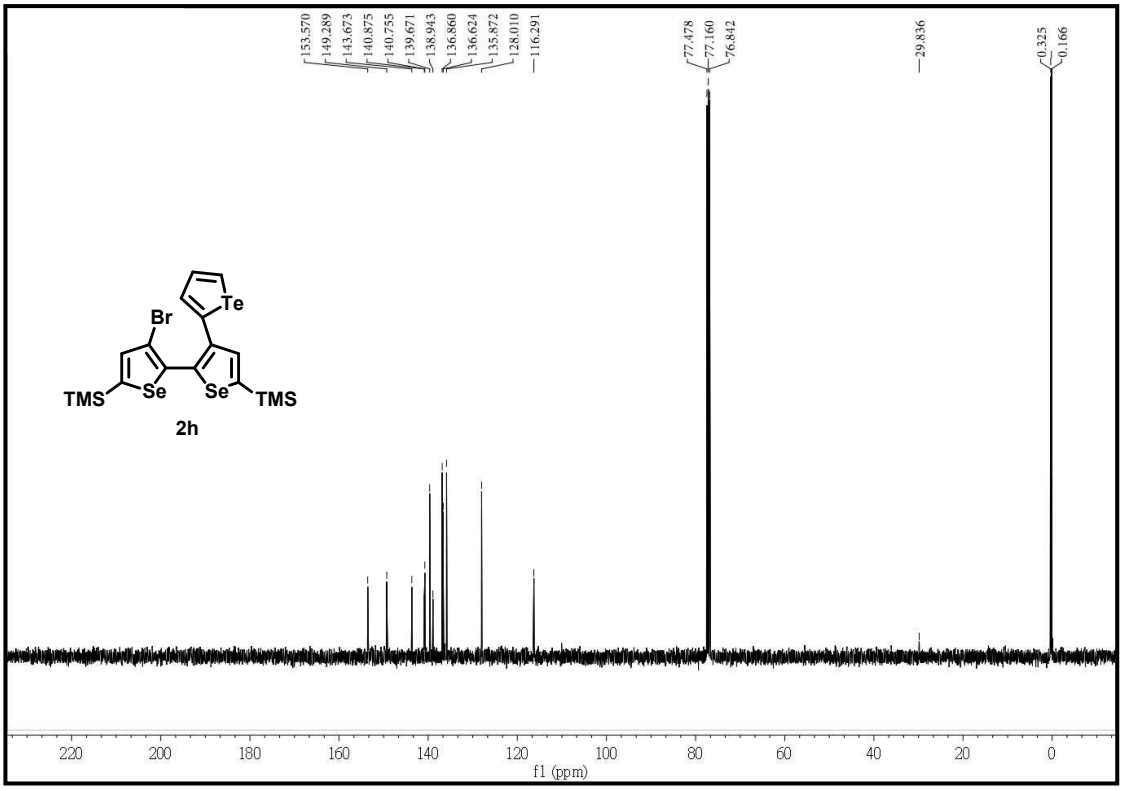
9.70
f1 (ppm)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136.860
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135.872
128.010
116.291
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77.160
76.842
29.836
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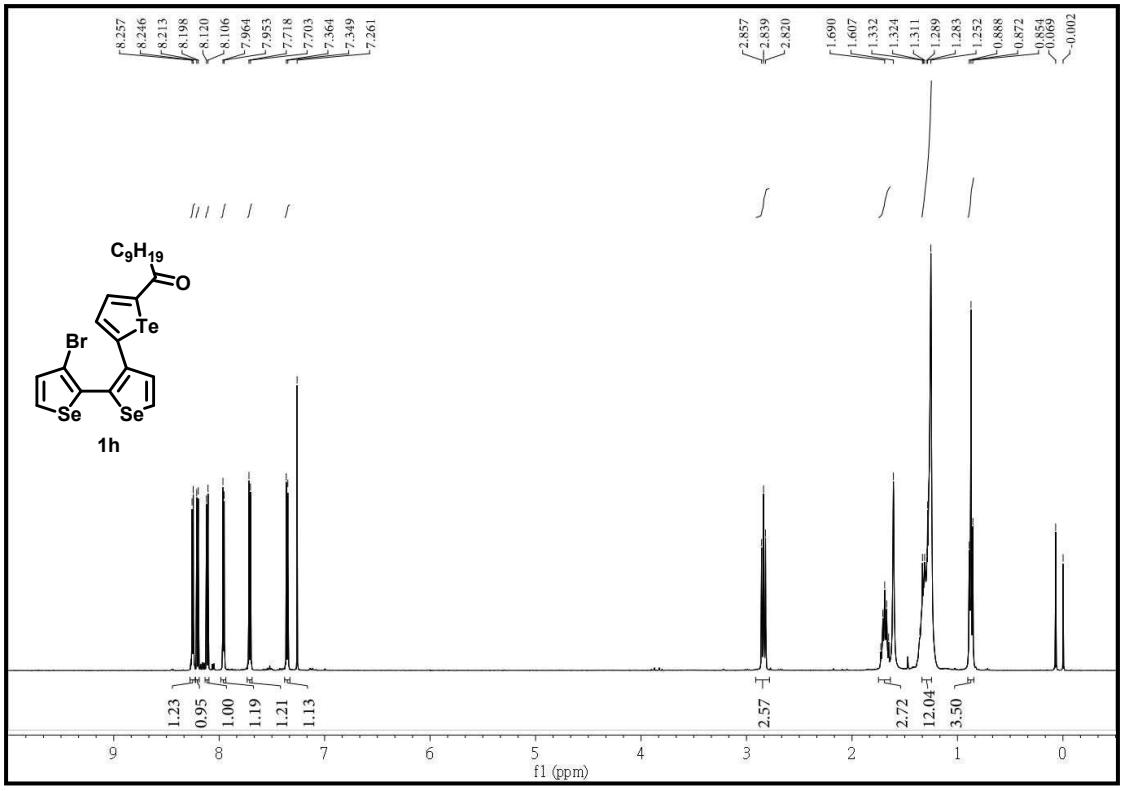
0.166
Br
Te
TMS
Se
Se
TMS
2h
f1 (ppm)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8.106
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7.953
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7.364
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7.261
2.857
2.839
2.820
1.690
1.607
1.332
1.324
1.311
1.289
1.283
1.252
0.888
0.872
0.854
0.069
-0.002
C9H19
O
Te
Br
Se
Se
1h
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1.00
1.19
1.21
1.13
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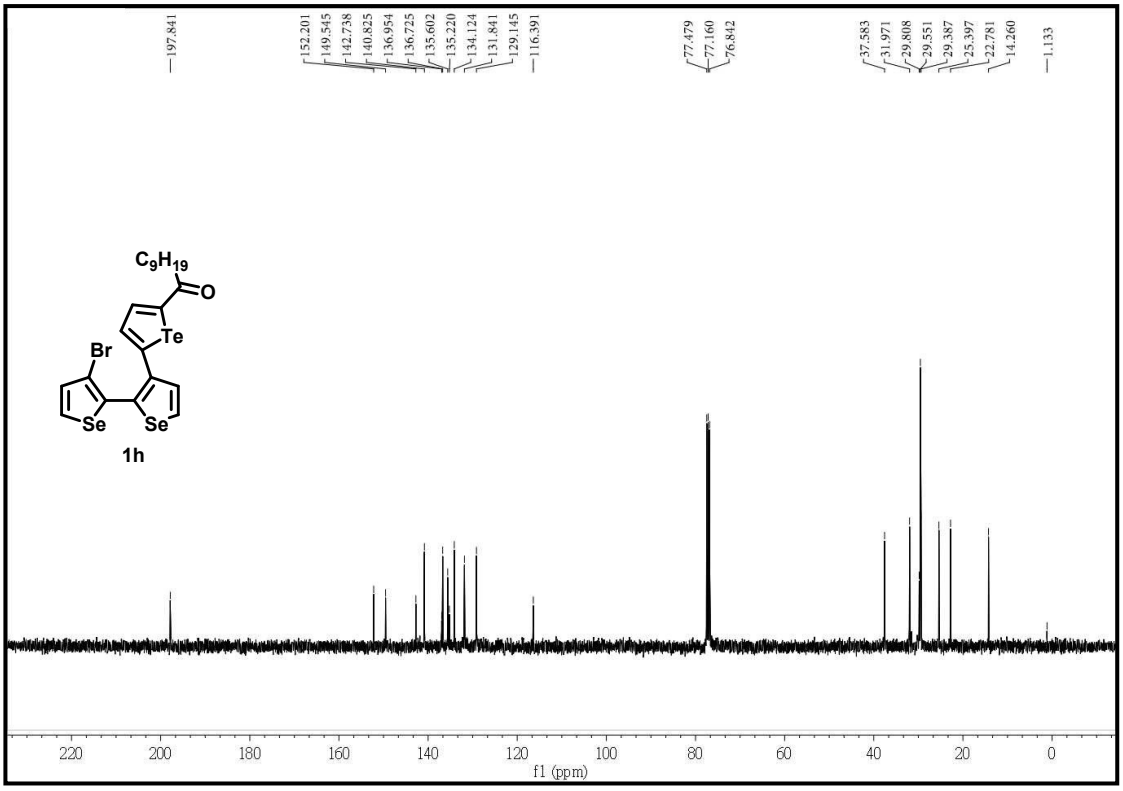
2.72
12.04
3.50
f1 (ppm)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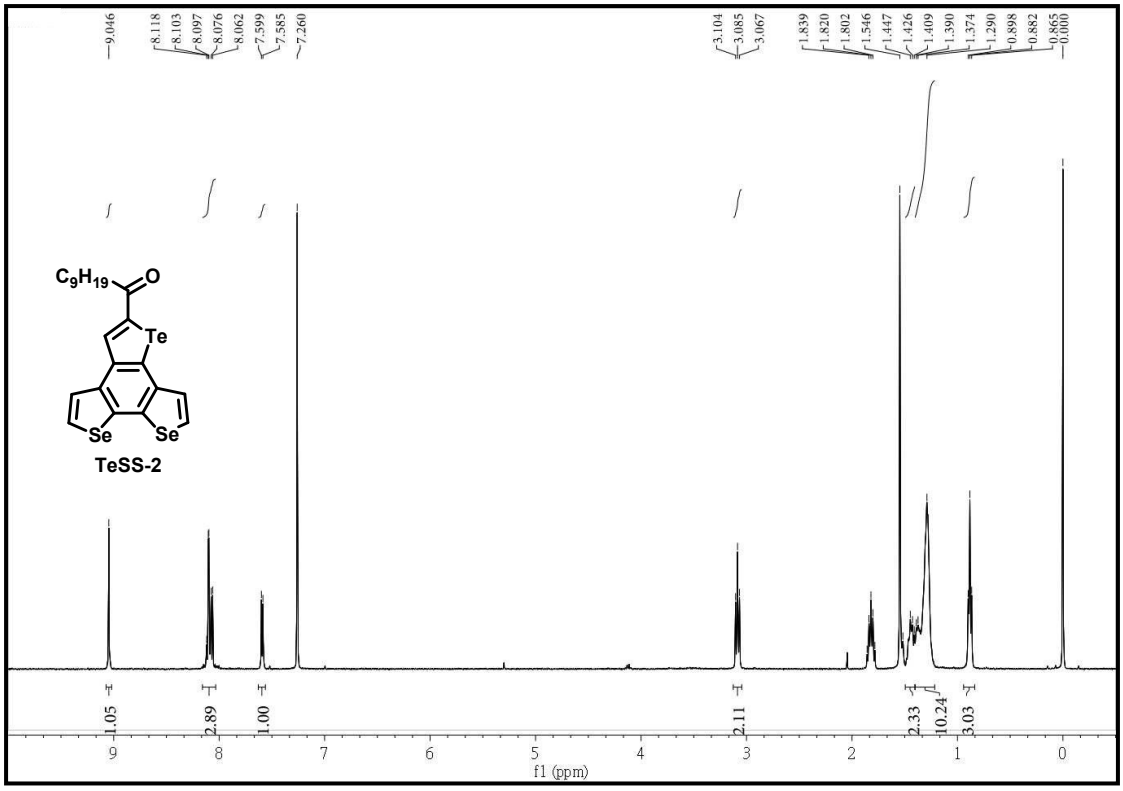
136.954
136.725
135.602
135.220
134.124
131.841
129.145
116.391
77.479
77.160
76.842
37.583
31.971
29.808
29.551
29.387
25.397
22.781
14.260
1.133
C9H19
O
Te
Br
Se
Se
1h
f1 (ppm)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8.118
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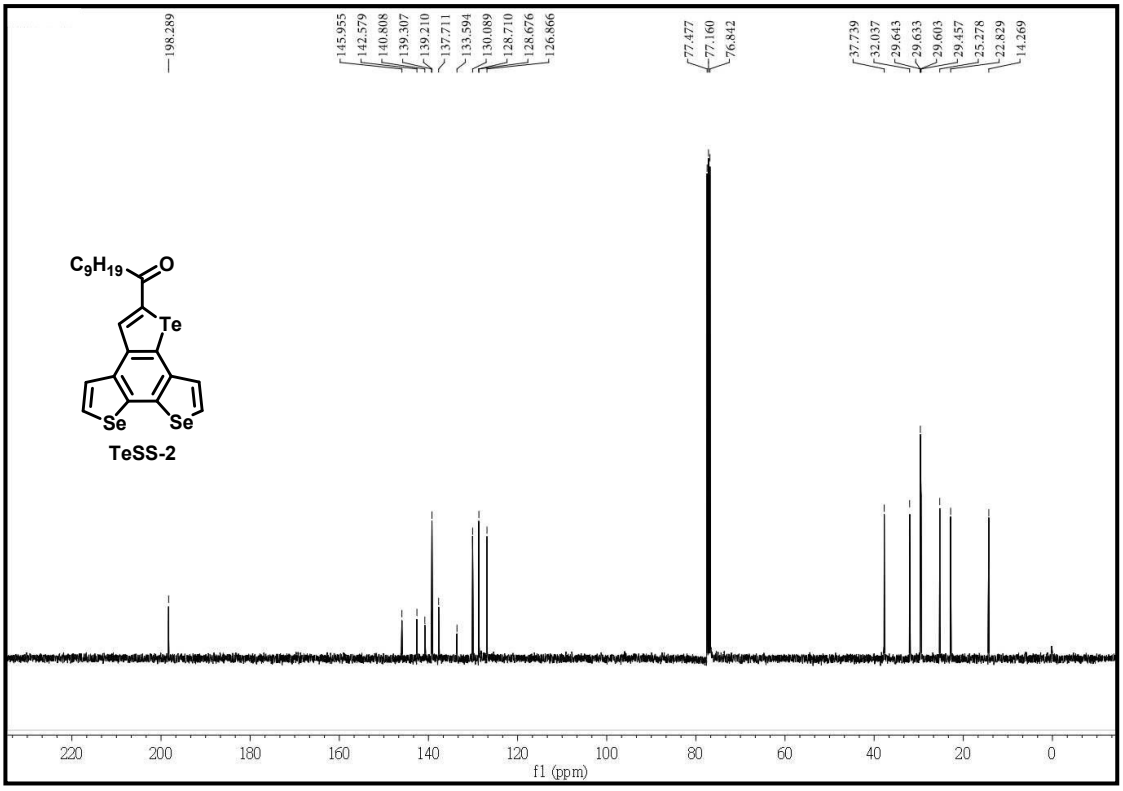
8.076
8.062
7.599
7.585
7.260
3.104
3.085
3.067
1.839
1.820
1.802
1.546
1.447
1.426
1.409
1.390
1.374
1.290
0.898
0.882
0.865
0.000
C9H19
O
Te
Se
Se
TeSS-2
1.05
2.89
1.00
2.11
2.33
10.24
3.03
f1 (ppm)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128.710
128.676
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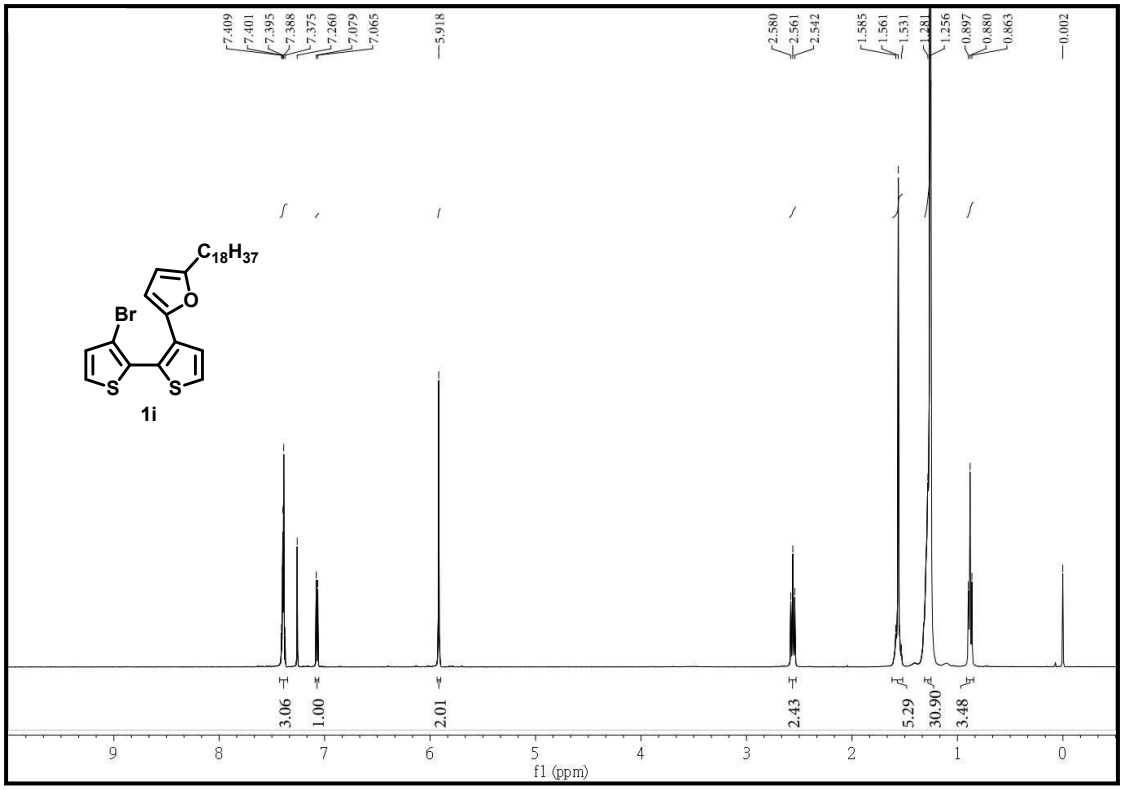
77.477
77.160
76.842
37.739
32.037
29.643
29.633
29.603
29.457
25.278
22.829
14.269
C9H19
O
Te
Se
Se
TeSS-2
f1 (ppm)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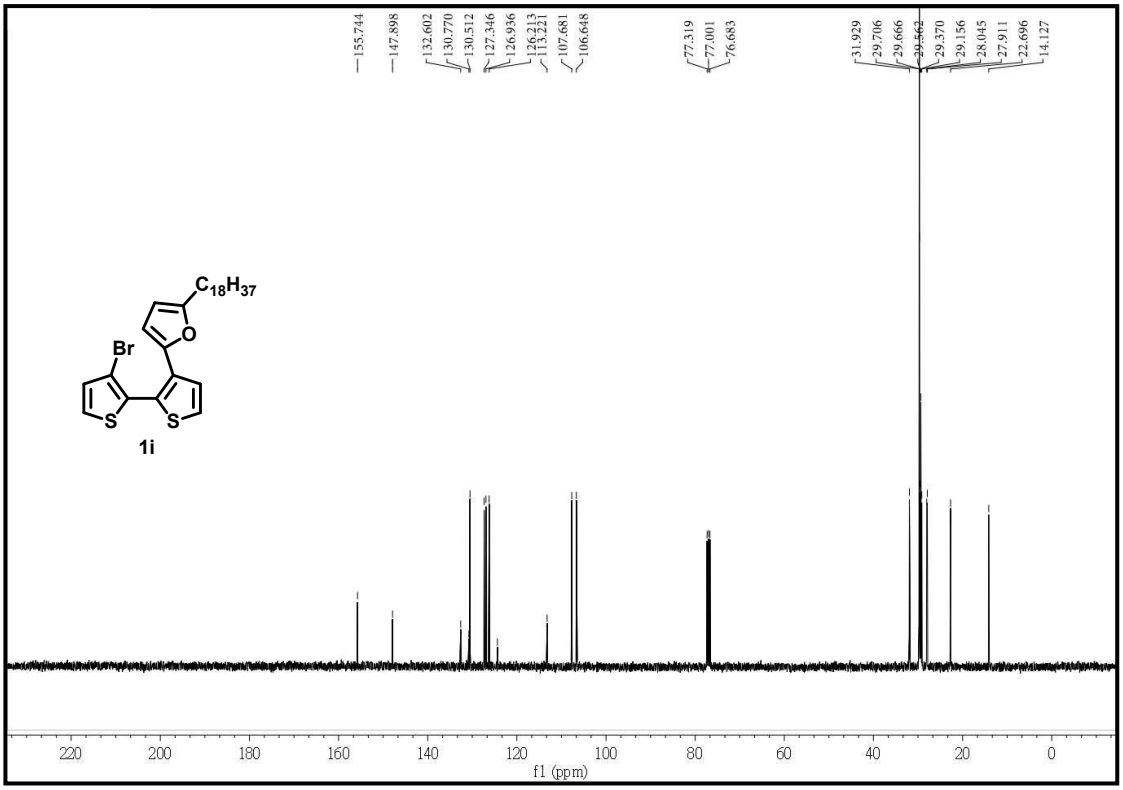
7.079
7.065
5.918
2.580
2.561
2.542
1.585
1.561
1.531
1.281
1.256
0.897
0.880
0.863
0.002
3.06
1.00
2.01
2.43
5.29
30.90
3.48
f1 (ppm)
Br
S
S
O
$C_{18}H_{37}$
1i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130.512
127.346
126.936
126.213
113.221
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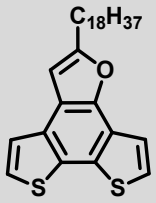
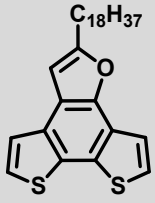
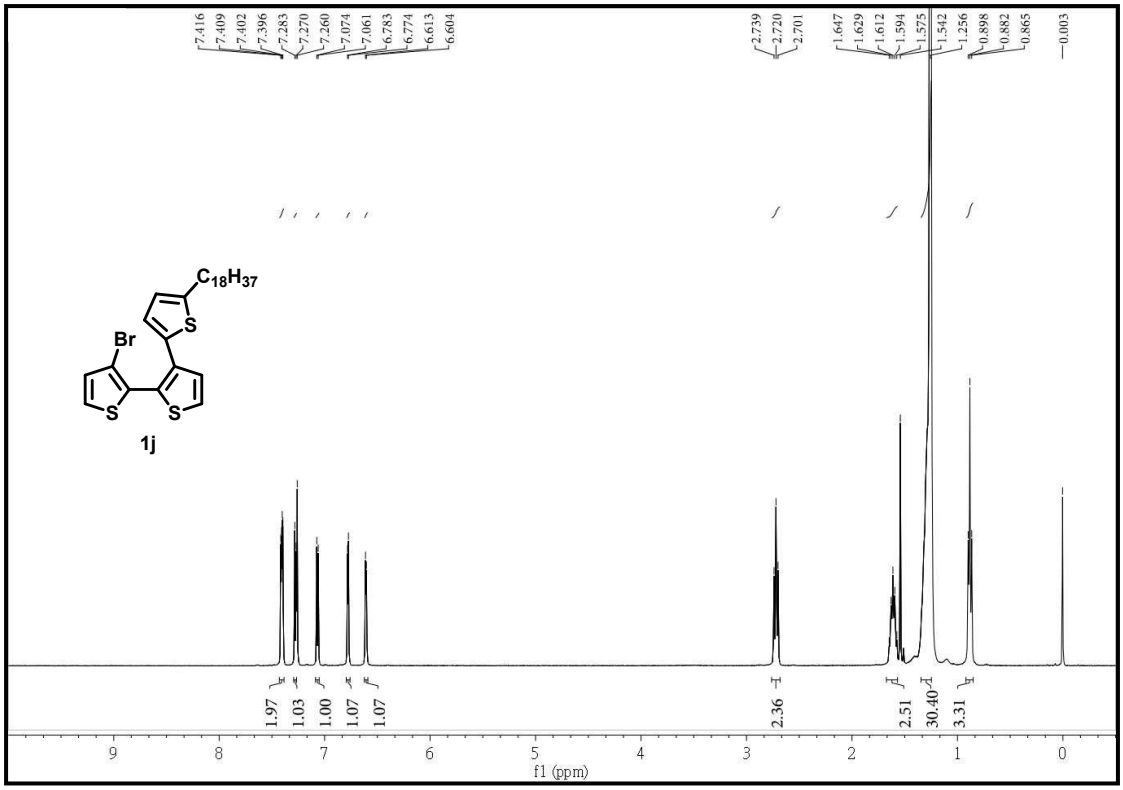
106.648
77.319
77.001
76.683
31.929
29.706
29.666
29.562
29.370
29.156
28.045
27.911
22.696
14.127
f1 (ppm)
Br
S
S
O
$C_{18}H_{37}$
1i



