Supporting Information for

Rational Design of Lamellar π–π Stacked Organic Crystalline Materials with Short Interplanar Distance

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1. General considerations:

All chemicals and solvents were purchased from commercial sources and used without further purification unless otherwise specified in the text. TLCs were run on aluminum-backed silica gel G254 TLC plates with 200 μm thickness from Sorbent Technologies, Inc. Column chromatography was carried out with silica gel (300-400 mesh).

All NMR spectral studies were carried out using $CDCl_3$ unless otherwise specified. ^1H and ^{19}F NMR were recorded on Bruker 400 MHz NMR spectrometer. MS spectra were recorded on a Varian 500-MS and GC-2010 plus Shimadzu mass spectrometer. Melting point was recorded on Vernier MLT-BTA melt station apparatus.

X-ray single crystal diffraction data were collected using Mo-Kα radiation (λ = 0.71073 Å) on a Bruker CCD APEXII diffractometer at 100 K. Structures were solved by direct methods using SHELXL-97 in conjunction with standard difference Fourier techniques and subsequently refined by full matrix least-squares analyses. All hydrogen atoms were placed in their ideal positions and all non-hydrogen atoms were refined anisotropically. Detailed crystal structure information is listed in attached cif files.

2. Synthesis and characterization:

Synthesis of 11,12-dibromo-dibenz[a, c] phenazine **2**:

A mixture of 4,5-dibromo-1,2-phenylenediamine (0.6 g, 2.3 mmol) and 9,10-phenanthrene quinone (0.47 g, 2.3 mmol) were added to the 250 ml one neck R.B. flask followed by 50 ml of glacial acetic acid. The mixture was refluxed for 20 hours; the reaction mixture was allowed to cool to room temperature. Filtered the yellow precipitate and washed with 30 ml of methanol and 30 ml of acetone to give crude product. Recrystallization with chloroform gave pure **2** as yellow crystals in a yield of 0.8 g (80 %) with mp > 250 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **2** in chloroform. ^1H NMR (400 MHz, $CDCl_3$): δ 9.35 (dd, J = 8.1, 1.5 Hz, 2H), 8.68 (s, 2H), 8.57 (d, J = 8.1 Hz, 2H), 7.85 (m, 2H), 7.78 (m, 2H); ESI-MS (positive ion mode); Calcd. For $[M+H]^+$: 439.1. Found 439.0.

Synthesis of 11,12-bis(perfluoropropyl)-dibenz[a, c] phenazine **3**:

A mixture of 11,12-dibromo-dibenz[a, c] phenazine **2** (0.13 g, 0.30 mmol), Cu powder (0.188 g, 3 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluoropropyl iodide (0.44 g, 1.48 mmol) was added and the reaction was carried out at 135 °C with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (30 ml), DI water (3x30 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. After column (hexane:chloroform in 3:1 ratio) and repeated recrystallization of crude product with chloroform gave pure **3** as yellow powder in a yield of 0.032 g (17.6%) with mp 258-260 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **3** in a mixture of chloroform and hexane (1:1 ratio). ^1H NMR (400 MHz, $CDCl_3$): δ

9.45 (dd, J = 8.1, 1.2 Hz, 2H), 8.84 (s, 2H), 8.62 (d, J= 8.1 Hz, 2H), 7.92 (m, 2H), 7.83 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.11 (dt, 12.2, 6.2 Hz, 6F), -103.05 (m, 4F), -122.03 (m, 4F); ESI-MS (positive ion mode); Calcd. For $[M+H]^+$: 617.4. Found 617.9.

Synthesis of 11,12-bis(perfluorobutyl)-dibenz[a, c] phenazine **4**:

A mixture of 11,12-dibromo-dibenz[a, c] phenazine **2** (0.14 g, 0.32 mmol), Cu powder (0.203 g, 3.2 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluorobutyl iodide (0.553 g, 1.6 mmol) was added and the reaction was carried out at 135 °C with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (2x35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (30 ml), DI water (3x30 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. After column (hexane:chloroform in 3:1 ratio) and repeated recrystallization of crude product with chloroform gave pure **4** as yellow powder in a yield of 0.03 g (13.2%) with mp 246-250 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **4** in a mixture of chloroform and hexane (1:1 ratio). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.44 (dd, J = 8.1, 1.5 Hz, 2H), 8.85 (s, 2H), 8.62 (d, J= 7.6 Hz, 2H), 7.92 (m, 2H), 7.83 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.84 (t, 9.54 Hz, 6F), -102.59 (m, 4F), -118.57 (m, 4F), -126.01 (m, 4F); EI-MS; m/z ($m^{+\cdot}$) 716.0 (calcd for $C_{28}H_{10}F_{18}N_2$: 716.36)

Synthesis of 11,12-bis(perfluorohexyl)-dibenz[a, c] phenazine **5**:

A mixture of 11,12-dibromo-dibenz[a, c] phenazine **2** (0.13 g, 0.30 mmol), Cu powder (0.188 g, 3 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluorohexyl iodide (0.66 g, 1.48 mmol) was added and the reaction was carried out at 135 °C with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (4x35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (70 ml), DI water (3x70 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. After column (hexane:chloroform in 3:1 ratio) and repeated recrystallization of crude product with chloroform gave pure **5** as yellow powder in a yield of 0.035 g (12.9%) with mp 224-228 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **5** in a mixture of chloroform and hexane (1:1 ratio). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.44 (dd, J = 7.9, 1.3 Hz, 2H), 8.85 (s, 2H), 8.62 (d, J= 8.1 Hz, 2H), 7.92 (m, 2H), 7.82 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.71 (t, 9.54 Hz, 6F), -102.44 (m, 4F), -117.60 (m, 4F), -121.87 (m, 4F), -122.62 (m, 4F), -126.04 (m, 4F); EI-MS; m/z ($m^{+\cdot}$) 916.0 (calcd for $C_{32}H_{10}F_{26}N_2$: 916.39)

Synthesis of 11,12-bis(perfluorooctyl)-dibenz[a, c] phenazine **6**:

A mixture of 11,12-dibromo-dibenz[a, c] phenazine **2** (0.13 g, 0.30 mmol), Cu powder (0.188 g, 3 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluorooctyl iodide (0.81 g, 1.48 mmol) was added and the reaction was carried out at 135 °C

with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (7x35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (120 ml), DI water (3x120 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. After column (hexane:chloroform in 3:1 ratio) and repeated recrystallization of crude product with chloroform gave pure **6** as yellow powder in a yield of 0.031 g (9.3%) with mp 198-202 °C ; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.45 (dd, J = 7.9, 1.3 Hz, 2H), 8.85 (s, 2H), 8.62 (d, J= 8.1 Hz, 2H), 7.91 (m, 2H), 7.82 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.92 (t, 9.54 Hz, 6F), -102.39 (m, 4F), -117.60 (m, 4F), -121.77 (m, 12F), -122.72 (m, 4F), -126.17 (m, 4F); ESI-MS (positive ion mode); Calcd. For $[M+H]^+$: 1117.4. Found 1117.2.

Synthesis of 11-perfluorobutyl-dibenz[a, c] phenazine **7**:

A mixture of 11-bromo-dibenz[a, c] phenazine (0.359 g, 1 mmol), Cu powder (0.317 g, 5 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluorobutyl iodide (0.761 g, 2.2 mmol) was added and the reaction was carried out at 135 °C with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (2x35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (30 ml), DI water (3x30 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. Recrystallization of crude product with chloroform gave pure **7** as yellow powder in a yield of 0.205 g (41.2%) with mp 180-182 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **7** in a mixture of chloroform and hexane (1:1 ratio). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.38 (td, J = 7.9, 1.6 Hz 2H), 8.64 (s, 1H), 8.56 (d, J= 8.2 Hz, 2H), 8.44 (d, J= 8.2 Hz, 1H), 7.97 (m, 1H), 7.83 (m, 2H), 7.76 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.88 (dt, 12.1, 6.3 Hz, 3F), -110.45 (m, 2F), -122.25 (m, 2F), -125.40 (m, 2F); EI-MS; m/z ($m^{+\cdot}$) 498.0 (calcd for $C_{24}H_{11}F_9N_2$: 498.34)

Synthesis of 9,10-dibromo-dithieno[2,3-a: 3',2'-c] phenazine **9**:

A mixture of 4,5-dibromo-1,2-phenylenediamine (0.15 g, 0.56 mmol) and thieno[3,2-e][1]benzothiophene-4,5-dione (0.124 g, 0.56 mmol) were added to the 100 ml one neck R.B. flask followed by 20 ml of glacial acetic acid. The mixture was refluxed for 20 hours and the reaction mixture was allowed to cool to room temperature. Filtered brown precipitate and washed with 20 ml of methanol and 10 ml of acetone to give **9** as brown powder in a yield of 0.22 g (88 %) with mp 276-280 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (s, 2H), 7.90 (d, J=5.4 Hz, 2H), 7.81 (d, J=5.1 Hz, 2H); ESI-MS (positive ion mode); Calcd. For $[M+H]^+$: 451.1. Found 450.9.

Synthesis of 9,10-bis(perfluorobutyl)-dithieno[2,3-a: 3',2'-c] phenazine **10**:

A mixture of 9,10-dibromo-dithieno[2,3-a: 3',2'-c] phenazine **9** (0.10 g, 0.22 mmol), Cu powder (0.141 g, 2.2 mmol), DMSO (1 ml), HFE-7200 (1 ml) were added to pressure tube. To this, perfluorobutyl iodide (0.384 g, 1.1 mmol) was added and the reaction was carried out at 135

°C with stirring for 24 hours. After 24 hours, the reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (2x35 ml) was added, sonicated for 15 minutes to dissolve the target product in dichloromethane and filtered the mixture. The filtrate was extracted with dichloromethane (30 ml), DI water (3x30 ml) to remove any residual DMSO. This methylene chloride solution was dried over Na_2SO_4, filtered and evaporated to get crude product. After column (hexane:chloroform in 3:1 ratio) and repeated recrystallization of crude product with chloroform gave pure **10** yellow powder in a yield of 0.045 g (27.7%) with mp 284-288 °C. Single crystals suitable for X-ray diffraction were grown by slow evaporation of saturated solution of **10** in a mixture of chloroform and hexane (1:1 ratio).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (s, 2H), 7.97 (d, J=5.3 Hz, 2H), 7.82 (d, J= 5 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -80.74 (t, 9.8 Hz, 6F), -102.53 (m, 4F), -118.47 (m, 4F), -125.95 (m, 4F); EI-MS; m/z ($m^{+\cdot}$) 728.0 (calcd for $C_{24}H_6F_{18}N_2S_2$: 728.4)

3. ^{1}H NMR, ^{19}F NMR, and MS spectra :

