Electronic Supplementary Material (ESI) for ChemComm.

BENZOTRIFURAN (BTFURAN): A BUILDING BLOCK FOR π-CONJUGATED SYSTEMS

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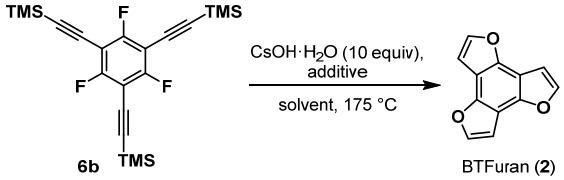
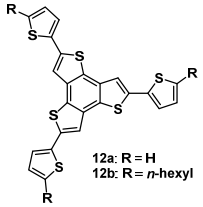
Supporting Information

Table S1. Optimization of BTFuran (2) Synthesis from Trialkyne 6b.



entry	solvent	additive (equiv)	time (h)	BTFuran (**2**) (%)
1	DMAc	-	4	41
2	DMAc	-	3	35
3	NMP	-	4	28
4	DMAc	KF (3)	4	25
5	DMAc	H_2O (10)	4	53
6	DMAc	H_2O (5)	2	47
7	DMAc	H_2O (10)	2	54
8	DMAc	H_2O (20)	2	46
9	DMAc	H_2O (30)	2	30

Table S2. Absorption Data and Theoretical Energy Calculations of Selected Compounds.



Cpd	λ_{max} [a] (nm)	ε [a] (10^4 $M^{-1}cm^{-1}$)	E_{HOMO} [b] (eV)	E_{LUMO} [b] (eV)	E_{gap} [b] (eV)
2	234	6.20±0.07	–5.94	–0.583	5.36
7c	243	7.8±0.2	–6.23	–1.08	5.16
8	340	10.2±0.3	–5.22[b]	–1.44[b]	3.79[b]
9a	321	11.4±0.1	–5.61	–1.83	3.78
9b	290	10.4±0.2	-	-	-
10	256,332	3.44±0.07	–5.59[b]	–1.65[b]	3.94[b]
11	334	5.4±0.1	–5.36[b]	–1.56[b]	3.80[b]
1	260[1] 288,267[2]	-	–5.94	–1.11	4.83
12a	343[1]	-	–5.51	–1.88	3.63
12b	357[2]	-	–5.28[b]	–1.69[b]	3.59[b]

[a]UV spectra recorded in CH_2Cl_2 (15 μM); [b]Calculations performed using a truncated structure where R = *n*-propyl.

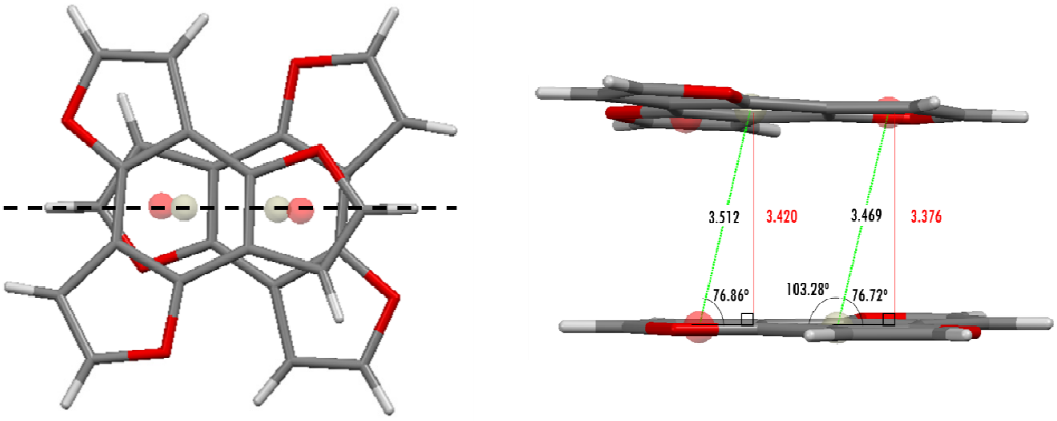


Figure S1. Estimation of intermolecular π-stacking distance in the crystal structure of BTFuran (**2**).

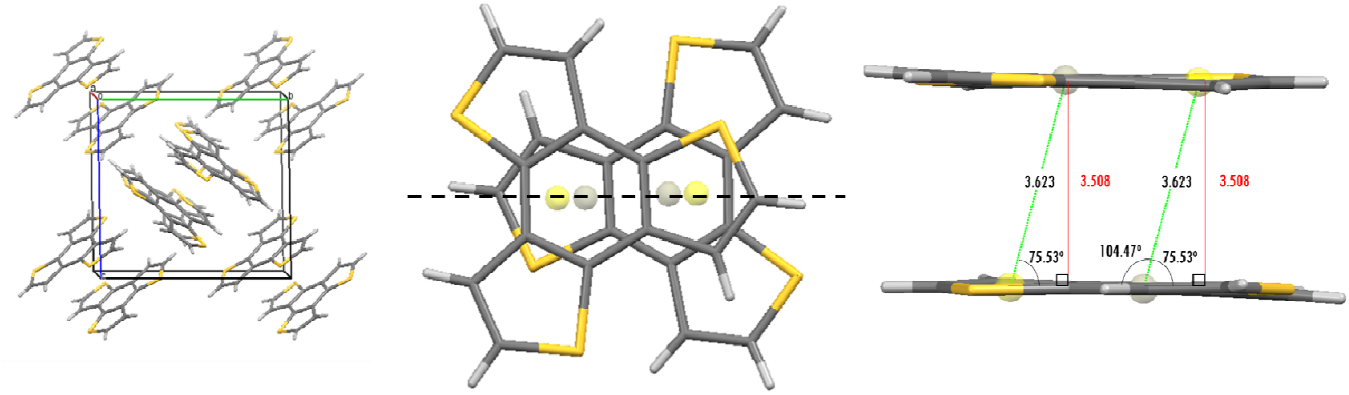
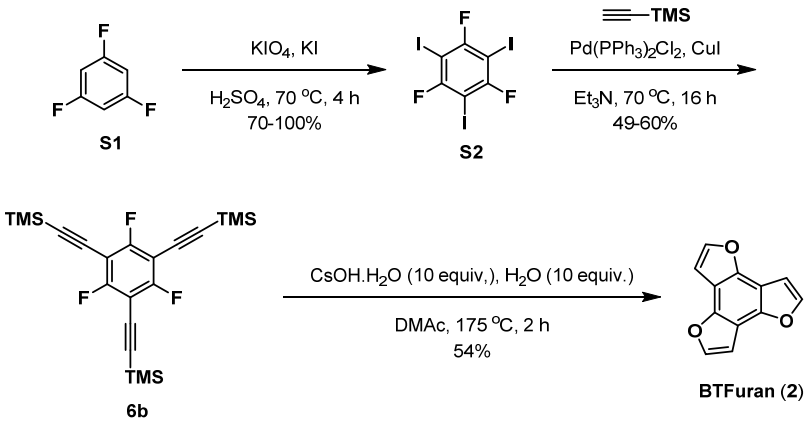


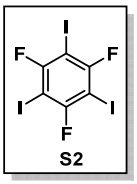
Figure S2. X-ray crystal structure of BTT (**1**, CSD entry: ERIKIZ)[2] and estimation of intermolecular π-stacking distance.

Experimental details

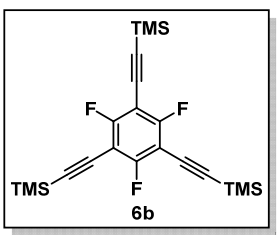
General information. DMF was degassed in 20 L drums and passed through two sequential purification columns (molecular sieves) under a positive argon atmosphere. Thin layer chromatography (TLC) was performed on aluminum backed SiO_2-60 F254 TLC plates with visualization via UV light. Flash column chromatography was performed using SiO_2-60 230−400 mesh silica gel and mobile phases as indicated within procedures. ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR were recorded on spectrometers operating at 500 MHz for ^{1}H, 471 MHz for ^{19}F, and at 126 MHz for ^{13}C. Chemical shifts (δ) are given in parts per million (ppm) relative to residual protonated solvent (DMSO-d_6: δ_H 2.50 ppm, δ_C 39.50 ppm; $CDCl_3$: δ_H 7.24 ppm, δ_C 77.0 ppm). Abbreviations used are s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), and m (multiplet). Electrospray ionization (ESI) or direct analysis in real time (DART) high-resolution mass spectra (HRMS) were recorded on an ESI-TOF instrument, operating in positive or negative ion mode as stated, with methanol as the carrier solvent for ESI experiments. Compounds 2-bromo-5-hexylthiophene, (5-hexylthiophen-2-yl)trimethylstannane, and 2-(5-hexylthiophen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane were prepared based on earlier literature procedures,[3] provided consistent ^{1}H and ^{13}C NMR data, and were used without further purification.

Synthesis of compounds



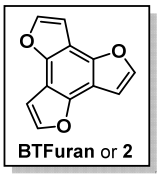


1,3,5-Trifluoro-2,4,6-triiodobenzene, **S2**: To a suspension of periodic acid (12.8 g, 56.2 mmol) in concentrated H_2SO_4 (85 mL), finely ground KI (28.0 g, 169 mmol) was added in small portions over 5 min. The dark mixture was stirred and cooled in an ice bath. 1,3,5-trifluorobenzene (**S1**, 5.00 g, 37.9 mmol) was added over 15 min by syringe. The ice bath was removed and the solution was heated to 70 °C for 4 h. The mixture was then cooled to rt, poured onto ice (855 g), and extracted with Et_2O (5 × 100 mL). The organic phase was washed with conc. aq. $Na_2S_2O_3$ (2 × 100 mL) and water (1 × 100 mL), dried over $MgSO_4$, and concentrated under reduced pressure to afford 15.5 g (30.3 mmol, 80% yield) of **S2** as off-white needles. NMR data matched with reported literature.[4] ^{13}C NMR ($CDCl_3$, 125 MHz): δ 64.0 (td, $^2J_{CF}$ = 34.4 and $^4J_{CF}$ = 4.2 Hz), 162.3 (dt, $^1J_{CF}$ = 242.5 and $^3J_{CF}$ = 7.5 Hz) ppm. ^{19}F NMR ($CDCl_3$, 500 MHz): -71.28 ppm.

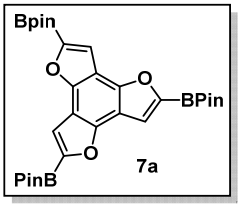


((2,4,6-Trifluorobenzene-1,3,5-triyl)tris(ethyne-2,1-diyl))tris (trimethylsilane), **6b**: **S2** (2.00 g, 3.90 mmol), $Pd(PPh_3)_2Cl_2$ (0.275 g, 0.392 mmol), and CuI (0.075 g, 0.40 mmol) were placed in a dry three-necked flask, followed by addition of Et_3N (100 mL). A solution of trimethylsilyl acetylene (1.94 mL,

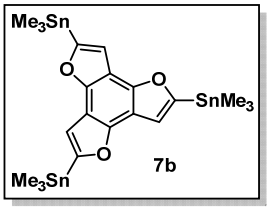
13.6 mmol) in Et_3N (50 mL) was then added dropwise. At the end of the addition, the mixture was warmed to 70 °C (oil bath temperature). After 1 h, THF (50 mL) was added, and the mixture was left stirring for 16 h under argon. The mixture was filtered over Celite® and purified by silica gel column chromatography using hexanes as the eluent. The obtained product was then recrystallized from hexanes to afford 0.880 g (2.09 mmol, 54% yield) of **6b** as white needles. NMR characterization of the compound matched previously reported data.[5] ^{1}H NMR ($CDCl_3$, 500 MHz): δ 1.54 (27H, s) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 88.7 (s), 99.7 (m), 106.9 (m), 163.1 (dt, $^1J_{CF}$ = 268.8 and $^3J_{CF}$ = 15.0 Hz) ppm; ^{19}F NMR ($CDCl_3$, 500 MHz): -99.53 ppm.



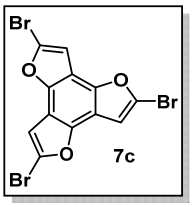
Benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, **BTFuran** or **2**: A mixture of **6b** (0.210 g, 0.500 mmol), $CsOH.H_2O$ (0.826 g, 5.00 mmol), and water (90 µL, 5.0 mmol) in DMAc (5 mL) was stirred at 175 °C for 2 h. After cooling to rt, water (5 mL) was added, and the organic layer was separated and extracted with CH_2Cl_2 (4 x 25 mL). The combined organic layers were dried over $MgSO_4$, and concentrated under reduced pressure. Purification by flash column chromatography on silica gel using CH_2Cl_2/hexanes 5:95 as the eluent afforded 53.7 mg (0.271 mmol, 54% yield) of **BTFuran** as a white solid. Scaling up the reaction compromises the yield of the reaction. Around 1 g of **BTFuran** can be obtained from 5-6 g of **6b** in a 35-45% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.14 (3H, d, J = 2.5 Hz), 7.72 (3H, d, J = 2.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 103.9, 109.2, 143.6, 146.6 ppm; DART-HRMS-ESI: *m/z* $[M+H]^+$ calcd for $[C_{12}H_7O_3]^+$: 199.0390; found: 199.0389.



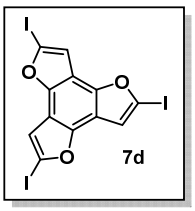
2,5,8-Tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 7a: To a solution of **BTFuran** (300 mg, 1.51 mmol) in THF (22.5 mL) at 0 °C was added *n*-BuLi (2.5 M soln. in hexanes, 2.7 mL) dropwise, and the mixture was stirred for 1 h at rt. The reaction was then cooled to -78 °C and *i*-PrOBPin (1.39 mL, 6.81 mmol) was added. The mixture was allowed to stir at 0 °C for 2 h. The reaction was quenched with 10% aq. HCl (20 mL) and extracted with $CHCl_3$ (3 x 30 mL). The organic extract was dried over Na_2SO_4, filtered and concentrated under vacuum. The crude was resuspended with MeOH, sonicated for 10 min and cooled down at 0 °C. The resulting solid was filtered and washed with cold MeOH to afford the product (0.389 g, 0.675 mmol, 45% yield) as an off-white powder. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.80 (3H, s), 1.41 (36H, s) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 151.2, 117.5, 110.2, 84.7, 25.0 ppm; HRMS-MALDI: *m/z* $[M^*]^+$ calcd for $[C_{30}H_{39}B_3O_9]^+$: 576.2873; found: 576.2901.



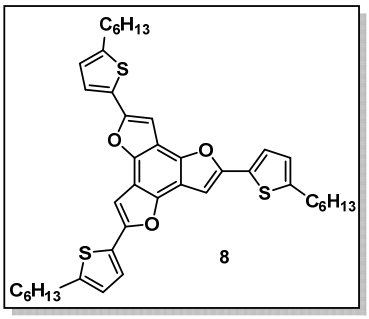
2,5,8-Tris(trimethylstannyl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 7b: To a solution of **BTFuran** (300 mg, 1.51 mmol) in THF (22.5 mL) at 0 °C was added *n*-BuLi (2.5 M soln. in hexanes, 2.7 mL) dropwise, and the mixture was stirred for 1 h at rt. The reaction was then cooled to -78 °C and Me_3SnCl (1.36 g, 6.81 mmol) was added. The mixture was allowed to stir at 0 °C for 2 h. The reaction was quenched with water (20 mL) and extracted with $CHCl_3$ (3 x 30 mL). The organic extract was dried over Na_2SO_4, filtered and concentrated under vacuum. The crude was resuspended with MeOH, sonicated for 10 min and cooled down at 0 °C. The resulting solid was filtered and washed with cold MeOH to afford the product (0.716 g, 1.04 mmol, 69% yield) as a white powder. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.30 (3H, s), 0.44 (27H, s) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 162.4, 150.3, 114.8, 109.2, –8.9 ppm; HRMS-ESI: *m/z* $[M+Na]^+$ calcd for $[C_{21}H_{30}NaO_3Sn_3]^+$: 710.9147; found: 710.9134.



2,5,8-Tribromobenzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 7c: BTFuran (75.0 mg, 0.378 mmol) was dissolved in dry THF (15 mL) and cooled to -78 ^{o}C. To this solution, an *n*-BuLi soln. (2.5 M in hexanes, 0.57 mL, 1.4 mmol) was added, and the solution was stirred for 30 min at rt. The solution was cooled down to -78 ^{o}C and a soln. of carbon tetrabromide (0.565 g, 1.70 mmol) in THF (7.5 mL) was added dropwise. After stirring for 5 min at -78 ^{o}C, the solution was allowed to warm to room temperature for 1 h. The reaction was quenched with water (20 mL), extracted with DCM (3 x 30 mL) and the combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo. The crude was resuspended in MeOH and the solid was filtered, washed with MeOH and dried under vacuum to afford the product (0.115 g, 0.264 mmol, 70% yield) as a brown solid. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.03 (3H, s) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 145.5, 128.5, 110.8, 105.5 ppm; DART-HRMS: *m/z* $[M+H]^+$ calcd for $[C_{12}H_4Br_3O_3]^+$: 434.7685; found: 434.7674.



2,5,8-Triiodobenzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 7d: BTFuran (50.0 mg, 0.252 mmol) was dissolved in dry THF (10 mL) and cooled to -78 ^{o}C. To this solution, an *n*-BuLi soln. (2.5 M in hexanes, 0.38 mL, 0.95 mmol) was added, and the solution was stirred for 30 min at rt. The solution was cooled down to -78 ^{o}C and a soln. of iodine (0.241 g, 0.946 mmol) in THF (5 mL) was added dropwise. After stirring for 5 min at -78 ^{o}C, the solution was allowed to warm to room temperature for 1 h. The reaction was quenched with water (20 mL), extracted with DCM (3 x 30 mL) and the combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo. The crude was resuspended in MeOH and the solid was filtered, washed with MeOH and dried under vacuum to afford the product (67.0 g, 0.116 mmol, 46% yield) as an off-white solid. ^{1}H NMR (DMSO-d_6, 50 ^{o}C, 500 MHz): δ 7.55 (3H, s) ppm; ^{13}C NMR (DMSO-d_6, 50 ^{o}C, 125 MHz): δ 146.7, 113.3, 110.4, 97.4 ppm; DART-HRMS: *m/z* $[M]^{+}$ calcd for $[C_{12}H_3I_3O_3]^{+}$: 575.7216; found: 575.7182.