FTT-1



FTT-1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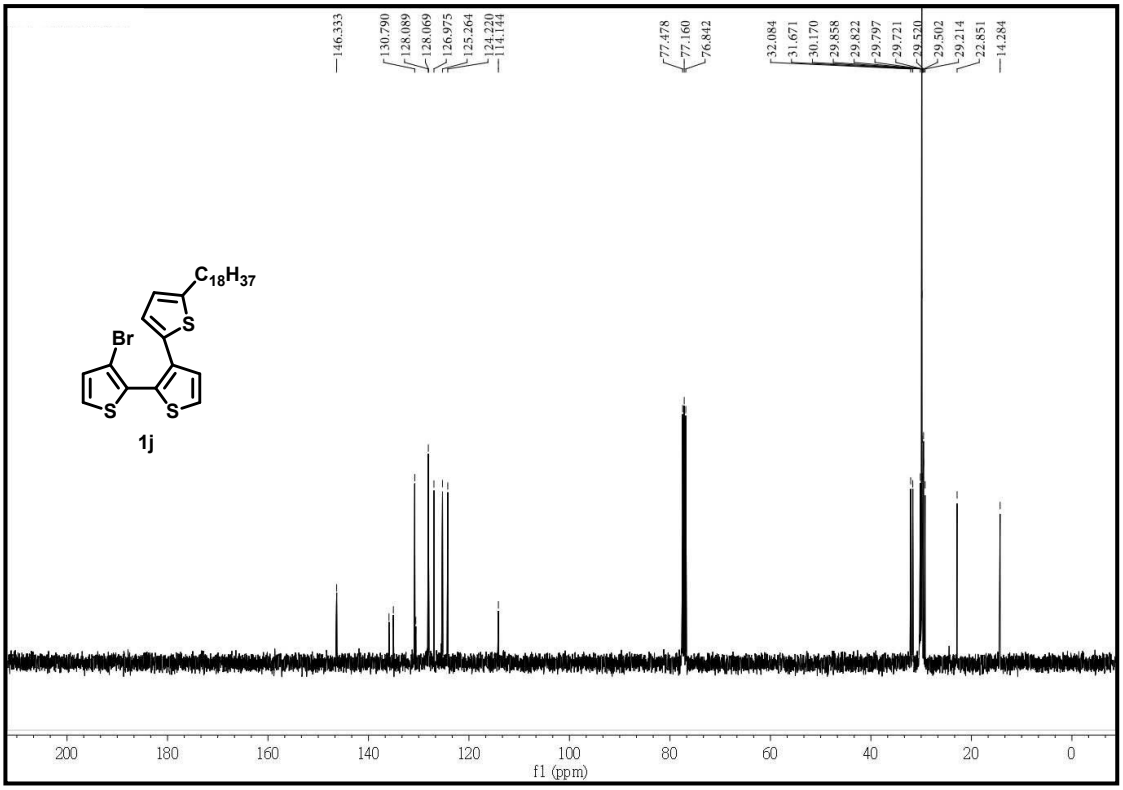
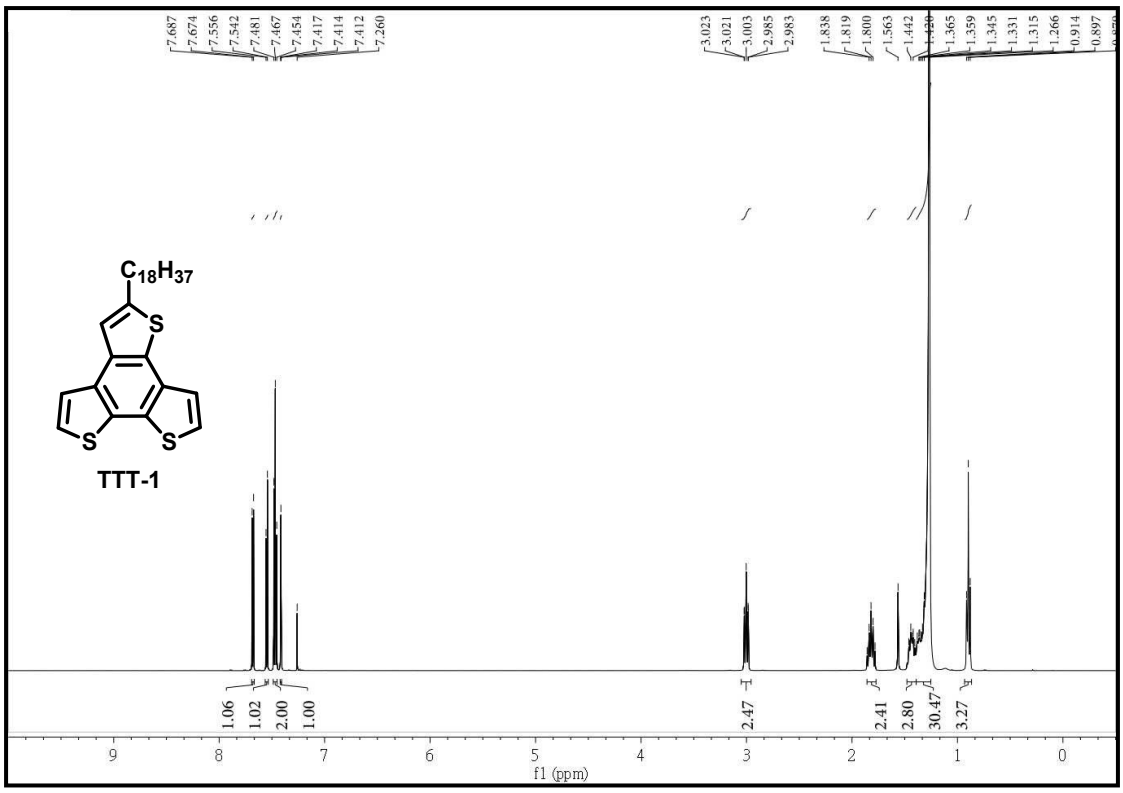
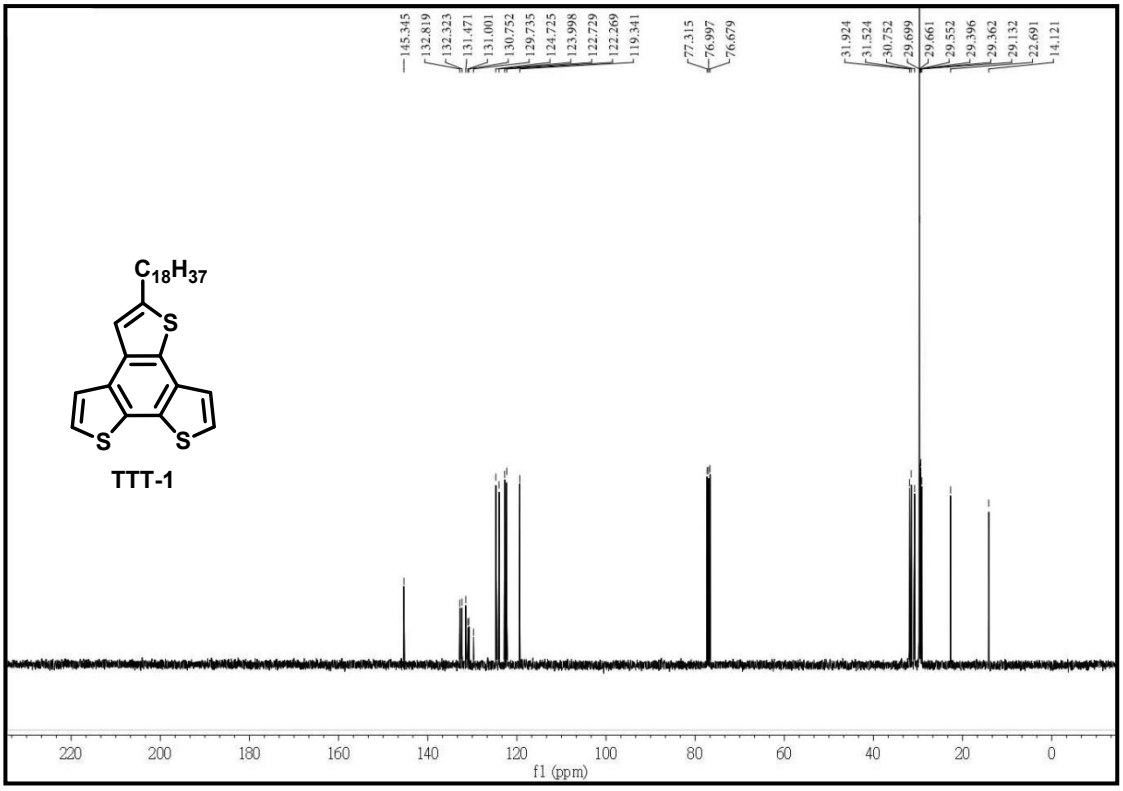
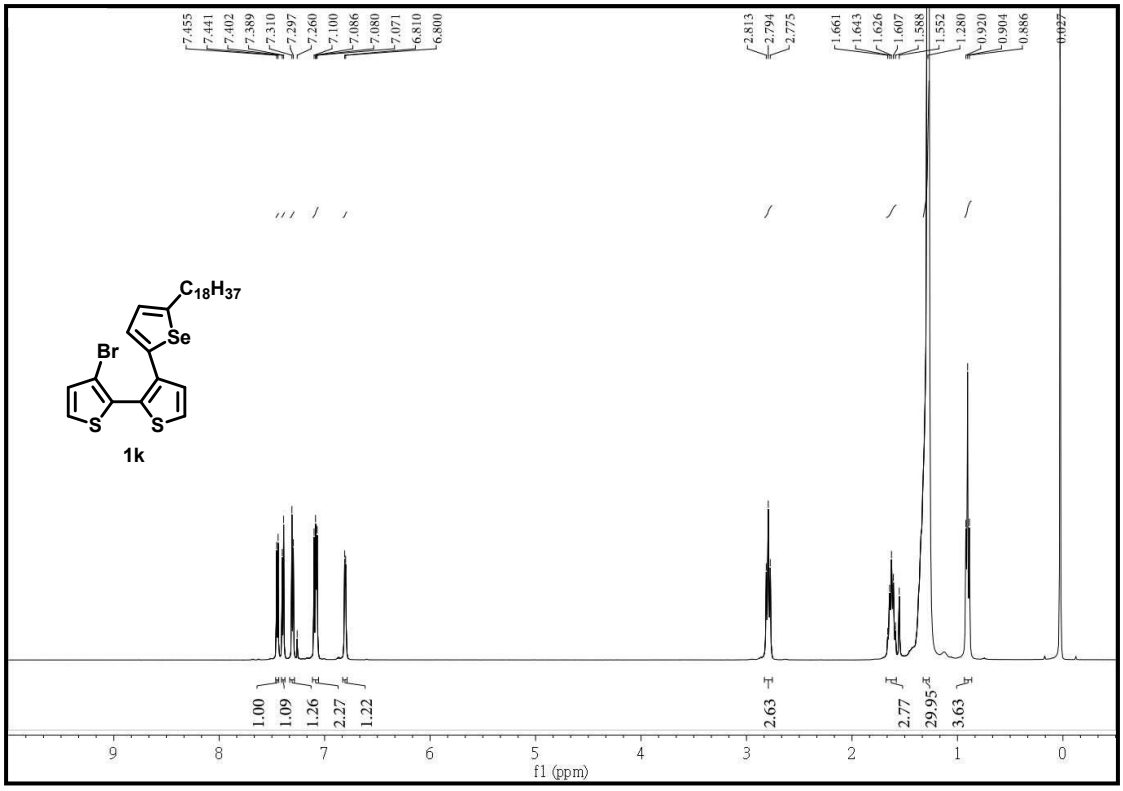
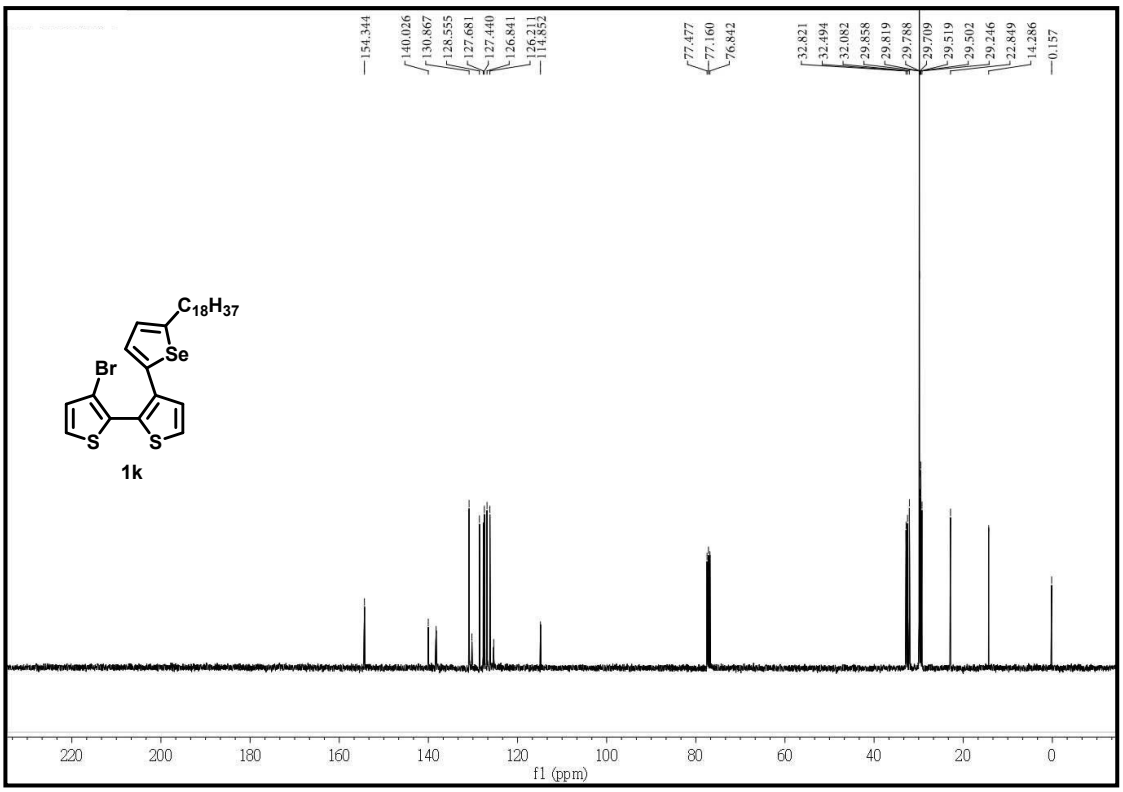
7.409
7.402
7.396
7.283
7.270
7.260
7.074
7.061
6.783
6.774
6.613
6.604
2.739
2.720
2.701
1.647
1.629
1.612
1.594
1.575
1.542
1.256
0.898
0.882
0.865
0.003
C18H37
Br
S
S
S
1j
1.97
1.03
1.00
1.07
1.07
2.36
2.51
30.40
3.31
f1 (ppm)