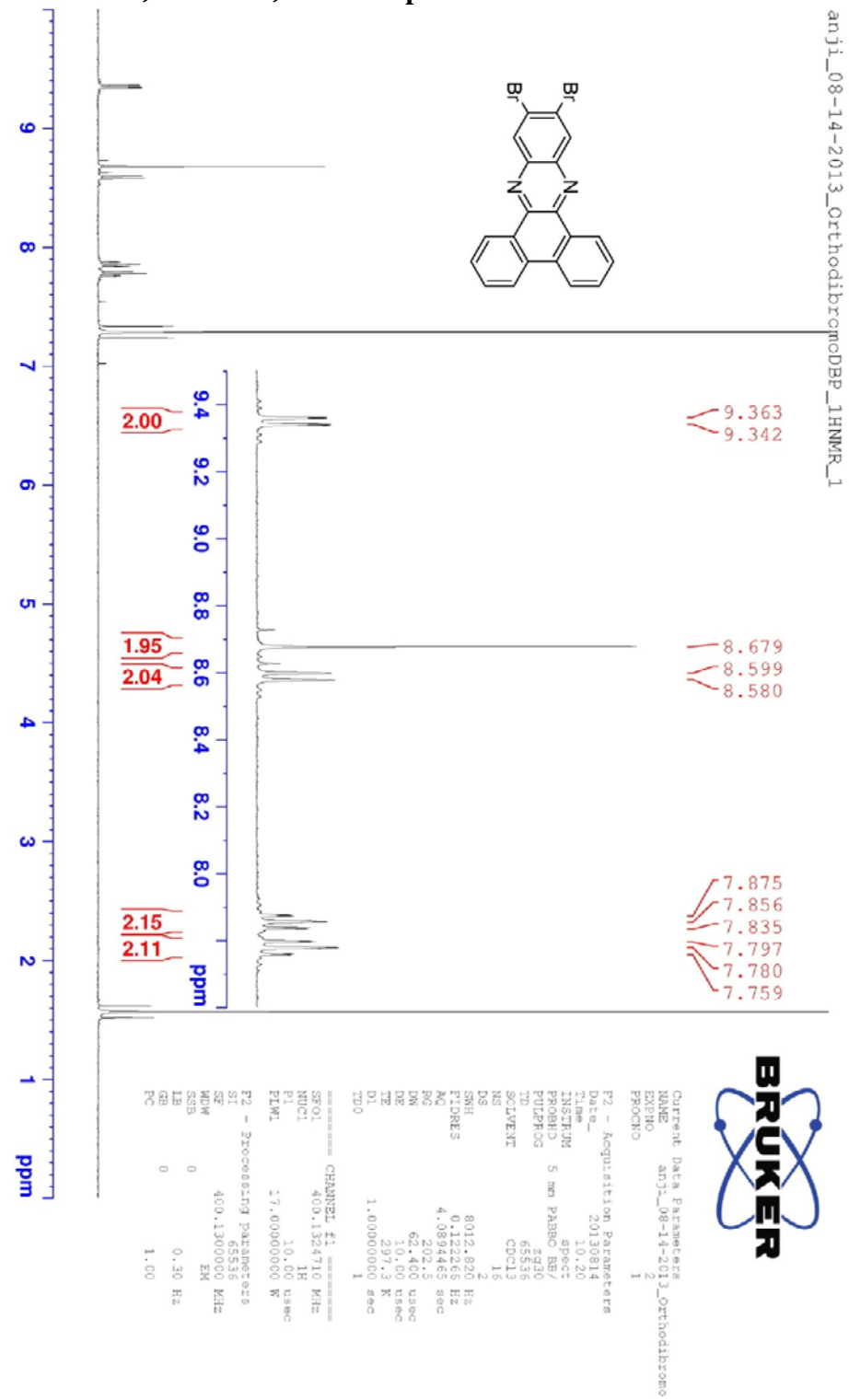


Figure S1: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**

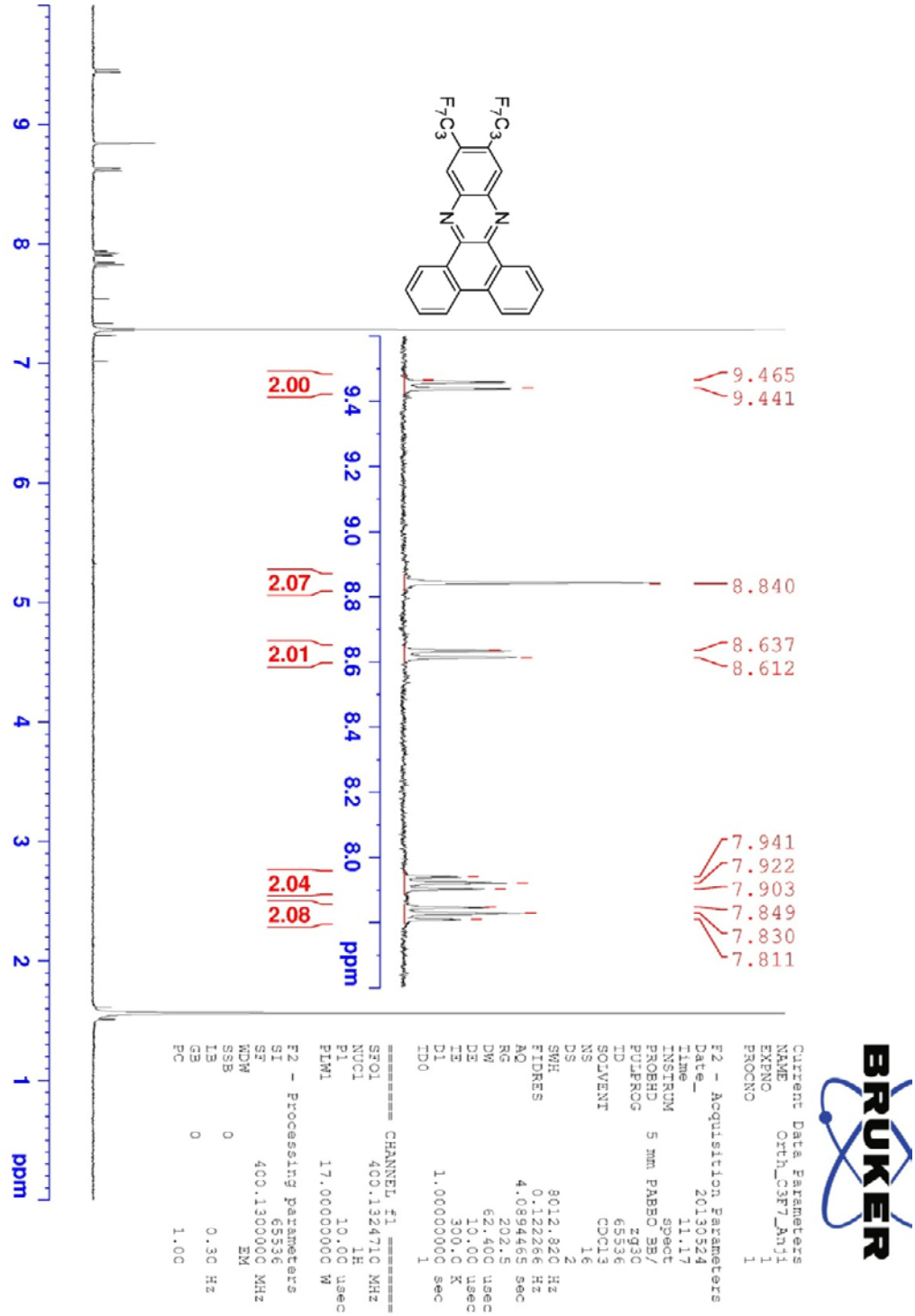


Figure S2: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**

Figure S3: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3**

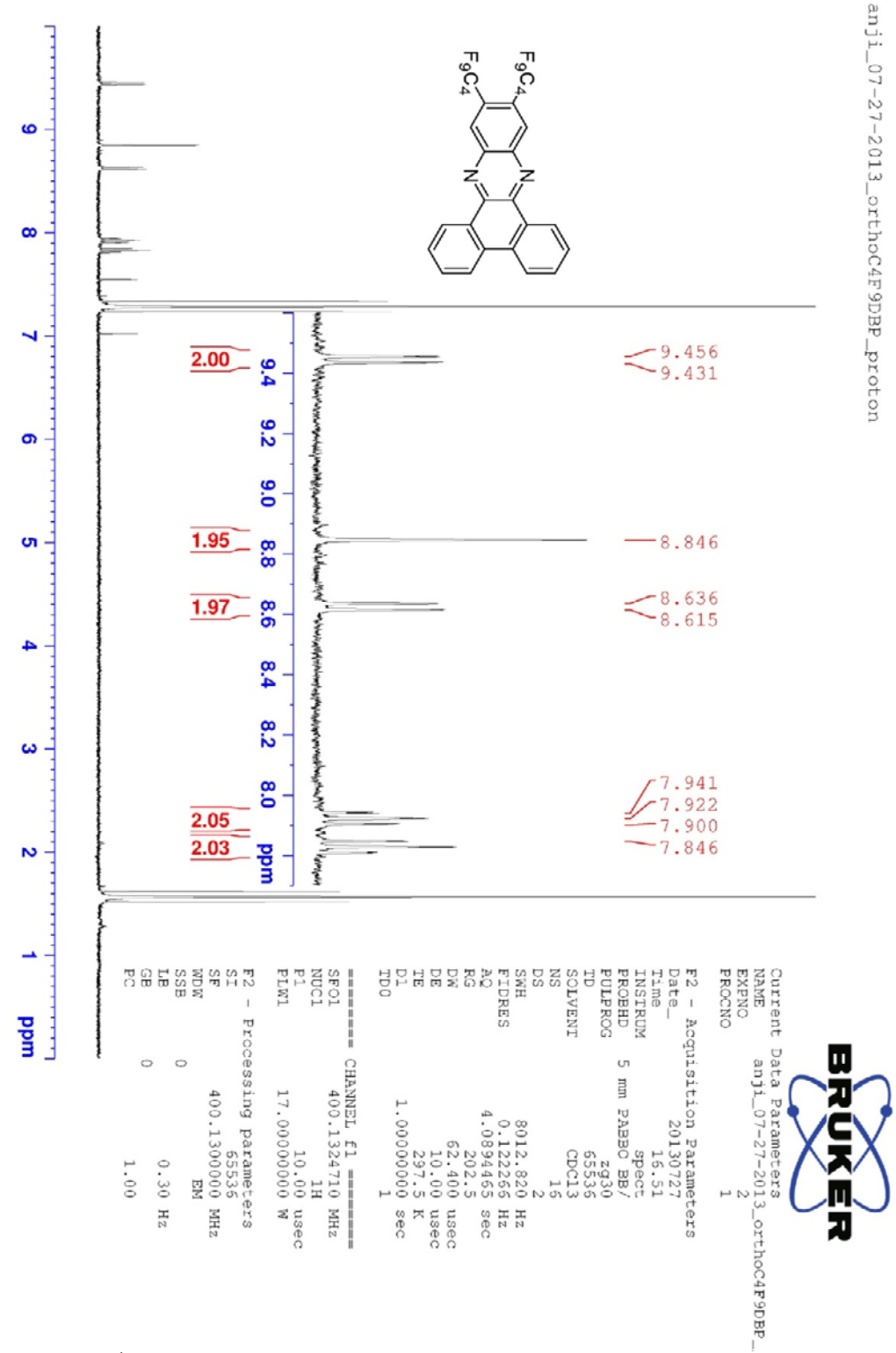


Figure S4: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**

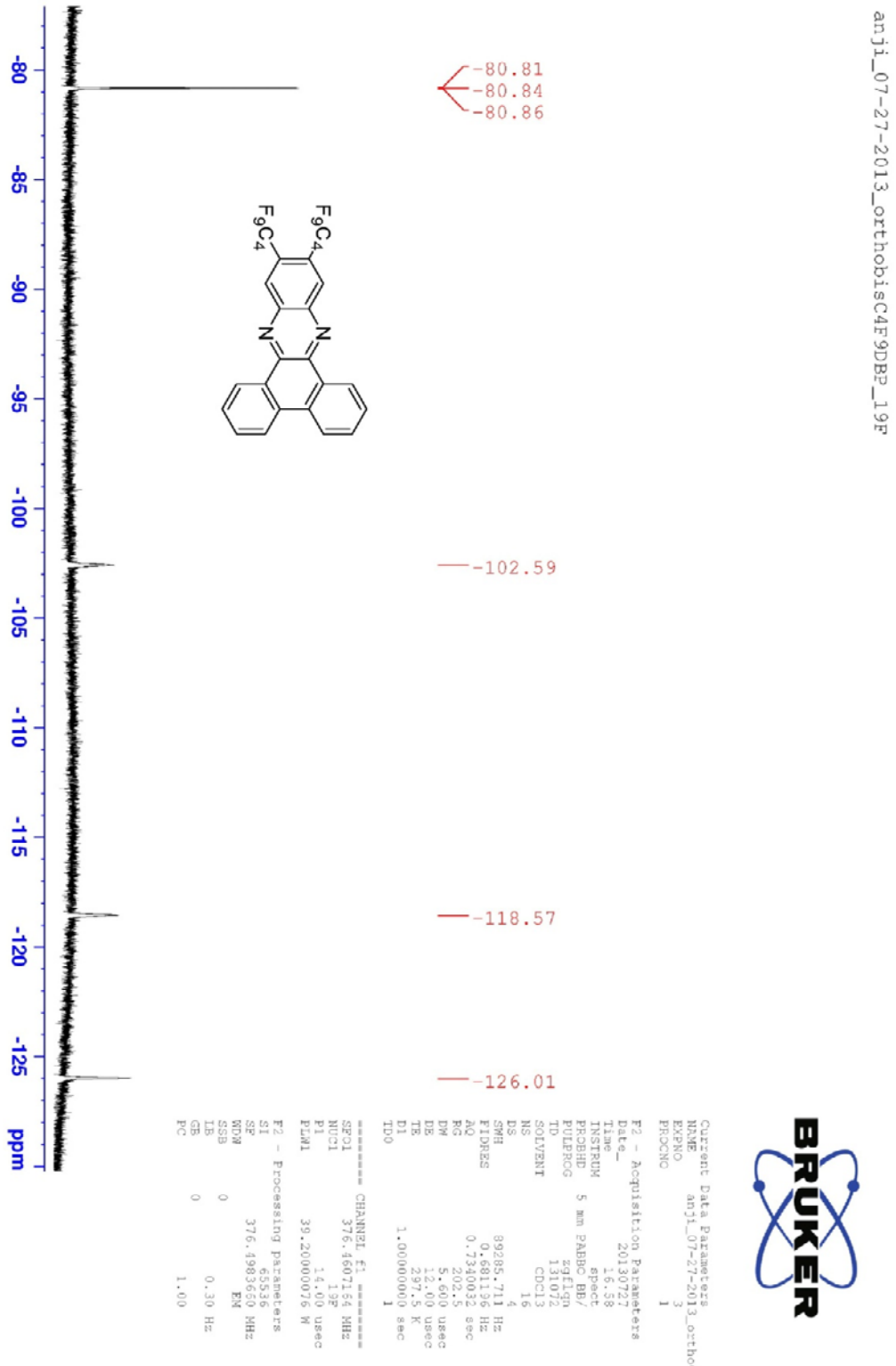


Figure S5: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **4**

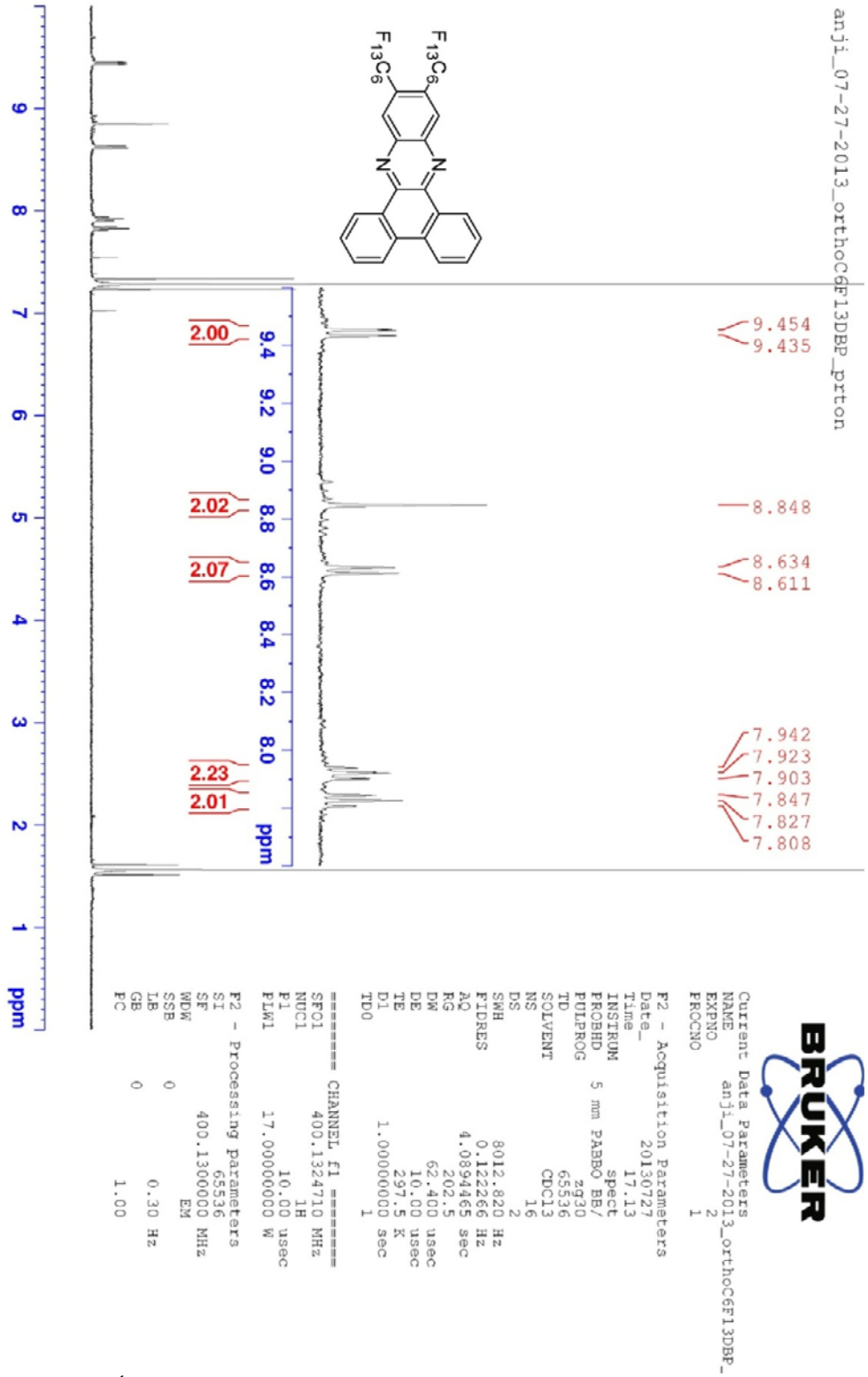