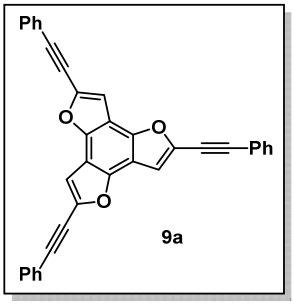
2,5,8-Tris(5-hexylthiophen-2-yl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 8:

a) *Stille coupling*: A 3-necked round-bottom flask equipped with a stirring bar and a reflux condenser was charged with **7c** (40.0 mg, 0.0920 mmol), DMF (7.6 mL), and (5-hexylthiophen-2-yl)trimethylstannane (110 mg, 0.331 mmol, 3.6 equiv). The mixture was deaerated with an argon stream for 15–20 min. $Pd(PPh_3)_4$ (15.9 mg, 0.0138 mmol, 15 mol%) was then added and the resulting mixture was stirred at 80 ^{o}C for 16 h. After the reaction period, brine was added (30 mL) and the mixture was extracted with DCM (3 x 30 mL). The organic phase was dried over Na_2SO_4, filtered, and concentrated. The crude product was adsorbed on silica and purified by column chromatography (SiO_2, hexanes as the eluent) to afford **8** (47.7 mg, 0.0684 mmol, 74% yield) as a white solid. Similar procedure and purification method were used for the reaction between **7b** (50.0 mg, 0.0728 mmol) and 2-bromo-5-hexylthiophene (65.0 mg, 0.262 mmol, 3.6 equiv), yielding **8** (30.1 mg, 0.0432 mmol) in 59% yield.

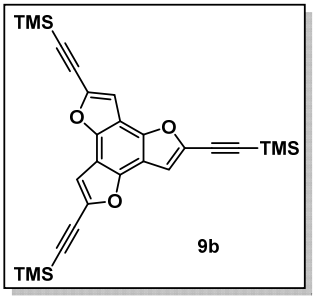
b) *Suzuki coupling:* A 3-necked round-bottom flask equipped with a stirring bar and a reflux condenser was charged with **7c** (50.0 mg, 0.0920 mmol), 2-(5-hexylthiophen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (97.4 mg, 0.331 mmol, 3.6 equiv), and DMF (8.0 mL). The mixture was deaerated with an argon stream for 15–20 min. $Pd(PPh_3)_4$ (15.9 mg, 0.0138 mmol, 15 mol%) was then added

and the mixture was stirred under argon for 10 min. A degassed solution of Na_2CO_3 (97.5 mg, 0.920 mmol) in water (1.4 mL) was added and the resulting mixture was stirred at 80 °C for 16 h. After the reaction period, water was added (30 mL) and the mixture was extracted with DCM (3 x 30 mL). The organic phase was dried over Na_2SO_4, filtered, and concentrated. The crude product was adsorbed on silica and purified by column chromatography (SiO_2, hexanes as the eluent) to afford **8** (46.5 mg, 0.0667 mmol, 73% yield) as a white solid. Similar procedure and purification method were used for the reaction between **7a** (50.0 mg, 0.0868 mmol) and 2-bromo-5-hexylthiophene (77.2 mg, 0.313 mmol, 3.6 equiv.), affording **8** (15.9 mg, 0.0228 mmol) in 26% yield.

8: ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.32 (d, J = 3.5 Hz, 1H), 7.13 (s, 1H), 6.79 (d, J = 3.6 Hz, 1H), 2.86 (t, J = 7.6 Hz, 2H), 1.73 (p, J = 7.5 Hz, 2H), 1.42 (p, J = 6.6 Hz, 2H), 1.38 – 1.31 (m, 4H), 0.92 (t, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 150.9, 146.7, 145.3, 130.8, 125.1, 124.0, 111.1 97.7, 31.8, 31.7, 30.3, 28.9, 22.8, 14.3 ppm; DART-HRMS: *m/z* $[M+H]^+$ calcd for $[C_{42}H_{49}O_3S_3]^+$: 697.2838; found: 697.2839.



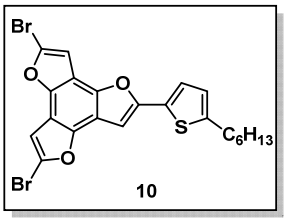
2,5,8-Tris(phenylethynyl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 9a: In a 10 mL round bottom flask equipped with a stirring bar and a reflux condenser was placed **7d** (46.8 mg, 0.0813 mmol), $Pd(PPh_3)_2Cl_2$ (8.6 mg, 0.0122 mmol, 15 mol%), piperidine (0.71 mL), and phenylacetylene (32 µL, 0.293 mmol, 3.6 equiv). The reaction was heated to 85 °C and stirred for 16 hours. After this time, the reaction was diluted with chloroform (20 mL) and washed with aq. sat. NH_4Cl. The aqueous phase was extracted with chloroform (2 x 20 mL). The combined organic phases were washed with 1 M HCl (30 mL), dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude product was adsorbed on silica and purified by column chromatography (0–20% DCM in hexanes) to afford **9a** (21.2 mg, 0.0425 mmol, 52% yield) as a white solid. Similar procedure and purification method were used for the reaction between **7c** (50.0 mg, 0.115 mmol) and phenylacetylene (45 µL, 0.41 mmol, 3.6 equiv), affording the product **9a** (21.3 mg, 0.0427 mmol) in 37% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.66-7.60 (m, 6H), 7.43-7.39 (m, 9H), 7.35 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 146.7, 138.4, 131.8, 129.3, 128.7, 121.9, 110.2, 108.74, 95.5, 79.4 ppm; DART-HRMS: *m/z* $[M+H]^+$ calcd for $[C_{36}H_{19}O_3]^+$: 499.1329; found: 499.1333.



2,5,8-Tris(trimethylsilylethynyl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran, 9b: To a degassed solution mixture of **7d** (53.0 mg, 0.0920 mmol), CuI (5.3 mg, 0.028 mmol, 30 mol%), and $Pd(PPh_3)_4$ (15.9 mg, 0.0138 mmol, 15 mol%) in Et_3N/THF (4:1 v/v, 9.5 mL) was added ethynyltrimethylsilane (87 µL, 0.626 mmol, 6.8 equiv). The reaction was rigorously stirred and heated to reflux for 16 h under argon. After the reaction period, water (20 mL) was added and the mixture was extracted with DCM (3 x 30 mL). The organic phase was dried over Na_2SO_4, filtered, and concentrated. The crude product was adsorbed on silica and purified by column chromatography (SiO_2, hexanes as the eluent) to afford **9b** (39.2 mg, 0.0805 mmol, 88% yield) as an oily white solid. Similar procedure and purification method were used for reaction between **7c** (40.0 mg, 0.920 mmol) and ethynyltrimethylsilane (87 µL, 0.63 mmol, 6.8 equiv), providing **9b** (19.3 mg, 0.0396 mmol) in 43% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.25 (s, 3H), 0.32 (s, 27H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 146.5, 138.0, 109.7, 109.1, 102.3, 93.7, 0.34 ppm; HRMS-ESI: *m/z* $[M+H]^+$ calcd for $[C_{27}H_{31}O_3Si_3]^+$: 487.1576; found: 487.1553.

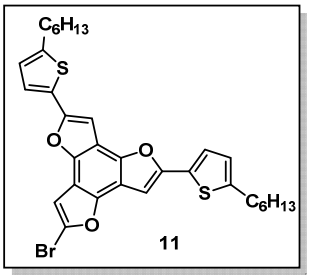
Stoichiometry control of Stille reaction:

General procedure: A 3-necked round-bottom flask equipped with a stirring bar and a reflux condenser was charged with the **7c** (50.0 mg, 0.0728 mmol), a solvent (6.0 mL), and trimethylstannylthiophene (65.0 mg, 0.262 mmol, 3.6 equiv). The mixture was deaerated using an argon stream for 15–20 min. $Pd(PPh_3)_4$ (25.0 mg, 0.0218 mmol, 10 mol%) was then added and the resulting mixture was stirred for 16 h at a certain temperature. After the reaction period, brine was added (30 mL) and the mixture was extracted with DCM (3 x 30 mL). The organic phase was dried over Na_2SO_4, filtered, and concentrated. The crude product was adsorbed on silica and purified by column chromatography (SiO_2, hexanes as the eluent) to afford pure fractions of desired products **10–11** along with recovered **7c** and **8** in different ratios (refer to Table 2 in the manuscript).



10

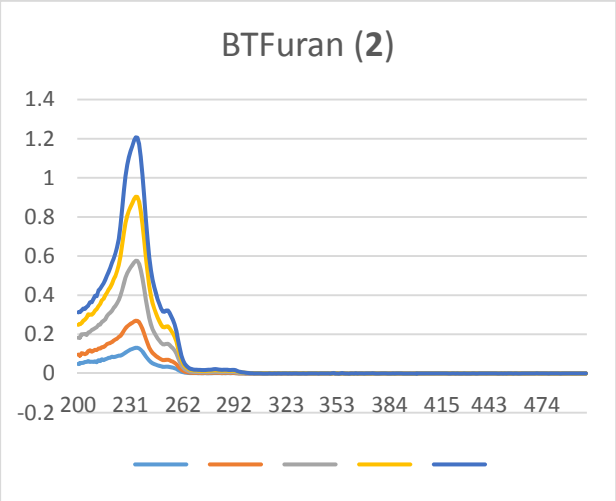
2,5-Dibromo-8-(5-hexylthiophen-2-yl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran (10): ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.29 (d, J = 3.6 Hz, 1H), 7.04 (s, 1H), 7.00 (s, 1H), 6.99 (s, 1H), 6.78 (d, J = 3.6 Hz, 1H), 2.84 (t, J = 7.6 Hz, 2H), 1.72 (p, J = 7.6 Hz, 2H), 1.46–1.29 (m, 6H), 0.92 (t, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz): δ 151.4, 147.2, 146.3, 145.5, 143.9, 130.1, 125.8, 125.1, 124.4, 111.0, 110.9, 110.3, 105.5, 105.3, 97.0, 31.7, 31.7, 30.3, 28.9, 22.7, 14.2. ppm; DART-HRMS: *m/z* $[M+H]^+$ calcd for $[C_{22}H_{19}Br_2O_3S]^+$: 522.9397; found: 522.9395.

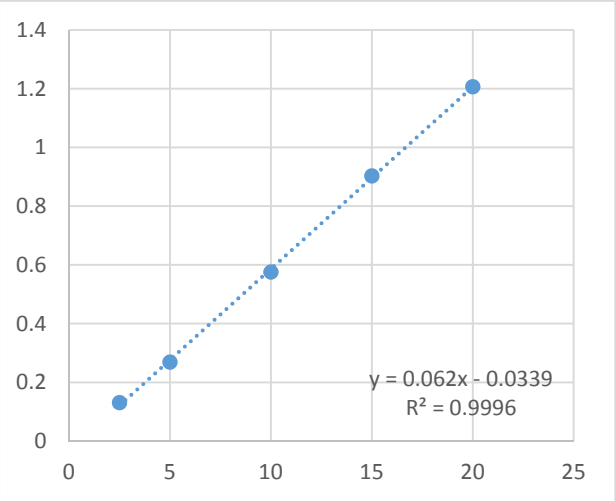


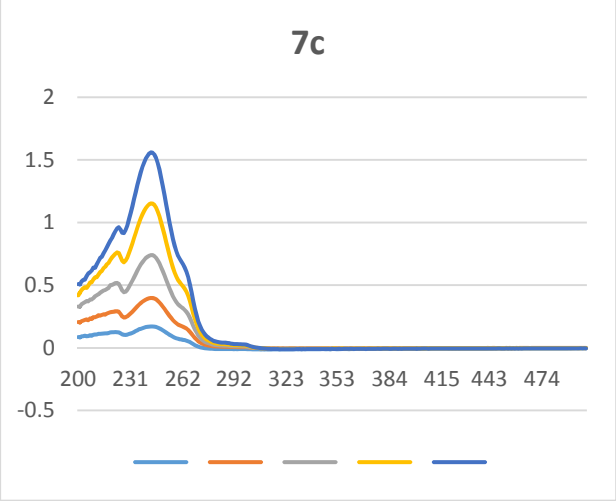
11

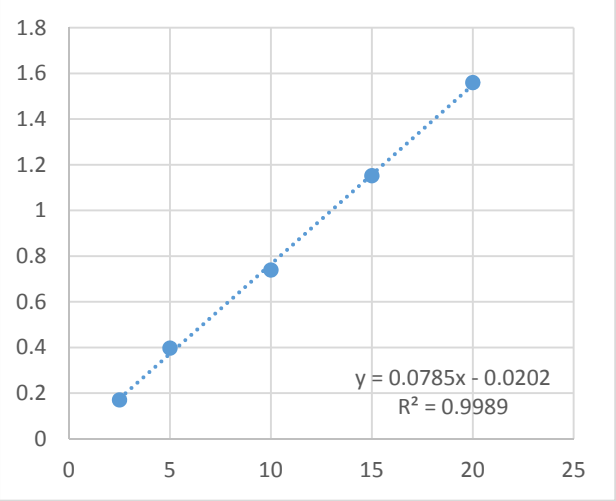
2-Bromo-5,8-bis(5-hexylthiophen-2-yl)benzo[1,2-*b*:3,4-*b*':5,6-*b*'']trifuran (11): ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.31 (d, J = 3.0 Hz, 2H), 7.11 (s, 1H), 7.07 (s, 1H), 7.05 (s, 1H), 6.79 (d, J = 3.5 Hz, 2H), 2.85 (t, J = 7.5 Hz, 4H), 1.73 (p, J = 7.6 Hz, 4H), 1.46–1.29 (m, 12H), 0.91 (t, J = 6.3 Hz, 6H) ppm; ^{13}C NMR ($CDCl_3$, 126 MHz): δ 151.1, 151.1, 146.8, 146.6, 145.0, 144.2, 130.5, 125.3, 125.0, 124.1, 111.3, 110.7, 110.6, 105.6, 97.4, 97.2, 31.7, 31.7, 30.3, 28.9, 22.7, 14.2 ppm; DART-HRMS: *m/z* $[M+H]^+$ calcd for $[C_{32}H_{34}BrO_3S_2]^+$: 609.1127; found: 609.1129.