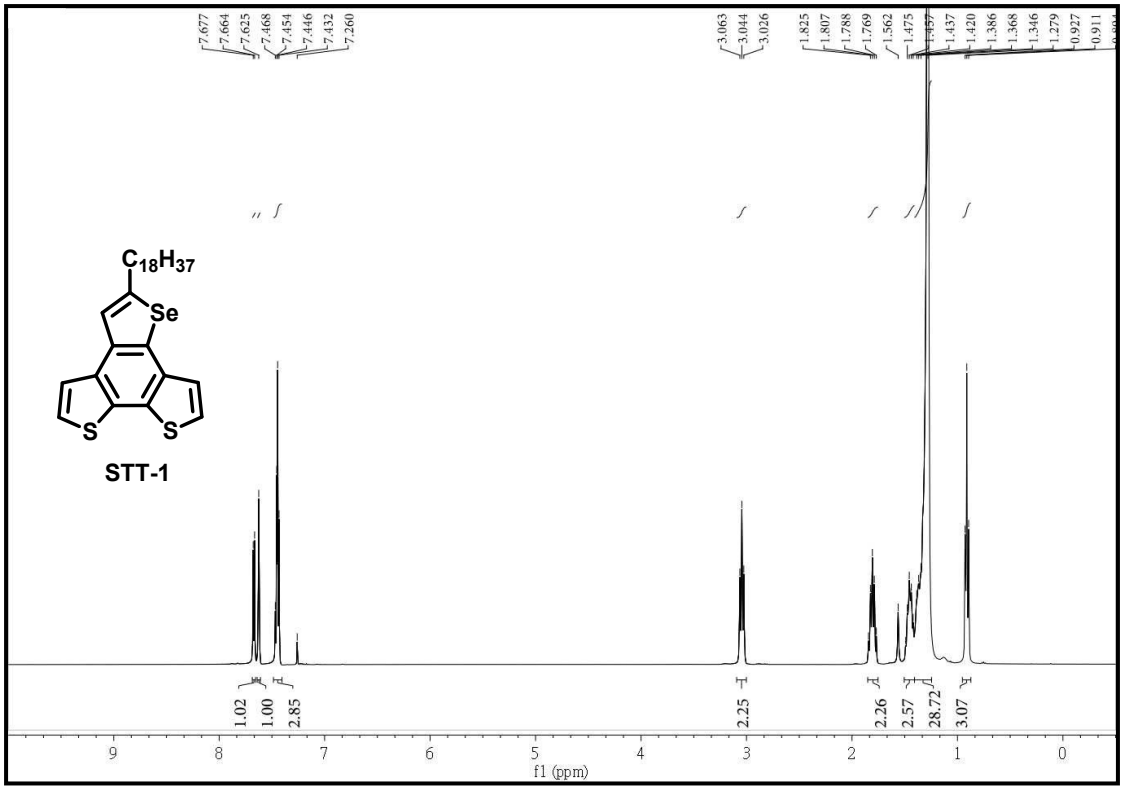

146.333
130.790
128.089
128.069
126.975
125.264
124.220
114.144
77.478
77.160
76.842
32.084
31.671
30.170
29.858
29.822
29.797
29.721
29.520
29.502
29.214
22.851
14.284
C18H37
Br
S
S
S
1j
f1 (ppm)

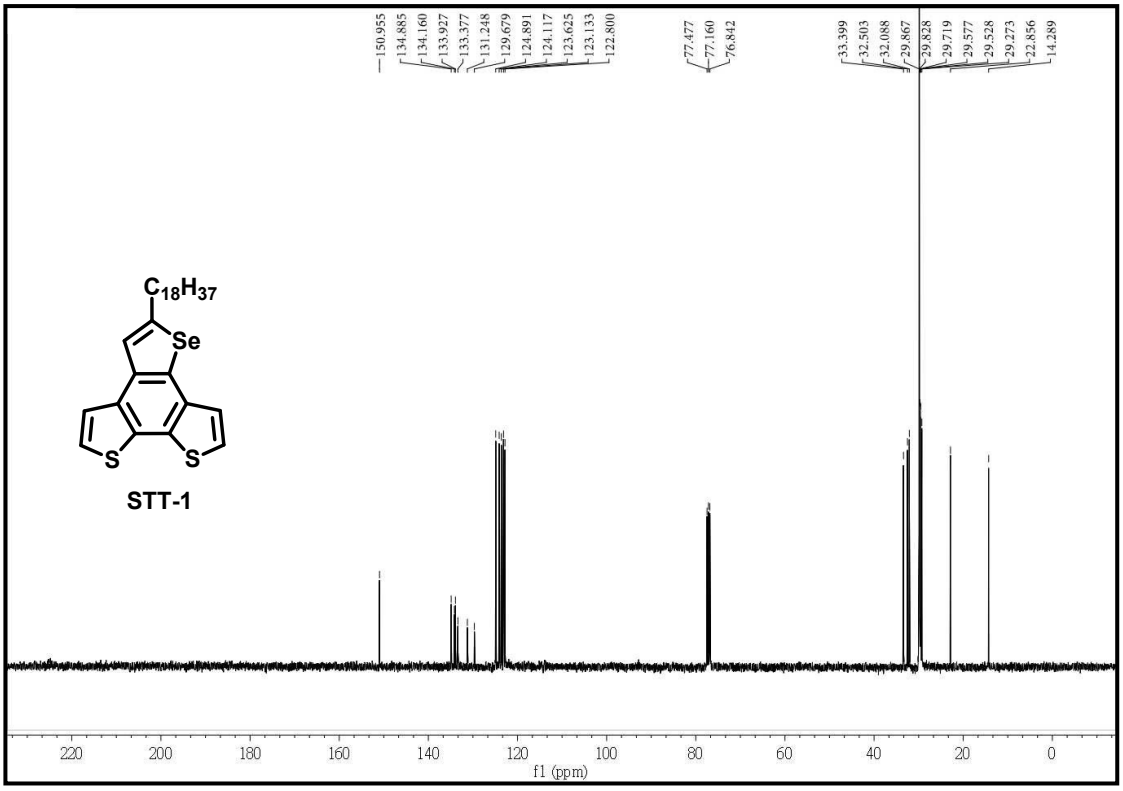

7.687
7.674
7.556
7.542
7.481
7.467
7.454
7.417
7.414
7.412
7.260
3.023
3.021
3.003
2.985
2.983
1.838
1.819
1.800
1.563
1.442
1.365
1.359
1.345
1.331
1.315
1.266
0.914
0.897
C18H37
S
S
S
TTT-1
1.06
1.02
2.00
1.00
2.47
2.41
2.80
30.47
3.27
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

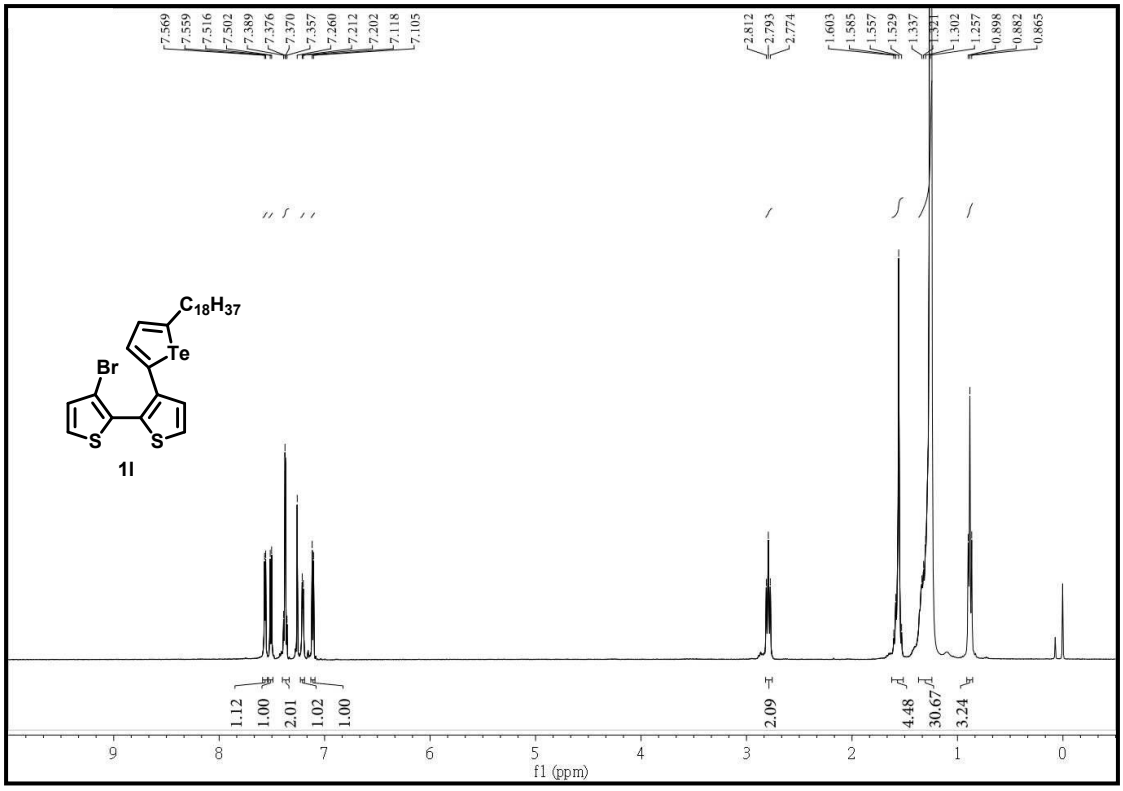

145.345
132.819
132.323
131.471
131.001
130.752
129.735
124.725
123.998
122.729
122.269
119.341
77.315
76.997
76.679
31.924
31.524
30.752
29.699
29.661
29.552
29.396
29.362
29.132
22.691
14.121
C18H37
S
S
S
TTT-1
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