Figure S6: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**

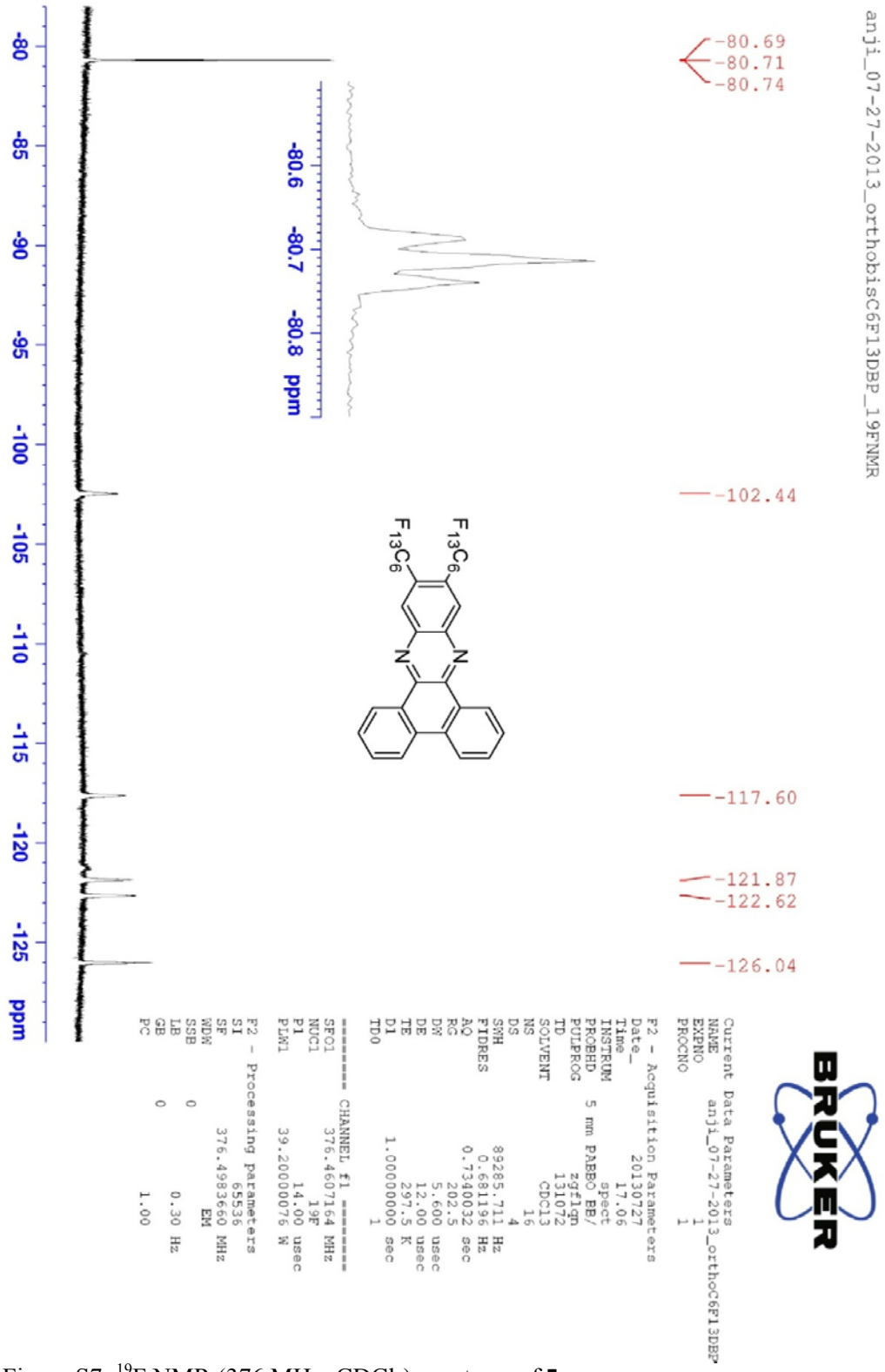


Figure S7: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **5**

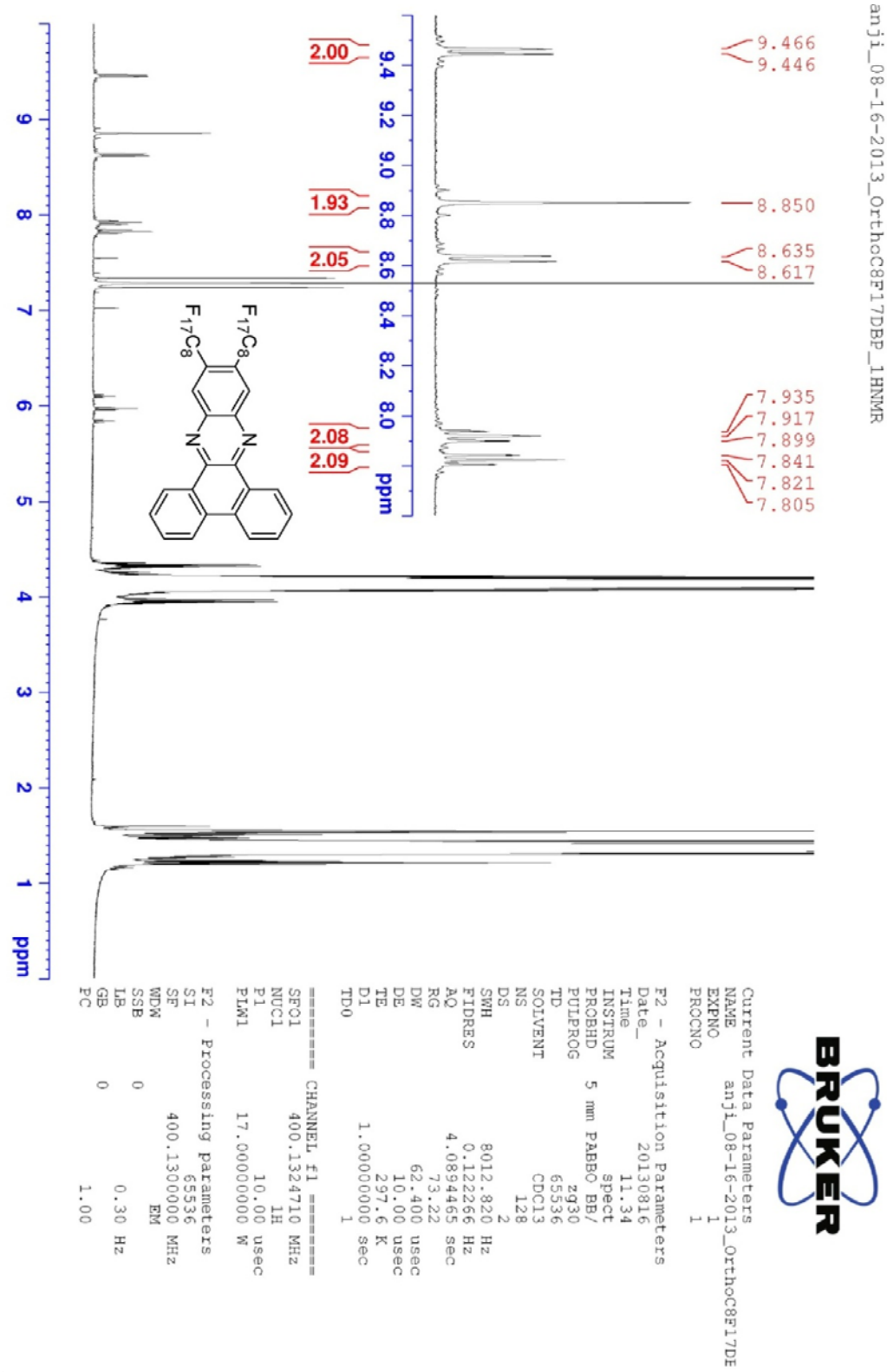


Figure S8: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**

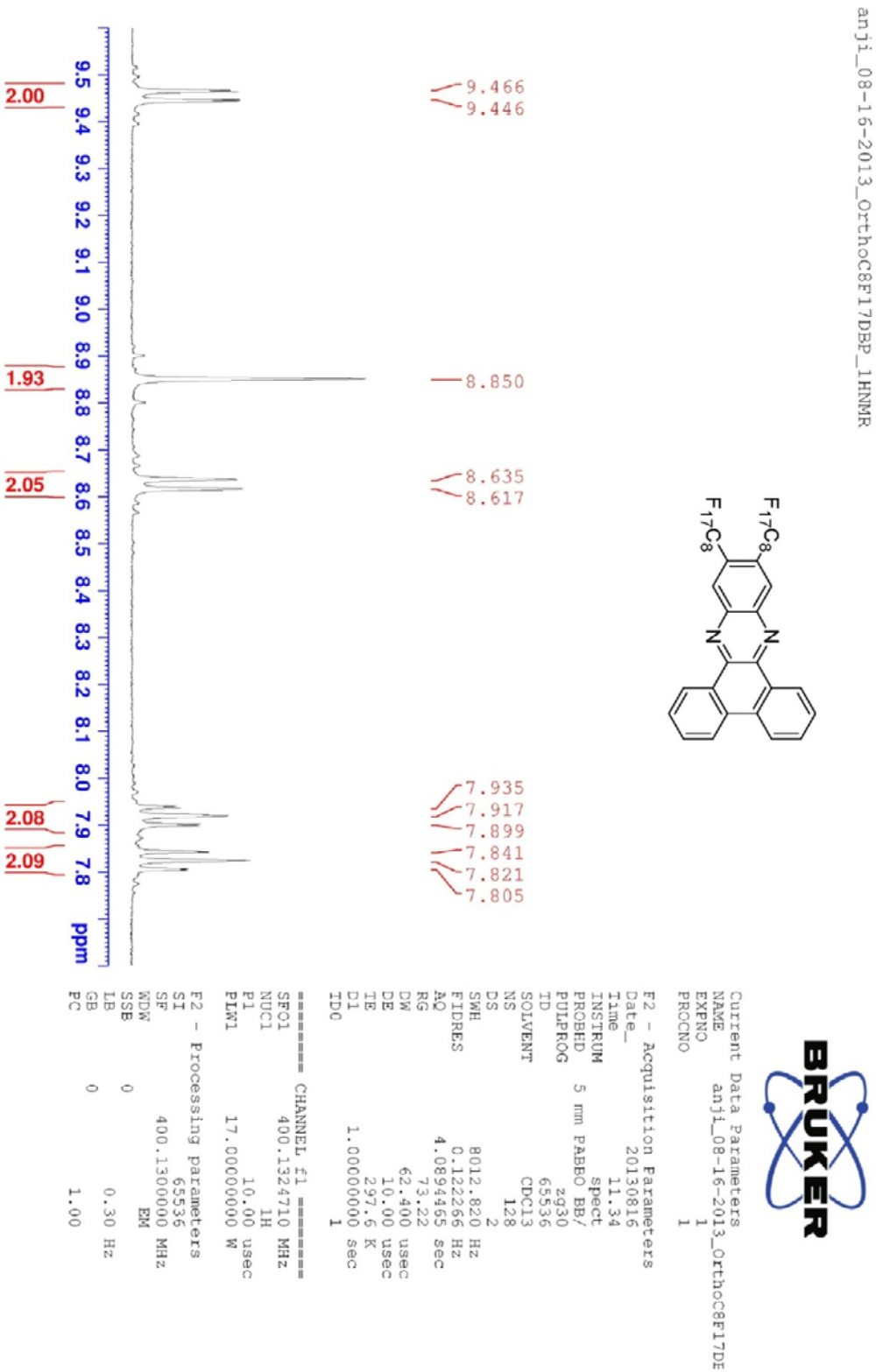


Figure S8: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6** (zoomed region)

Figure S9: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **6**

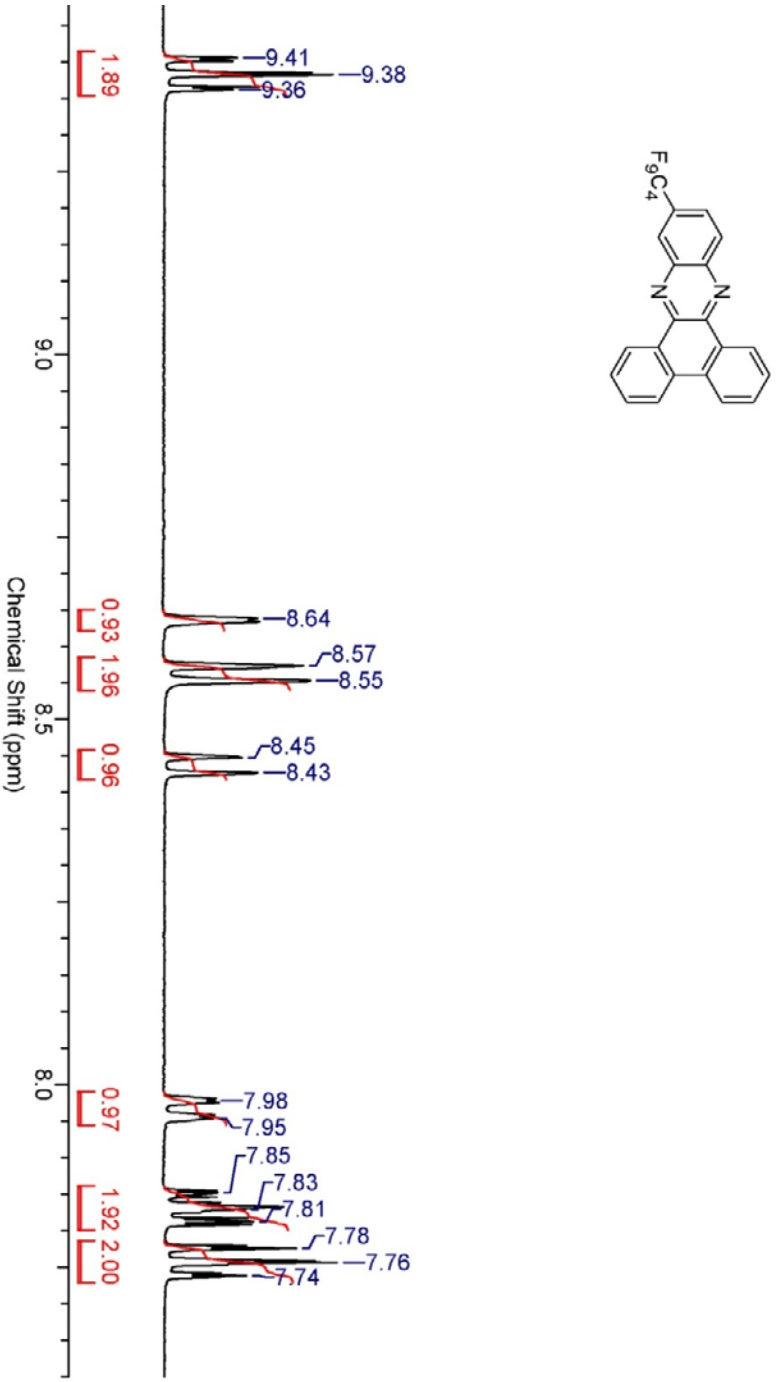


Figure S10: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7** (zoomed region)