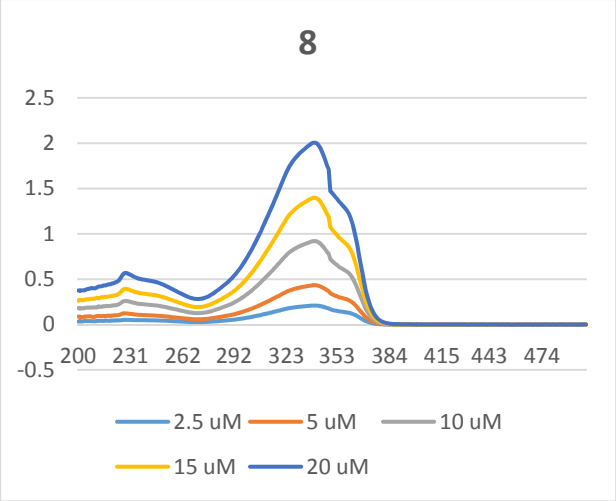
UV-Vis spectra

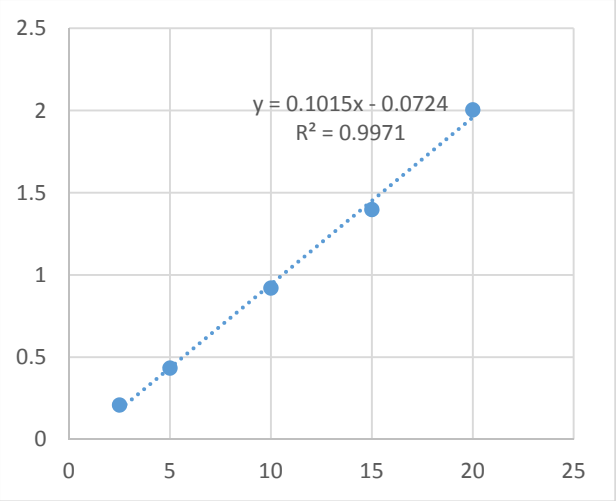


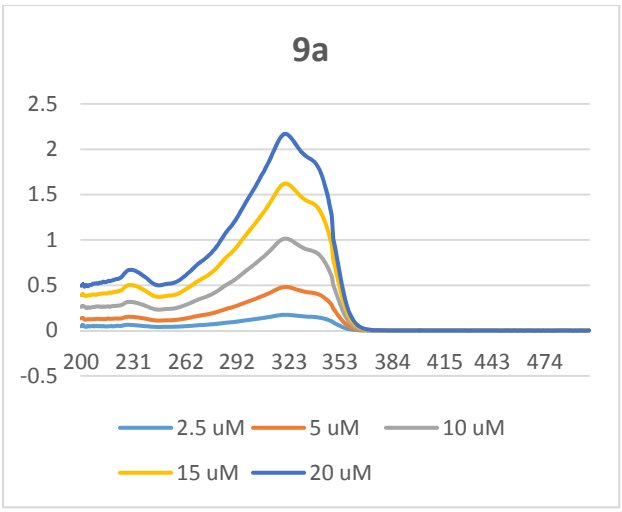


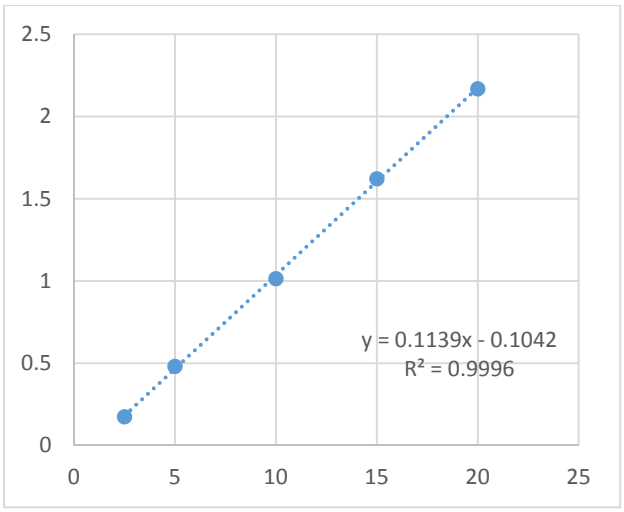


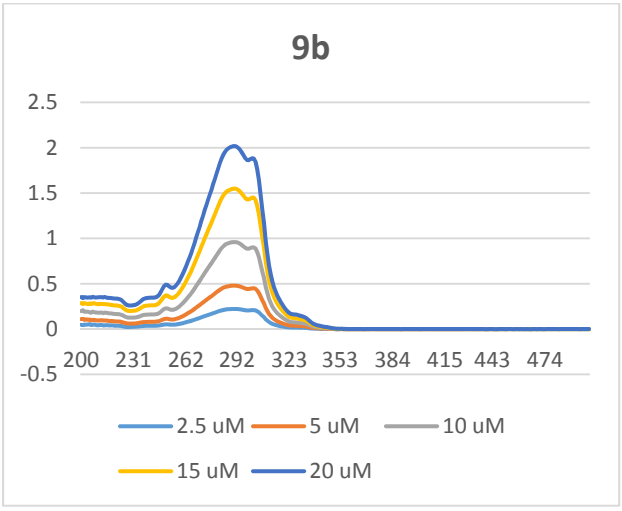


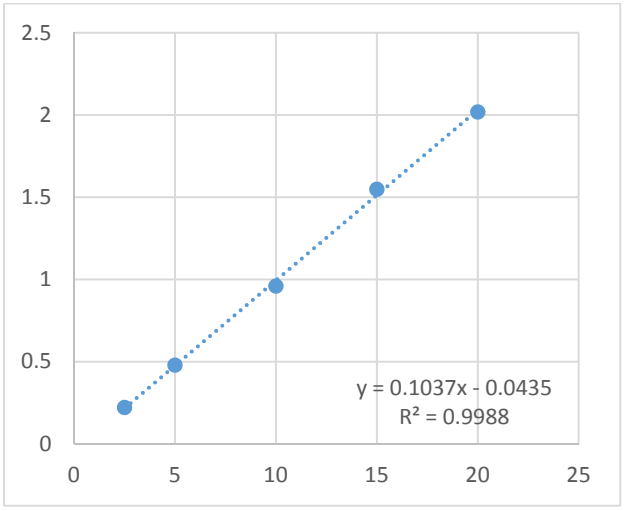


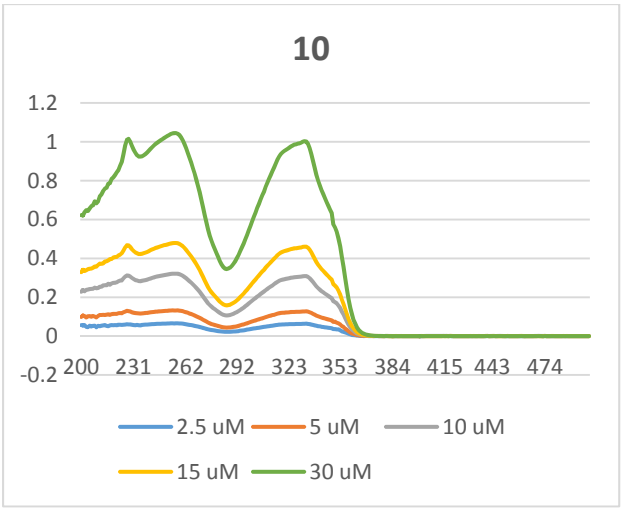


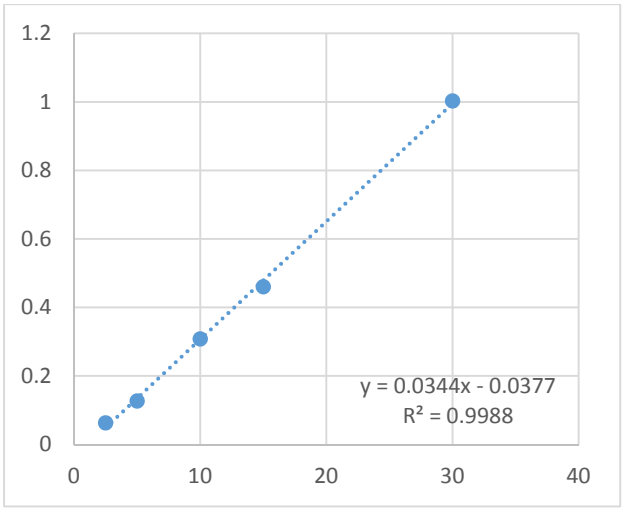

9a
2.5
2
1.5
1
0.5
0
-0.5
200 231 262 292 323 353 384 415 443 474
2.5 uM
5 uM
10 uM
15 uM
20 uM

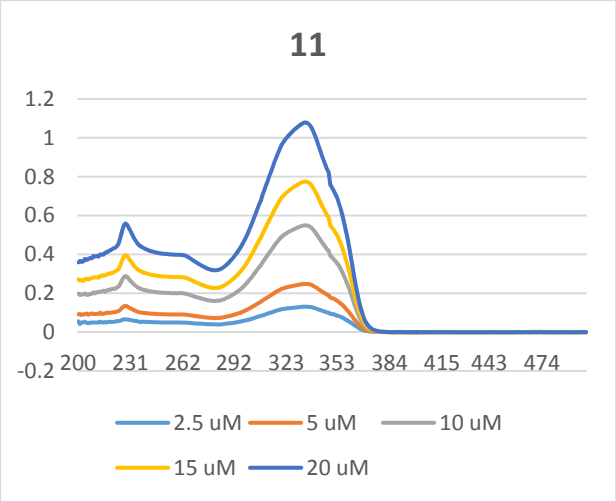

2.5
2
1.5
1
0.5
0
0 5 10 15 20 25
y = 0.1139x - 0.1042
R² = 0.9996

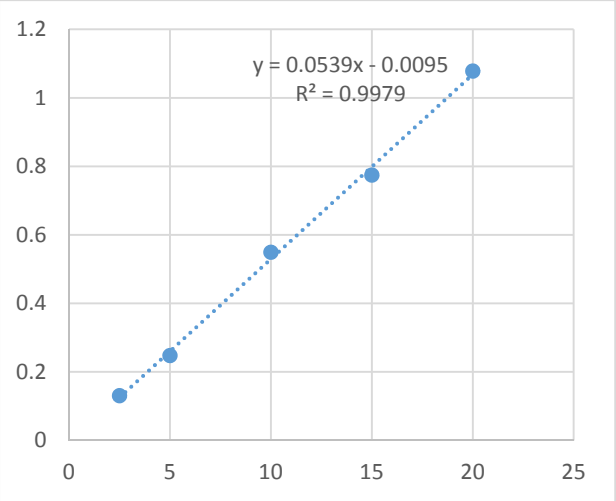

9b
2.5
2
1.5
1
0.5
0
-0.5
200 231 262 292 323 353 384 415 443 474
2.5 uM
5 uM
10 uM
15 uM
20 uM


2.5
2
1.5
1
0.5
0
0 5 10 15 20 25
y = 0.1037x - 0.0435
R² = 0.9988


10
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
200 231 262 292 323 353 384 415 443 474
2.5 uM
5 uM
10 uM
15 uM
30 uM


1.2
1
0.8
0.6
0.4
0.2
0
0 10 20 30 40
y = 0.0344x - 0.0377
R² = 0.9988


11
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
200 231 262 292 323 353 384 415 443 474
2.5 uM
5 uM
10 uM
15 uM
20 uM


y = 0.0539x - 0.0095
R² = 0.9979
1.2
1
0.8
0.6
0.4
0.2
0
0 5 10 15 20 25

Electrochemical Analysis

Electrochemical measurements were conducted using a Princeton Applied Research Versastat II potentiostat and Model 270 analysis software. A single-compartment three-electrode cell was employed using a platinum disk (3 mm^2) working electrode, platinum wire counter electrode, and Ag/AgCl reference electrode. All measurements were collected in 0.2 M $TBAPF_6$/dichloromethane electrolyte solution and the scan rate was 100 mVs^{-1}. $TBAPF_6$ was recrystallized twice from ethanol, ferrocene was sublimed, and all materials dried under vacuum prior to use. DCM was collected from an Innovative Technologies solvent system, sparged with Ar, and passed over two columns of 5Å activated sieves. E_{HOMO} for BTFuran was estimated from the onset of the oxidation potential (E_{onset}^{ox} ~ 1.28 V) as $E_{HOMO} = -(E_{onset}^{ox} + 4.8)$ eV = –6.1 eV.

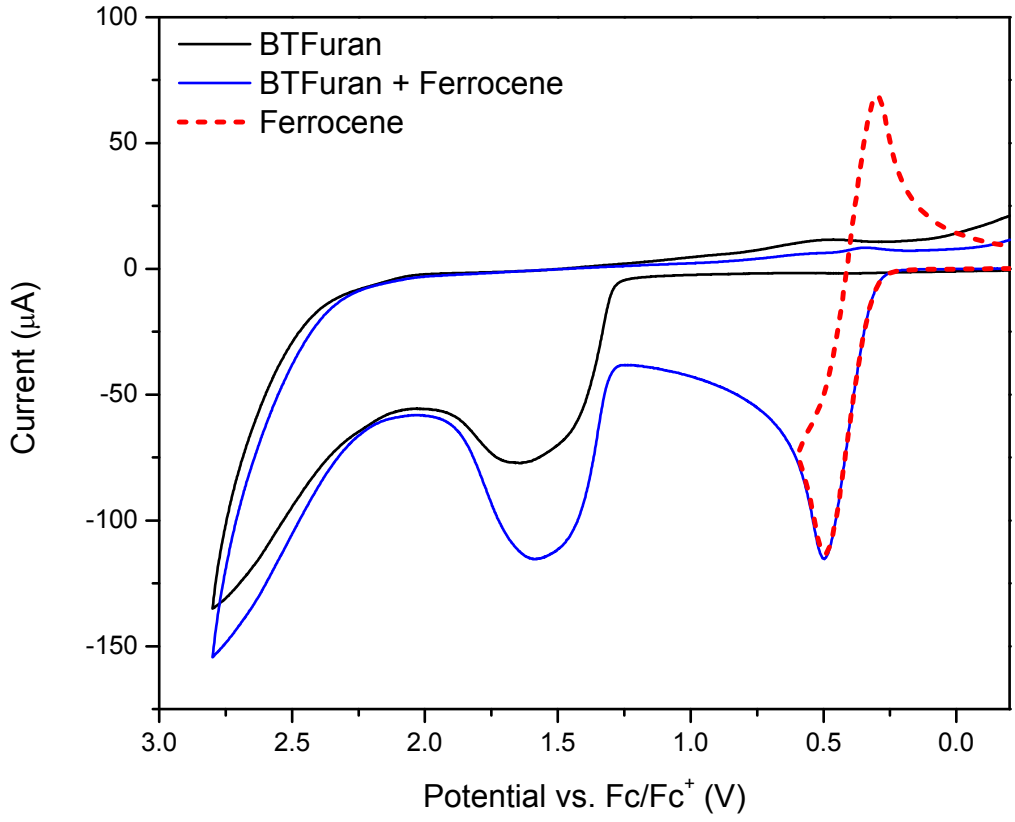
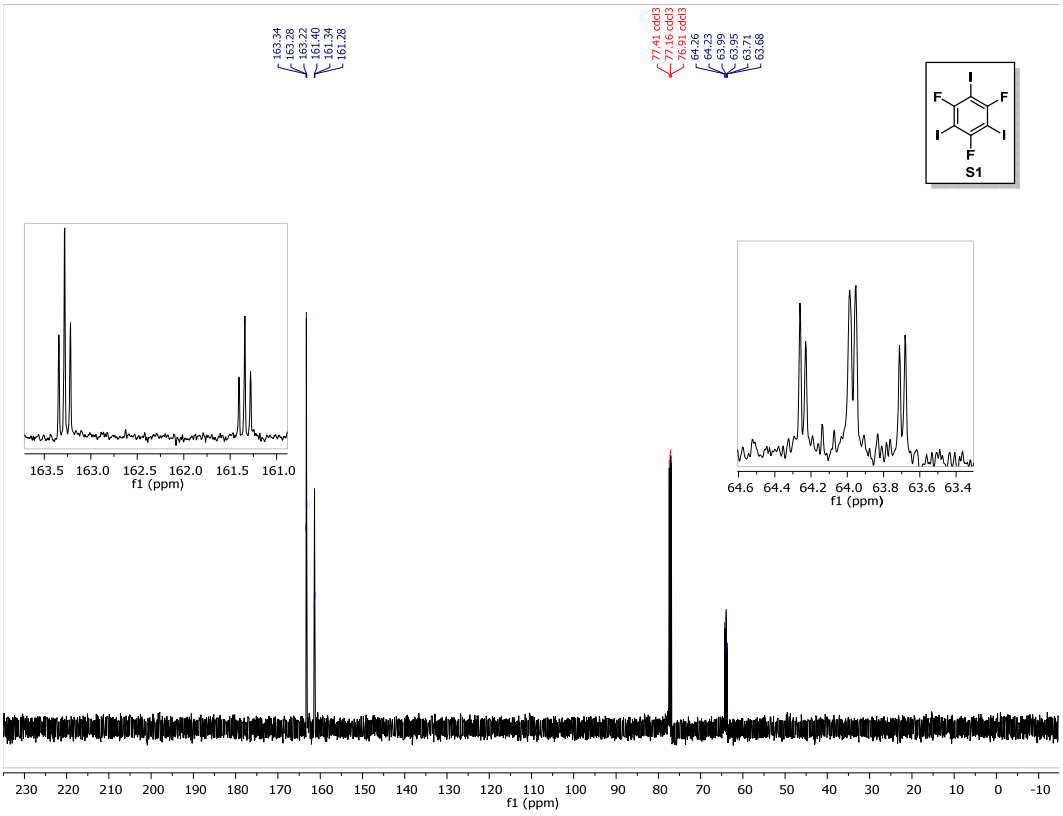
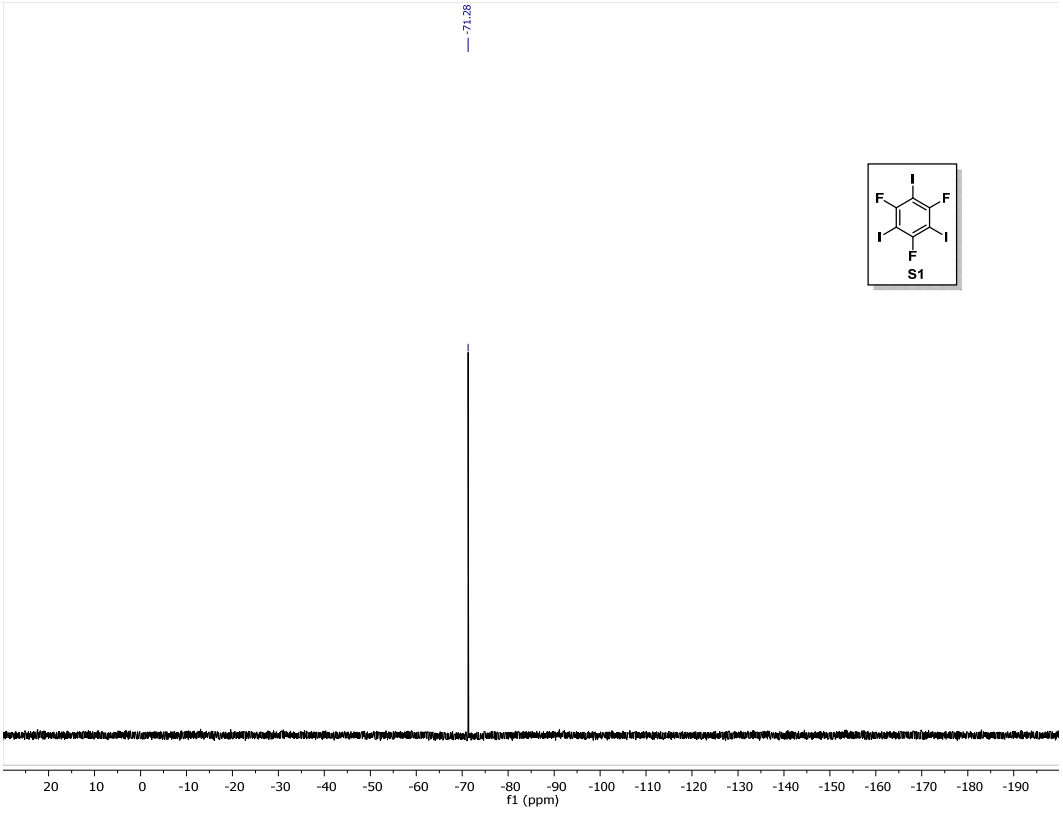
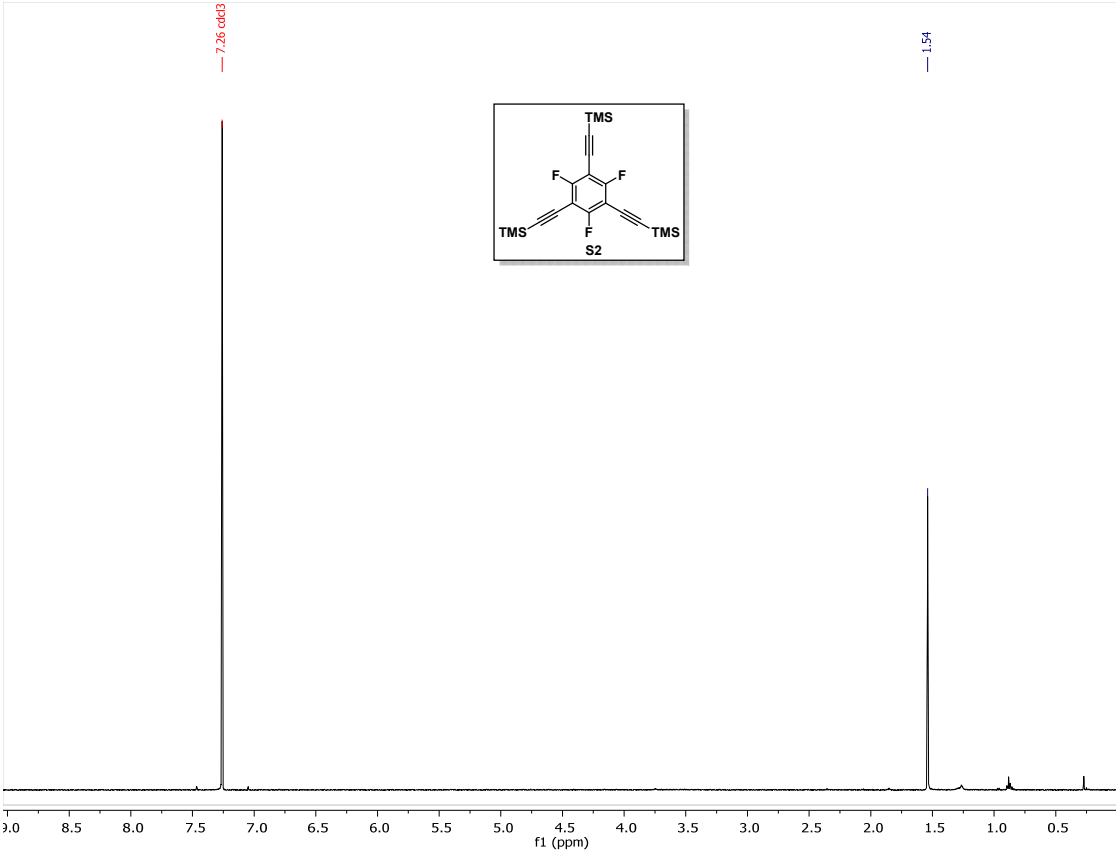