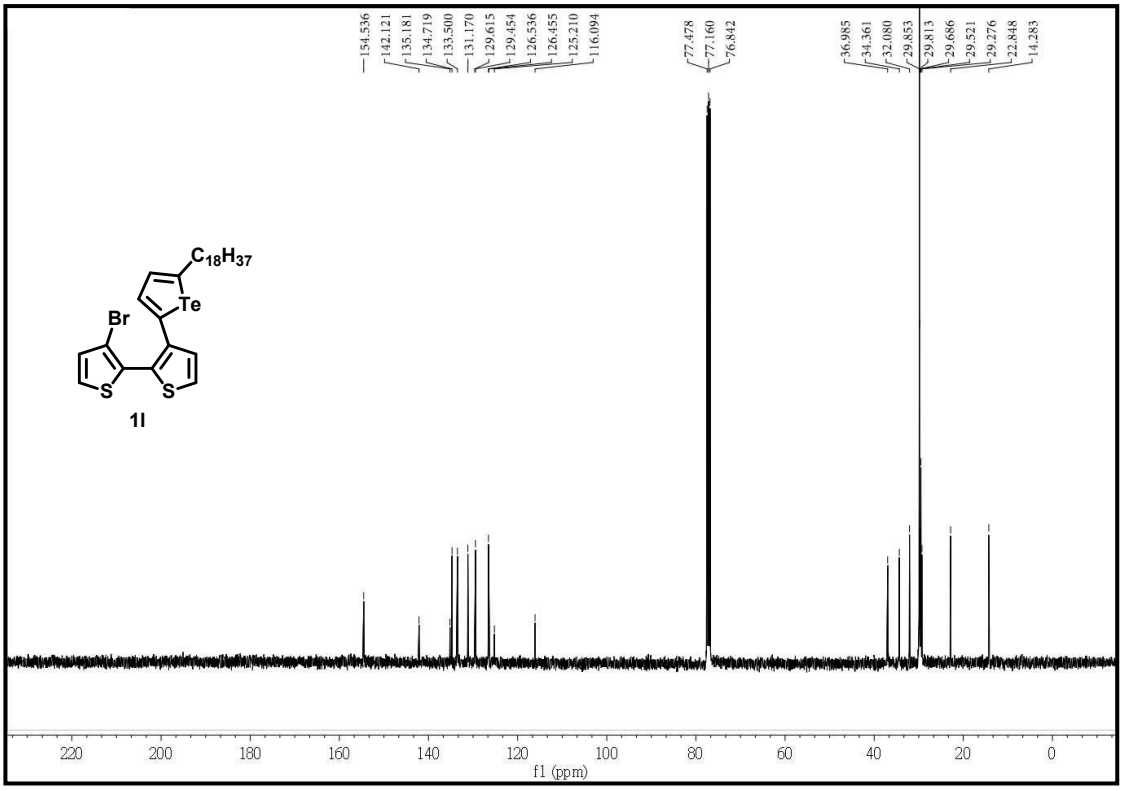

7.455
7.441
7.402
7.389
7.310
7.297
7.260
7.100
7.086
7.080
7.071
6.810
6.800
2.813
2.794
2.775
1.661
1.643
1.626
1.607
1.588
1.552
1.280
0.920
0.904
0.886
0.027
C18H37
Se
Br
S
S
1k
1.00
1.09
1.26
2.27
1.22
2.63
2.77
29.95
3.63
f1 (ppm)

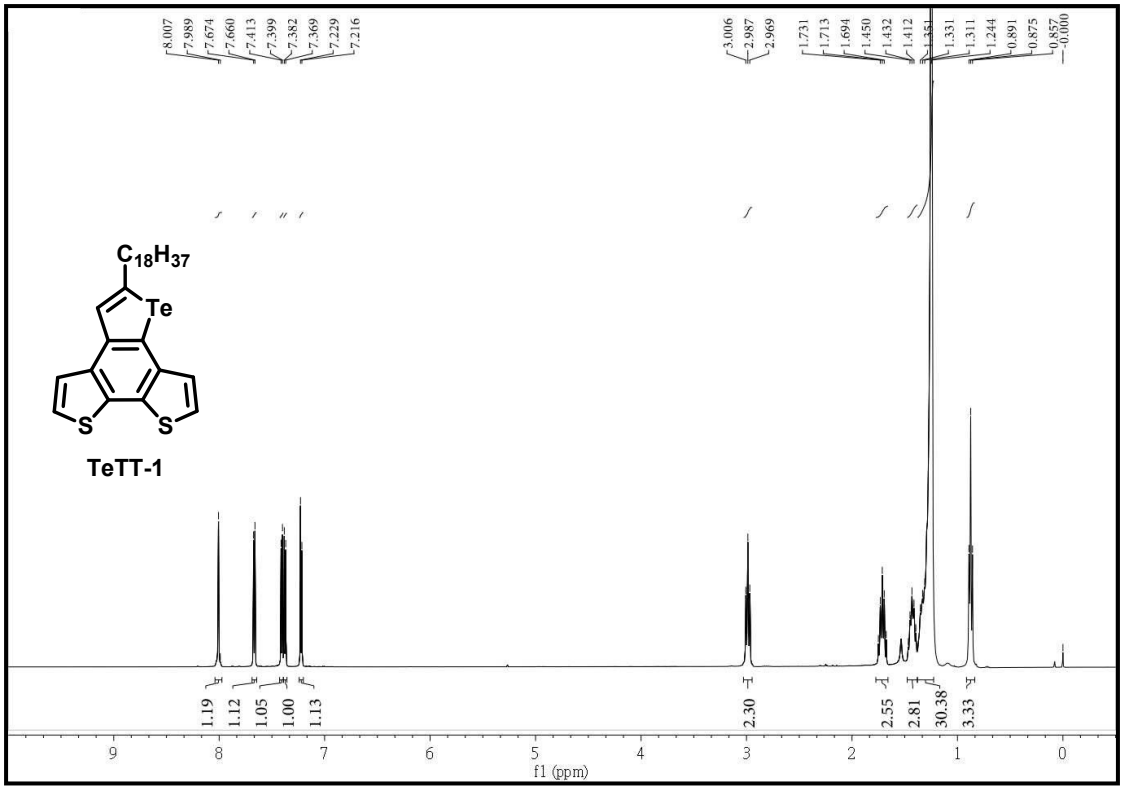

154.344
140.026
130.867
128.555
127.681
127.440
126.841
126.211
114.852
77.477
77.160
76.842
32.821
32.494
32.082
29.858
29.819
29.788
29.709
29.519
29.502
29.246
22.849
14.286
0.157
C18H37
Se
Br
S
S
1k
f1 (ppm)


7.677
7.664
7.625
7.468
7.454
7.446
7.432
7.260
3.063
3.044
3.026
1.825
1.807
1.788
1.769
1.562
1.475
1.437
1.420
1.386
1.368
1.346
1.279
0.927
0.911
C18H37
Se
S
S
STT-1
1.02
1.00
2.85
2.25
2.26
2.57
28.72
3.07
f1 (ppm)


150.955
134.885
134.160
133.927
133.377
131.248
129.679
124.891
124.117
123.625
123.133
122.800
77.477
77.160
76.842
33.399
32.503
32.088
29.867
29.828
29.719
29.577
29.528
29.273
22.856
14.289
C18H37
Se
S
S
STT-1
f1 (ppm)


7.569
7.559
7.516
7.502
7.389
7.376
7.370
7.357
7.260
7.212
7.202
7.118
7.105
2.812
2.793
2.774
1.603
1.585
1.557
1.529
1.337
1.321
1.302
1.257
0.898
0.882
0.865
C18H37
Te
Br
S
S
1l
1.12
1.00
2.01
1.02
1.00
2.09
4.48
30.67
3.24
f1 (ppm)


154.536
142.121
135.181
134.719
133.500
131.170
129.615
129.454
126.536
126.455
125.210
116.094
77.478
77.160
76.842
36.985
34.361
32.080
29.853
29.813
29.686
29.521
29.276
22.848
14.283
C18H37
Te
Br
S
S
1l
f1 (ppm)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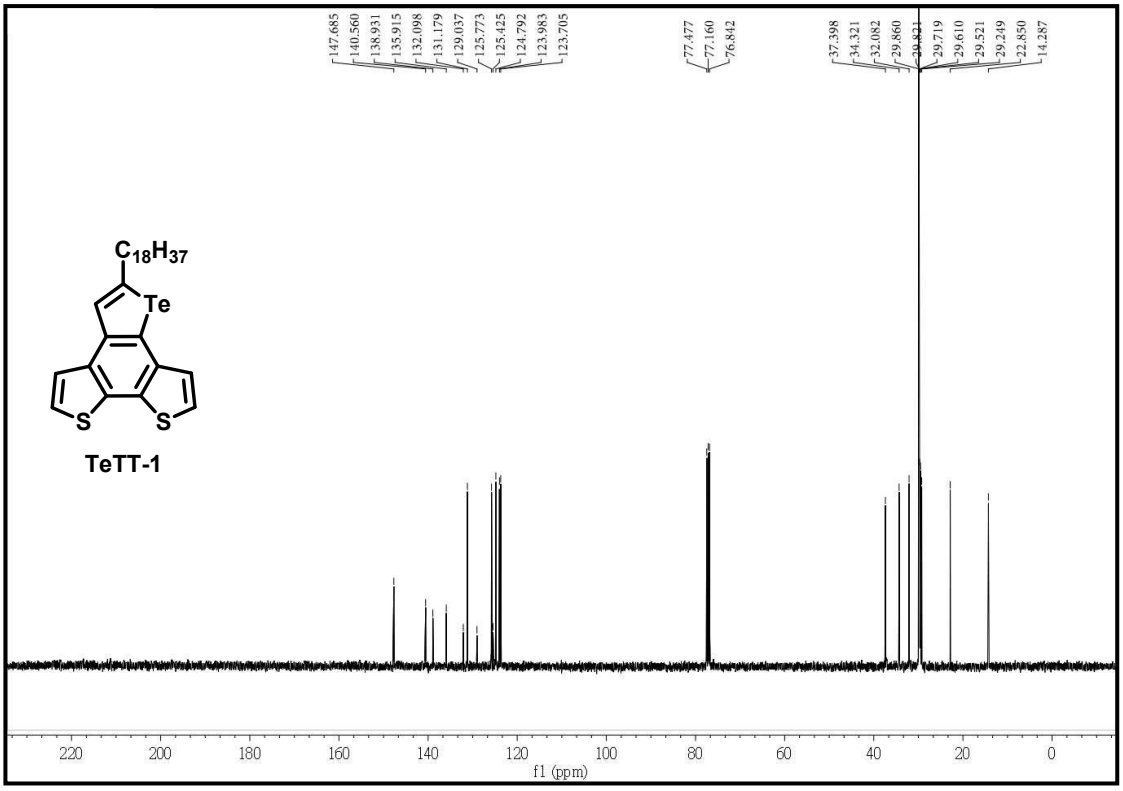
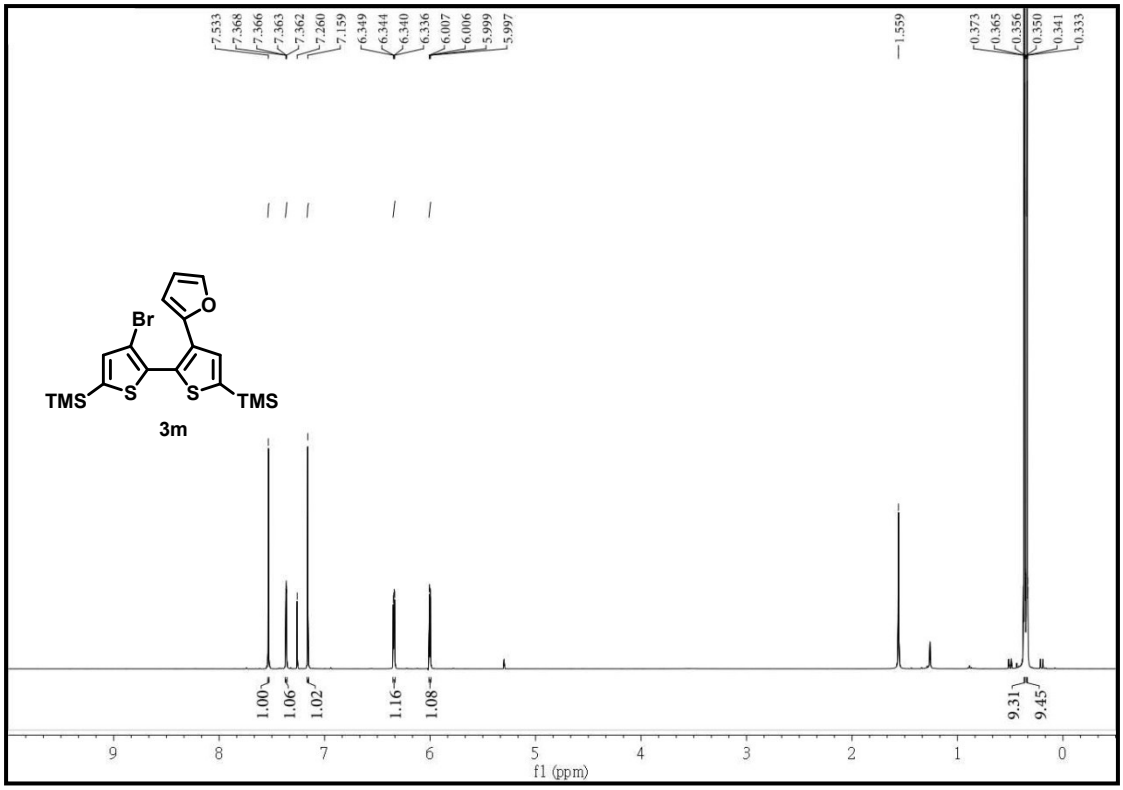
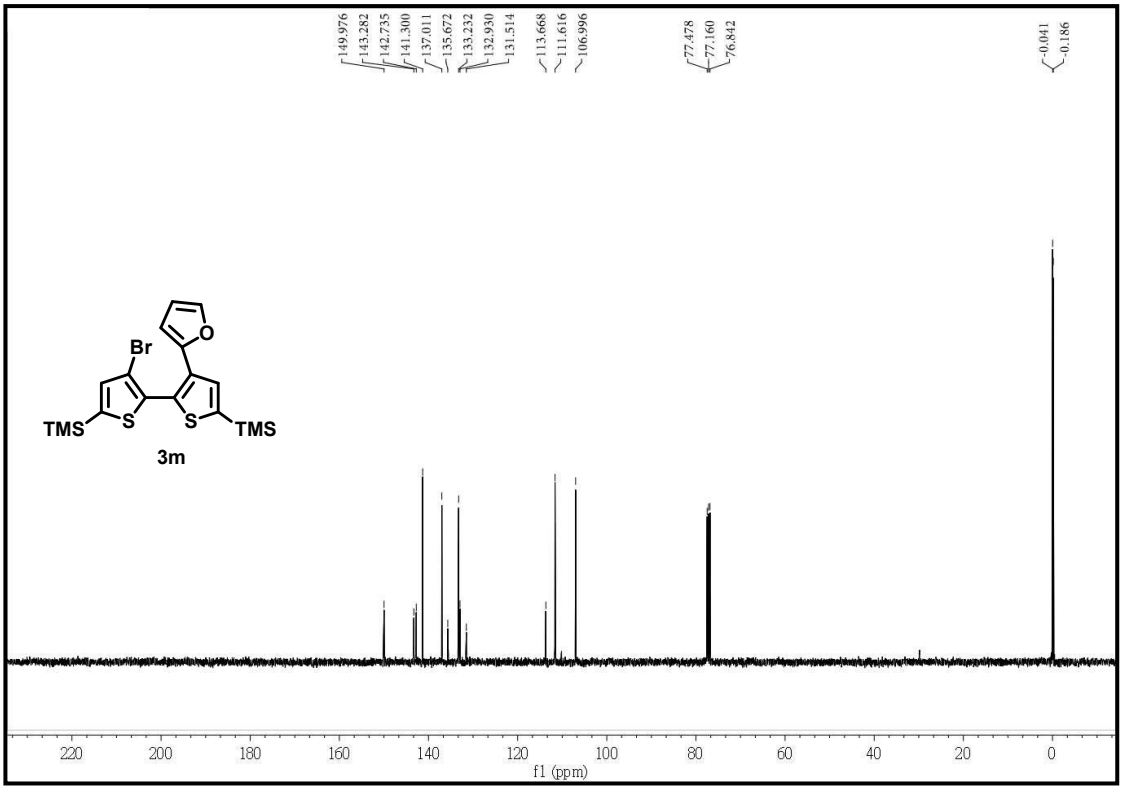
7.989
7.674
7.660
7.413
7.399
7.382
7.369
7.229
7.216
3.006
2.987
2.969
1.731
1.713
1.694
1.450
1.432
1.412
1.331
1.311
1.244
0.891
0.875
0.857
-0.000
C18H37
Te
S
S
TeTT-1
1.19
1.12
1.05
1.00
1.13
2.30
2.55
2.81
30.38
3.33
f1 (ppm)