Figure S11: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **7**

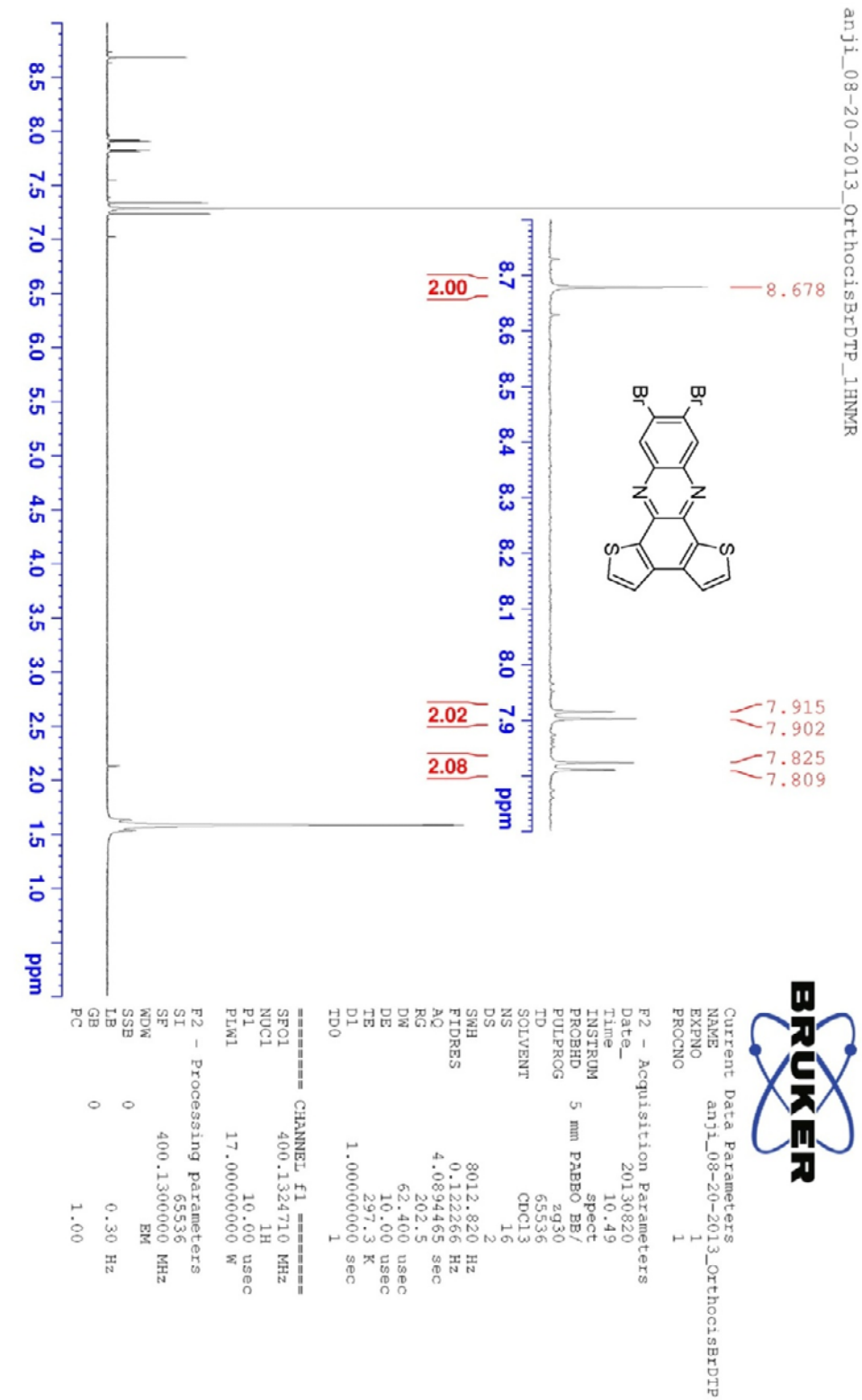


Figure S12: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9**

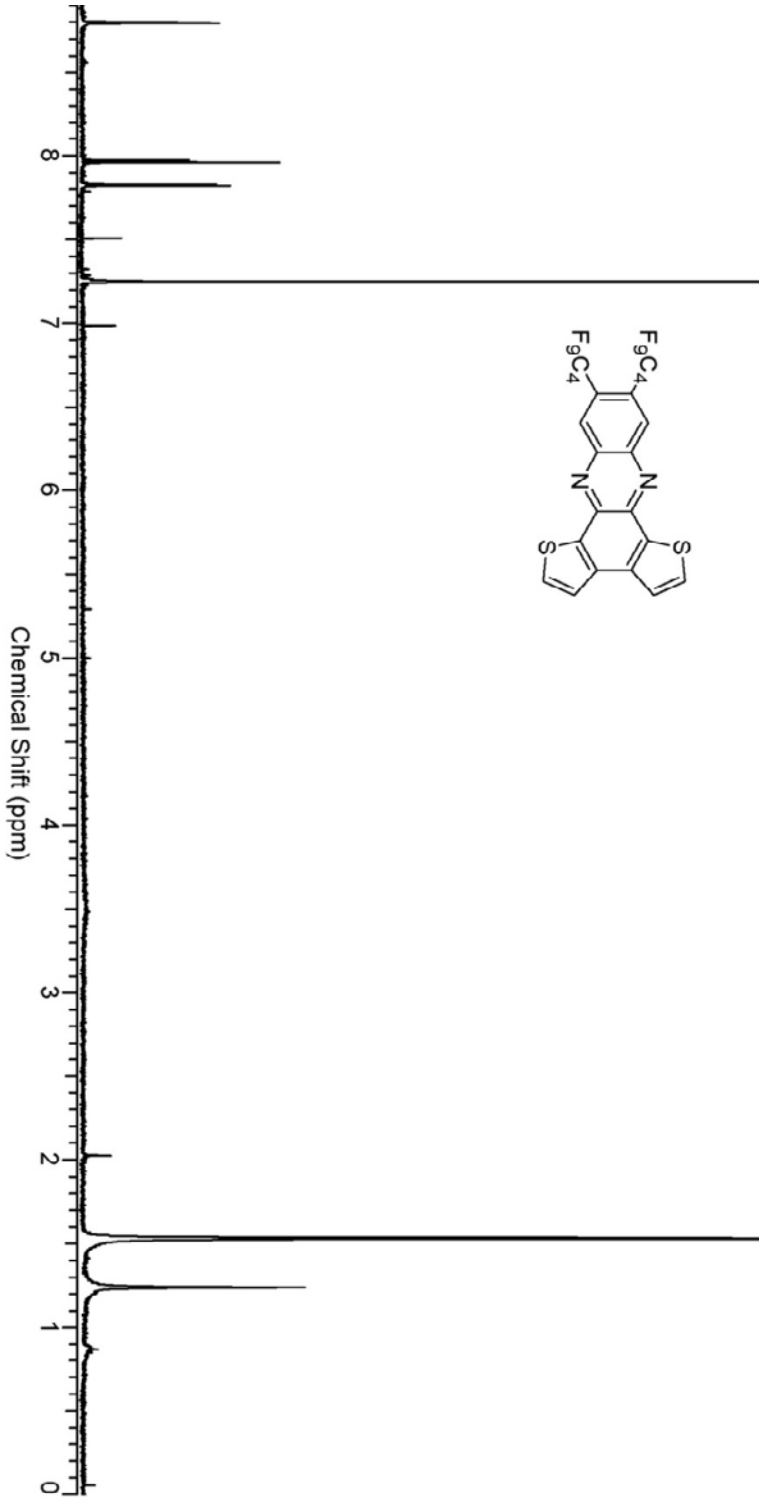


Figure S13: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10**

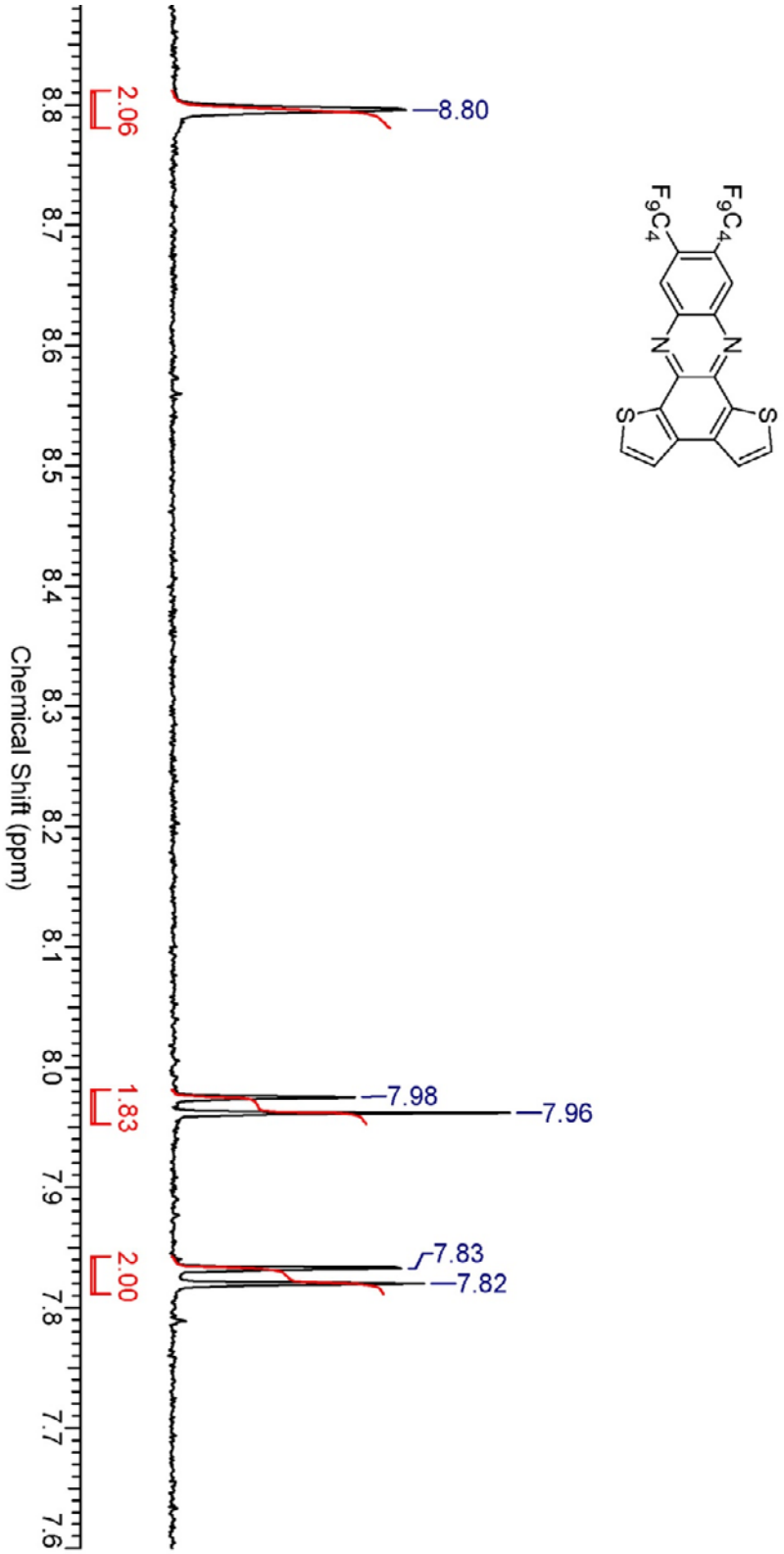


Figure S13: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10** (Zoomed aromatic region)