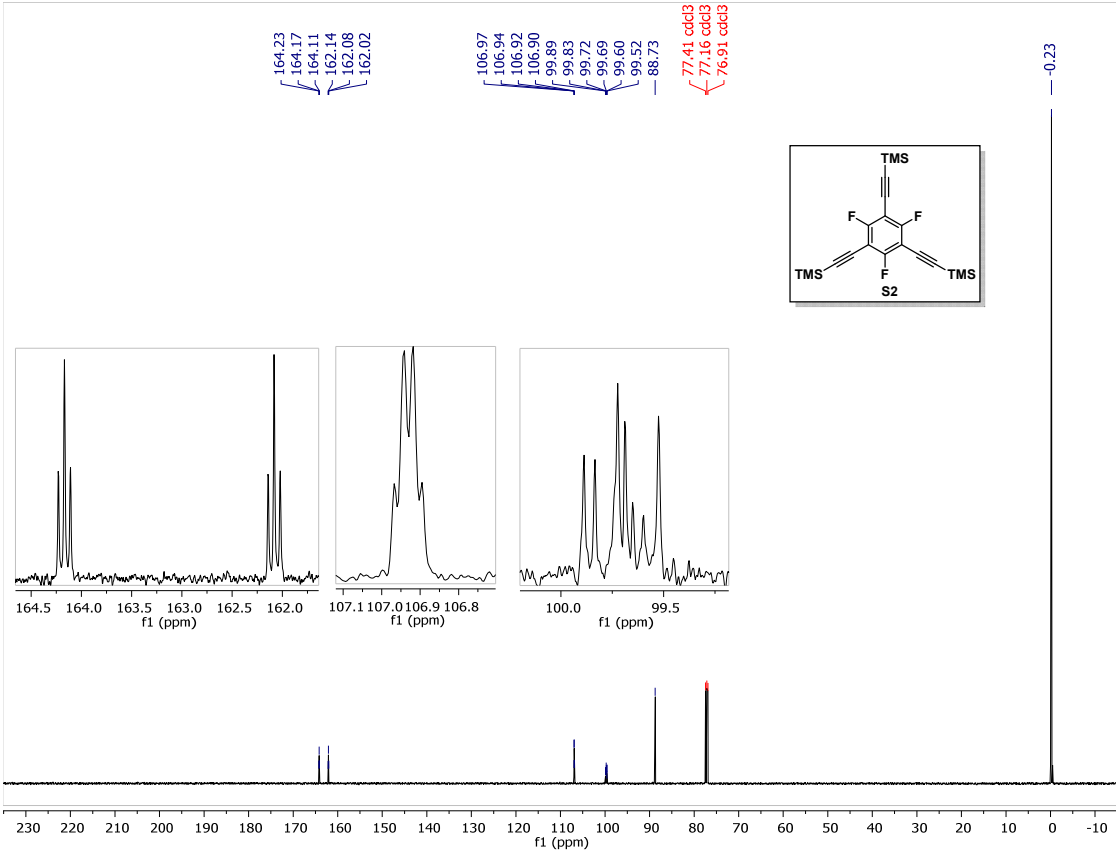
Figure S3. Cyclic voltammogram of 1 mM BTFuran (black solid line) and 1 mM BTFuran doped with ferrocene scanned in the ferrocenium/ferrocene potential window (red dashed line) and full potential window (blue solid line). The oxidation of ferrocene to ferrocenium was irreversible in the presence of BTFuran, suggesting that ferrocenium may react with BTFuran under oxidative electrochemical conditions and become effectively "trapped". This was observed in both ambient and oxygen-free (performed in glovebox, data not shown) atmosphere.

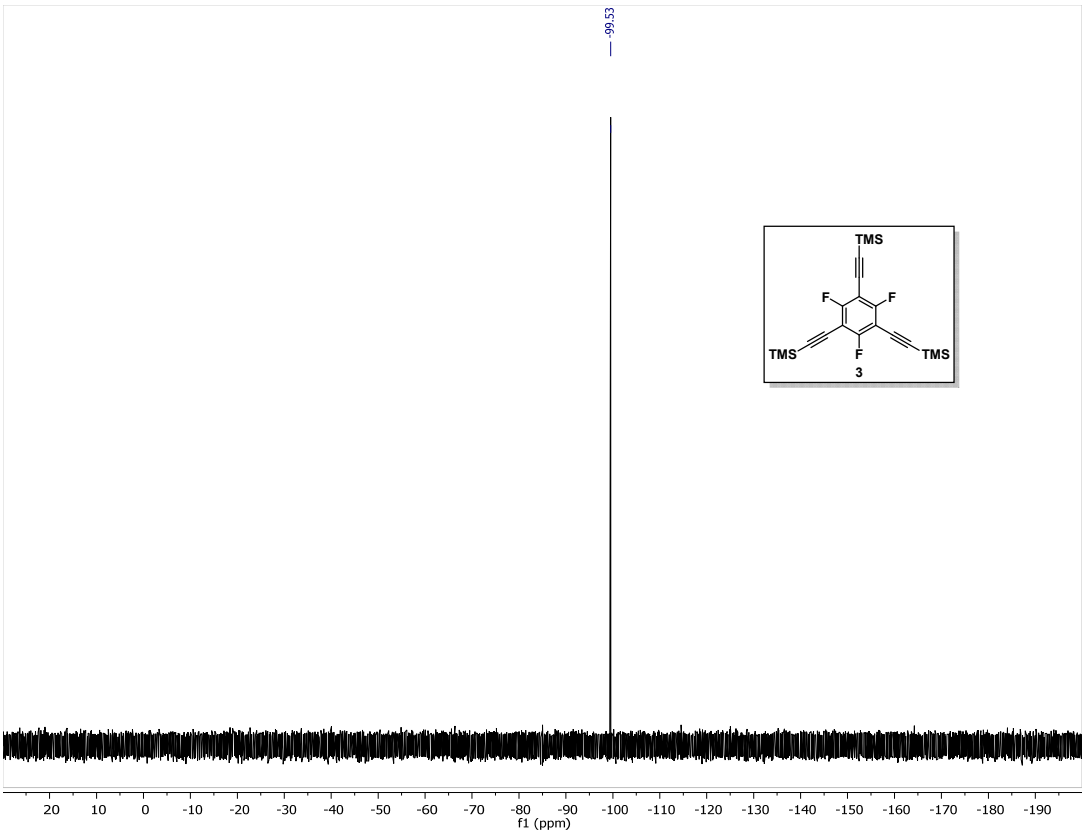
NMR spectra

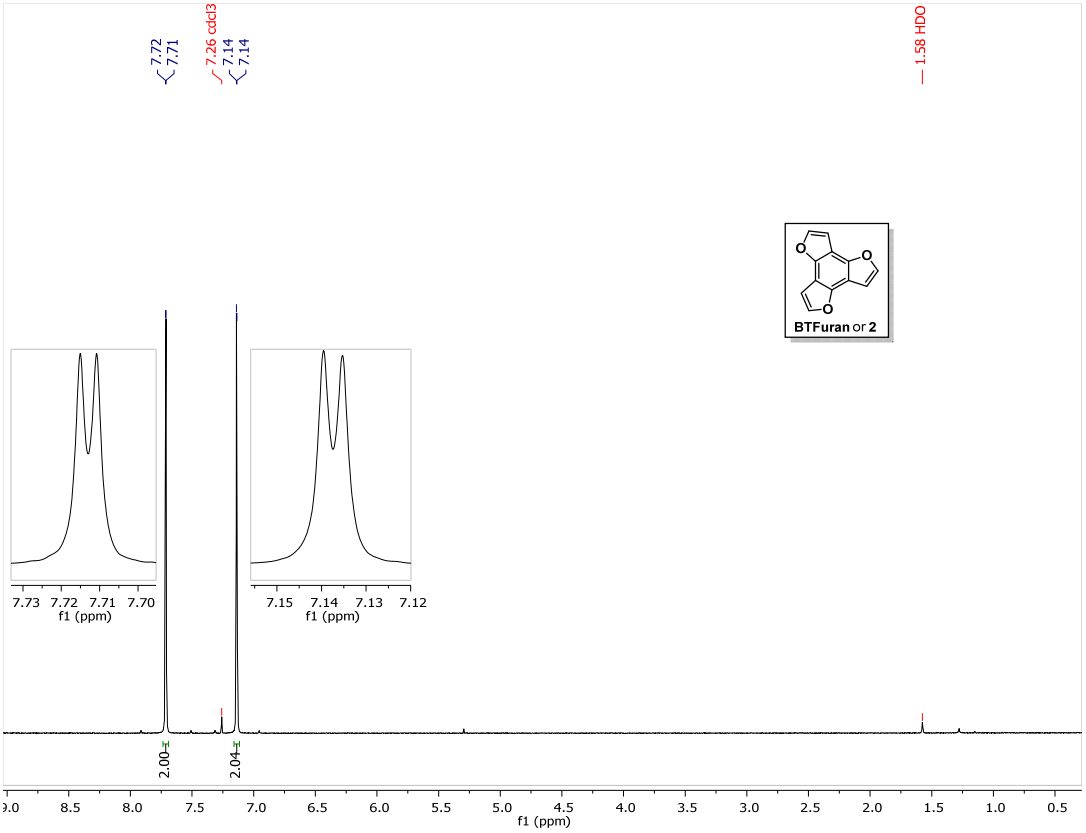

163.34
163.28
163.22
161.40
161.34
161.28
77.41 cdd3
77.16 cdd3
76.91 cdd3
64.26
64.23
63.99
63.95
63.71
63.68
S1
163.5 163.0 162.5 162.0 161.5 161.0
f1 (ppm)
64.6 64.4 64.2 64.0 63.8 63.6 63.4
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

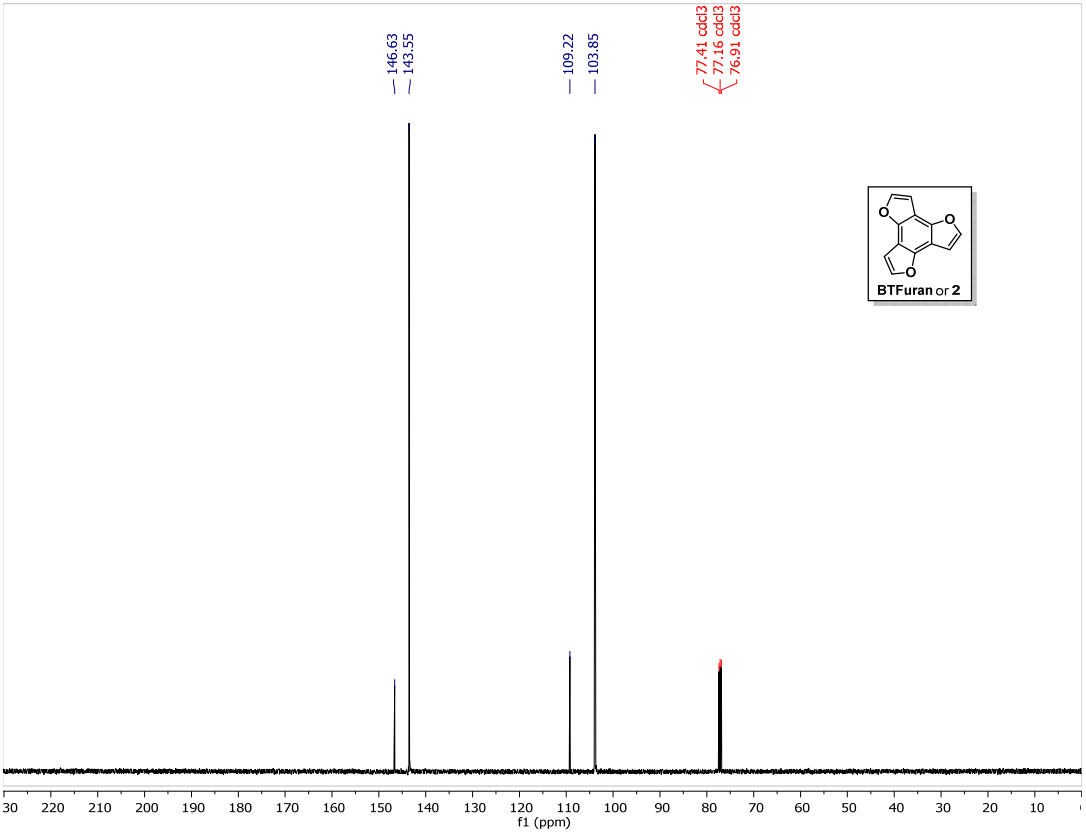

-71.28
S1
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

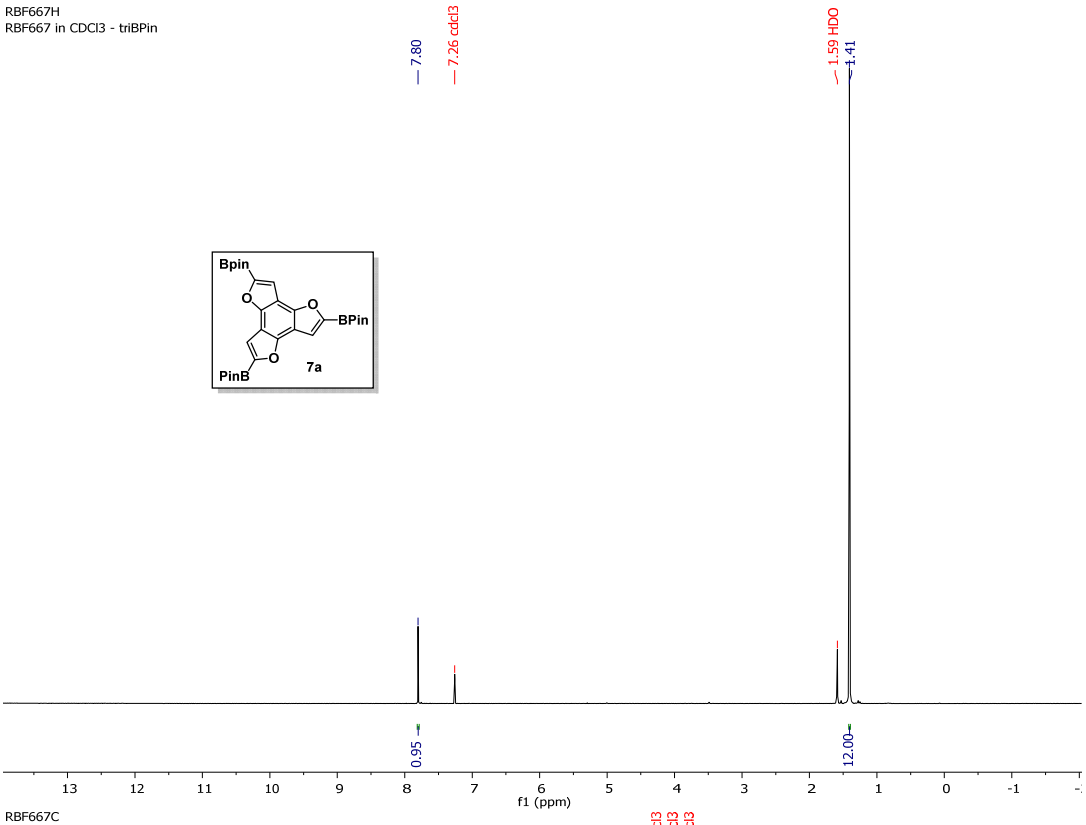

7.26 cdcl3
1.54
TMS
F
F
TMS
F
TMS
S2
f1 (ppm)

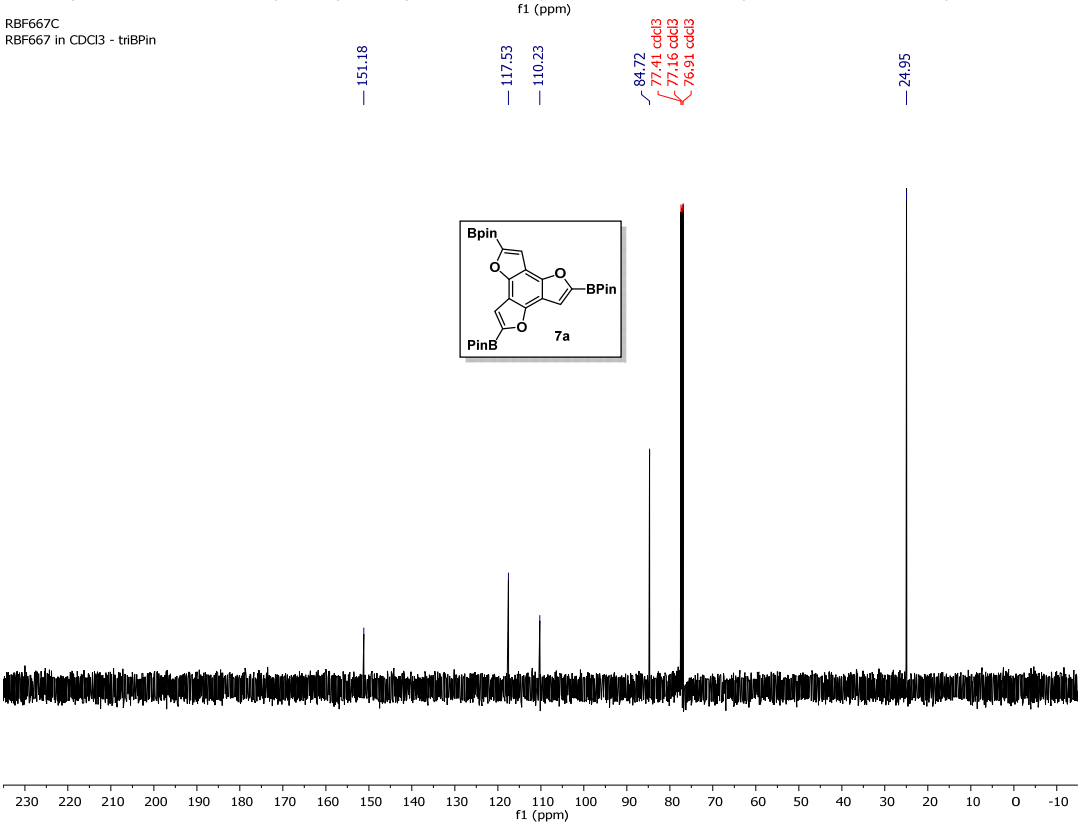

164.23
164.17
164.11
162.14
162.08
162.02
106.97
106.94
106.92
106.90
99.89
99.83
99.72
99.69
99.60
99.52
88.73
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
-0.23
TMS
F
F
TMS
F
TMS
S2
164.5 164.0 163.5 163.0 162.5 162.0
f1 (ppm)
107.1 107.0 106.9 106.8
f1 (ppm)
100.0 99.5
f1 (ppm)
f1 (ppm)