147.685
140.560
138.931
135.915
132.098
131.179
129.037
125.773
125.425
124.792
123.983
123.705
77.477
77.160
76.842
37.398
34.321
32.082
29.860
29.821
29.719
29.610
29.521
29.249
22.850
14.287
C18H37
Te
S
S
TeTT-1
f1 (ppm)


7.533
7.368
7.366
7.363
7.362
7.260
7.159
6.349
6.344
6.340
6.336
6.007
6.006
5.999
5.997
1.559
0.373
0.365
0.356
0.350
0.341
0.333
Br
O
S
S
TMS
TMS
3m
1.00
1.06
1.02
1.16
1.08
9.31
9.45
f1 (ppm)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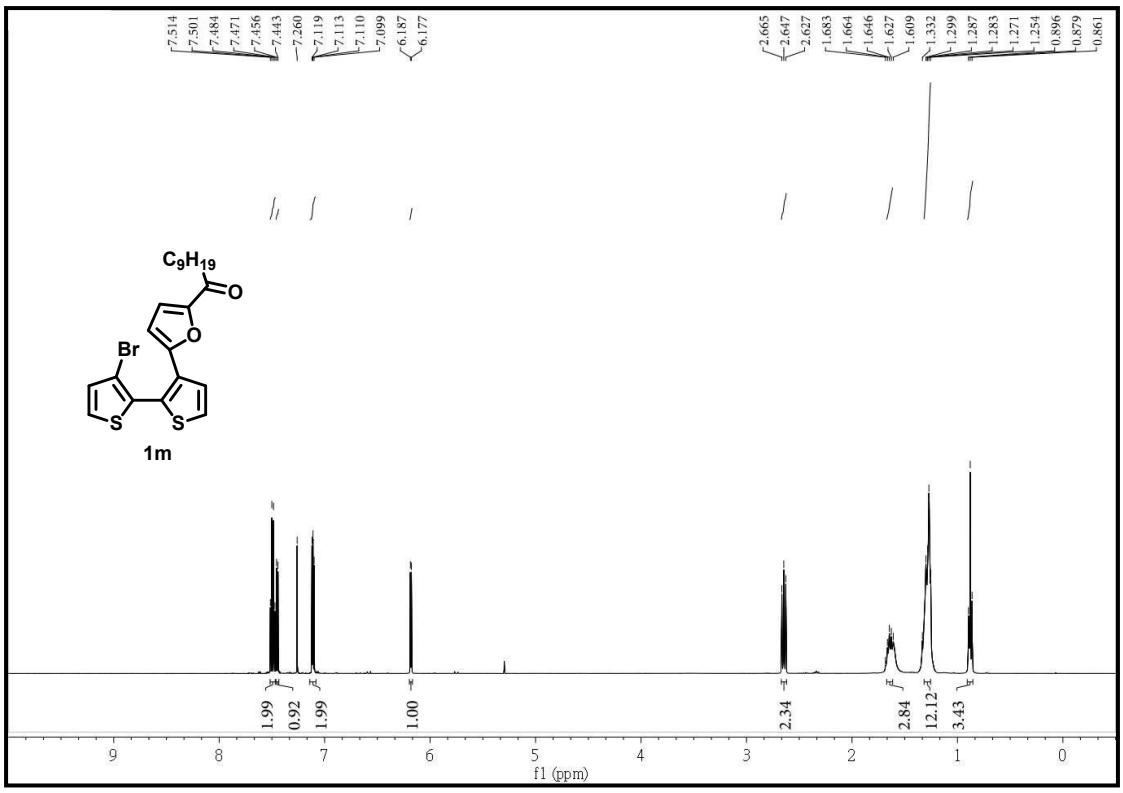
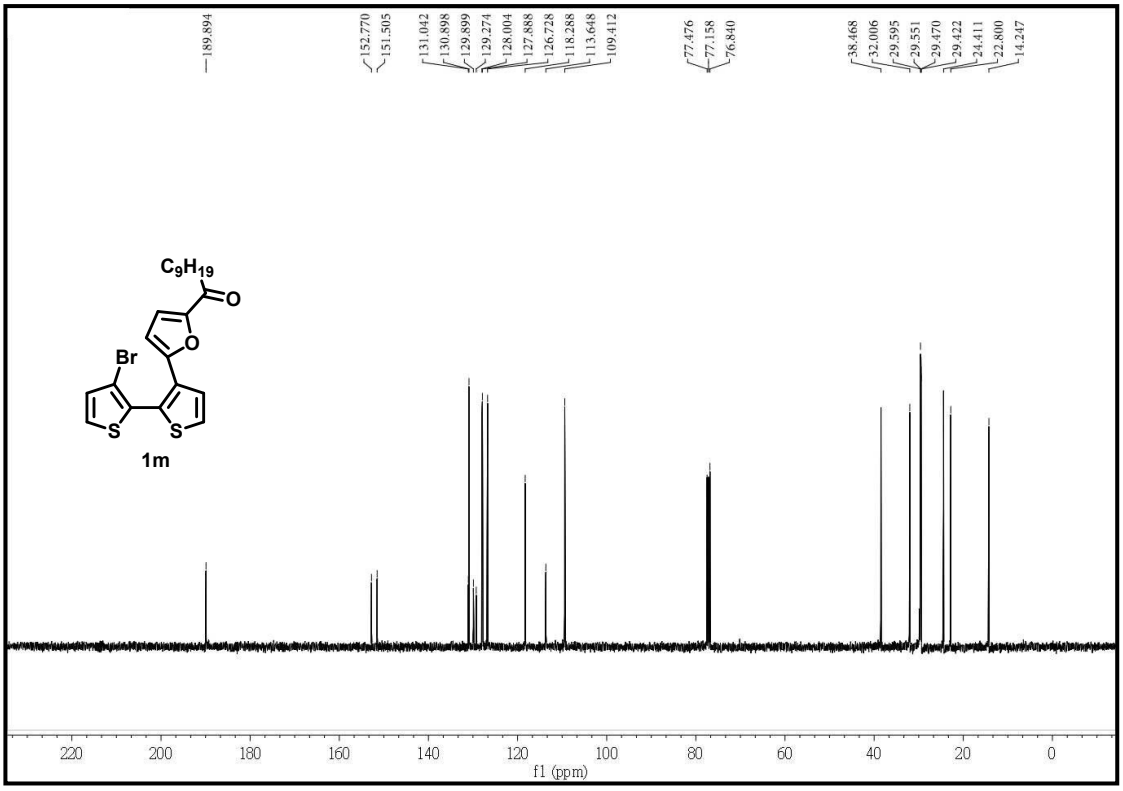
142.735
141.300
137.011
135.672
133.232
132.930
131.514
113.668
111.616
106.996
77.478
77.160
76.842
-0.041
-0.186
Br
O
S
S
TMS
TMS
3m
f1 (ppm)