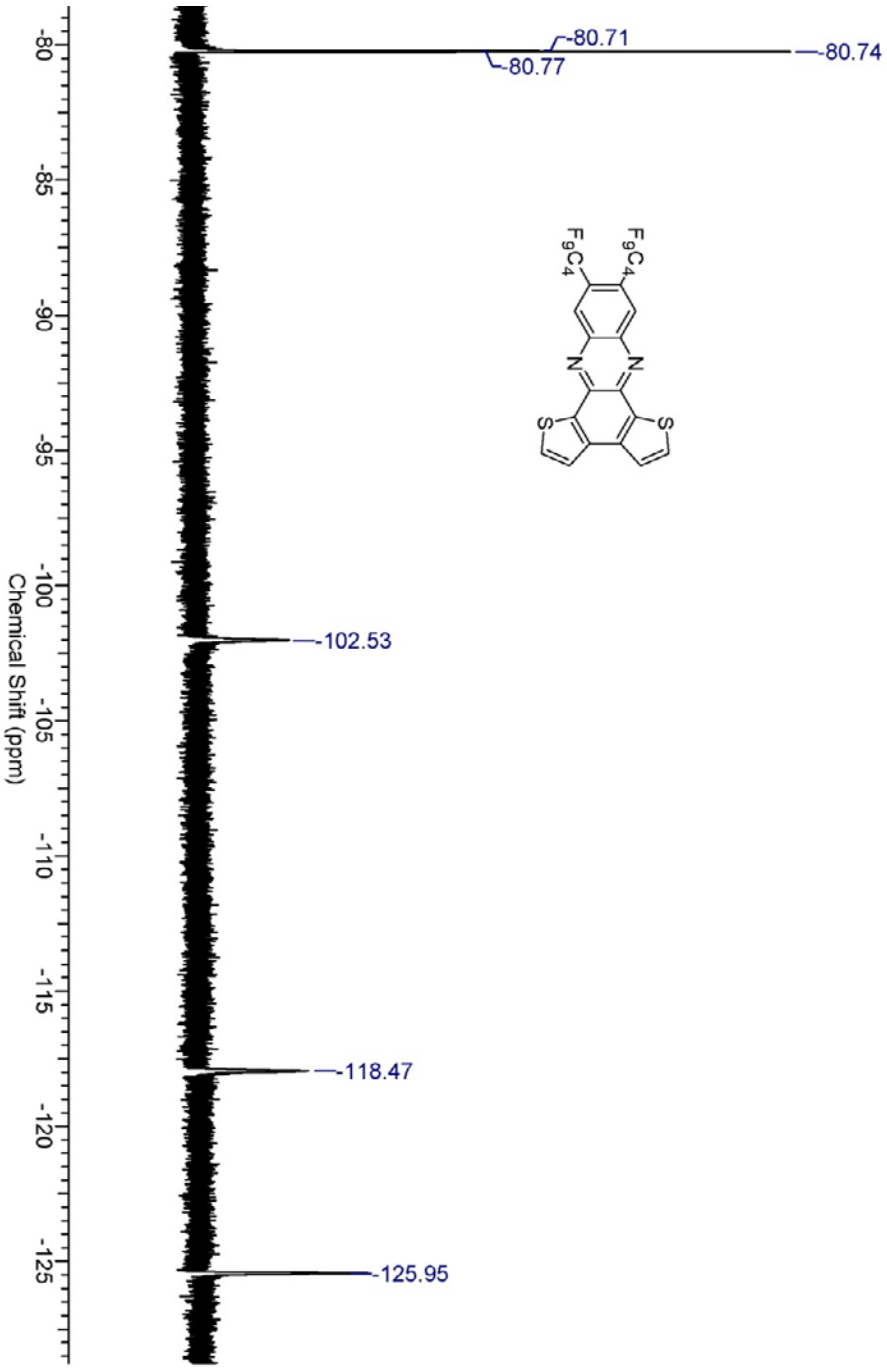


Figure S14: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **10**

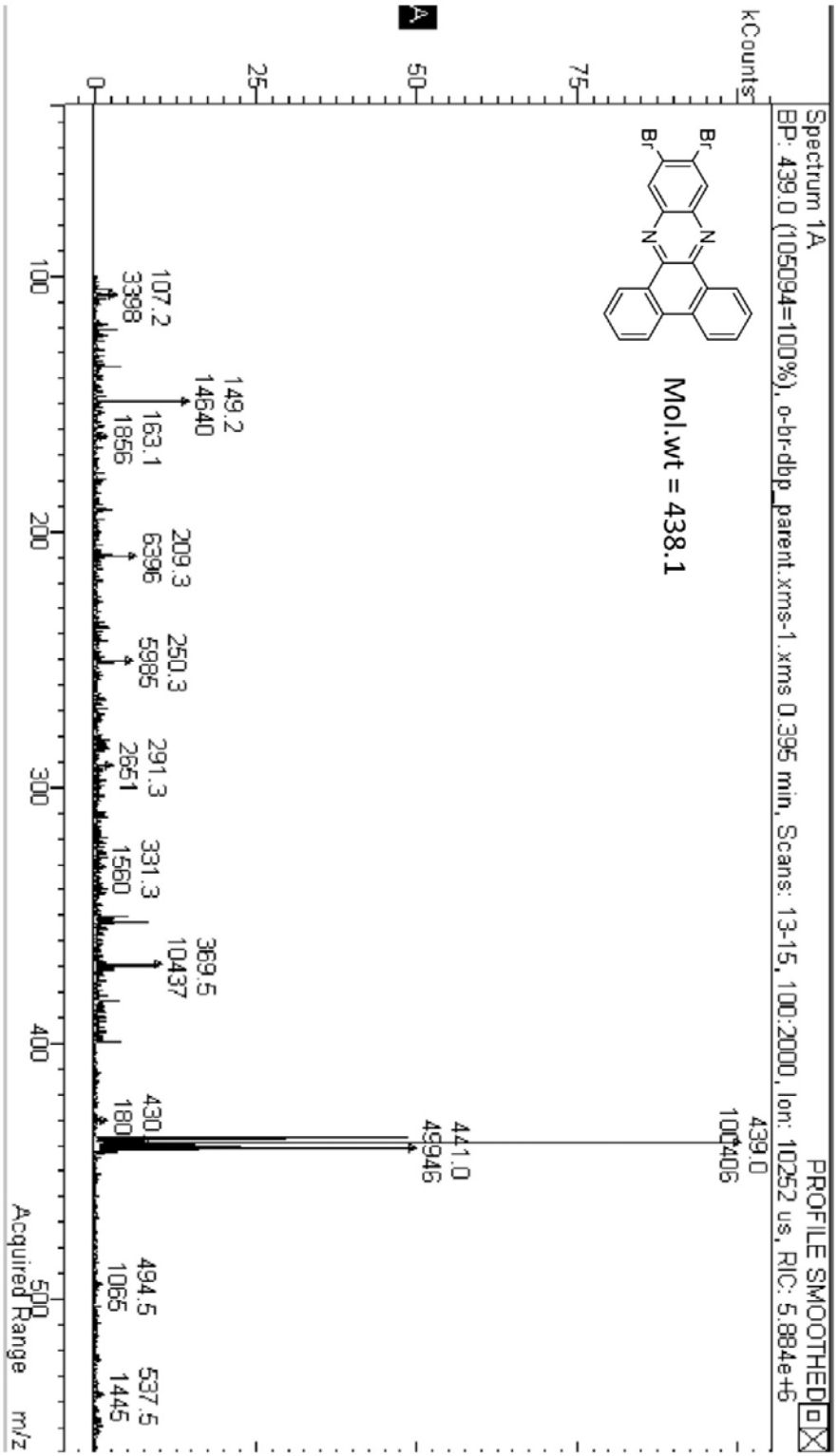


Figure S15: ESI-MS spectrum of **2**

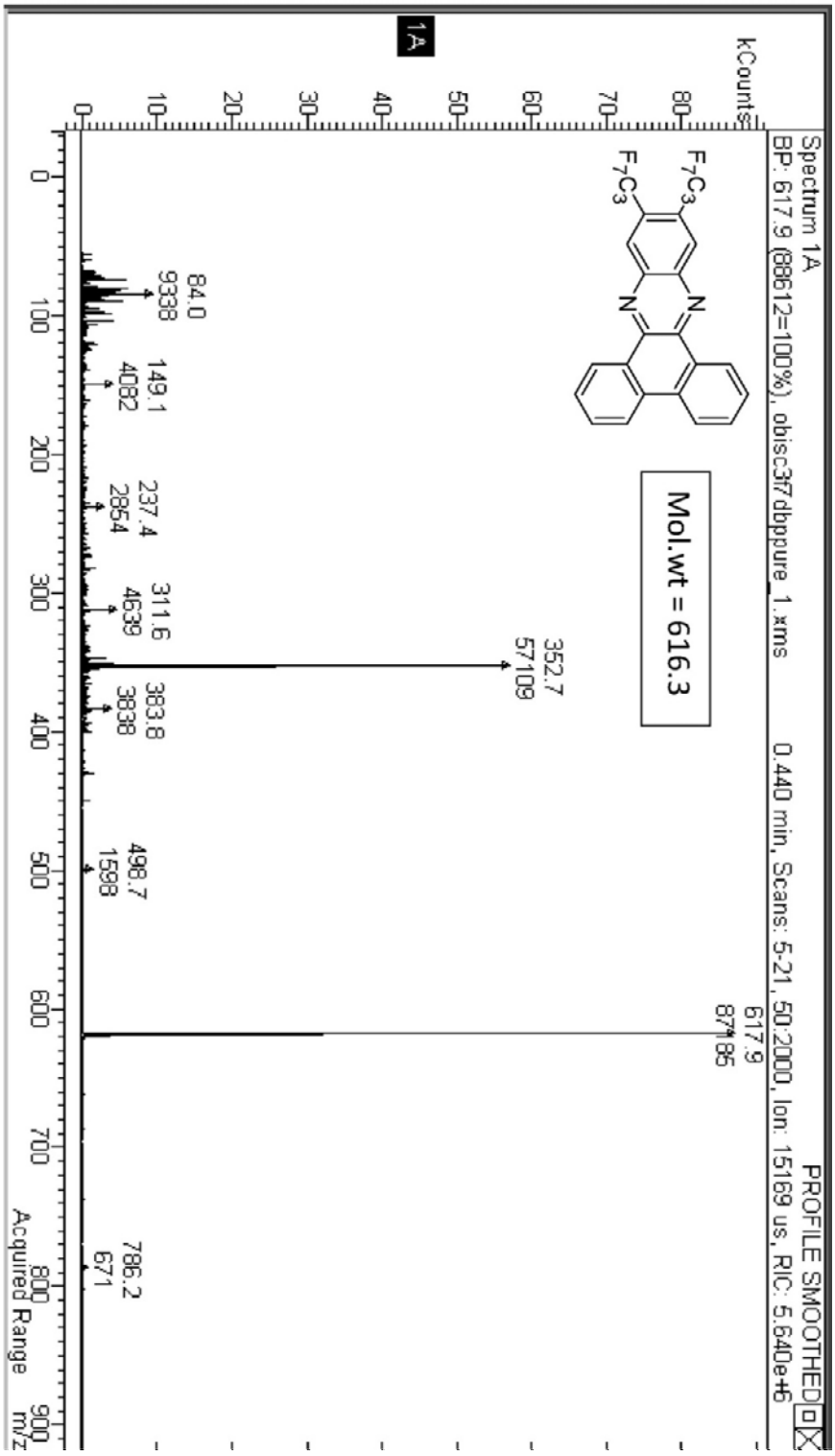


Figure S16: ESI-MS spectrum of **3**

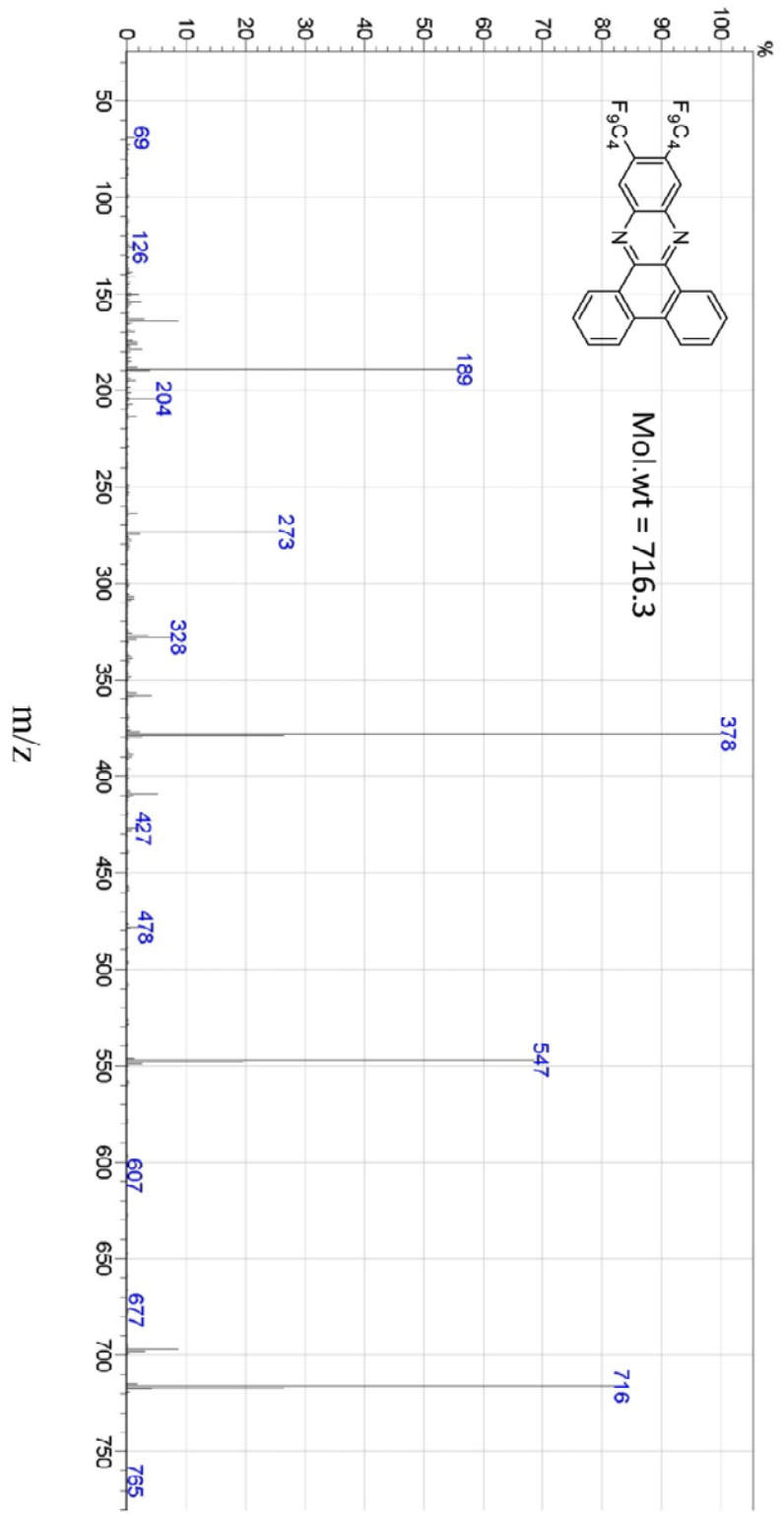


Figure S17: EI-MS spectrum of **4**

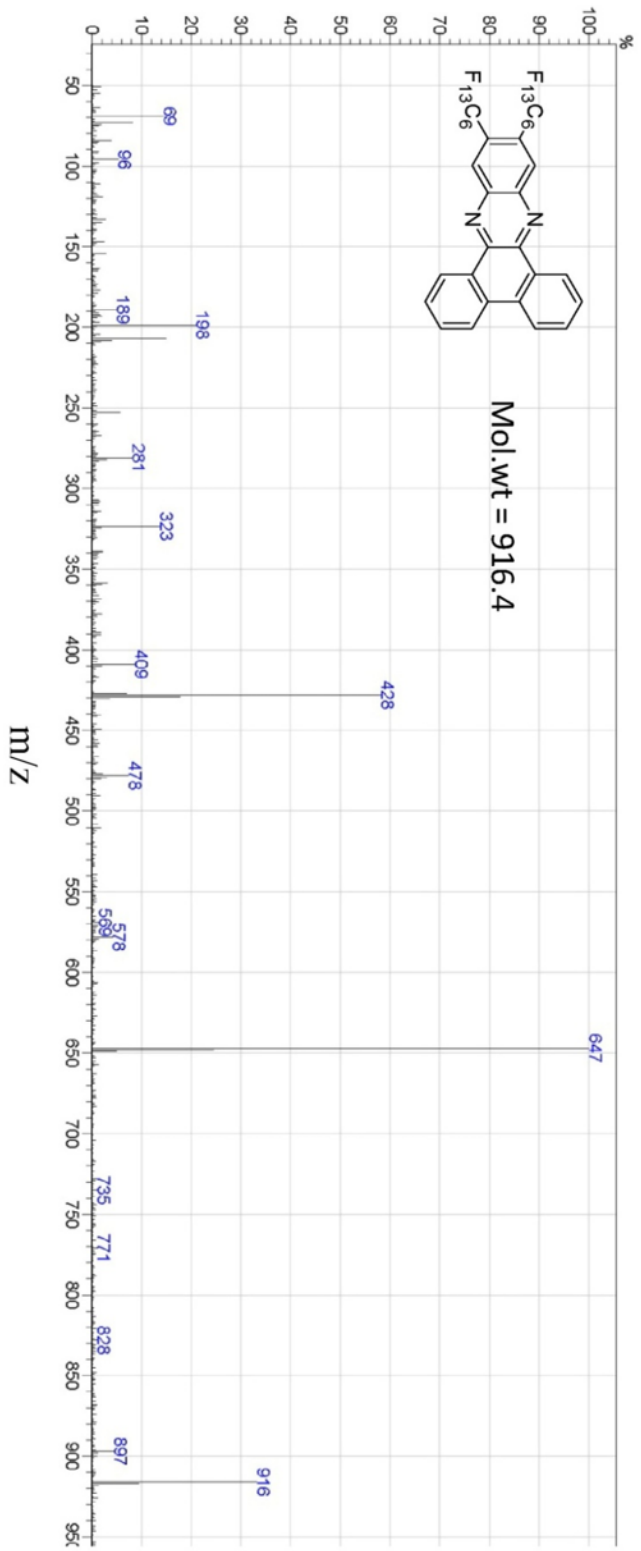


Figure S18: EI-MS spectrum of **5**

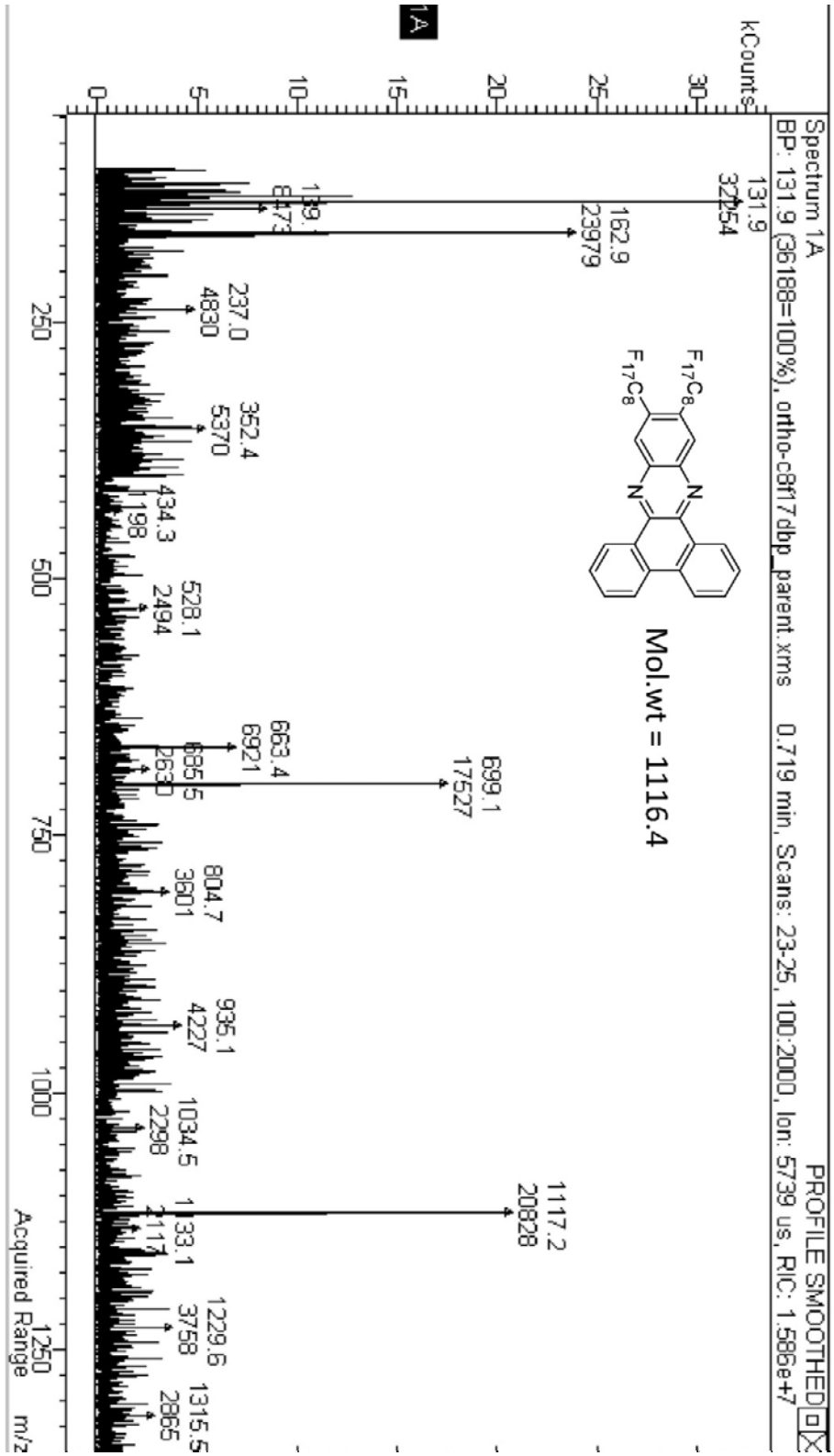


Figure S19: ESI-MS spectrum of **6**

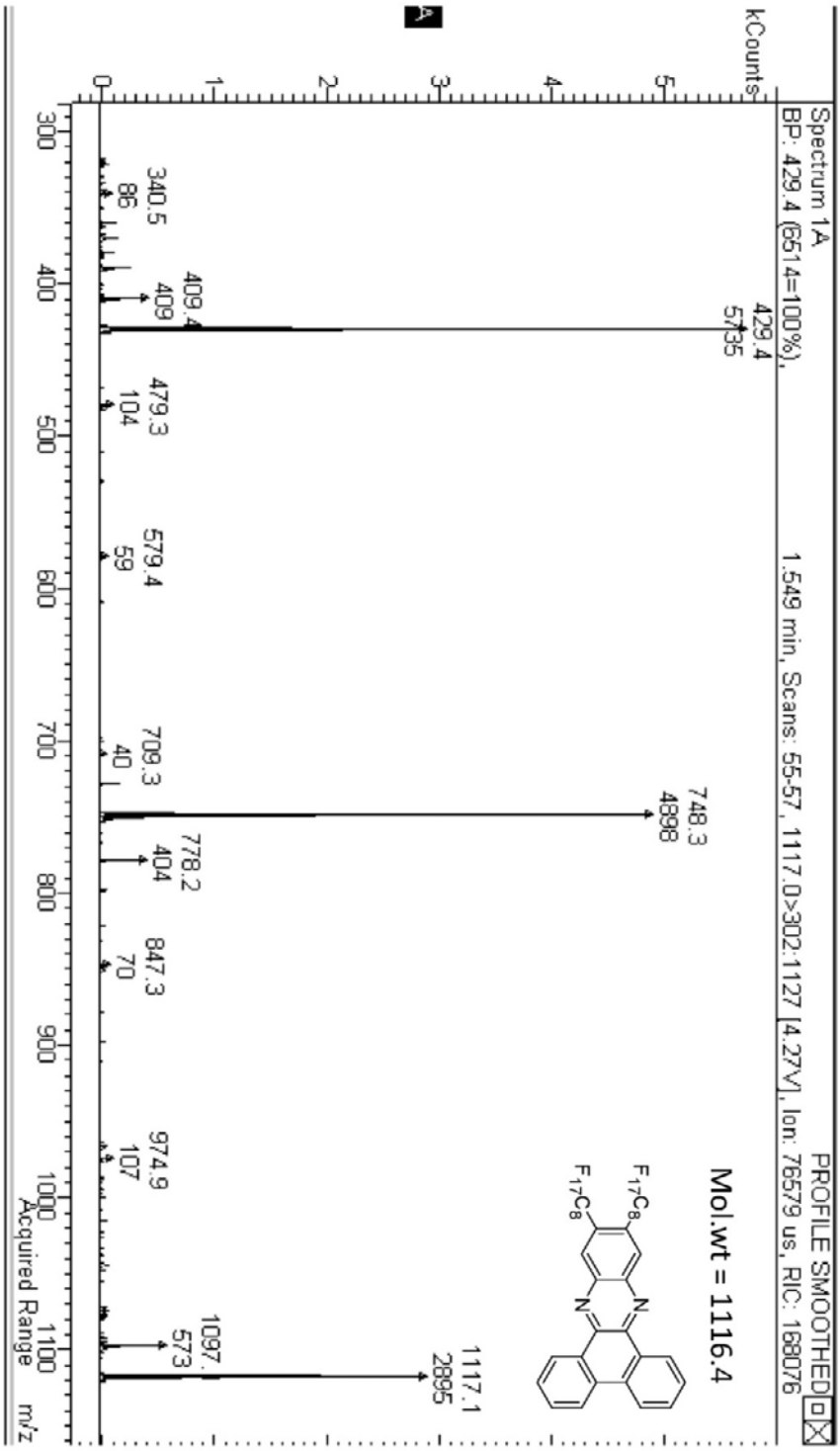


Figure S19: ESI-MS spectrum of **6** (Fragmentation of 1117 peak)