-99.53
TMS
F
F
TMS
F
TMS
3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

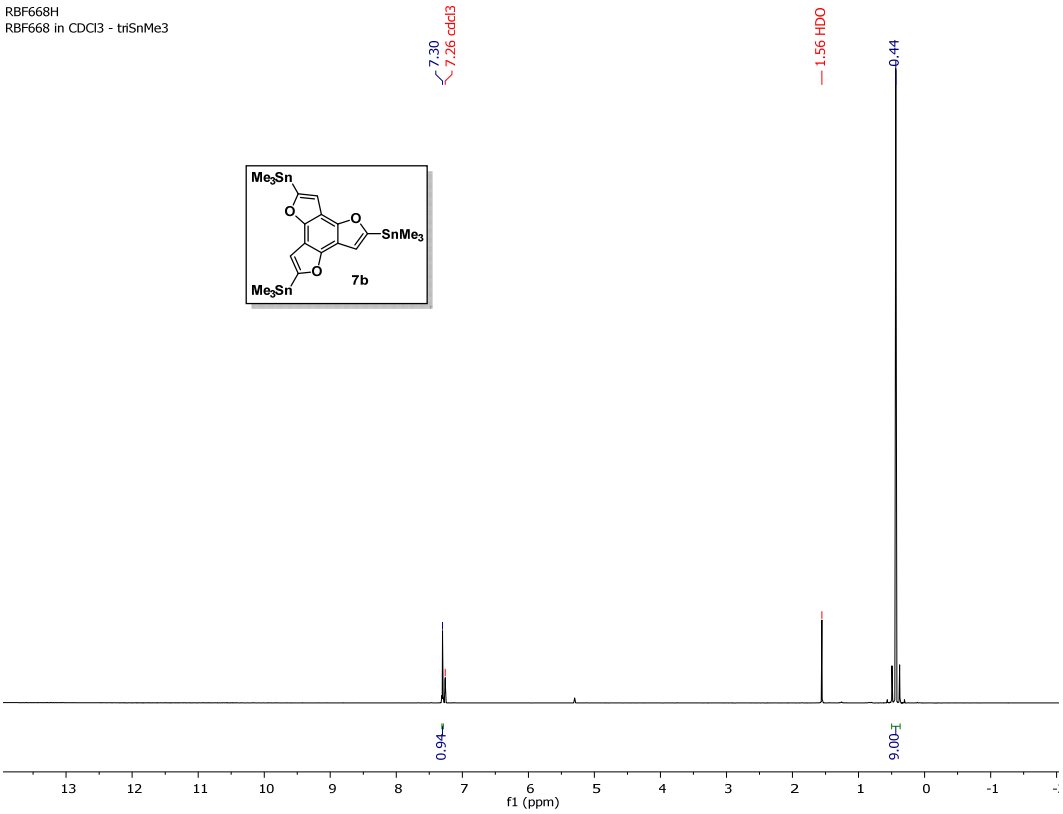

7.72
7.71
7.26 cdcl3
7.14
7.14
1.58 HDO
BTFuran or 2
7.73 7.72 7.71 7.70
f1 (ppm)
7.15 7.14 7.13 7.12
f1 (ppm)
2.00
2.04
f1 (ppm)


146.63
143.55
109.22
103.85
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
BTFuran or 2
f1 (ppm)

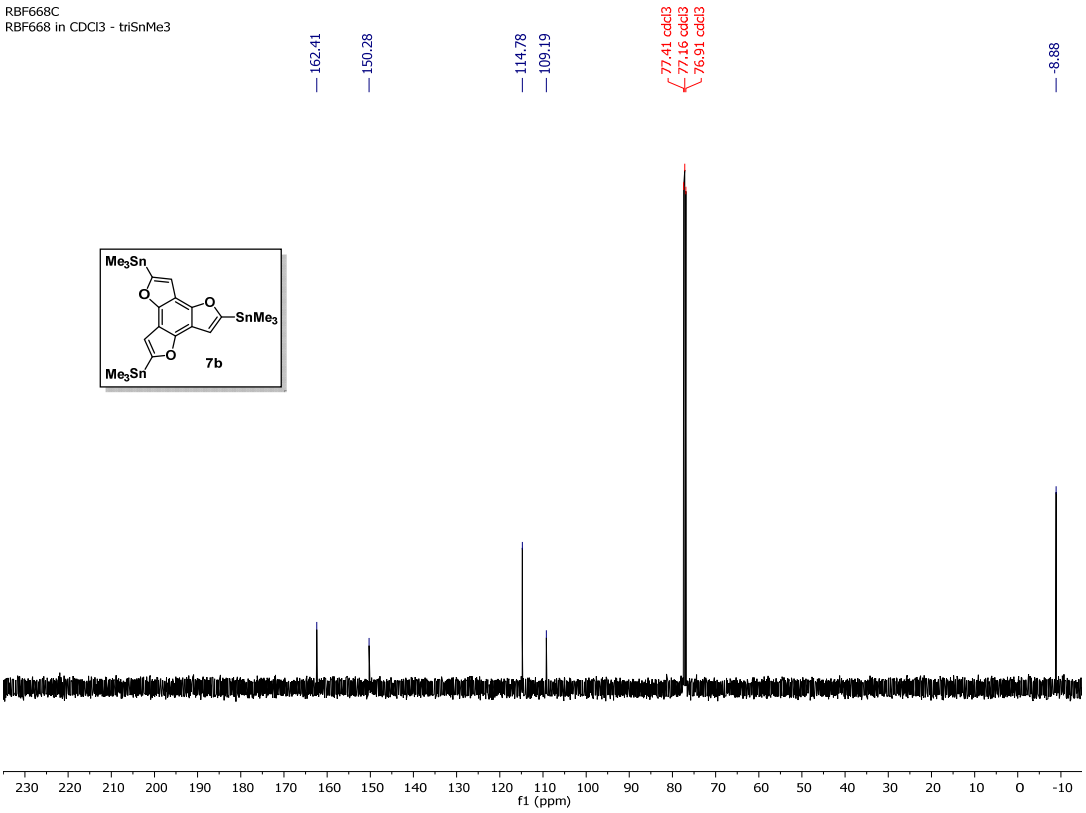

RBF667H
RBF667 in CDCl3 - triBPin
7.80
7.26 cdcl3
1.59 HDO
1.41
Bpin
BPin
PinB
7a
0.95
12.00
f1 (ppm)


RBF667C
RBF667 in CDCl3 - triBPin
151.18
117.53
110.23
84.72
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
24.95
Bpin
BPin
PinB
7a
f1 (ppm)

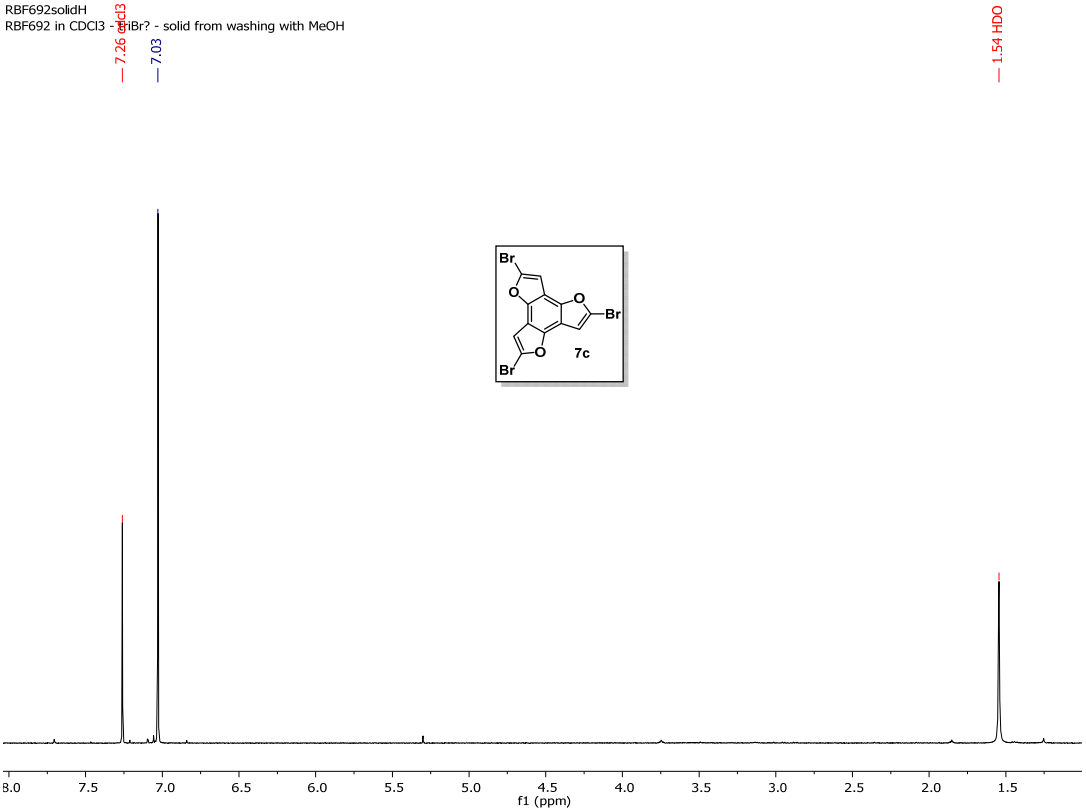
RBF668H
RBF668 in CDCl3 - triSnMe3



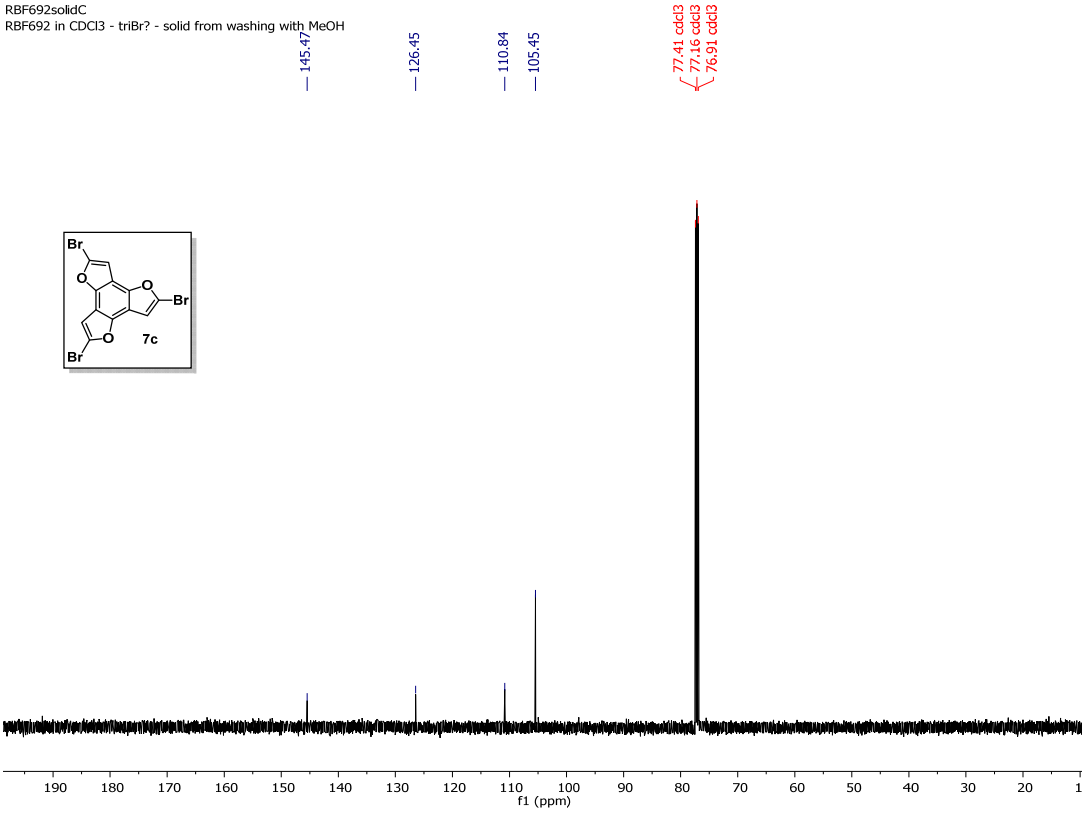
RBF668C
RBF668 in CDCl3 - triSnMe3



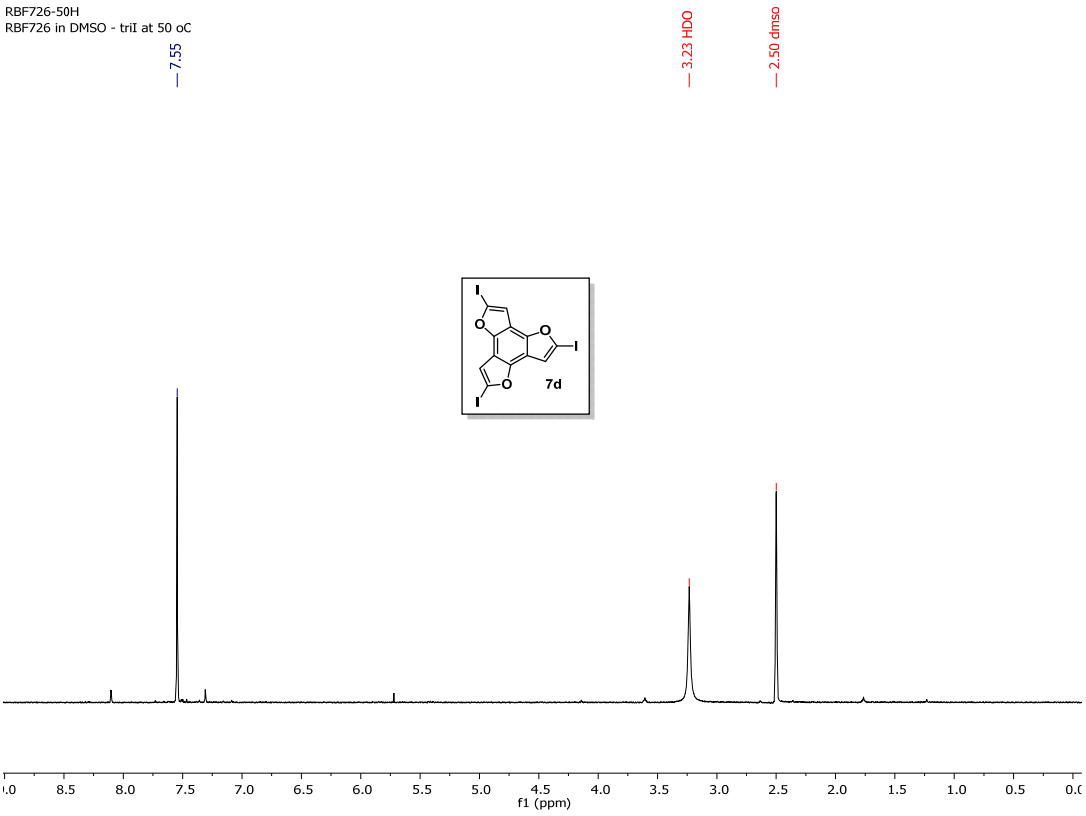
RBF692solidH
RBF692 in CDCl3 - triBr? - solid from washing with MeOH



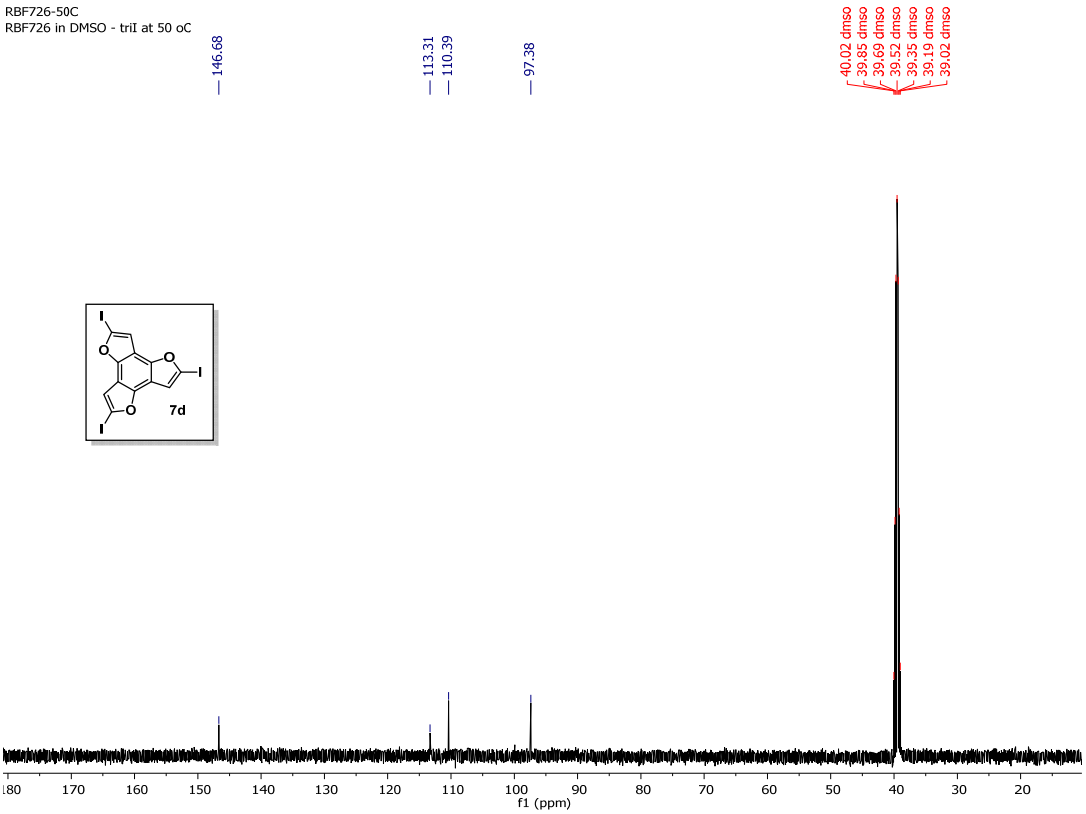
RBF692solidC
RBF692 in CDCl3 - triBr? - solid from washing with MeOH