7.514
7.501
7.484
7.471
7.456
7.443
7.260
7.119
7.113
7.110
7.099
6.187
6.177
2.665
2.647
2.627
1.683
1.664
1.646
1.627
1.609
1.332
1.299
1.287
1.283
1.271
1.254
0.896
0.879
0.861
C9H19
O
O
Br
S
S
1m
1.99
0.92
1.99
1.00
2.34
2.84
12.12
3.43
f1 (ppm)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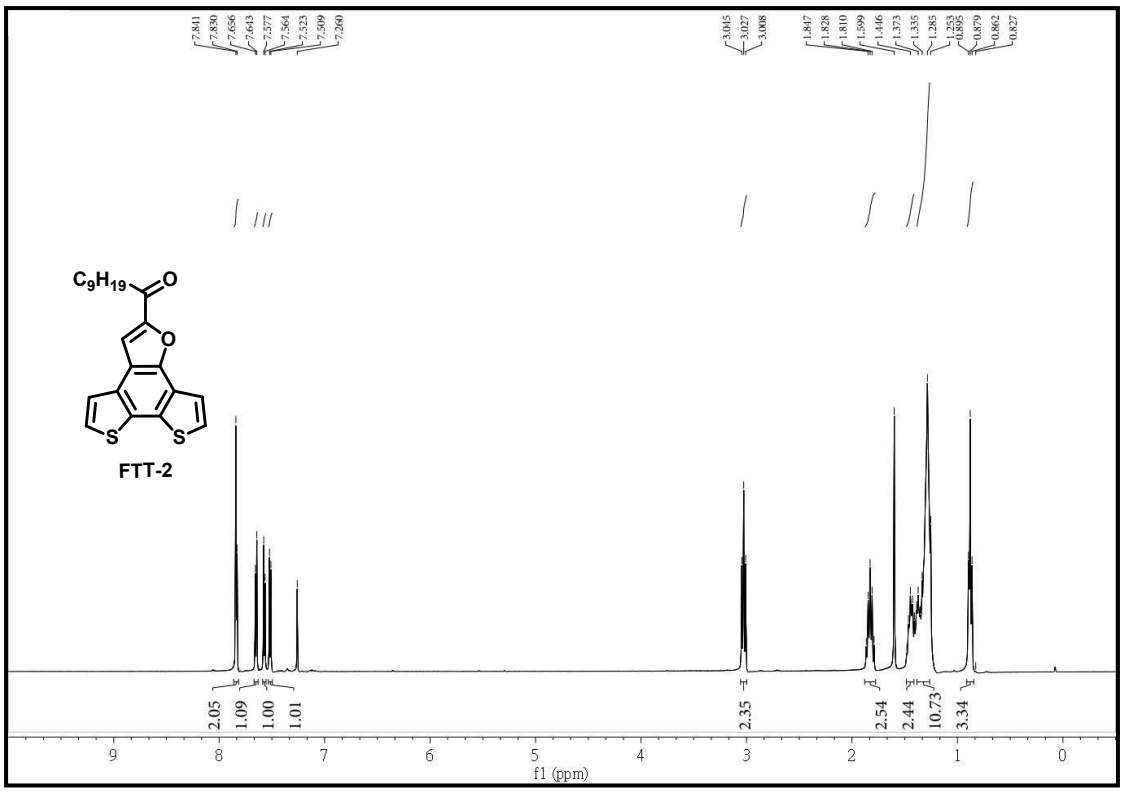
152.770
151.505
131.042
130.898
129.899
129.274
128.004
127.888
126.728
118.288
113.648
109.412
77.476
77.158
76.840
38.468
32.006
29.595
29.551
29.470
29.422
24.411
22.800
14.247
C9H19
O
O
Br
S
S
1m
f1 (ppm)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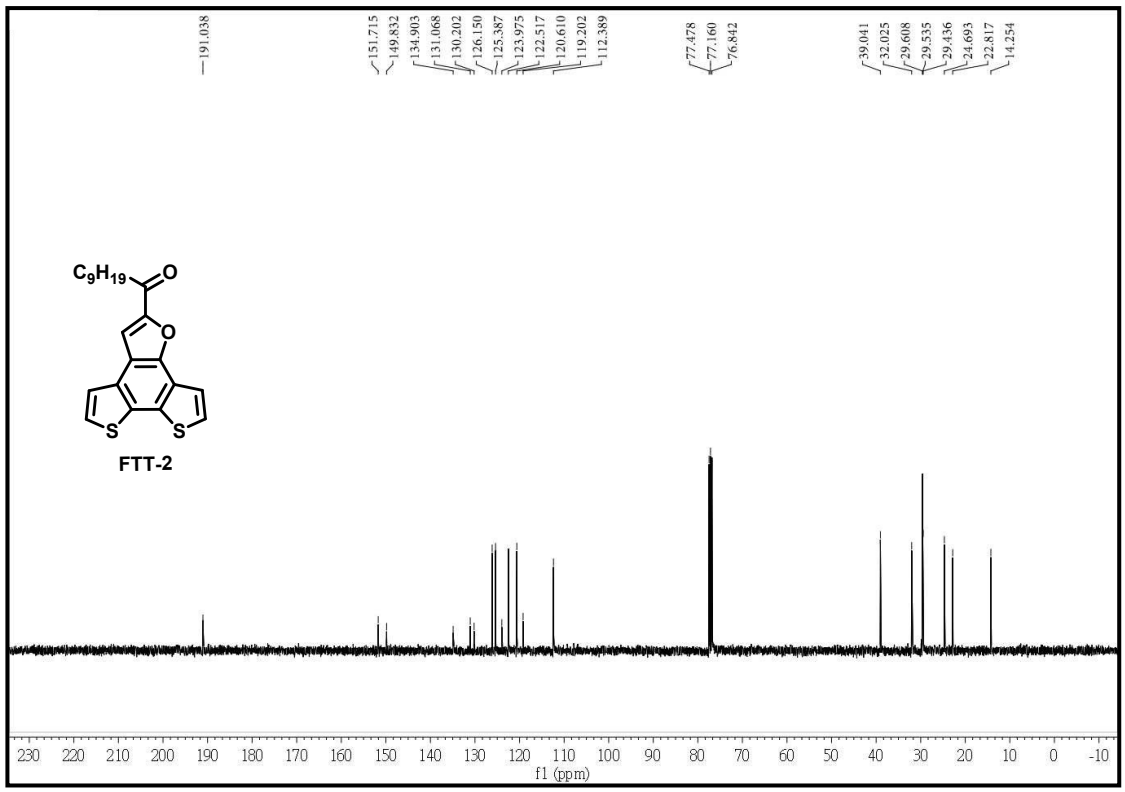
7.830
7.656
7.643
7.577
7.564
7.523
7.509
7.260
3.045
3.027
3.008
1.847
1.828
1.810
1.599
1.446
1.373
1.335
1.285
1.253
0.895
0.879
0.862
0.827
C9H19
O
O
S
S
FTT-2
2.05
1.09
1.00
1.01
2.35
2.54
2.44
10.73
3.34
f1 (ppm)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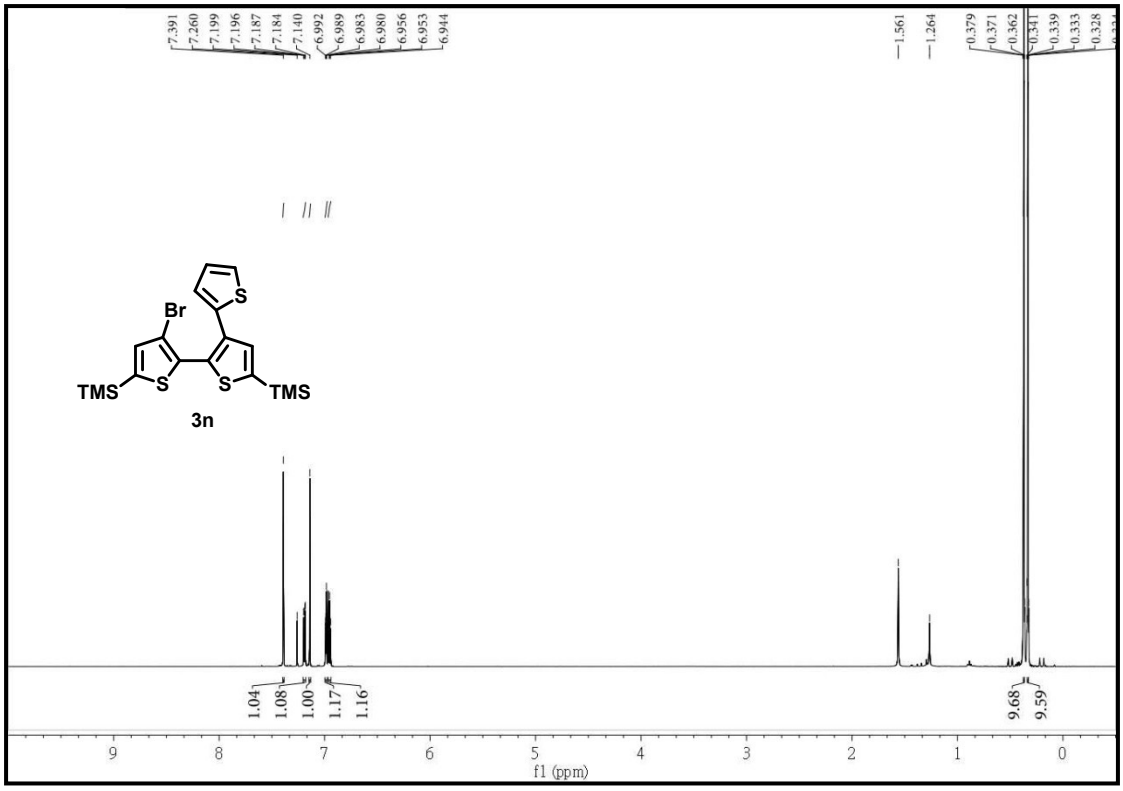
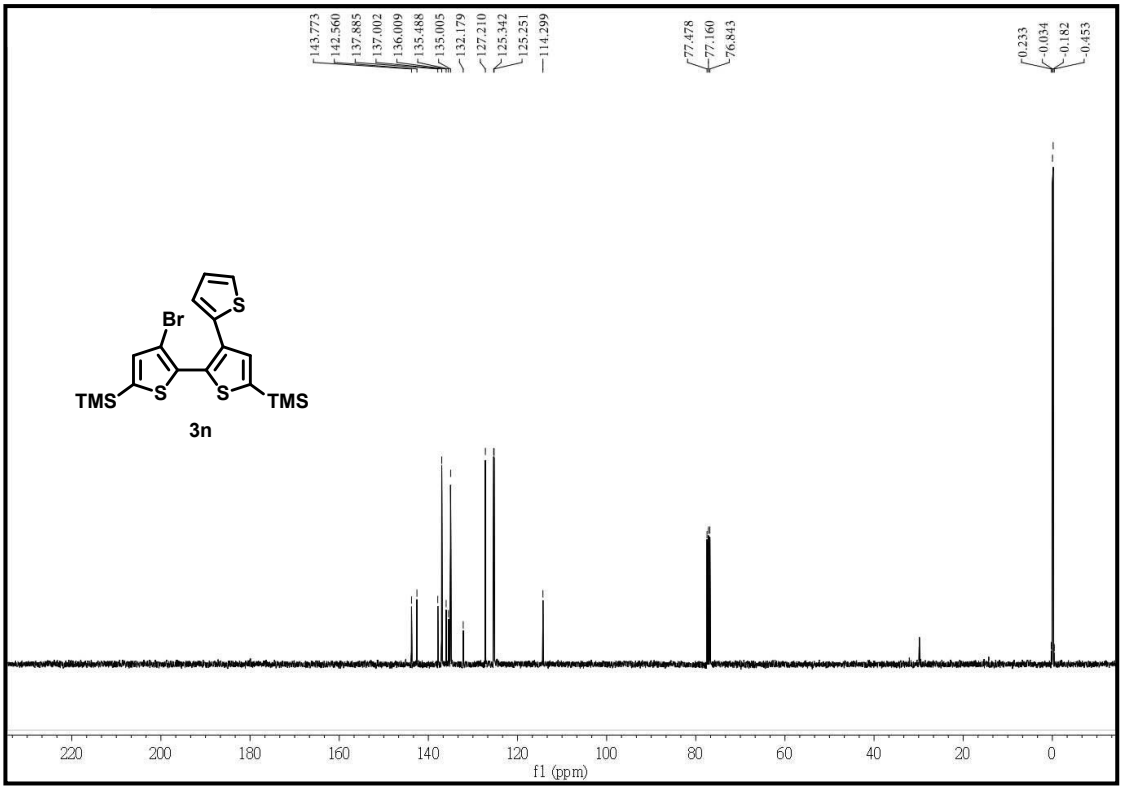
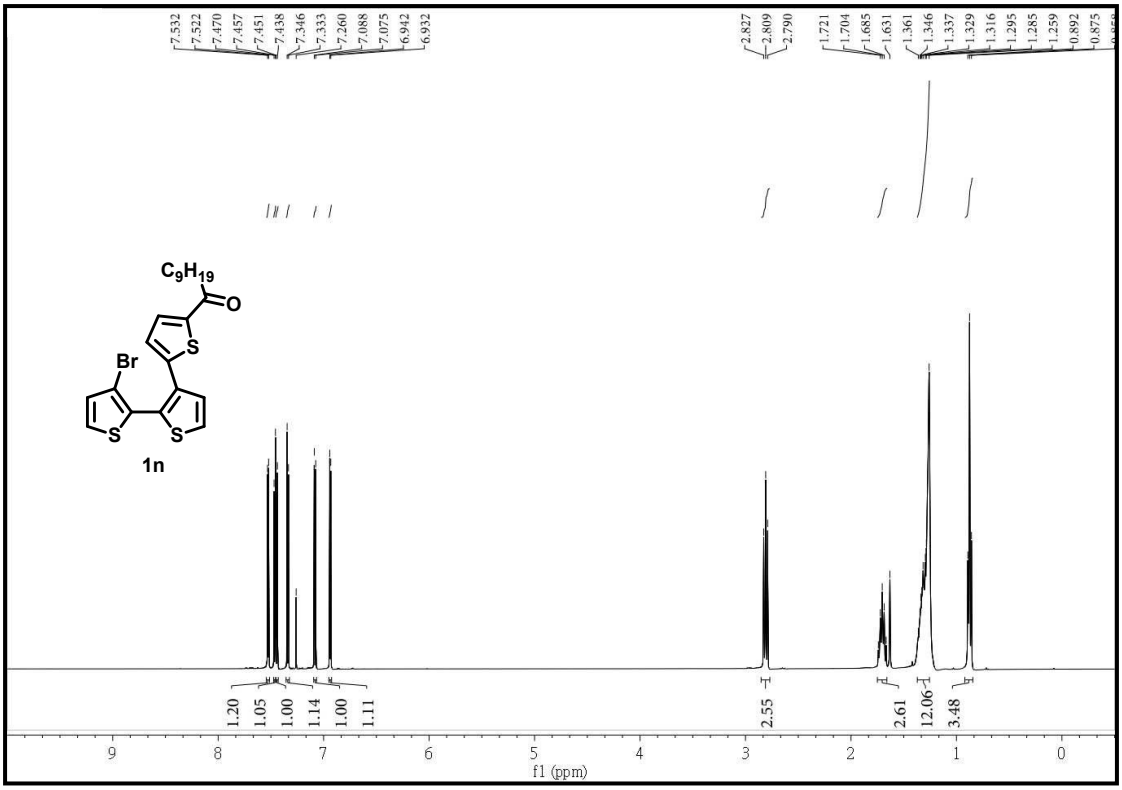
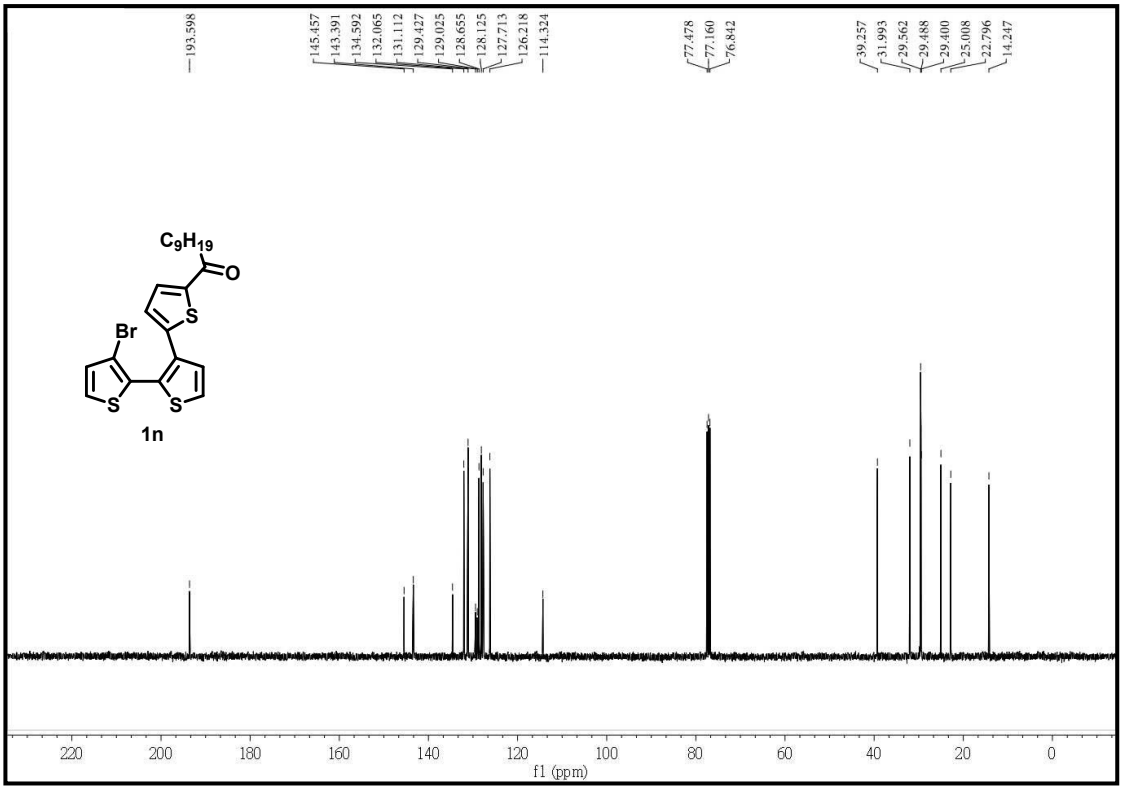
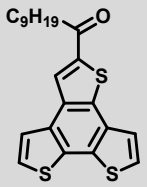
151.715
149.832
134.903
131.068
130.202
126.150
125.387
123.975
122.517
120.610
119.202
112.389
77.478
77.160
76.842
39.041
32.025
29.608
29.535
29.436
24.693
22.817
14.254
C9H19
O
O
S
S
FTT-2
f1 (ppm)


7.391
7.260
7.199
7.196
7.187
7.184
7.140
6.992
6.989
6.983
6.980
6.956
6.953
6.944
1.561
1.264
0.379
0.371
0.362
0.341
0.339
0.333
0.328
Br
S
TMS
S
S
TMS
3n
1.04
1.08
1.00
1.17
1.16
9.68
9.59
f1 (ppm)

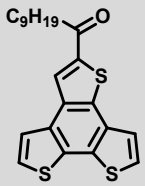

143.773
142.560
137.885
137.002
136.009
135.488
135.005
132.179
127.210
125.342
125.251
114.299
77.478
77.160
76.843
0.233
-0.034
-0.182
-0.453
Br
S
TMS
S
S
TMS
3n
f1 (ppm)


7.532
7.522
7.470
7.457
7.451
7.438
7.346
7.333
7.260
7.088
7.075
6.942
6.932
2.827
2.809
2.790
1.721
1.704
1.685
1.651
1.361
1.346
1.337
1.329
1.316
1.295
1.285
1.259
0.892
0.875
C9H19
O
S
Br
S
S
1n
1.20
1.05
1.00
1.14
1.00
1.11
2.55
2.61
12.06
3.48
f1 (ppm)

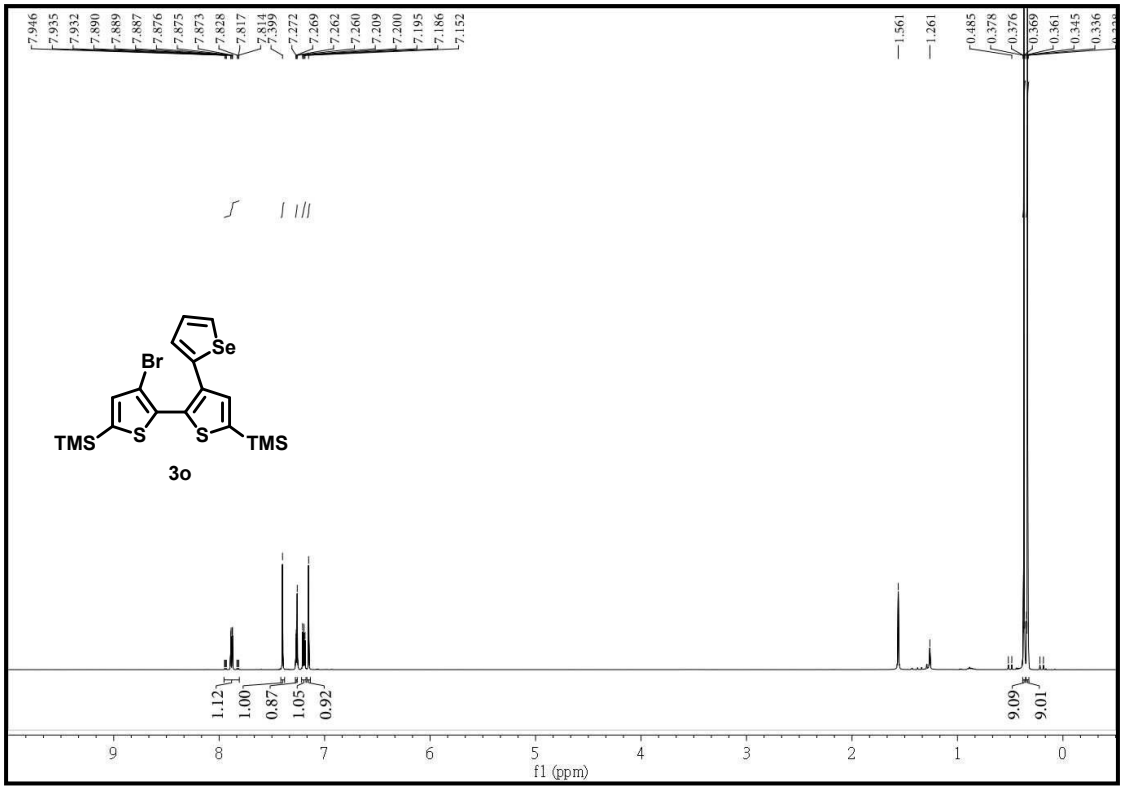

193.598
145.457
143.391
134.592
132.065
131.112
129.427
129.025
128.655
128.125
127.713
126.218
114.324
77.478
77.160
76.842
39.257
31.993
29.562
29.488
29.400
25.008
22.796
14.247
C9H19
O
S
Br
S
S
1n
f1 (ppm)