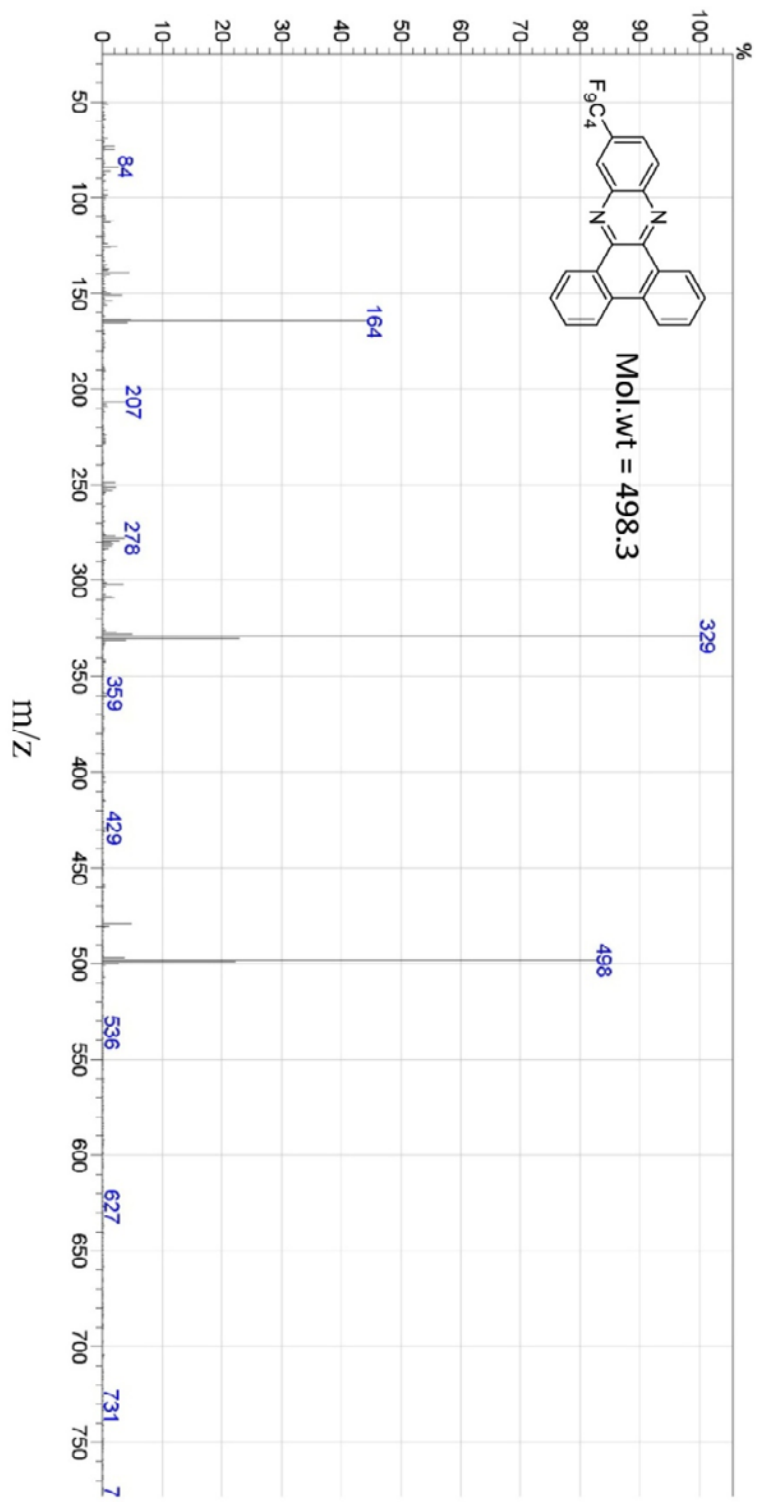


Figure S20: EI-MS spectrum of **7**

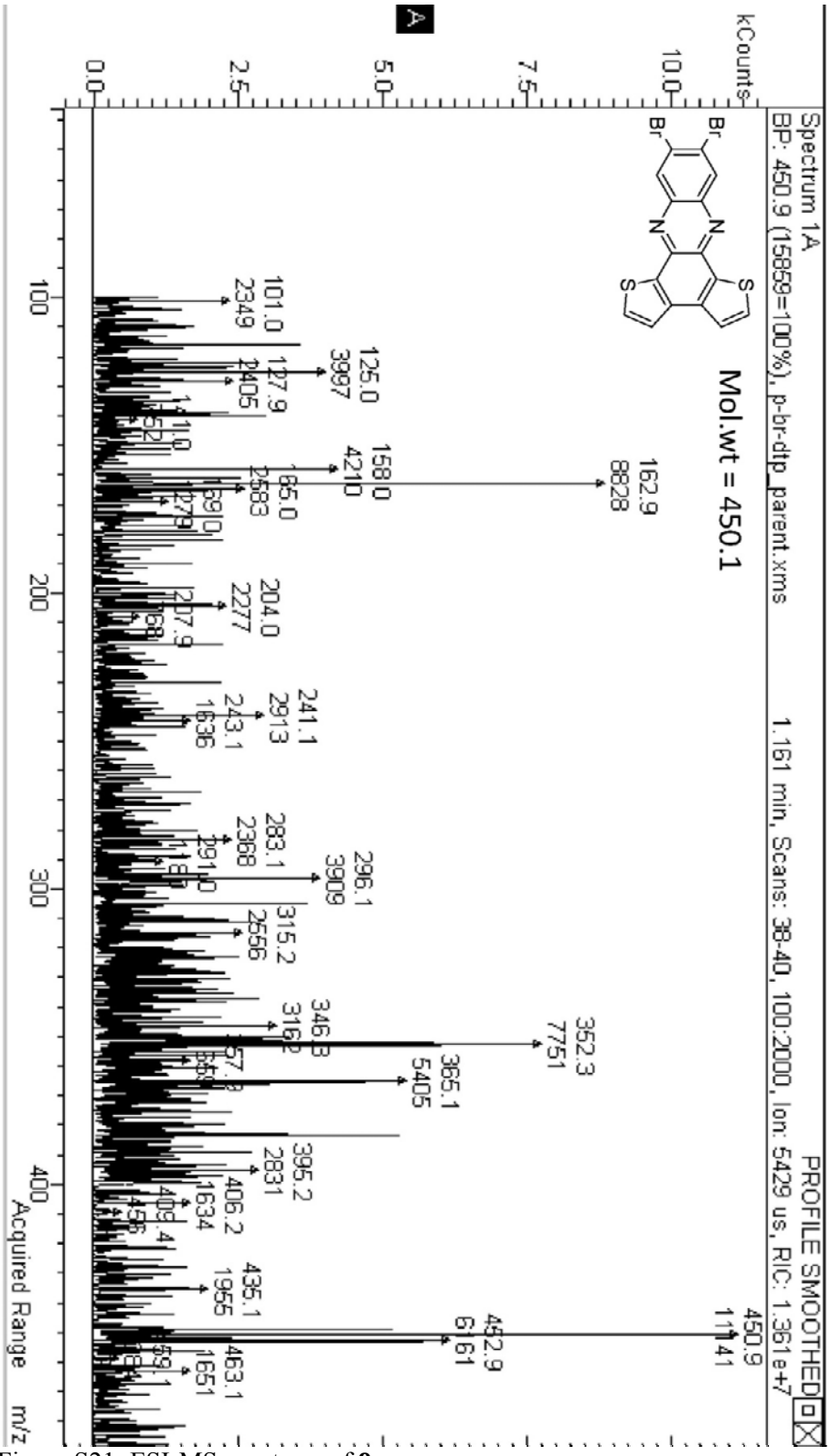


Figure S21: ESI-MS spectrum of **9**

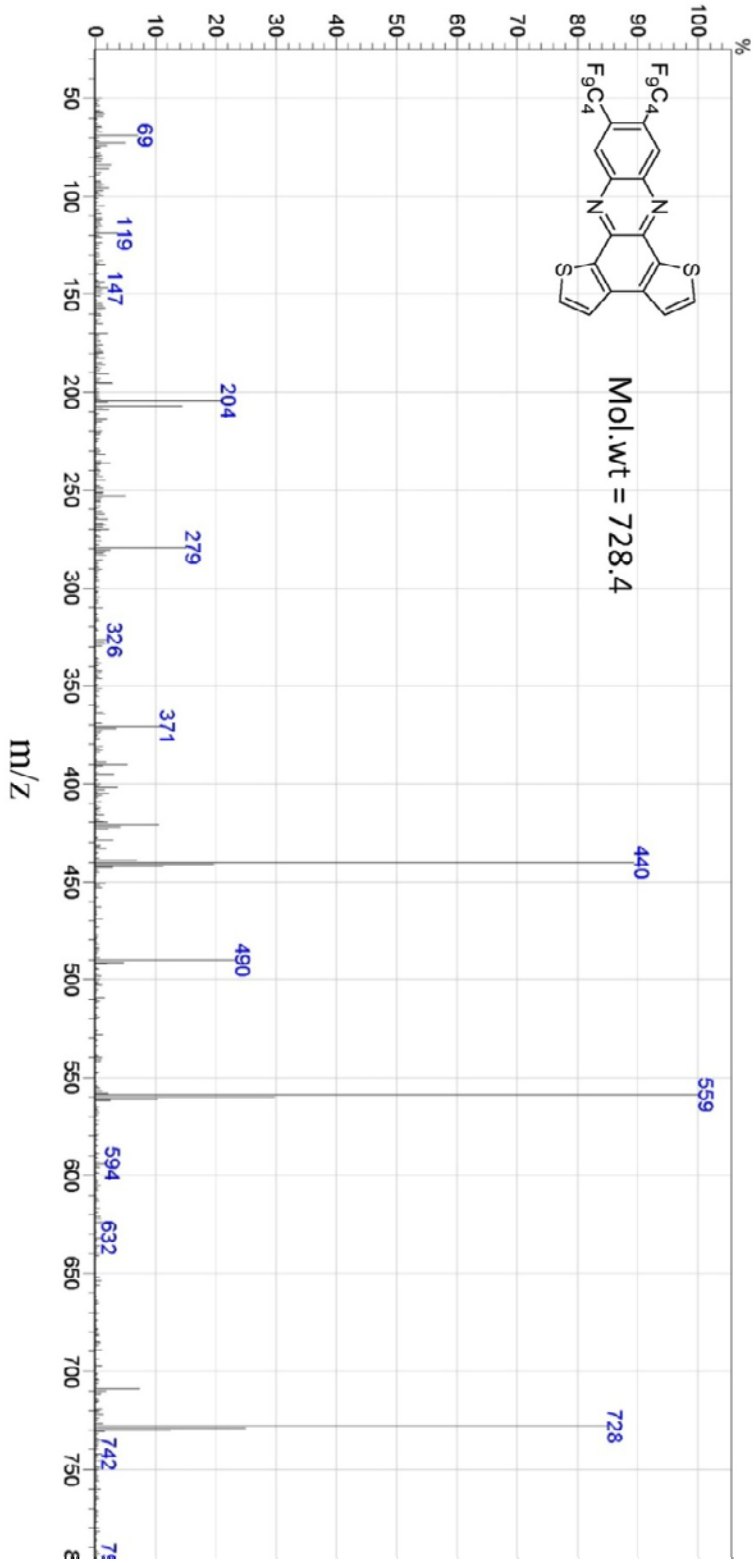


Figure S22: EI-MS spectrum of **10**

4. Crystal structures, short contacts and intermolecular distances:

Table S1: F-F short contact distances and DFT-D (B97D/TZV) estimated Rf-Rf chain interaction energies within the same π–π stacked column of crystal molecules

Compounds	**Distance of (F-F) short contacts (Å)**	**Interaction energies (kcal/mol)**
3	2.666 (F002-F002)	-3.88
4	2.794 (F3-F12)	-6.63
5	2.664 (F5-F11)	-9.99
	2.666 (F8-F16)	
	2.863 (F9-F22)	
10	2.842 (F003-F006)	-7.13
	2.902 (F007-F7)	

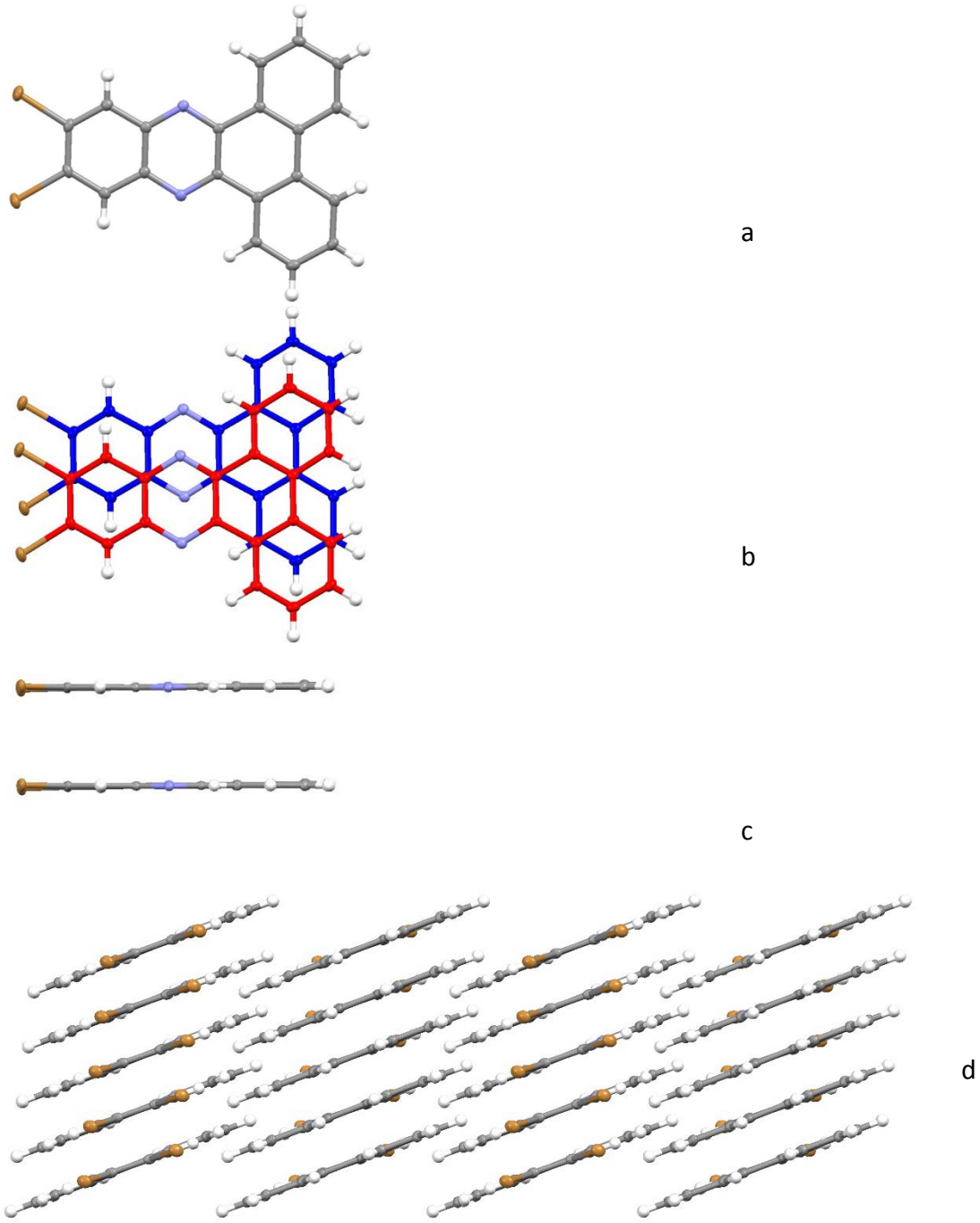


Figure S23: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, (d) crystal packing along b axis of **2**: (color code: brown, Br; light blue, N; gray, C; white, H).

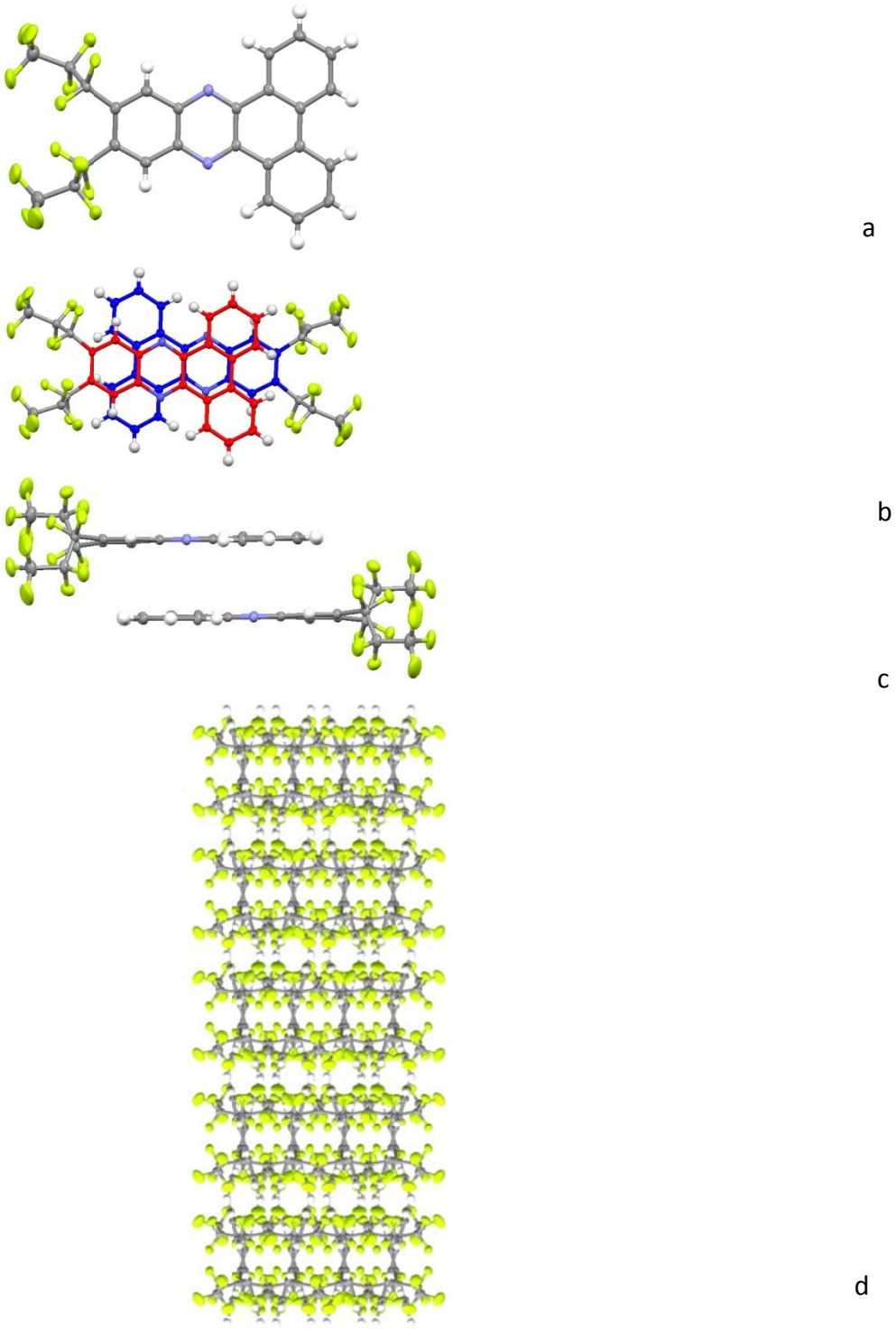


Figure S24: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, (d) crystal packing along b axis of **3**: (color code: light green, F; light blue, N; gray, C; white, H).

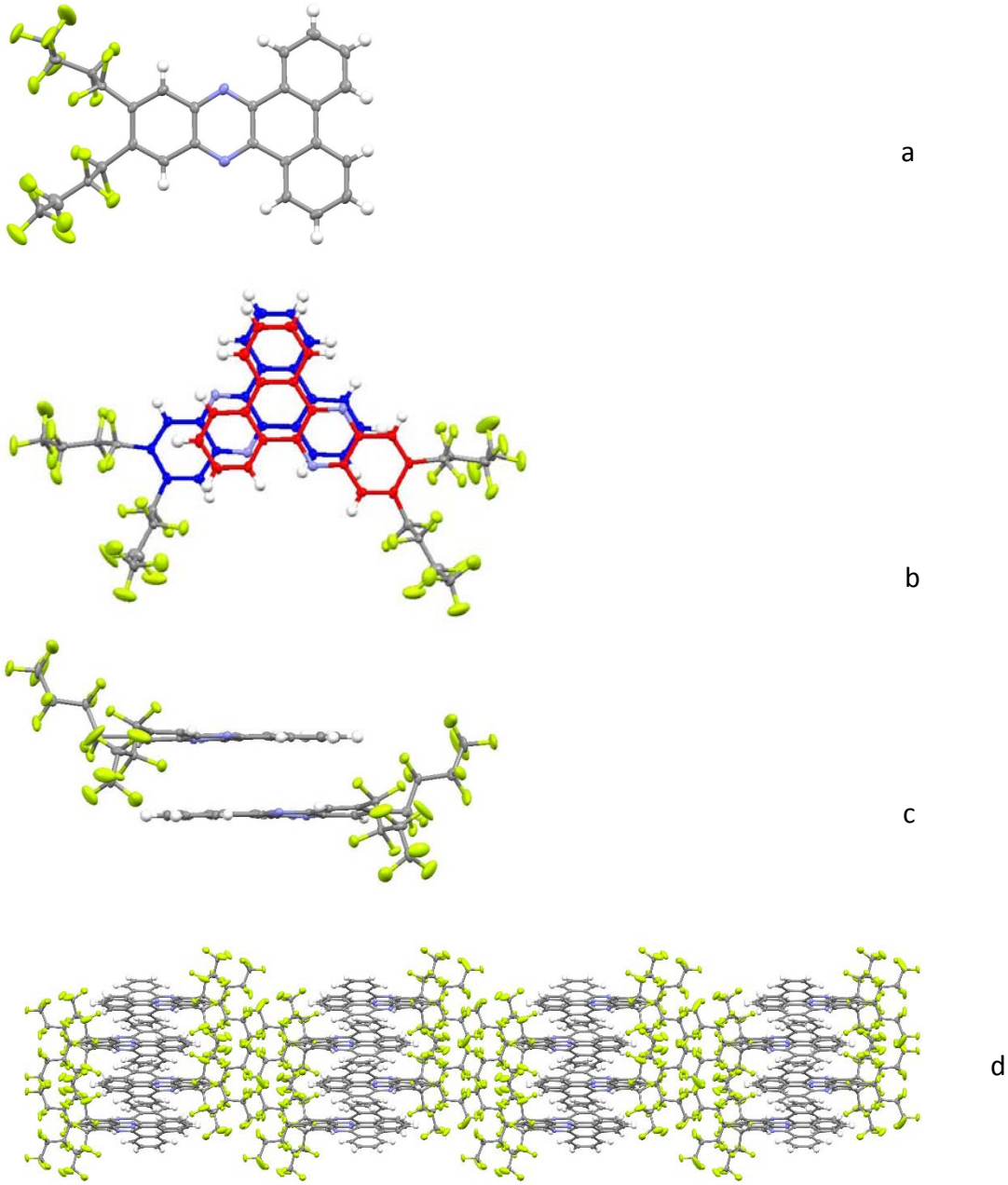


Figure S25: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, (d) crystal packing along b axis of **4**: (color code: light green, F; light blue, N; gray, C; white, H).