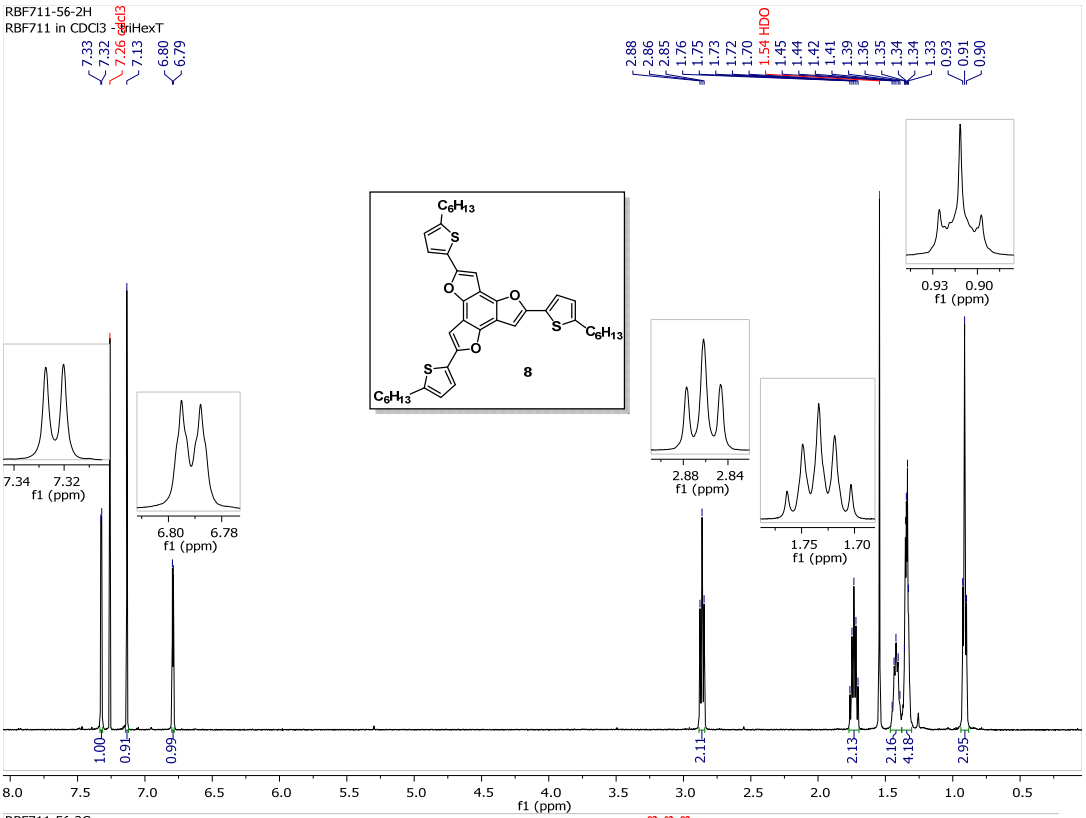


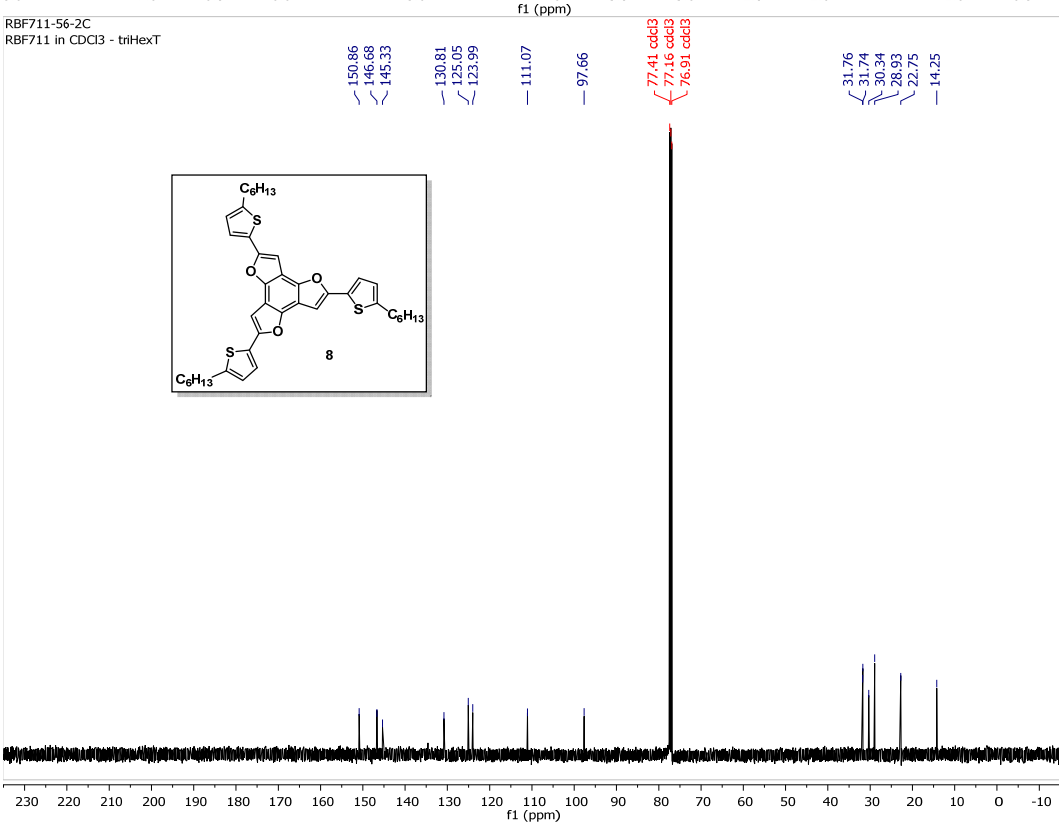
RBF726-50H
RBF726 in DMSO - triI at 50 oC

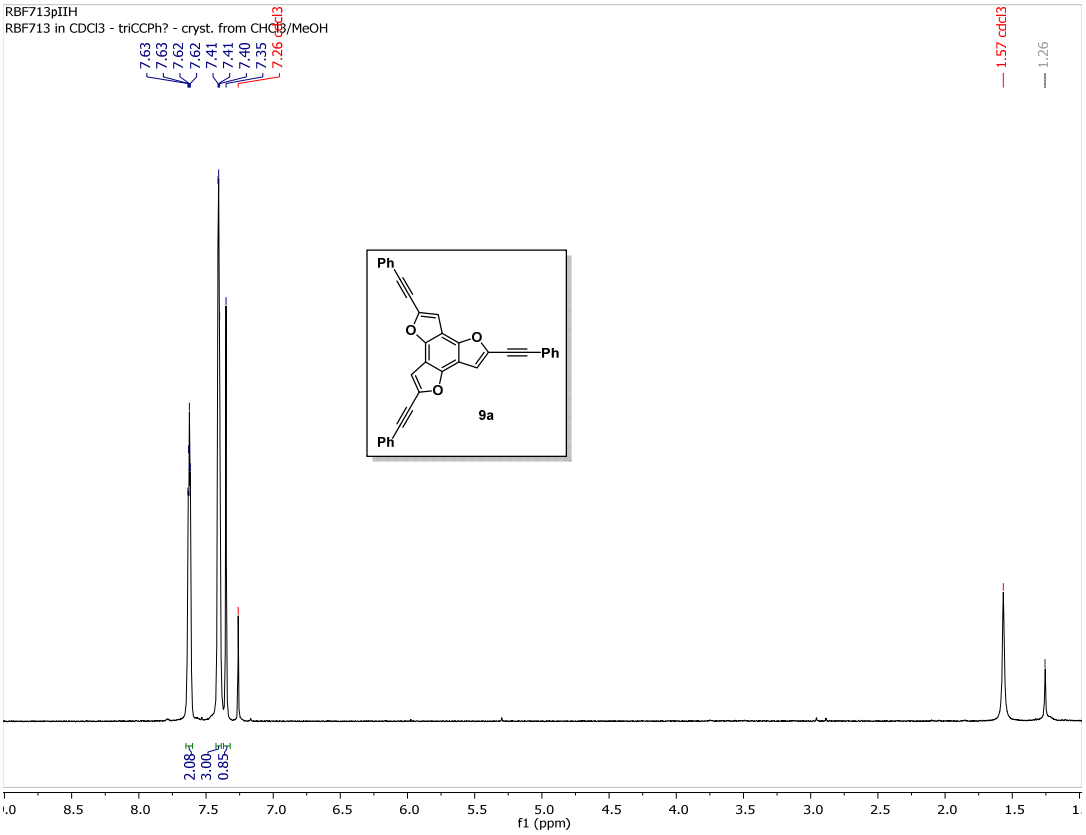


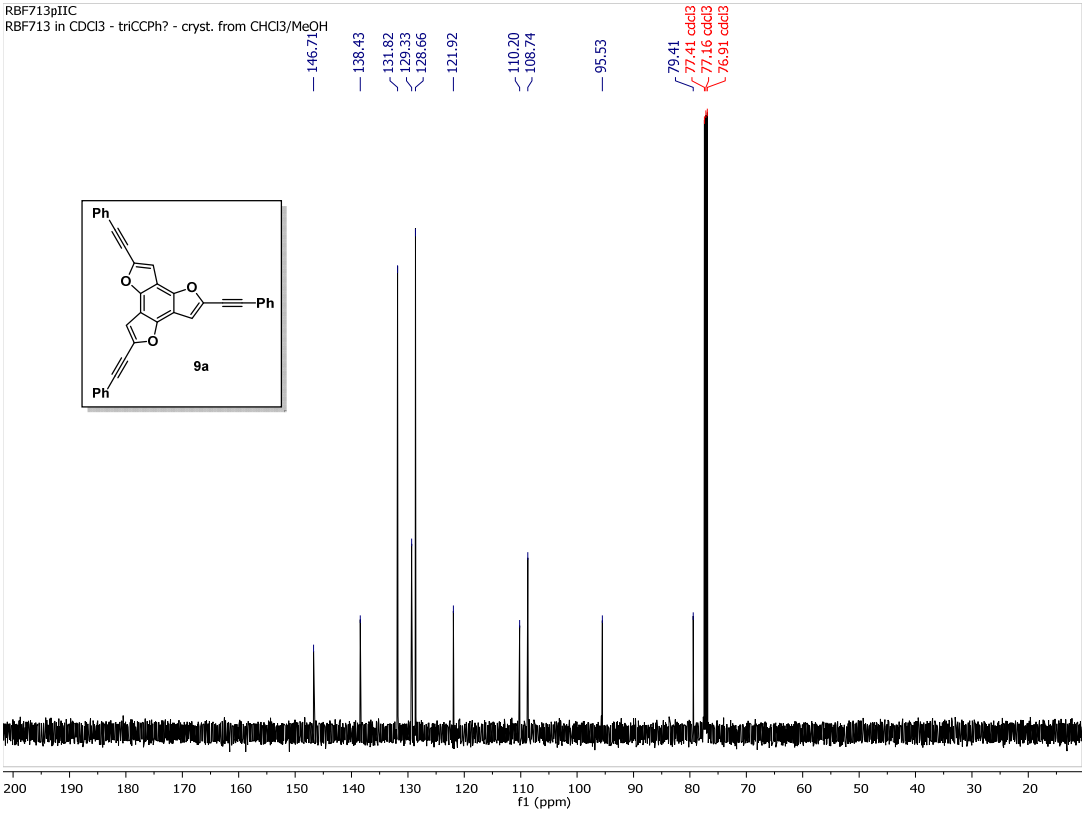
RBF726-50C
RBF726 in DMSO - triI at 50 oC

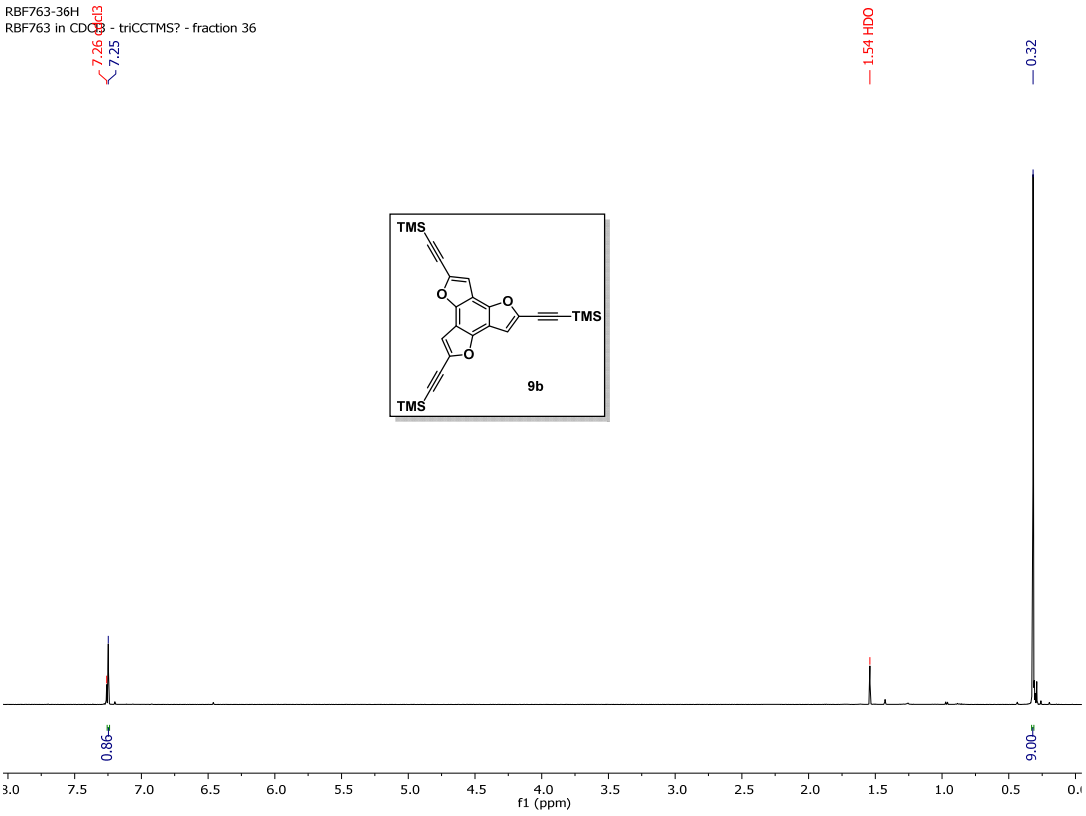


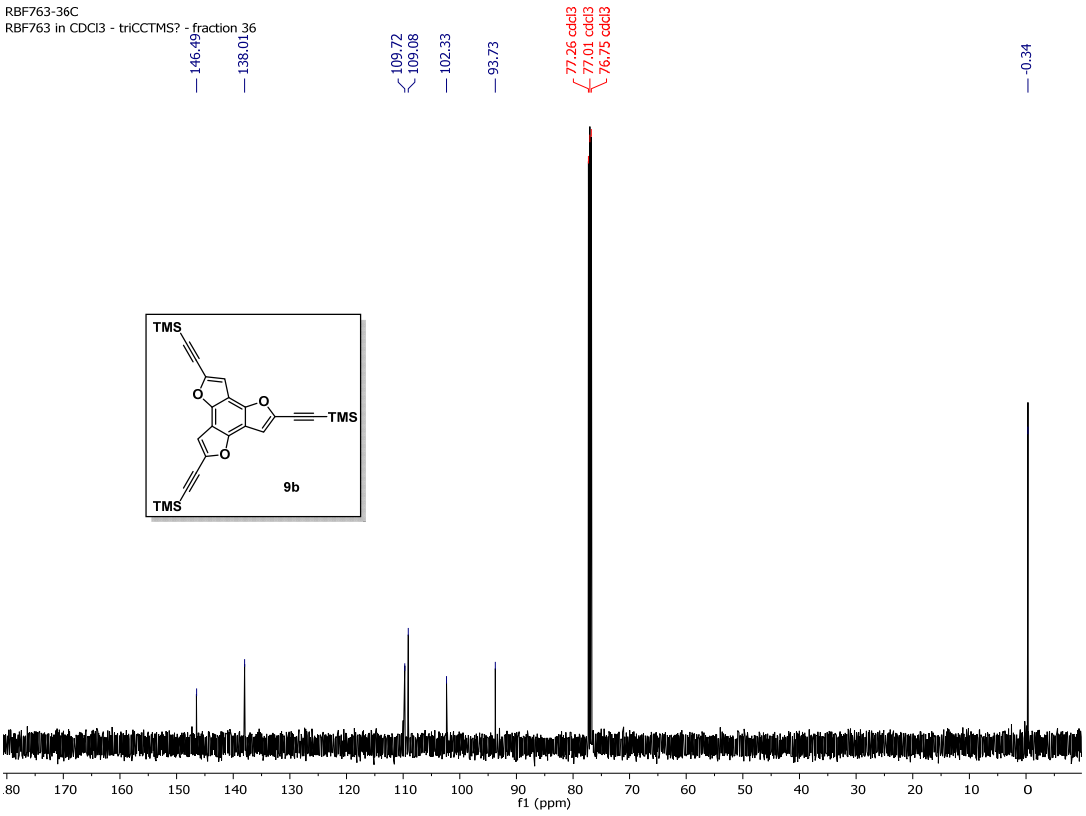

RBF711-56-2H
RBF711 in CDCl3 - triHexT
7.33
7.32
7.26 cdcl3
7.13
6.80
6.79
2.88
2.86
2.85
1.76
1.75
1.73
1.72
1.70
1.54 HDO
1.45
1.44
1.42
1.41
1.39
1.36
1.35
1.34
1.34
1.33
0.93
0.91
0.90
8
7.34 7.32
f1 (ppm)
6.80 6.78
f1 (ppm)
2.88 2.84
f1 (ppm)
1.75 1.70
f1 (ppm)
0.93 0.90
f1 (ppm)
1.00
0.91
0.99
2.11
2.13
2.16
4.18
2.95
f1 (ppm)

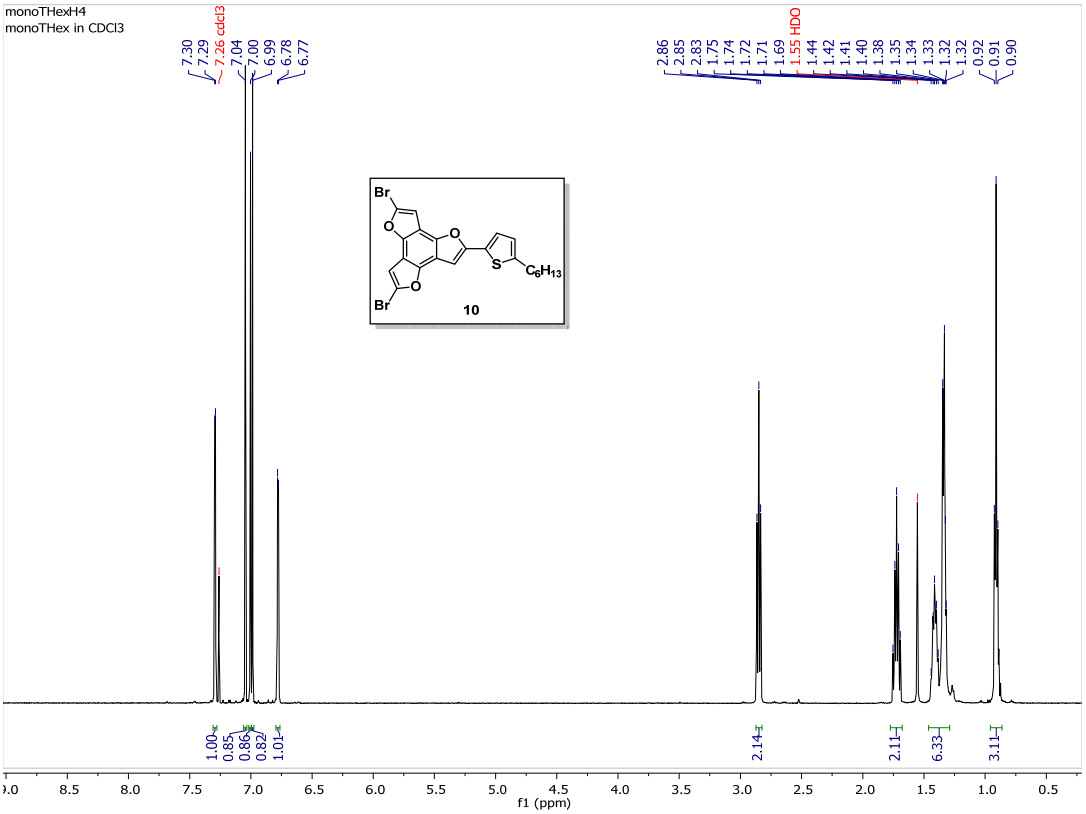

RBF711-56-2C
RBF711 in CDCl3 - triHexT
150.86
146.68
145.33
130.81
125.05
123.99
111.07
97.66
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
31.76
31.74
30.34
28.93
22.75
14.25
8
f1 (ppm)