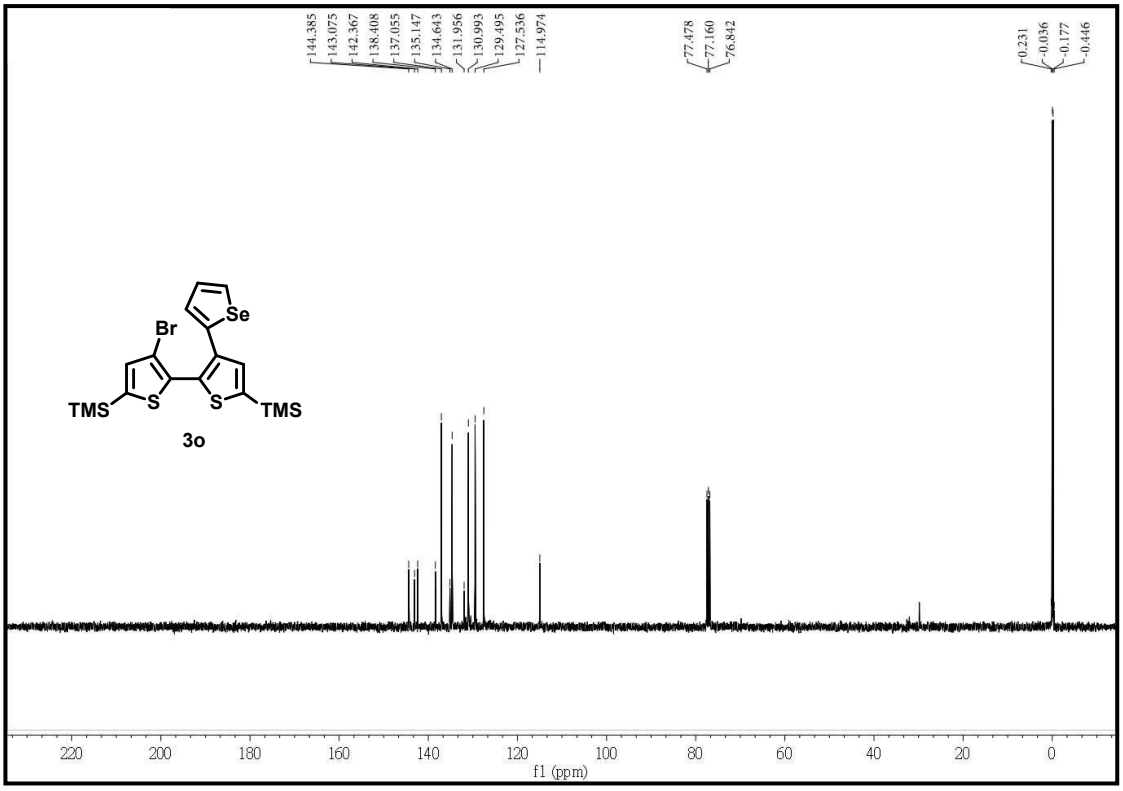


TTT-2



TTT-2


7.946
7.935
7.932
7.890
7.889
7.887
7.876
7.875
7.873
7.828
7.817
7.814
7.399
7.272
7.269
7.262
7.260
7.209
7.200
7.195
7.186
7.152
1.561
1.261
0.485
0.378
0.376
0.369
0.361
0.345
0.336
Br
Se
TMS
S
S
TMS
3o
1.12
1.00
0.87
1.05
0.92
9.09
9.01
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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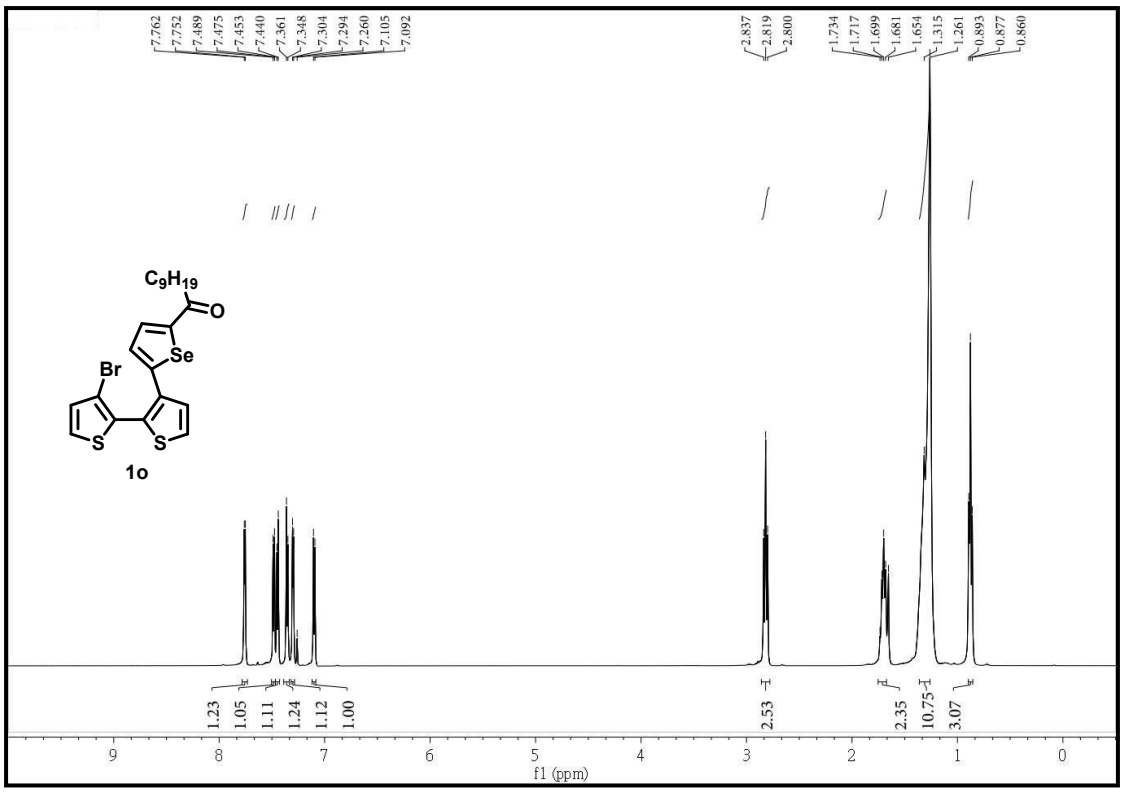
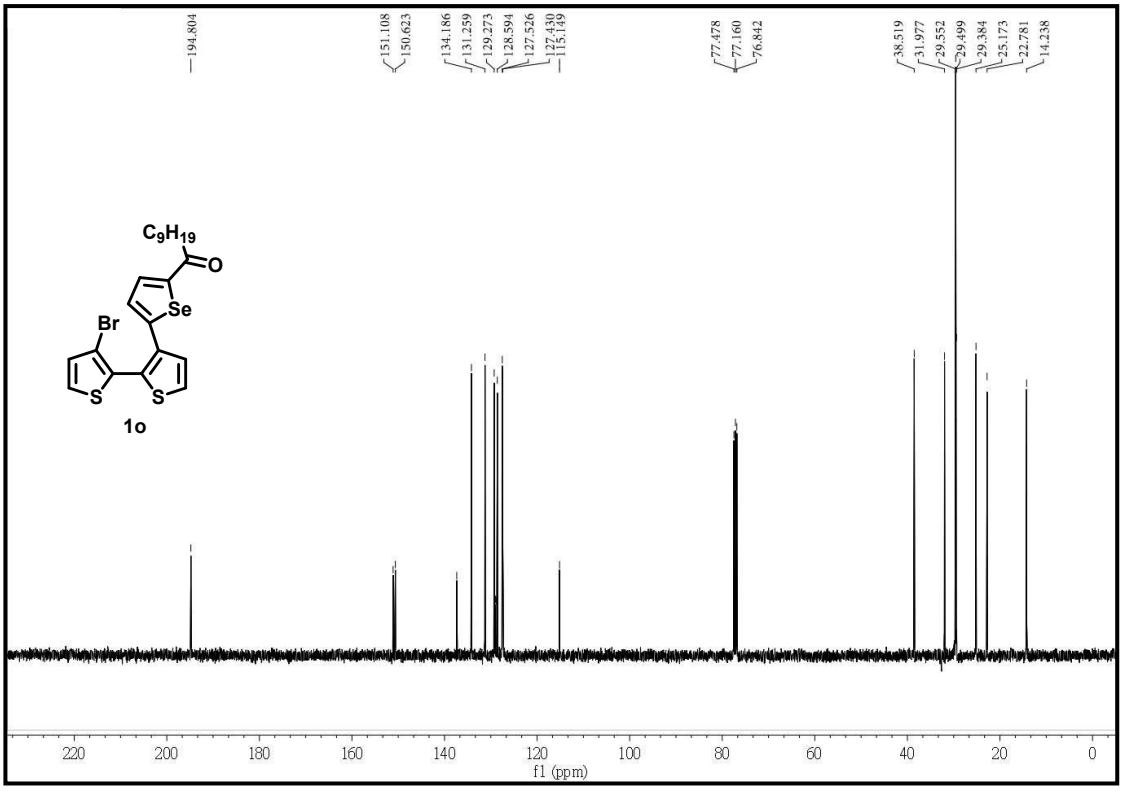
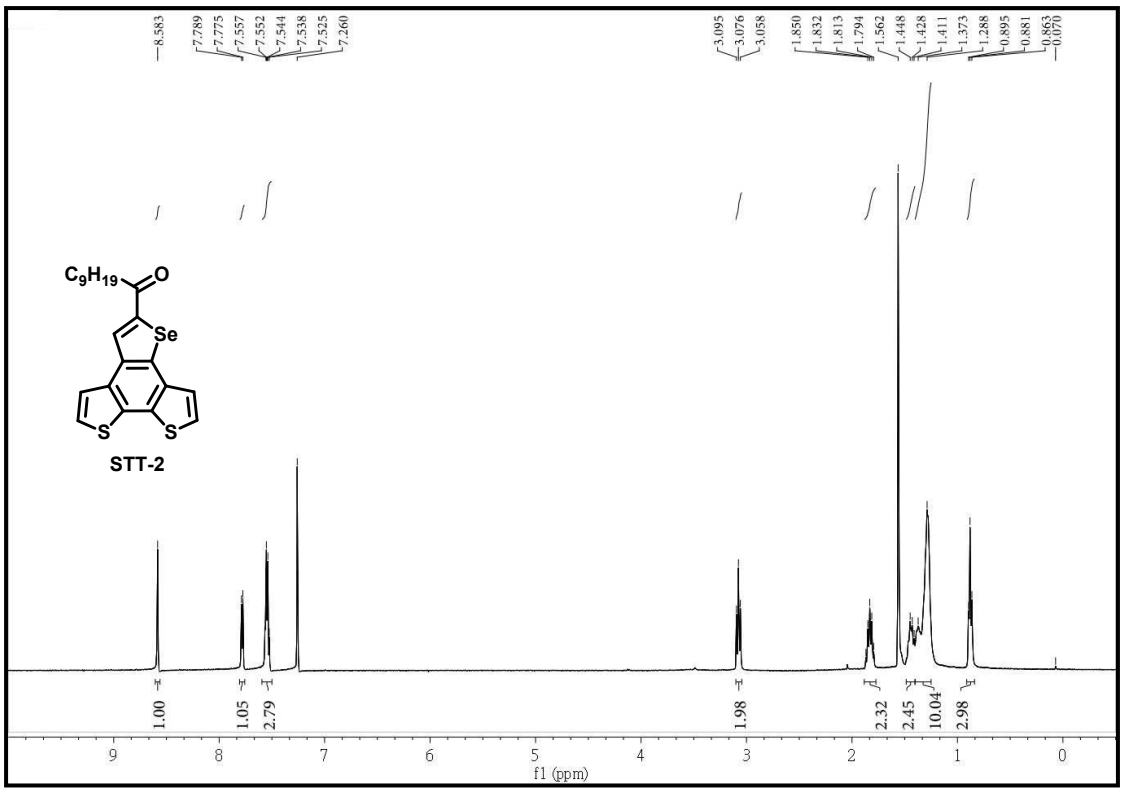
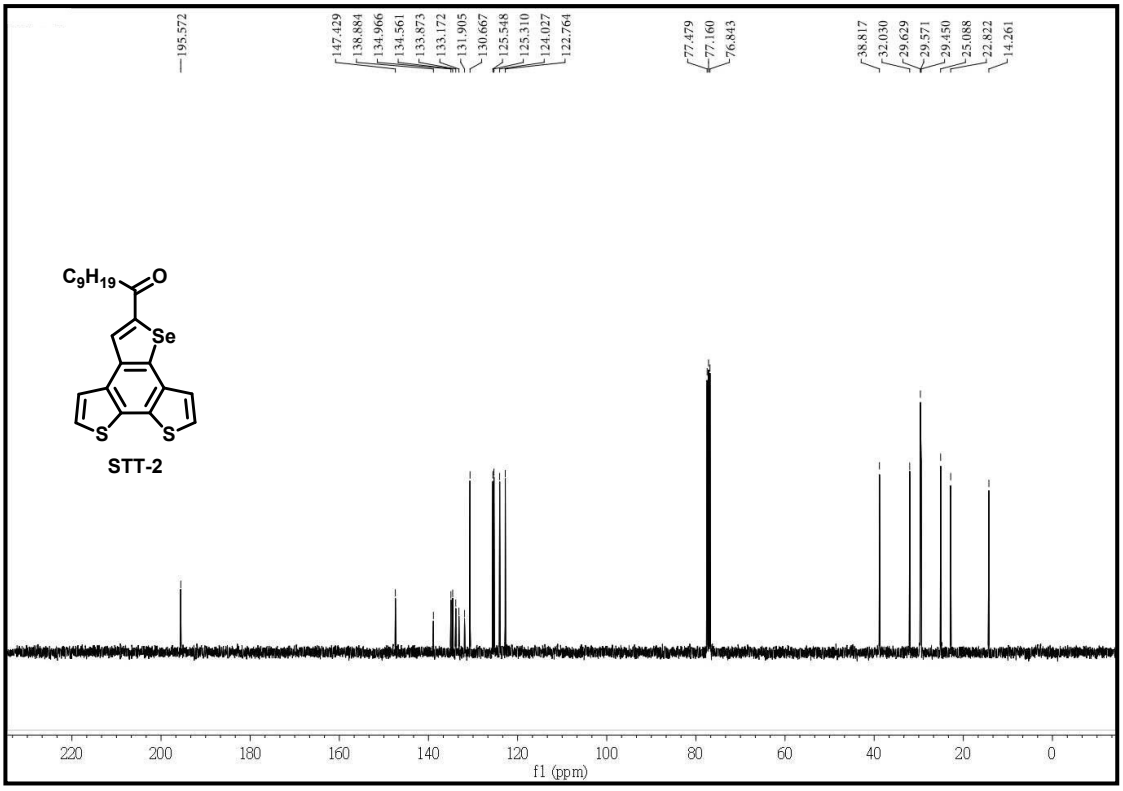
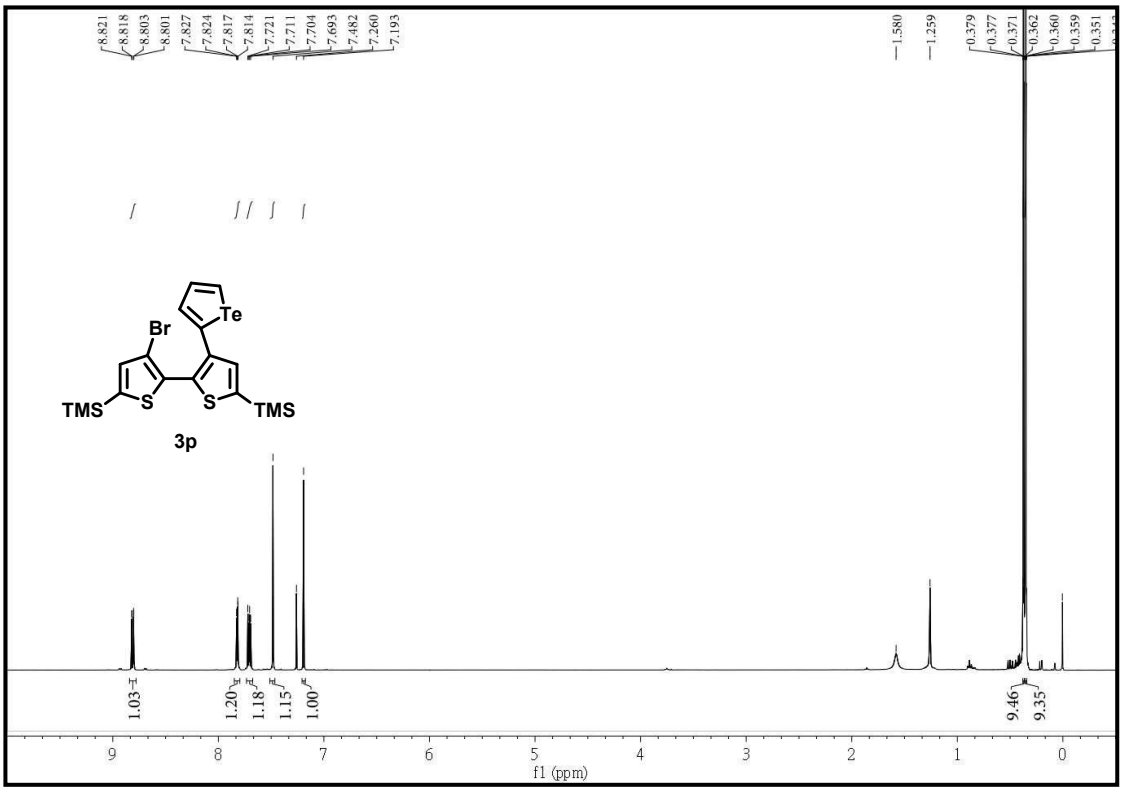
143.075
142.367
138.408
137.055
135.147
134.643
131.956
130.993
129.495
127.536
114.974
77.478
77.160
76.842
0.231
-0.036
-0.177
-0.446
Br
Se
TMS
S
S
TMS
3o
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