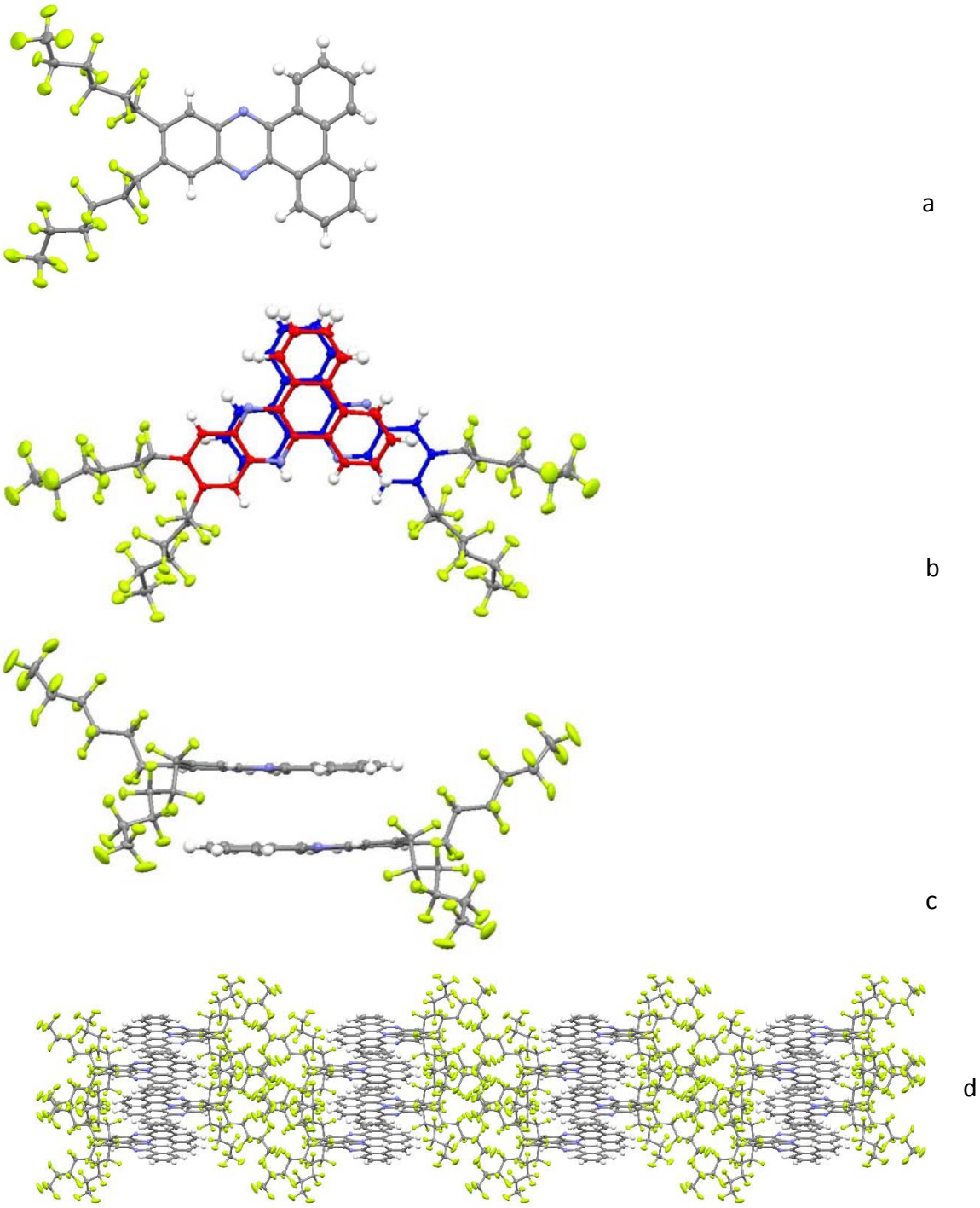


Figure S26: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, (d) crystal packing along b axis of **5**: (color code: light green, F; light blue, N; gray, C; white, H).

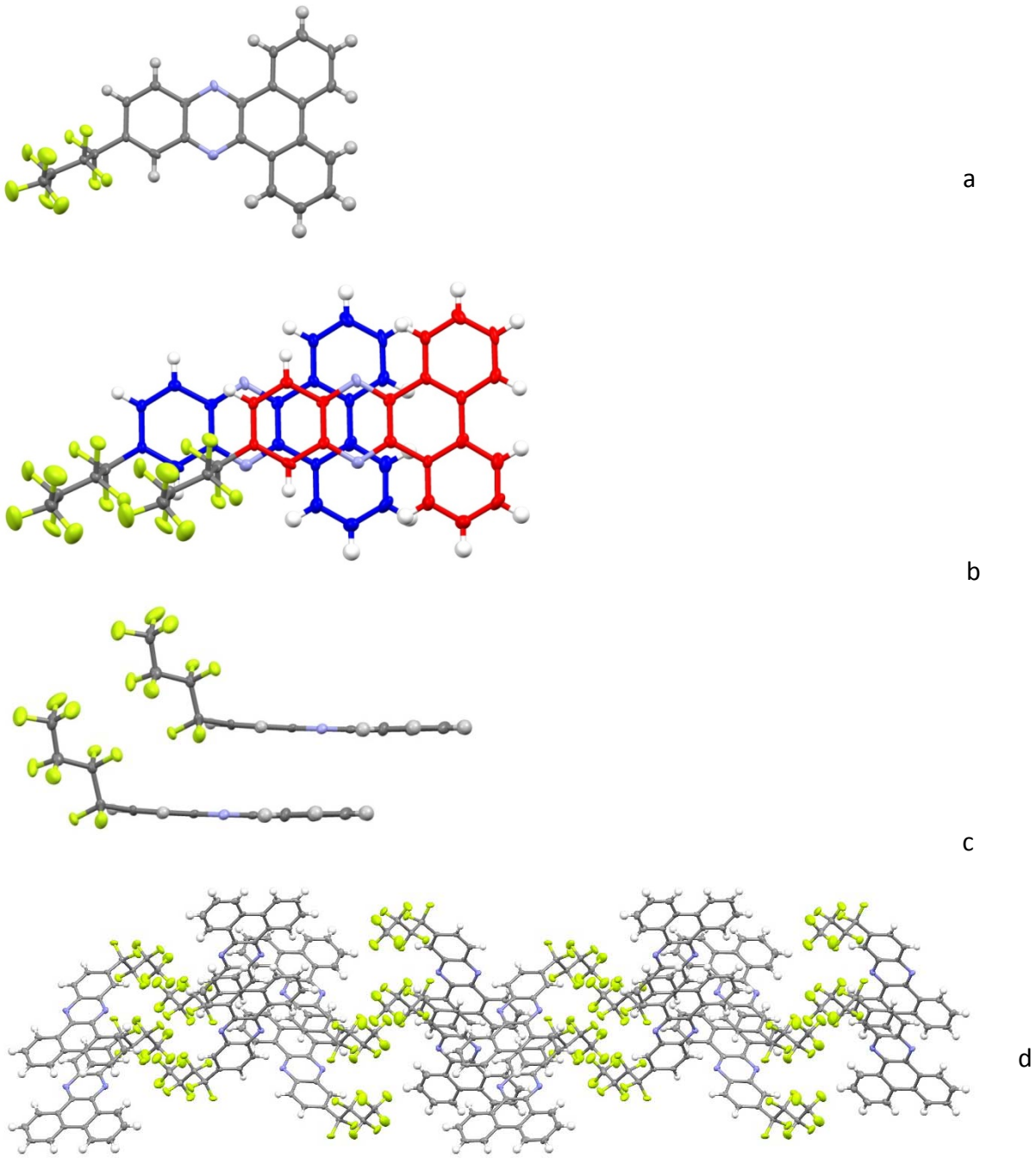


Figure S27: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, (d) crystal packing along b axis of **7**: (color code: light green, F; light blue, N; gray, C; white, H).

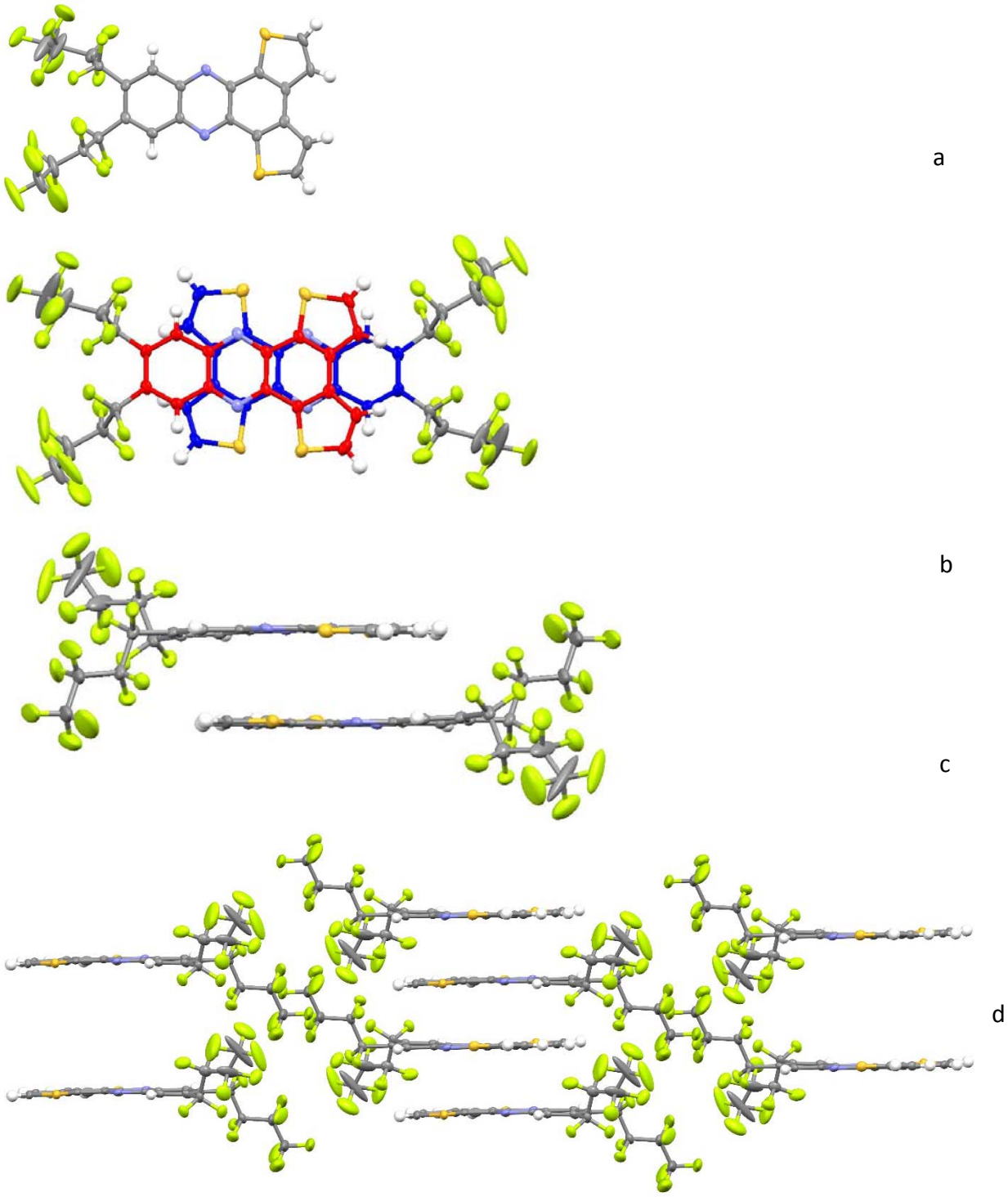


Figure S28: (a) Crystal structure, (b) topview dimer (overlapped dibenzphenazine rings are highlighted in red and blue colors, (c) sideview dimer, and (d) crystal packing (viewed along b axix) of **10**: (color code: light green, F; yellow, S; light blue, N; gray, C; white, H).

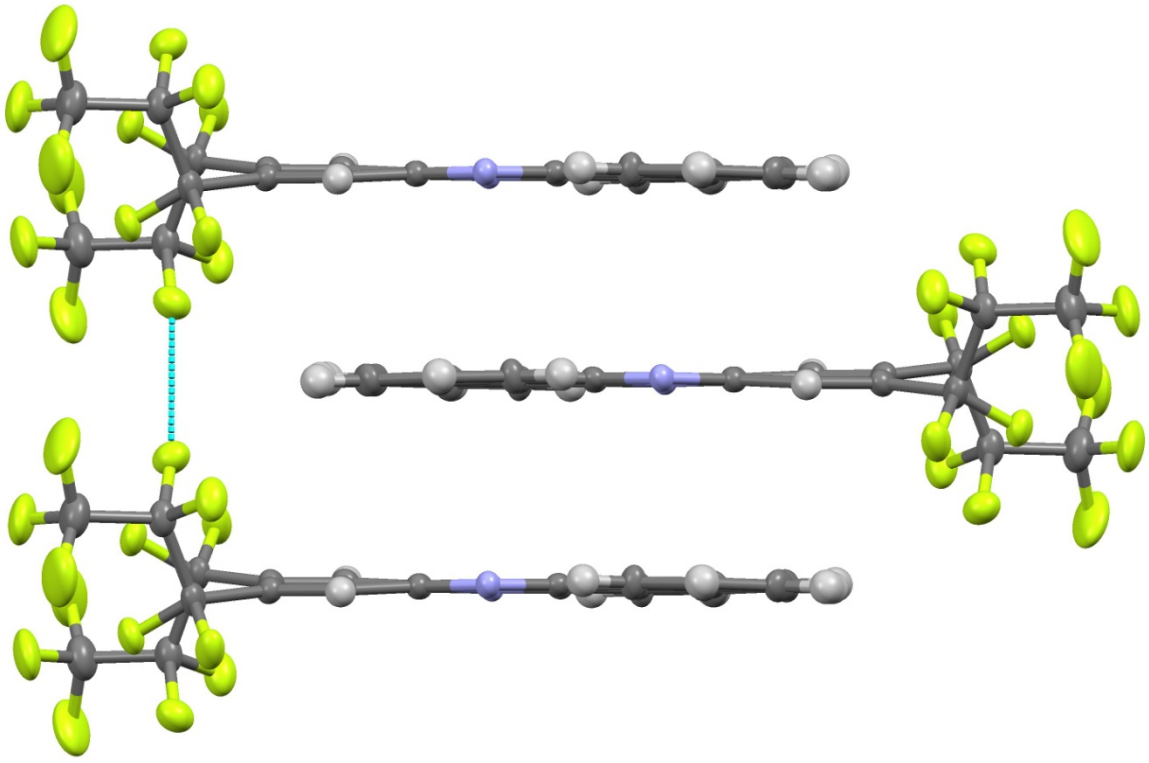


Figure S29: F-F short contact (C_{sp3}-F-F-C_{sp3} attractive intermolecular interactions) observed between alternative molecules of **3** in crystal packing: (color code: light green, F; light blue, N; gray, C; white, H).

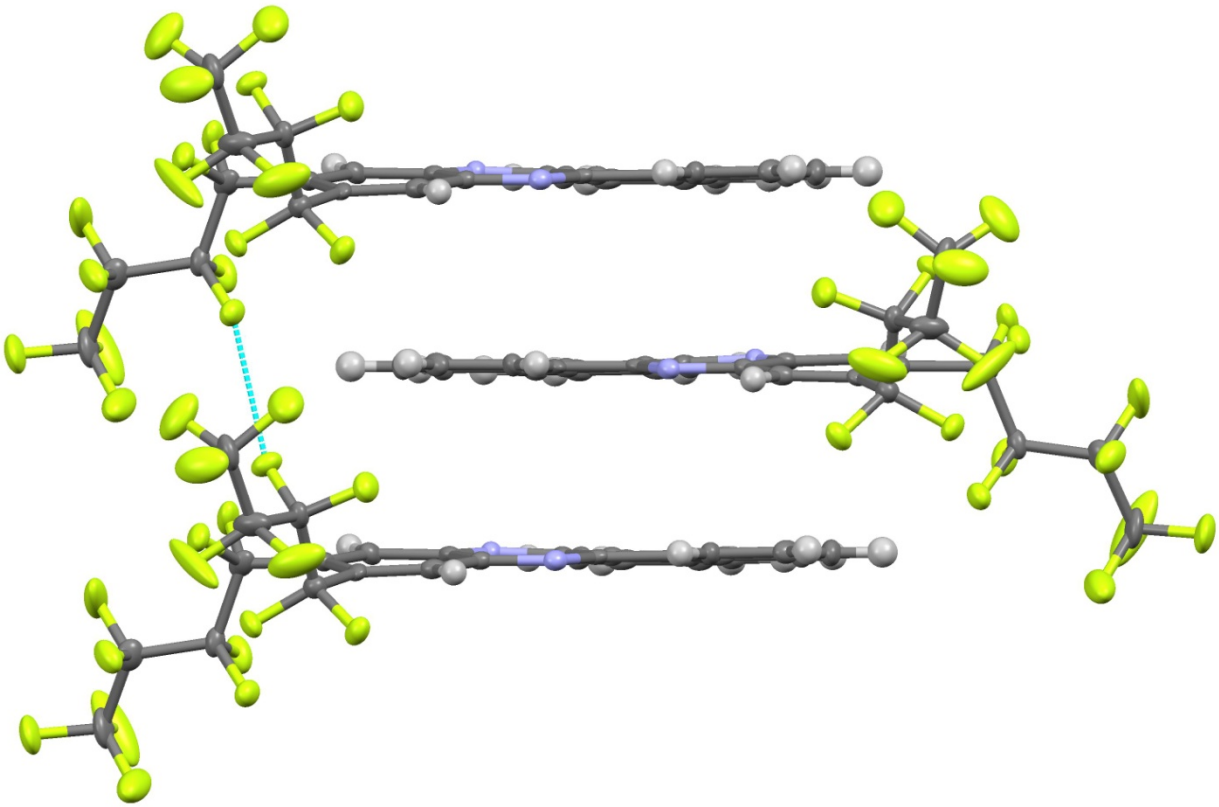


Figure S30: F-F short contact (C_{sp3}-F-F-C_{sp3} attractive intermolecular interactions) observed between alternative molecules of **4** in crystal packing: (color code: light green, F; light blue, N; gray, C; white, H).