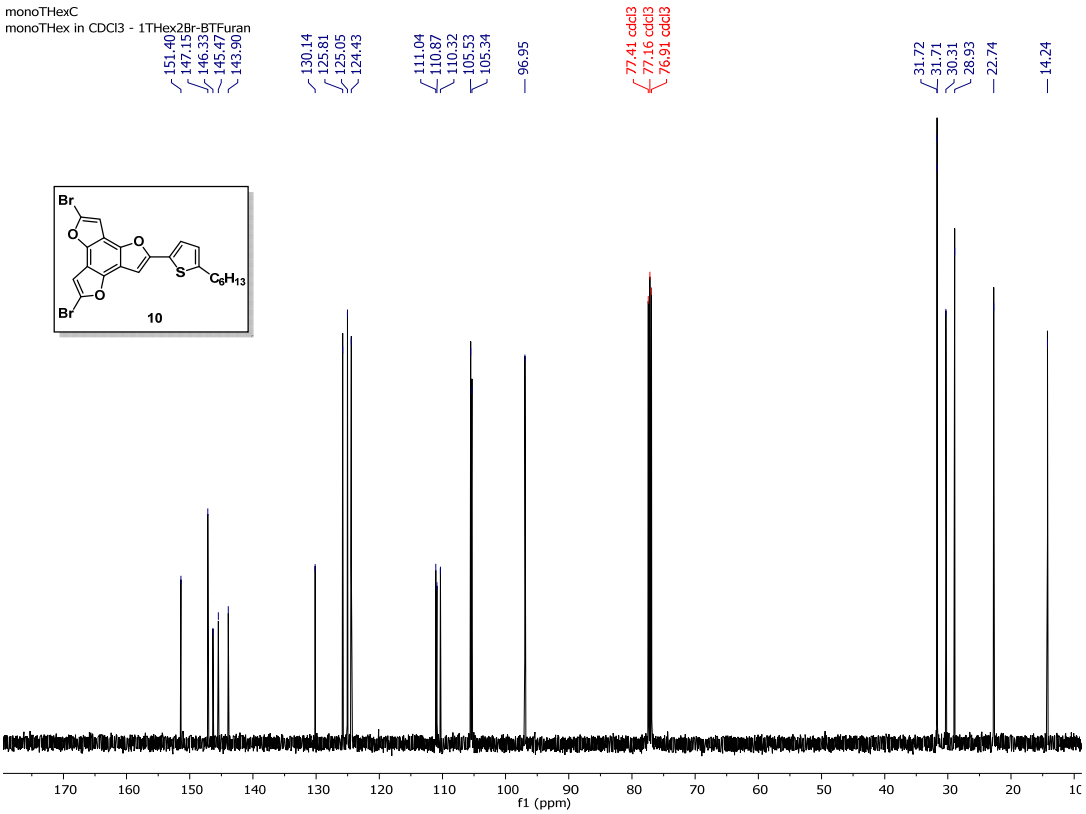

RBF713pIIH
RBF713 in CDCl3 - triCCPh? - cryst. from CHCl3/MeOH
7.63
7.63
7.62
7.62
7.41
7.41
7.40
7.35
7.26 cdcl3
1.57 cdcl3
1.26
Ph
O
O
Ph
O
Ph
9a
2.08
3.00
0.85
f1 (ppm)

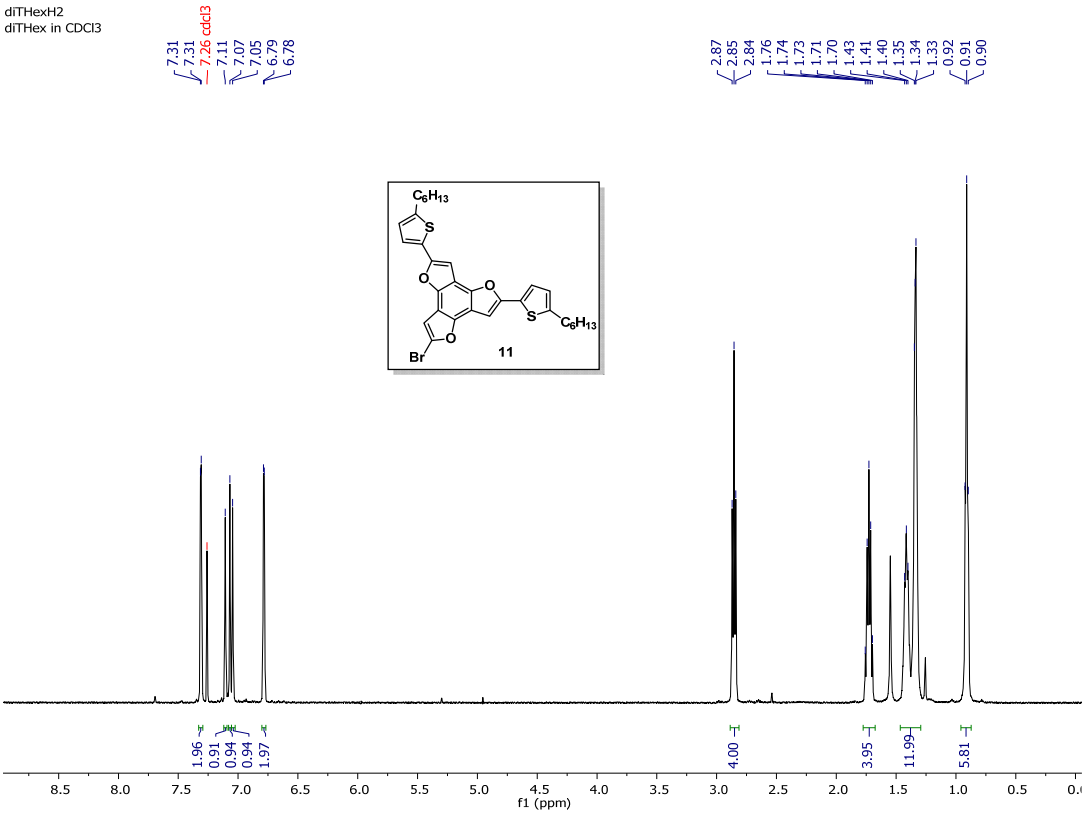

RBF713pIIC
RBF713 in CDCl3 - triCCPh? - cryst. from CHCl3/MeOH
146.71
138.43
131.82
129.33
128.66
121.92
110.20
108.74
95.53
79.41
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
Ph
O
O
Ph
O
Ph
9a
f1 (ppm)

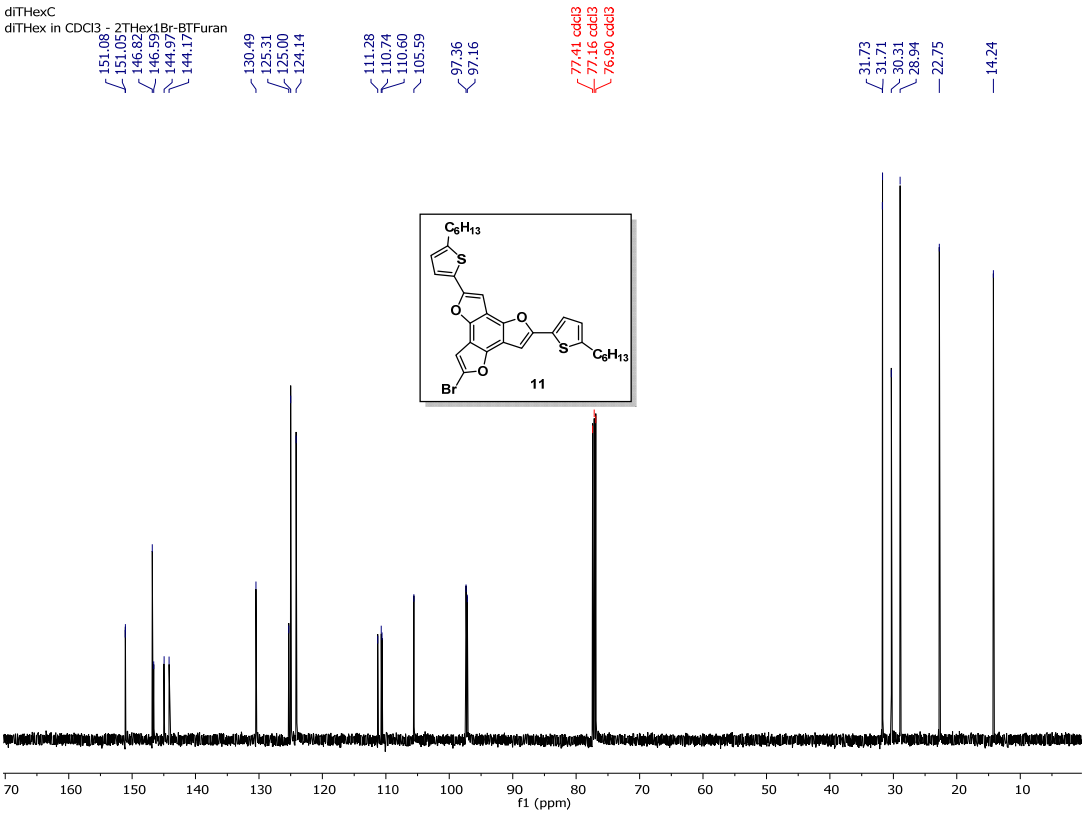

RBF763-36H
RBF763 in CDCl3 - triCCTMS? - fraction 36
7.26 cdcl3
7.25
1.54 HDO
0.32
TMS
TMS
TMS
9b
0.86
9.00
f1 (ppm)


RBF763-36C
RBF763 in CDCl3 - triCCTMS? - fraction 36
146.49
138.01
109.72
109.08
102.33
93.73
77.26 cdcl3
77.01 cdcl3
76.75 cdcl3
-0.34
TMS
TMS
TMS
9b
f1 (ppm)


monoTHexH4
monoTHex in CDCl3
7.30
7.29
7.26 cdcl3
7.04
7.00
6.99
6.78
6.77
2.86
2.85
2.83
1.75
1.74
1.72
1.71
1.69
1.55 HDO
1.44
1.42
1.41
1.40
1.38
1.35
1.34
1.33
1.32
1.32
0.92
0.91
0.90
Br
O
O
O
S
C6H13
Br
10
1.00
0.85
0.86
0.82
1.01
2.14
2.11
6.33
3.11
f1 (ppm)


monoTHexC
monoTHex in CDCl3 - 1THex2Br-BTFuran
151.40
147.15
146.33
145.47
143.90
130.14
125.81
125.05
124.43
111.04
110.87
110.32
105.53
105.34
96.95
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
31.72
31.71
30.31
28.93
22.74
14.24
Br
O
O
O
S
C6H13
Br
10
f1 (ppm)


diTHexH2
diTHex in CDCl3
7.31
7.31
7.26 cdcl3
7.11
7.07
7.05
6.79
6.78
2.87
2.85
2.84
1.76
1.74
1.73
1.71
1.70
1.43
1.41
1.40
1.35
1.34
1.33
0.92
0.91
0.90
11
1.96
0.91
0.94
0.94
1.97
4.00
3.95
11.99
5.81
f1 (ppm)


diTHexC
diTHex in CDCl3 - 2THex1Br-BTFuran
151.08
151.05
146.82
146.59
144.97
144.17
130.49
125.31
125.00
124.14
111.28
110.74
110.60
105.59
97.36
97.16
77.41 cdcl3
77.16 cdcl3
76.90 cdcl3
31.73
31.71
30.31
28.94
22.75
14.24
11
f1 (ppm)

X-ray crystallography details

X-ray intensity data were collected at 100 K on a Bruker DUO diffractometer using MoKα radiation (λ = 0.71073 Å) and an APEXII CCD area detector.

Raw data frames were read by program SAINT[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces.

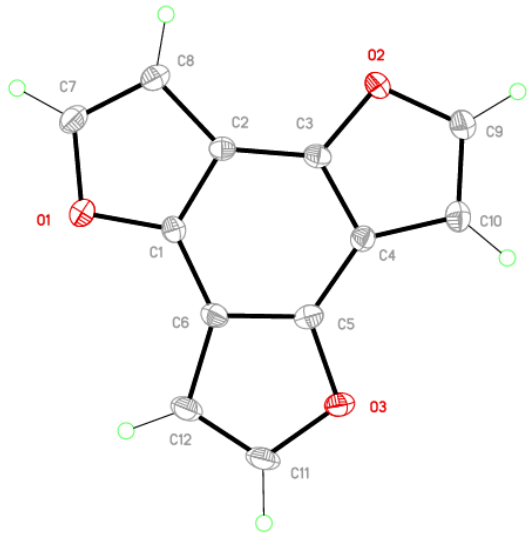
The structure was solved and refined in *SHELXTL2014* (Bruker-AXS, Madison, Wisconsin, USA), using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. Although the value of the Flack x parameter, 0.5(2), suggests the presence of higher symmetry, the fact that the X-ray source is Mo and the error is very high, and the absence of heavy atoms, indicate that it is not reliable to distinguish between space groups P6(5), P6(1), or any higher symmetry space group. Additionally, the molecules are not chiral. In the final cycle of refinement, 1972 reflections (of which 1897 are observed with $I > 2\sigma(I)$) were used to refine 136 parameters and the resulting R1, wR2 and S (goodness of fit) were 2.99%, 7.83%, and 1.110, respectively. The refinement was carried out by minimizing the wR2 function using F2 rather than F values. R1 is calculated to provide a reference to the conventional R value but its function is not minimized.

The structure was solved and refined in SHELXTL6.1, using full-matrix least-squares refinement.

Table S3. Crystal data and structure refinement for BTFuran.

Identification code	renan2	
Empirical formula	C12 H6 O3	
Formula weight	198.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_5	
Unit cell dimensions	a = 8.7768(4) Å	α = 90°.
	b = 8.7768(4) Å	β = 90°.
	c = 19.3349(9) Å	γ = 120°.
Volume	1289.87(13) $Å^3$	
Z	6	
Density (calculated)	1.531 Mg/m^3	
Absorption coefficient	0.111 mm^{-1}	
F(000)	612	
Crystal size	0.228 x 0.129 x 0.114 mm^3	
Theta range for data collection	2.680 to 27.461°.	
Index ranges	-11≤h≤11, -11≤k≤11, -24≤l≤25	
Reflections collected	24932	
Independent reflections	1972 [R(int) = 0.0225]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Analytical	
Max. and min. transmission	0.9948 and 0.9883	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1972 / 1 / 136	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0299, wR2 = 0.0783 [1897]	
R indices (all data)	R1 = 0.0313, wR2 = 0.0789	
Absolute structure parameter	0.5(2)	
Largest diff. peak and hole	0.320 and -0.184 $e.Å^{-3}$	

Table S4. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2× 10^3) for BTFuran. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.



	x	y	z	U(eq)
O(1)	3526(2)	316(2)	1517(1)	18(1)
O(2)	-1766(2)	480(2)	1780(1)	18(1)
O(3)	3734(2)	5776(2)	1803(1)	20(1)
C(1)	2779(3)	1351(3)	1604(1)	14(1)
C(2)	954(3)	328(3)	1631(1)	14(1)
C(3)	25(2)	1234(3)	1728(1)	14(1)
C(4)	834(3)	3051(3)	1787(1)	14(1)
C(5)	2676(3)	3986(3)	1749(1)	16(1)
C(6)	3695(3)	3194(3)	1661(1)	16(1)
C(7)	2131(3)	-1396(3)	1483(1)	19(1)
C(8)	566(3)	-1465(3)	1545(1)	18(1)
C(9)	-2080(3)	1862(3)	1866(1)	19(1)
C(10)	-568(3)	3435(3)	1880(1)	18(1)
C(11)	5441(3)	6095(3)	1752(1)	23(1)
C(12)	5491(3)	4601(3)	1663(1)	21(1)

Cartesian coordinates of minimized geometries (in Å)

BTT (**1**)

Atom	X	Y	Z
S	-1.368068	2.810448	0.000000
C	-0.517969	1.296044	0.000000
C	-1.406201	0.214875	0.000000
C	-2.779045	0.641335	0.000000
C	-2.898654	1.993348	0.000000
C	0.889860	1.111344	0.000000
C	1.381255	-0.198609	0.000000
C	0.517713	-1.325953	0.000000
C	-0.862239	-1.096462	0.000000
C	0.833168	-2.728578	0.000000
C	-0.278451	-3.507313	0.000000
S	-1.750608	-2.588226	0.000000
S	3.117537	-0.221544	0.000000
C	3.176999	1.512694	0.000000
C	1.946560	2.086054	0.000000
H	1.783325	3.158212	0.000000
H	4.137301	2.010897	0.000000
H	1.843294	-3.123290	0.000001
H	-0.327503	-4.588060	0.000000
H	-3.625582	-0.036615	0.000000
H	-3.810592	2.575325	0.000000

BTFuran (**2**)

Atom	X	Y	Z
C	-2.158101	-1.851224	0.000001
C	-1.203671	-0.770855	0.000001
C	0.060880	-1.379086	0.000001
O	-0.073830	-2.739218	0.000000
C	-1.425223	-2.995157	-0.000003
C	-1.224727	0.636889	0.000001
C	-0.065751	1.427950	0.000002
C	1.163968	0.742270	0.000002
C	1.269532	-0.656949	0.000001
C	-0.524292	2.794668	-0.000001
C	-1.881432	2.731677	-0.000001
O	-2.335422	1.433367	-0.000001
C	2.682373	-0.943330	0.000003
C	3.306564	0.263359	-0.000004
O	2.409206	1.305688	0.000001
H	4.346584	0.553216	-0.000009
H	3.158046	-1.913963	0.000004
H	-2.652545	3.487334	-0.000002
H	0.078329	3.692068	0.000000
H	-1.694234	-4.040762	-0.000005
H	-3.236543	-1.777862	0.000004