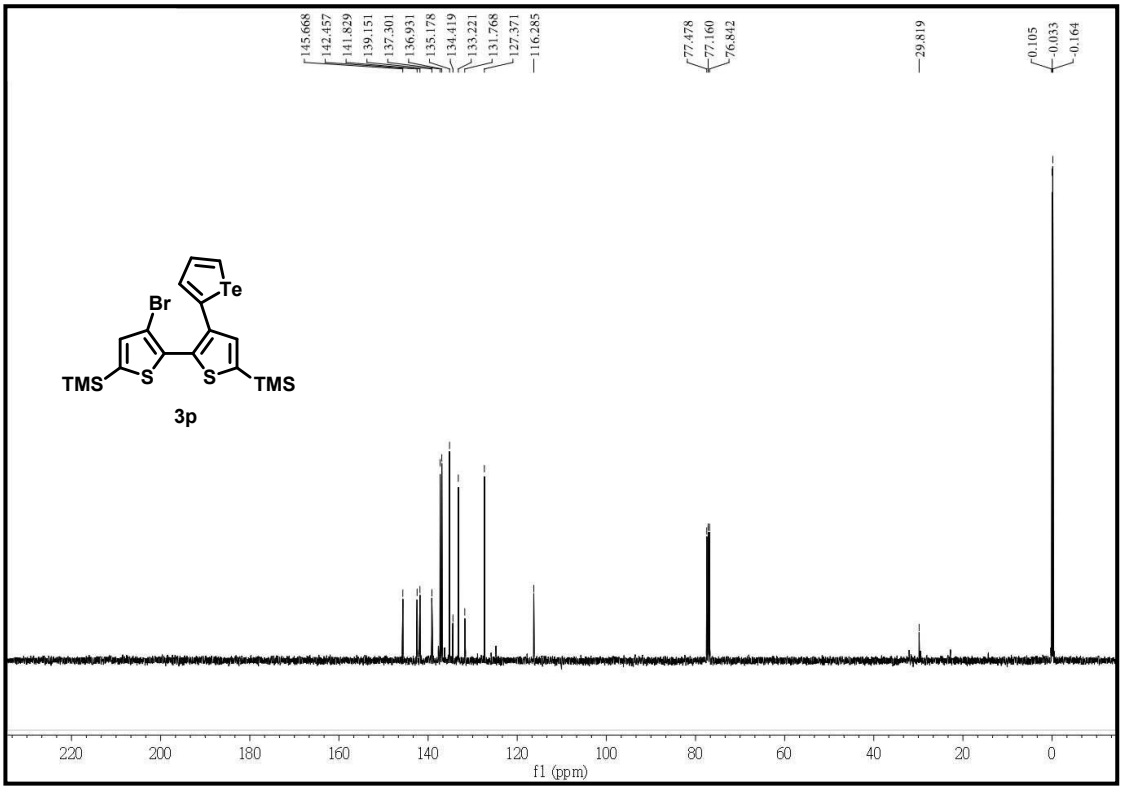

7.762
7.752
7.489
7.475
7.453
7.440
7.361
7.348
7.304
7.294
7.260
7.105
7.092
2.837
2.819
2.800
1.734
1.717
1.699
1.681
1.654
1.315
1.261
0.893
0.877
0.860
C9H19
O
Se
Br
S
S
1o
1.23
1.05
1.11
1.24
1.12
1.00
2.53
2.35
10.75
3.07
f1 (ppm)

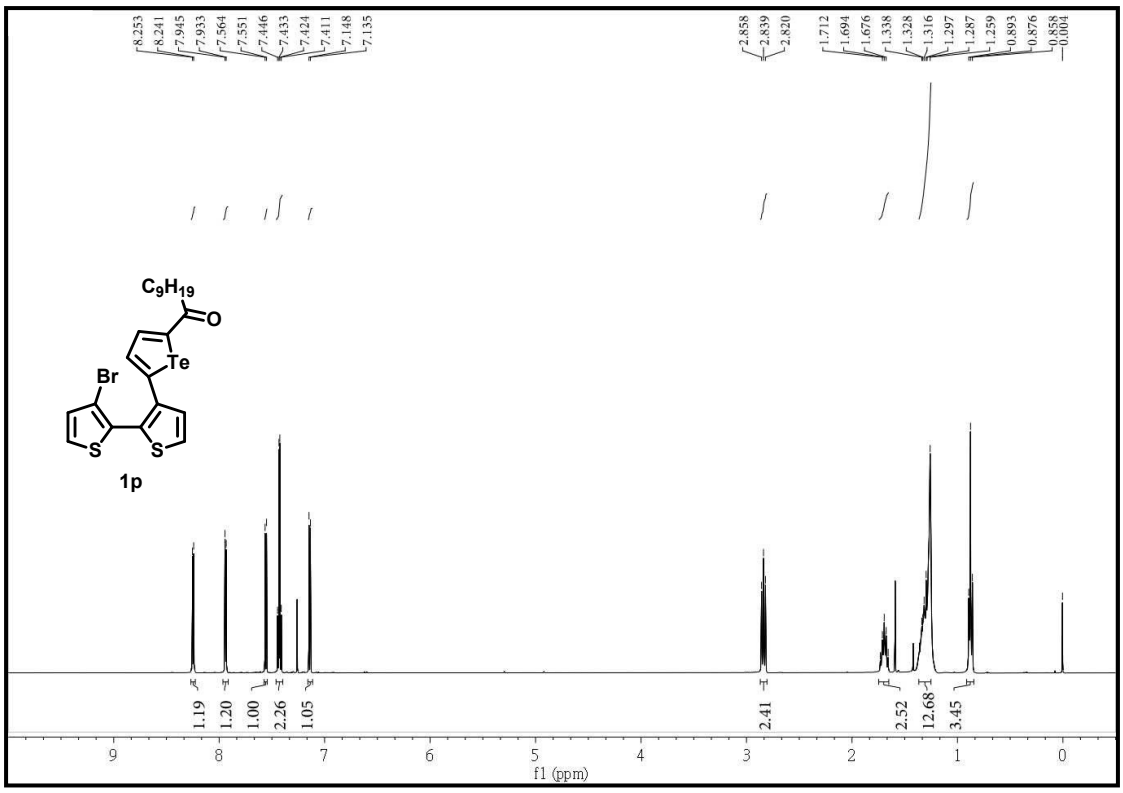

194.804
151.108
150.623
134.186
131.259
129.273
128.594
127.526
127.430
115.149
77.478
77.160
76.842
38.519
31.977
29.552
29.499
29.384
25.173
22.781
14.238
C9H19
O
Se
Br
S
S
1o
f1 (ppm)

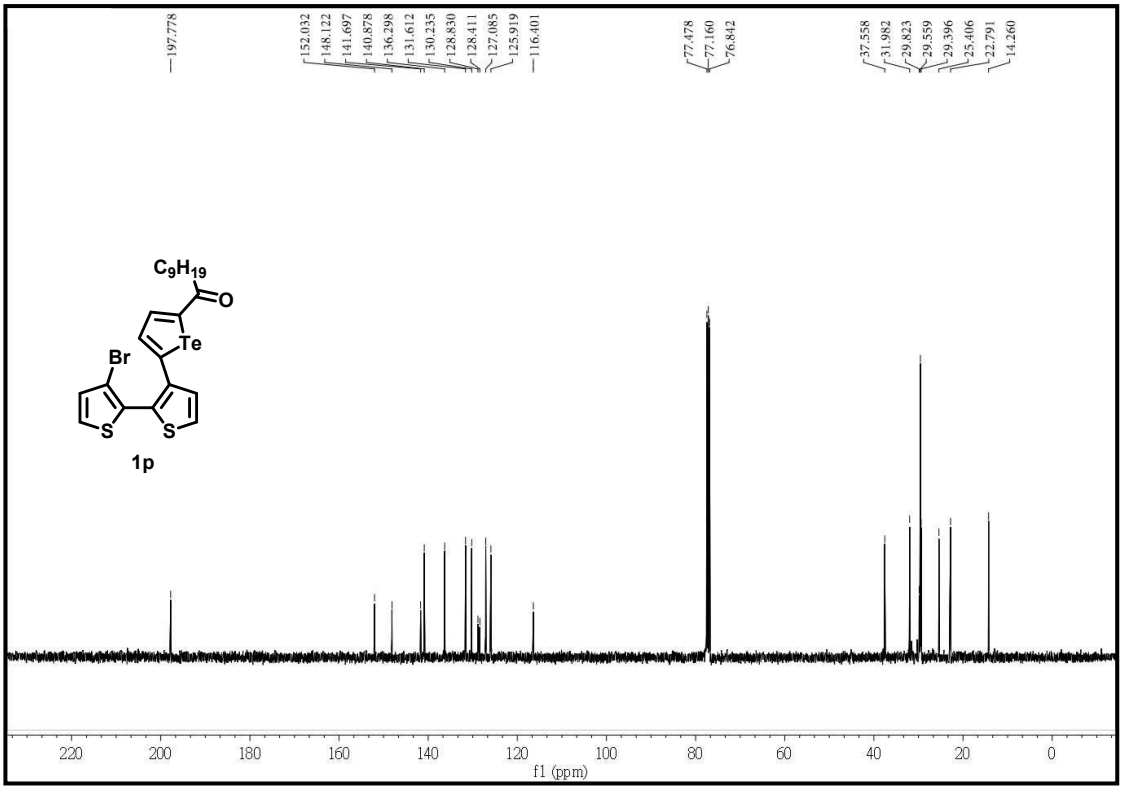

8.583
7.789
7.775
7.557
7.552
7.544
7.538
7.525
7.260
3.095
3.076
3.058
1.850
1.832
1.813
1.794
1.562
1.448
1.428
1.411
1.373
1.288
0.895
0.881
0.863
0.070
C9H19
O
Se
S
S
STT-2
1.00
1.05
2.79
1.98
2.32
2.45
10.04
2.98
f1 (ppm)

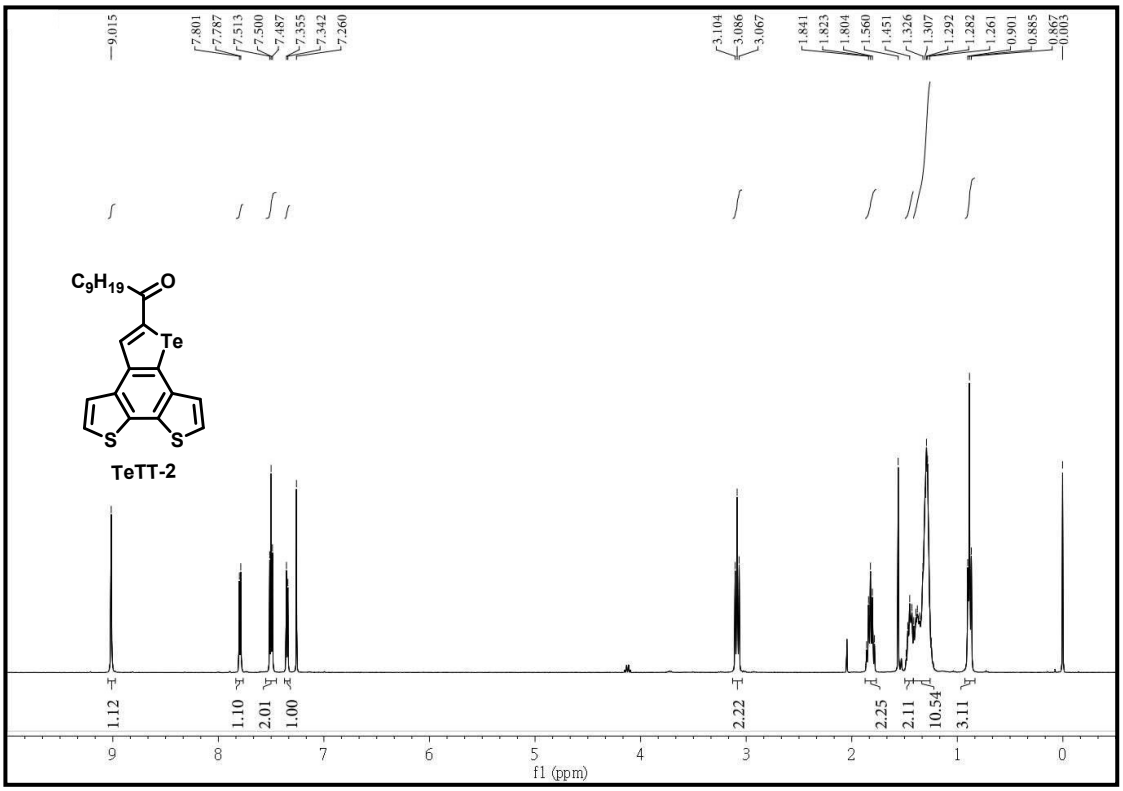

195.572
147.429
138.884
134.966
134.561
133.873
133.172
131.905
130.667
125.548
125.310
124.027
122.764
77.479
77.160
76.843
38.817
32.030
29.629
29.571
29.450
25.088
22.822
14.261
C9H19
O
Se
S
S
STT-2
f1 (ppm)

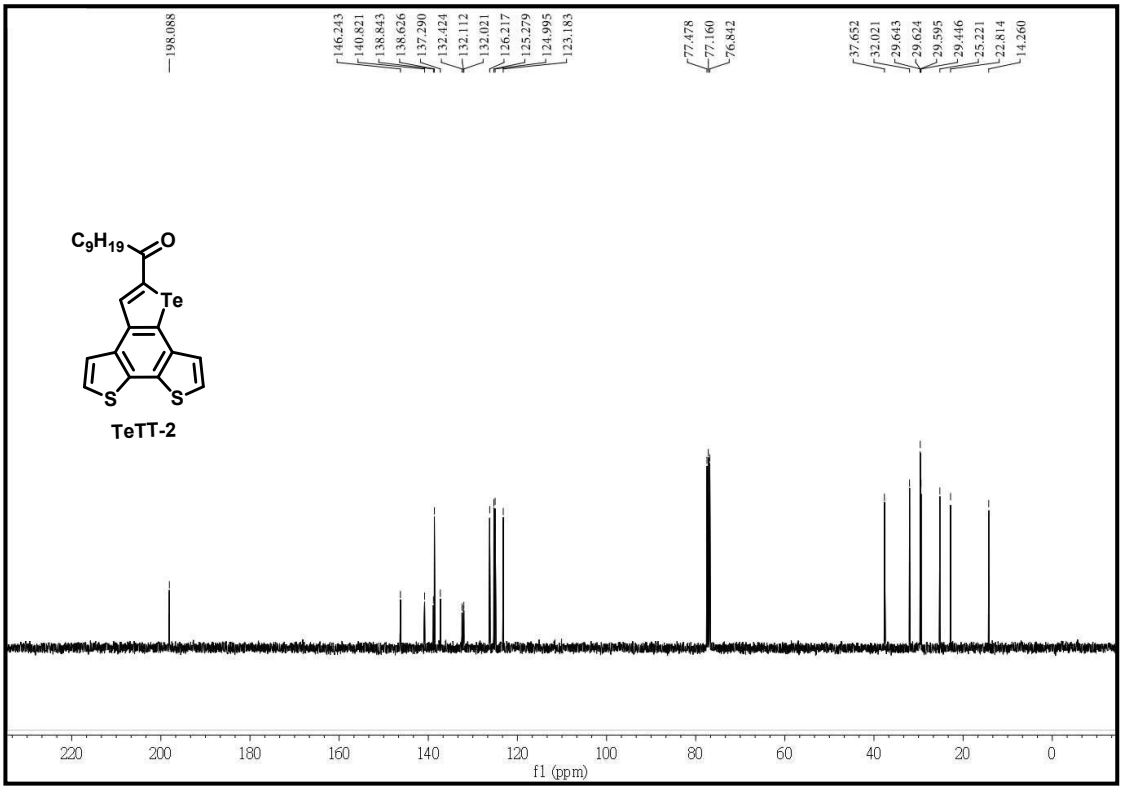

8.821
8.818
8.803
8.801
7.827
7.824
7.817
7.814
7.721
7.711
7.704
7.693
7.482
7.260
7.193
1.580
1.259
0.379
0.377
0.371
0.362
0.360
0.359
0.351
Te
Br
TMS
S
S
TMS
3p
1.03
1.20
1.18
1.15
1.00
9.46
9.35
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


145.668
142.457
141.829
139.151
137.301
136.931
135.178
134.419
133.221
131.768
127.371
116.285
77.478
77.160
76.842
29.819
0.105
-0.033
-0.164
Te
Br
TMS
S
S
TMS
3p
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


8.253
8.241
7.945
7.933
7.564
7.551
7.446
7.433
7.424
7.411
7.148
7.135
2.858
2.839
2.820
1.712
1.694
1.676
1.338
1.328
1.316
1.297
1.287
1.259
0.893
0.876
0.858
0.004
C9H19
O
Te
Br
S
S
1p
1.19
1.20
1.00
2.26
1.05
2.41
2.52
12.68
3.45
f1 (ppm)


197.778
152.032
148.122
141.697
140.878
136.298
131.612
130.235
128.830
128.411
127.085
125.919
116.401
77.478
77.160
76.842
37.558
31.982
29.823
29.559
29.396
25.406
22.791
14.260
C9H19
O
Te
Br
S
S
1p
f1 (ppm)


9.015
7.801
7.787
7.513
7.500
7.487
7.355
7.342
7.260
3.104
3.086
3.067
1.841
1.823
1.804
1.560
1.451
1.326
1.307
1.292
1.282
1.261
0.901
0.885
0.867
0.003
C9H19
O
Te
S
S
TeTT-2
1.12
1.10
2.01
1.00
2.22
2.25
2.11
10.54
3.11
f1 (ppm)


198.088
146.243
140.821
138.843
138.626
137.290
132.424
132.112
132.021
126.217
125.279
124.995
123.183
77.478
77.160
76.842
37.652
32.021
29.643
29.624
29.595
29.446
25.221
22.814
14.260
C9H19
O
Te
S
S
TeTT-2
f1 (ppm)