7c

Atom	X	Y	Z
C	-2.159975	1.849037	-0.000001
C	-1.204451	0.769636	-0.000001
C	0.059483	1.379147	-0.000001
O	-0.076604	2.739142	0.000000
C	-1.428256	2.993712	0.000003
C	-1.224081	-0.638129	-0.000001
C	-0.064305	-1.428016	-0.000002
C	1.164719	-0.741091	-0.000002
C	1.268866	0.658234	-0.000001
C	-0.521461	-2.795198	0.000001
C	-1.878664	-2.733581	0.000001
O	-2.333969	-1.435732	0.000001
C	2.681416	0.946046	-0.000003
C	3.306829	-0.260010	0.000004
O	2.410527	-1.303247	-0.000001
H	3.156106	1.917160	-0.000004
H	0.082068	-3.691987	0.000000
H	-3.238342	1.774583	-0.000004
Br	-1.906030	4.842991	0.000007
Br	-3.241486	-4.071795	0.000003
Br	5.147227	-0.770928	0.000013

8' (**8** with a shorter propyl chain)

Atom	X	Y	Z
C	0.733921	2.740277	-0.000017
C	0.557593	1.315820	-0.000011
C	-0.831240	1.101517	-0.000005
O	-1.489329	2.298168	-0.000007
C	-0.521803	3.289325	-0.000014
C	1.370451	0.168579	-0.000010
C	0.861595	-1.141364	-0.000005
C	-0.538383	-1.271737	0.000001
C	-1.418363	-0.176057	0.000001
C	2.007088	-2.006261	-0.000006
C	3.110447	-1.193312	-0.000013
O	2.735823	0.140159	-0.000015
C	-2.740148	-0.735547	0.000008
C	-2.587837	-2.097550	0.000011
O	-1.245710	-2.440004	0.000007
H	-3.678166	-0.198183	0.000010
H	2.010591	-3.087272	-0.000003
H	1.668394	3.283754	-0.000023
C	4.529617	-1.447744	-0.000017
C	5.558973	-0.532818	-0.000021
S	5.163249	-3.082761	-0.000013
C	6.849800	-1.139326	-0.000024
H	5.390081	0.538008	-0.000022
C	6.820865	-2.511631	-0.000022

H	7.771451	-0.567492	-0.000027
C	-1.010822	4.645673	-0.000018
C	-2.317740	5.079997	-0.000030
S	0.088768	6.011586	-0.000003
C	-2.437482	6.501183	-0.000031
H	-3.160770	4.398466	-0.000038
C	-1.234357	7.161884	-0.000020
H	-3.393238	7.013999	-0.000040
C	-3.518329	-3.198882	0.000018
C	-3.241617	-4.547982	0.000024
S	-5.250873	-2.928732	0.000021
C	-4.412921	-5.361702	0.000030
H	-2.230045	-4.937709	0.000024
C	-5.586324	-4.649585	0.000030
H	-4.379552	-6.445802	0.000035
C	-7.011968	-5.138972	0.000034
H	-7.536169	-4.731501	0.876403
H	-7.536169	-4.731517	-0.876342
C	7.958263	-3.500722	-0.000028
H	7.868135	-4.158416	-0.876461
H	7.868117	-4.158449	0.876378
C	-0.946379	8.641453	-0.000024
H	-0.331714	8.892397	0.876347
H	-0.331768	8.892403	-0.876431
C	-7.145293	-6.666799	0.000048
H	-6.678945	-7.109631	-0.887470
H	-6.678944	-7.109615	0.887573
C	9.347412	-2.850890	-0.000001
H	9.496896	-2.225425	-0.887511
H	9.496872	-2.225449	0.887530
C	-2.203967	9.519262	0.000018
H	-2.820275	9.335768	-0.887502
H	-2.820228	9.335749	0.887566
C	-8.632454	-7.066741	0.000053
H	-8.714893	-8.133561	0.000037
H	-9.107870	-6.672286	0.873715
H	-9.107885	-6.672259	-0.873588
C	10.438556	-3.937630	-0.000003
H	11.403155	-3.474548	-0.001959
H	10.336518	-4.545508	0.874625
H	10.334127	-4.547907	-0.872675
C	-1.808857	11.007714	0.000021
H	-1.229850	11.223036	-0.873642
H	-2.692387	11.611266	0.000046
H	-1.229810	11.223023	0.873660

9a

Atom	X	Y	Z
C	-1.017365	-2.654950	-0.000038
C	-0.324005	-1.398382	-0.000039
C	-1.322127	-0.409818	-0.000049

O	-2.556469	-0.987869	-0.000052
C	1.010428	-0.946520	-0.000035
C	1.367871	0.412113	-0.000044
C	0.309360	1.341778	-0.000054
C	-1.045886	0.971595	-0.000057
C	2.802693	0.439971	-0.000044
O	2.128278	-1.726296	-0.000028
C	-1.787647	2.200041	-0.000072
O	0.425550	2.699822	-0.000067
H	-2.860185	2.327337	-0.000085
H	3.449574	1.304964	-0.000059
H	-0.591558	-3.647593	-0.000041
C	-2.357526	-2.357060	-0.000044
C	3.214599	-0.869487	-0.000029
C	-0.859853	3.211765	-0.000075
C	-3.478166	-3.185067	0.000041
C	4.491839	-1.425946	0.000067
C	-1.017063	4.595997	-0.000001
C	-4.465671	-3.896878	0.000132
C	5.602365	-1.924620	0.000165
C	-1.141951	5.806906	0.000081
C	-5.789709	-4.408210	0.000067
C	-6.892127	-3.530972	-0.000159
C	-6.016418	-5.798491	0.000184
C	-8.191667	-4.038116	0.000053
H	-6.720819	-2.458277	0.000150
C	-7.319732	-6.295999	-0.000090
H	-5.169341	-6.478594	0.000293
C	-8.409653	-5.419636	-0.000095
H	-9.037329	-3.354222	0.000171
H	-7.486234	-7.370786	-0.000220
H	-9.424120	-5.811433	0.000055
C	6.718041	-2.801862	0.000098
C	6.526931	-4.197667	-0.000116
C	8.028928	-2.286212	0.000199
C	7.627221	-5.055197	0.000090
H	5.517409	-4.598702	0.000204
C	9.122841	-3.151903	-0.000077
H	8.180060	-1.210402	0.000295
C	8.926158	-4.536530	-0.000068
H	7.471935	-6.131670	0.000218
H	10.131722	-2.745718	-0.000218
H	9.781094	-5.208650	0.000080
C	-0.929417	7.210405	0.000043
C	0.379067	7.732804	-0.000179
C	-2.024720	8.096255	0.000179
C	0.582712	9.112812	0.000064
H	1.225735	7.052325	0.000110
C	-1.810858	9.474754	-0.000068
H	-3.035075	7.697280	0.000281
C	-0.509353	9.986637	-0.000061

H	1.595678	9.508720	0.000189
H	-2.661541	10.152381	-0.000181
H	-0.346736	11.061936	0.000116

9b

Atom	X	Y	Z
O	2.738226	-0.006691	0.001062
C	1.383250	0.092451	0.001604
C	0.798826	-1.185696	0.001178
C	1.888978	-2.114522	0.000273
C	3.038218	-1.366274	0.000336
C	0.632986	1.285947	0.002320
C	-0.766063	1.152700	0.002806
C	-1.424408	-0.093735	0.002407
C	-0.609938	-1.238903	0.001529
O	-1.358265	2.375404	0.003400
C	-0.331054	3.315522	0.003005
C	0.892043	2.694538	0.002444
O	-1.373536	-2.362853	0.000951
C	-2.700945	-1.942387	0.001388
C	-2.773894	-0.573089	0.002408
C	-0.700602	4.673398	0.002877
C	-1.007821	5.837696	0.002036
Si	-1.487059	7.623076	-0.001341
C	0.038657	8.635312	-0.469643
C	-3.694459	-2.940189	0.000745
C	-4.566208	-3.797805	0.000017
Si	-5.880970	-5.097429	-0.001164
C	-5.683663	-6.145132	-1.561611
C	4.399452	-1.726103	-0.000371
C	5.578879	-2.049131	-0.000784
Si	7.363688	-2.531135	-0.000932
C	8.211401	-1.673154	1.453944
C	-7.558631	-4.227128	0.013412
C	-5.666827	-6.164602	1.543797
C	8.133089	-1.978783	-1.636407
C	7.458577	-4.409931	0.180942
C	-2.089610	8.087639	1.728855
C	-2.866801	7.861808	-1.270330
H	1.851194	3.192150	0.002084
H	-3.684087	0.009250	0.002913
H	1.839883	-3.193935	-0.000251
H	-7.682399	-3.585498	-0.867264
H	-8.375984	-4.959993	0.012307
H	-7.673369	-3.598172	0.904377
H	-4.680915	-6.644465	1.561766
H	-6.426632	-6.956348	1.578029
H	-5.762977	-5.566015	2.457518
H	-6.443202	-6.937088	-1.597080
H	-5.790693	-5.535283	-2.466630
H	-4.697649	-6.623834	-1.596761

H	8.044923	-0.893991	-1.770651
H	9.199783	-2.236207	-1.671353
H	7.642362	-2.461303	-2.490133
H	6.998315	-4.743209	1.118817
H	8.503219	-4.747431	0.180887
H	6.942616	-4.916467	-0.643551
H	9.278923	-1.927396	1.487415
H	8.128386	-0.582518	1.375135
H	7.763685	-1.973601	2.408774
H	-1.304450	7.933364	2.478662
H	-2.388370	9.143469	1.766417
H	-2.955545	7.482786	2.023561
H	-2.535893	7.576759	-2.276108
H	-3.185781	8.911746	-1.305148
H	-3.744294	7.252522	-1.022541
H	-0.194233	9.708103	-0.474790
H	0.857882	8.473687	0.241258
H	0.404066	8.366198	-1.467895

10' (**10** with a shorter propyl chain)

Atom	X	Y	Z
C	-0.692315	-2.750451	-0.000024
C	-0.537805	-1.323461	-0.000017
C	0.847541	-1.087877	-0.000006
O	1.523854	-2.274315	-0.000006
C	0.571693	-3.280281	-0.000017
C	-1.368171	-0.188863	-0.000019
C	-0.879590	1.128797	-0.000010
C	0.518234	1.280634	0.000001
C	1.414934	0.198565	0.000003
C	-2.038406	1.975858	-0.000017
C	-3.129056	1.145909	-0.000024
O	-2.733812	-0.181607	-0.000027
C	2.727997	0.778311	0.000015
C	2.554827	2.137811	0.000021
O	1.207611	2.459643	0.000011
H	3.674196	0.255520	0.000019
H	-2.058827	3.056684	-0.000015
H	-1.618566	-3.307843	-0.000033
C	3.468481	3.253166	0.000033
C	3.171118	4.597809	0.000037
S	5.204879	3.010013	0.000044
C	4.329582	5.429649	0.000050
H	2.153641	4.971854	0.000032
C	5.514252	4.736030	0.000055
H	4.278441	6.513024	0.000055
C	6.932912	5.245024	0.000067
H	7.464112	4.845144	0.876781
H	7.464122	4.845158	-0.876648
C	7.055670	6.776177	0.000080
H	6.541491	7.183437	-0.880539

H	6.541480	7.183423	0.880698
C	8.516809	7.240674	0.000092
H	8.582737	8.334927	0.000101
H	9.051206	6.874835	0.886108
H	9.051217	6.874849	-0.885922
Br	-4.844499	1.425638	-0.000032
Br	1.186876	-4.905870	-0.000019

11' (**11** with a shorter propyl chain)

Atom	X	Y	Z
C	-2.812282	0.933011	-0.000027
C	-1.417354	1.271167	-0.000020
C	-0.726291	0.047600	-0.000009
O	-1.613379	-0.990720	-0.000009
C	-2.882468	-0.435751	-0.000020
C	-0.631239	2.436862	-0.000022
C	0.774024	2.423664	-0.000013
C	1.390522	1.159980	-0.000002
C	0.676306	-0.050325	0.000000
C	1.178318	3.800949	-0.000020
C	0.027908	4.545856	-0.000027
O	-1.087151	3.724174	-0.000030
C	1.666678	-1.089268	0.000012
C	2.887076	-0.465685	0.000018
O	2.733375	0.910884	0.000008
H	1.495427	-2.156637	0.000016
H	2.188286	4.186392	-0.000018
H	-3.650554	1.615599	-0.000036
C	-3.978225	-1.372771	-0.000022
C	-3.921536	-2.748820	-0.000022
S	-5.644994	-0.828582	-0.000025
C	-5.207991	-3.364252	-0.000024
H	-2.985690	-3.295983	-0.000020
C	-6.252459	-2.473446	-0.000027
H	-5.348051	-4.439738	-0.000024
C	4.246036	-0.947360	0.000030
C	5.410374	-0.211965	0.000034
S	4.605633	-2.663428	0.000041
C	6.585542	-1.020034	0.000047
H	5.417526	0.872064	0.000029
C	6.334373	-2.369651	0.000052
H	7.587499	-0.604824	0.000052
C	7.293960	-3.531918	0.000064
H	7.097729	-4.167190	0.876778
H	7.097745	-4.167195	-0.876651
C	-7.738420	-2.726309	-0.000032
H	-8.191408	-2.239664	0.876730
H	-8.191396	-2.239695	-0.876817
C	8.776130	-3.128593	0.000077
H	8.985071	-2.506834	-0.880542
H	8.985054	-2.506828	0.880695

C	-8.126541	-4.212550	-0.000009
H	-7.691082	-4.703142	-0.880610
H	-7.691088	-4.703112	0.880612
C	9.708245	-4.345904	0.000089
H	10.760105	-4.037151	0.000098
H	9.545125	-4.972649	0.886105
H	9.545142	-4.972655	-0.885925
C	-9.646188	-4.415686	-0.000011
H	-10.108953	-3.962693	-0.886036
H	-9.901284	-5.481835	0.000006
H	-10.108961	-3.962663	0.885994
Br	-0.290177	6.254603	-0.000035

12a

Atom	X	Y	Z
C	0.000000	1.397518	0.000000
C	1.238561	0.710481	0.000000
C	-1.234575	0.717385	0.000000
C	1.210286	-0.698759	0.000000
C	-1.210286	-0.698759	0.000000
C	-0.003986	-1.427866	0.000000
S	-0.235980	3.131669	0.000000
C	-1.996358	2.939369	0.000000
C	-2.349614	1.615226	0.000000
C	-2.850744	4.109094	0.000000
S	-4.600615	3.954433	0.000000
C	-4.806243	5.677020	0.000000
C	-3.604544	6.329892	0.000000
C	-2.493106	5.440981	0.000000
S	-2.594115	-1.770199	0.000000
C	-1.547389	-3.198582	0.000000
C	-0.224020	-2.842439	0.000000
C	-2.133208	-4.523363	0.000000
S	-1.124332	-5.961466	0.000000
C	-2.513322	-7.000839	0.000000
C	-3.679576	-6.286572	0.000000
C	-3.465474	-4.879583	0.000000
S	2.830095	-1.361470	0.000000
C	3.543747	0.259213	0.000000
C	2.573634	1.227212	0.000000
C	4.983951	0.414269	0.000000
S	5.724947	2.007032	0.000000
C	7.319565	1.323819	0.000000
C	7.284119	-0.043320	0.000000
C	5.958580	-0.561397	0.000000
H	-3.382142	1.281629	0.000000
H	-5.802171	6.099064	0.000000
H	-3.511075	7.410346	0.000000
H	-1.460592	5.774268	0.000000
H	0.581147	-3.569836	0.000000
H	-2.380859	-8.074360	0.000000

H	-4.662011	-6.745853	0.000000
H	-4.270366	-4.152044	0.000000
H	2.800995	2.288206	0.000000
H	8.183030	1.975296	0.000000
H	8.173085	-0.664493	0.000000
H	5.730958	-1.622224	0.000000

12b' (**12b** with a shorter propyl chain)

Atom	X	Y	Z
S	-1.444867	-2.790909	-0.000432
C	-0.548092	-1.287625	-0.000509
C	-1.418058	-0.177483	-0.000442
C	-2.797075	-0.567292	-0.000455
C	-2.989959	-1.926004	-0.000502
C	0.861136	-1.140820	-0.000590
C	1.387403	0.167730	-0.000636
C	0.555634	1.314723	-0.000583
C	-0.840722	1.116400	-0.000452
C	0.907611	2.703874	-0.000765
C	-0.172583	3.550279	-0.000667
S	-1.694257	2.644816	-0.000248
S	3.137622	0.143343	-0.000691
C	3.161587	-1.627242	-0.000806
C	1.888602	-2.139932	-0.000719
H	1.683650	-3.205736	-0.000847
H	1.933307	3.058635	-0.001118
H	-3.617046	0.143715	-0.000562
C	-0.193748	4.999061	-0.000751
C	-1.276711	5.851220	-0.003594
S	1.297846	5.929948	0.003109
C	-0.919771	7.231452	-0.002729
H	-2.304572	5.502262	-0.006393
C	0.434452	7.454150	0.000679
H	-1.652109	8.031410	-0.004680
C	-4.234194	-2.668486	-0.000570
C	-4.431249	-4.032380	-0.002511
S	-5.785911	-1.841642	0.002011
C	-5.805265	-4.412827	-0.001993
H	-3.615441	-4.748417	-0.004386
C	-6.674728	-3.350944	0.000317
H	-6.132291	-5.446903	-0.003360
C	4.427243	-2.332621	-0.000887
C	5.706271	-1.819637	-0.003065
S	4.489293	-4.089891	0.002070
C	6.723992	-2.817935	-0.002421
H	5.916886	-0.754781	-0.005183
C	6.240885	-4.102492	0.000207
H	7.782817	-2.583149	-0.003923
C	1.197557	8.753952	0.002589
H	1.863127	8.785777	-0.871895
H	1.858214	8.786071	0.880786

C	-8.181985	-3.338922	0.001509
H	-8.541154	-2.778652	-0.873636
H	-8.539788	-2.781458	0.879004
C	6.986957	-5.412209	0.001634
H	6.682933	-6.004350	-0.873390
H	6.684959	-6.001292	0.879422
C	-8.815822	-4.735328	-0.000228
H	-8.522961	-5.309543	0.886191
H	-8.524341	-5.306713	-0.888927
C	0.303444	10.000013	-0.000114
H	-0.341159	10.032336	0.885658
H	-0.336215	10.032043	-0.889472
C	8.512856	-5.258462	-0.000397
H	8.859810	-4.719292	-0.889263
H	8.861872	-4.716265	0.885817
C	9.183107	-6.644954	0.001198
H	8.883056	-7.187163	-0.871086
H	10.246586	-6.527010	-0.000423
H	8.885374	-7.184032	0.876213
C	-10.351319	-4.617647	0.001157
H	-10.669081	-4.086107	-0.871422
H	-10.784033	-5.596246	-0.000025
H	-10.667713	-4.088821	0.875878
C	1.171329	11.272165	0.002108
H	0.538998	12.135322	-0.002057
H	1.784942	11.283778	0.878604
H	1.793059	11.281293	-0.868678

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