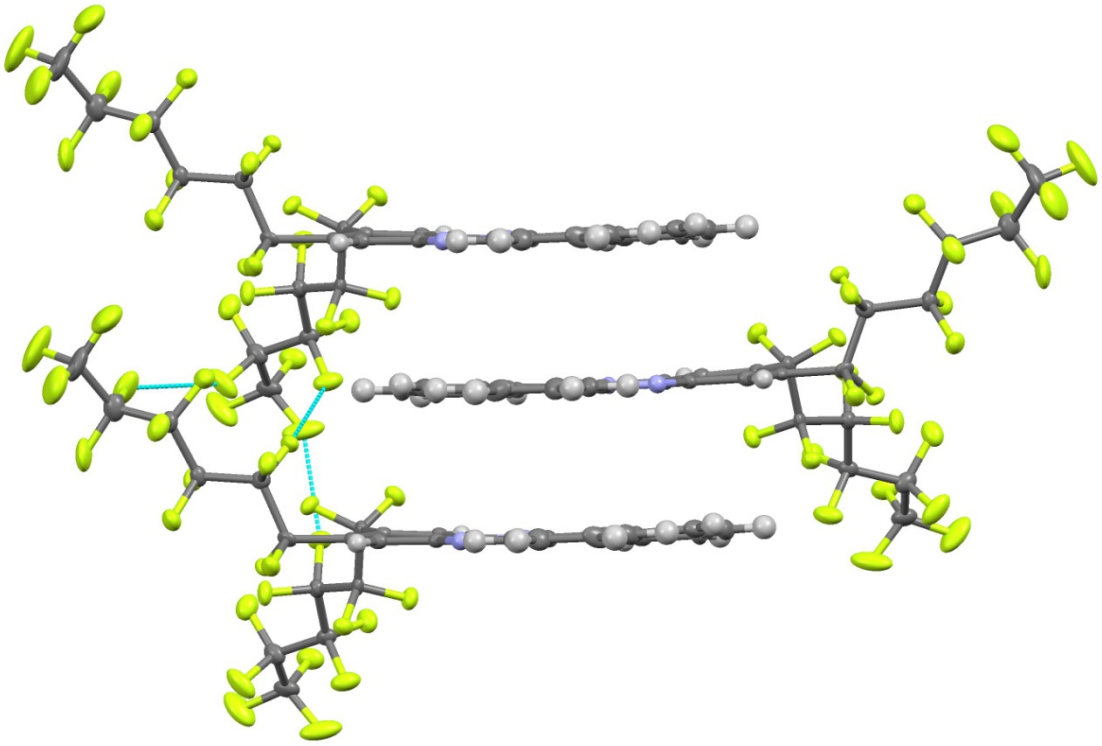


Figure S31: F-F short contact (C_{sp3}-F-F-C_{sp3} attractive intermolecular interactions) observed between alternative molecules of **5** in crystal packing: (color code: light green, F; light blue, N; gray, C; white, H).

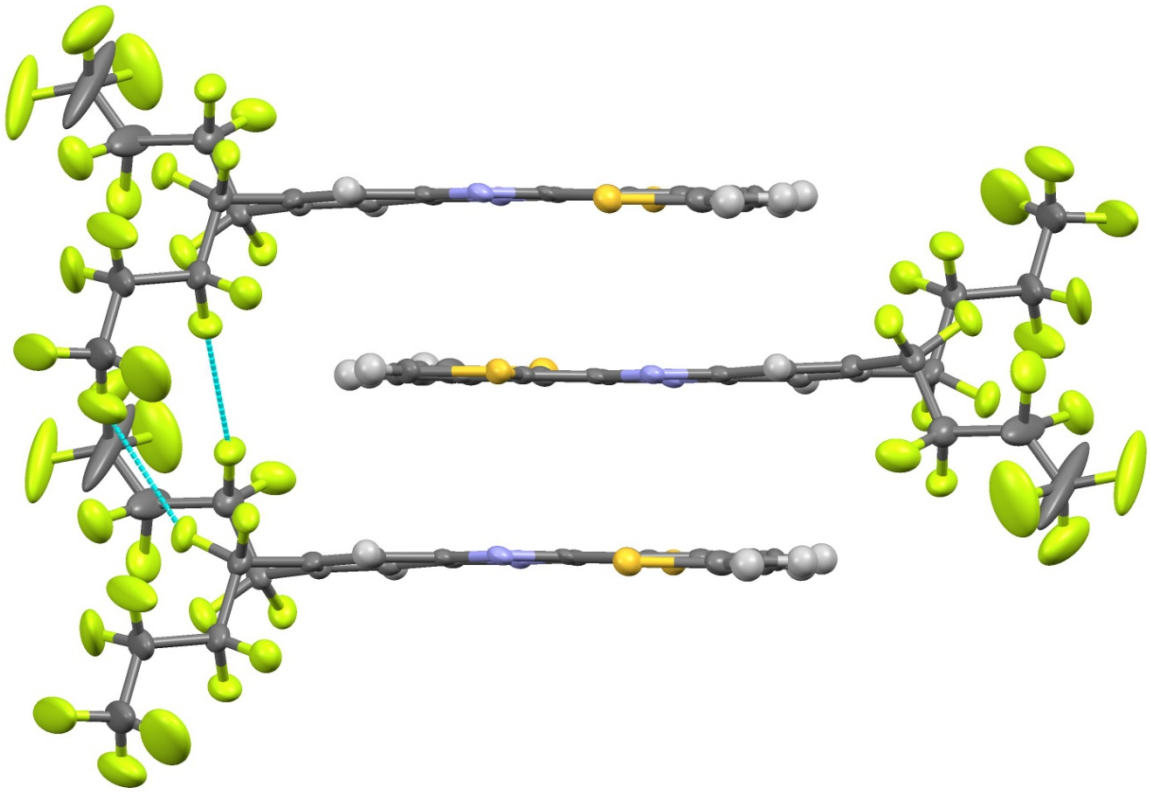


Figure S32: F-F short contact (C_{sp3}-F-F-C_{sp3} attractive intermolecular interactions) observed between alternative molecules of **10** in crystal packing: (color code: light green, F; yellow, S; light blue, N; gray, C; white, H).

5. Computational methods and general procedures

All computational calculations were done on a 744 CPU cluster computer (USD HPC) at the University of South Dakota supercomputing facility. Gaussian-09 program[1] and Gaussview interface program were used for all the calculations and post-processing of results. Frontier orbital maps of representative dimers were calculated using B97-D/TZV level of theory. The interaction energies of dimer molecules and between Rf-Rf chains of selected monomer molecules were calculated using long-range DFT with M06-2X/TZVP level of functional and theory. To calculate interaction energies in the solid state, we took structural coordinates from the crystal structure (adjacent molecules) and calculated single point energy of dimers with M06-2X/TZVP level of theory. Single point energy for monomers was calculated under similar conditions by removing one monomer molecule from the reduced crystal structure. The interaction energies were calculated by the following equation from the final energy output of the single point calculations:

$$\Delta E = E_{dimer} - 2(E_{monomer})$$

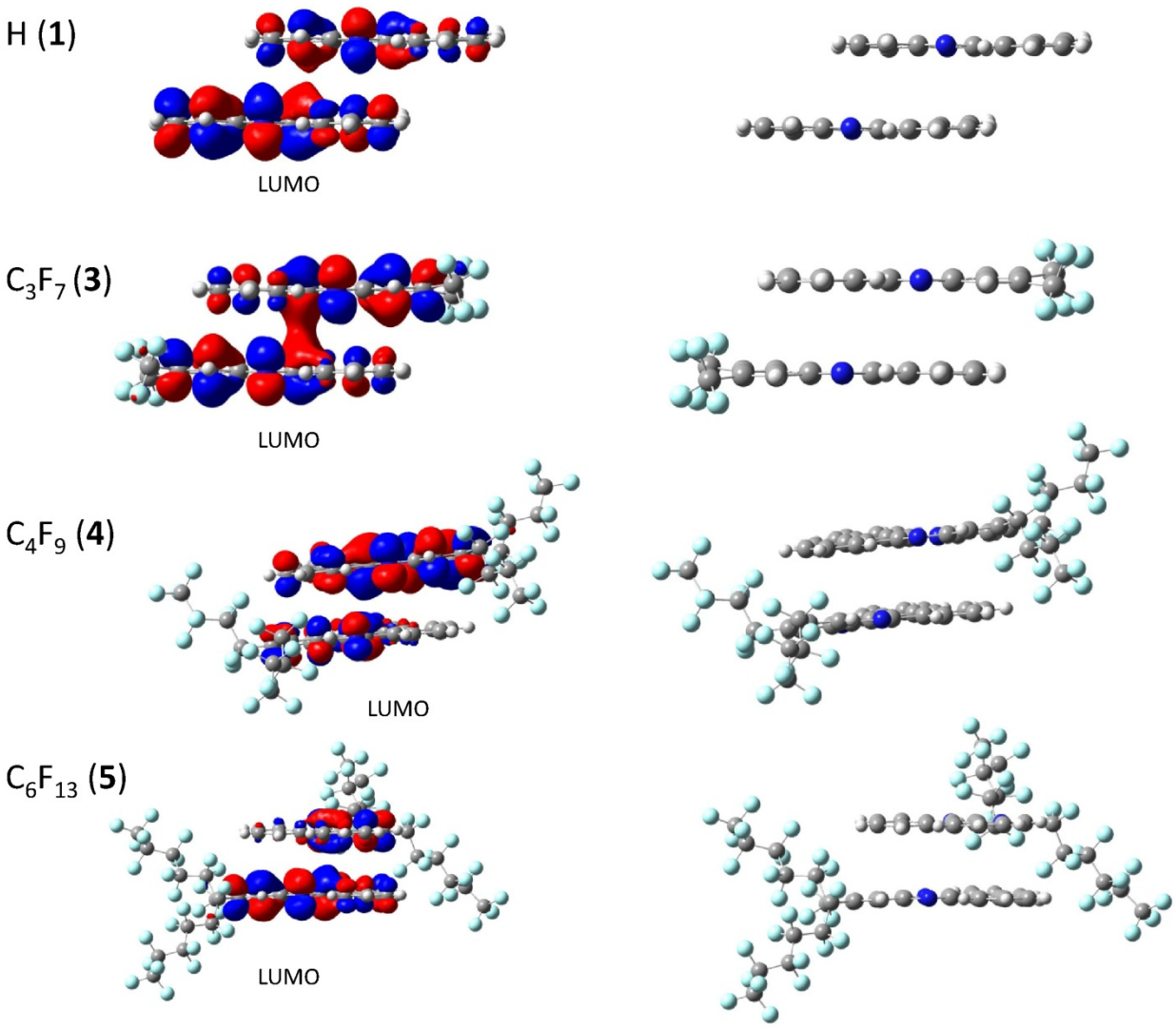
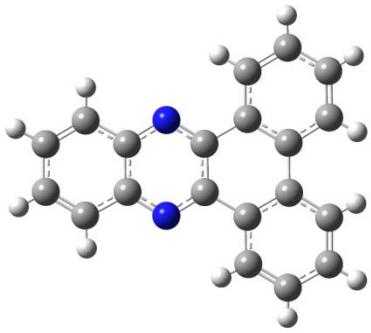


Figure S33: Change in LUMO (molecular orbital overlapping) of dimers by change in the length of Rf (perfluoroalkyl) chain

5.1. Molecular coordinates and total energies of monomer and dimers of crystal structures

Monomer (1):



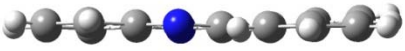
Coordinates of crystal structure geometry

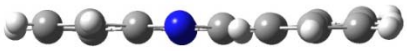
N	-3.53243	-8.58486	9.45536
N	-3.76821	-6.96509	11.76505
C	-1.6561	-7.94637	7.4556
C	-0.71872	-7.67093	6.50713
C	0.1539	-6.58911	6.68493
C	0.07047	-5.82597	7.82754
C	-0.04197	-4.25962	10.33821
C	-0.10985	-3.55334	11.51463
C	-1.10372	-3.82103	12.44763
C	-2.02557	-4.81955	12.19757
C	-5.57873	-8.33426	12.51685
C	-6.40004	-9.42067	12.33941
C	-6.25858	-10.2437	11.20165
C	-5.31445	-9.98535	10.26217
C	-0.8721	-6.09768	8.82203
C	-0.95812	-5.30538	10.06658
C	-1.95147	-5.5814	11.01972
C	-2.86916	-6.71563	10.82143
C	-4.58382	-8.03771	11.56496
C	-4.45065	-8.8448	10.4094
C	-2.75361	-7.51482	9.64394
C	-1.7587	-7.19271	8.6313
H	-2.25927	-8.59793	7.36877
H	-0.73063	-8.10822	5.72927
H	0.79282	-6.36479	6.01331
H	0.65291	-5.14411	7.91887
H	0.62182	-4.03113	9.72196
H	0.52854	-2.96698	11.70842
H	-1.11927	-3.36765	13.29219
H	-2.75672	-4.96747	12.8176
H	-5.64298	-7.78079	13.32096
H	-7.10943	-9.66783	12.99917
H	-6.79852	-10.98473	11.11518

H	-5.18698	-10.5223	9.4595

Total electronic energy: -878.00639821

Dimer (1):





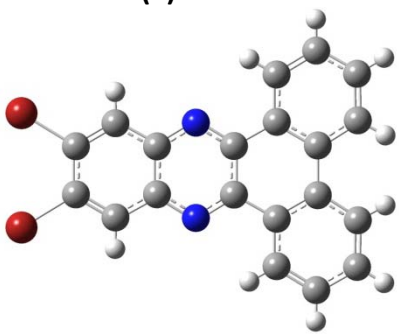
Coordinates of crystal structure geometry

N	-3.53243	-8.58486	9.45536
N	-3.76821	-6.96509	11.76505
C	-1.6561	-7.94637	7.4556
C	-0.71872	-7.67093	6.50713
C	0.1539	-6.58911	6.68493
C	0.07047	-5.82597	7.82754
C	-0.04197	-4.25962	10.33821
C	-0.10985	-3.55334	11.51463
C	-1.10372	-3.82103	12.44763
C	-2.02557	-4.81955	12.19757
C	-5.57873	-8.33426	12.51685
C	-6.40004	-9.42067	12.33941
C	-6.25858	-10.2437	11.20165
C	-5.31445	-9.98535	10.26217
C	-0.8721	-6.09768	8.82203
C	-0.95812	-5.30538	10.06658
C	-1.95147	-5.5814	11.01972
C	-2.86916	-6.71563	10.82143
C	-4.58382	-8.03771	11.56496
C	-4.45065	-8.8448	10.4094
C	-2.75361	-7.51482	9.64394
C	-1.7587	-7.19271	8.6313
H	-2.25927	-8.59793	7.36877
H	-0.73063	-8.10822	5.72927
H	0.79282	-6.36479	6.01331
H	0.65291	-5.14411	7.91887
H	0.62182	-4.03113	9.72196
H	0.52854	-2.96698	11.70842
H	-1.11927	-3.36765	13.29219
H	-2.75672	-4.96747	12.8176
H	-5.64298	-7.78079	13.32096
H	-7.10943	-9.66783	12.99917
H	-6.79852	-10.98473	11.11518
H	-5.18698	-10.5223	9.4595
N	1.64937	-8.58486	9.45536
N	1.41359	-6.96509	11.76505

C	3.5257	-7.94637	7.4556
C	4.46308	-7.67093	6.50713
C	5.3357	-6.58911	6.68493
C	5.25227	-5.82597	7.82754
C	5.13983	-4.25962	10.33821
C	5.07195	-3.55334	11.51463
C	4.07808	-3.82103	12.44763
C	3.15623	-4.81955	12.19757
C	-0.39693	-8.33426	12.51685
C	-1.21824	-9.42067	12.33941
C	-1.07678	-10.2437	11.20165
C	-0.13265	-9.98535	10.26217
C	4.3097	-6.09768	8.82203
C	4.22368	-5.30538	10.06658
C	3.23033	-5.5814	11.01972
C	2.31264	-6.71563	10.82143
C	0.59798	-8.03771	11.56496
C	0.73115	-8.8448	10.4094
C	2.42819	-7.51482	9.64394
C	3.4231	-7.19271	8.6313
H	2.92253	-8.59793	7.36877
H	4.45117	-8.10822	5.72927
H	5.97462	-6.36479	6.01331
H	5.83471	-5.14411	7.91887
H	5.80362	-4.03113	9.72196
H	5.71034	-2.96698	11.70842
H	4.06253	-3.36765	13.29219
H	2.42508	-4.96747	12.8176
H	-0.46118	-7.78079	13.32096
H	-1.92763	-9.66783	12.99917
H	-1.61672	-10.98473	11.11518
H	-0.00518	-10.5223	9.4595

Total electronic energy: -1756.03954560

Monomer (2):

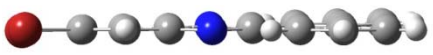


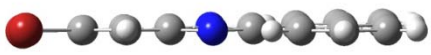
Coordinates of crystal structure geometry

Br	9.63144	59.62502	24.17569
C	9.22527	58.01141	25.06954
C	9.24405	55.60648	25.08217
N	9.57141	54.45237	24.46018
C	9.25224	53.32268	25.07409
C	10.20579	52.05913	23.18121
H	10.4078	52.86901	22.77272
C	9.61314	49.64969	24.40434
H	9.42672	48.83158	24.80784
C	9.53287	56.83843	24.45915
H	9.93783	56.84799	23.62203
C	10.52673	50.88323	22.55025
H	10.93793	50.89545	21.71623
C	9.26172	50.83675	25.06087
C	9.577	52.05382	24.43608
C	10.23139	49.672	23.16916
H	10.45135	48.87142	22.74774
Br	8.21219	59.62502	27.25322
C	8.61836	58.01141	26.35937
C	8.59957	55.60648	26.34674
N	8.27222	54.45237	26.96873
C	8.59139	53.32268	26.35482
C	7.63784	52.05913	28.2477
H	7.43583	52.86901	28.65619
C	8.23049	49.64969	27.02457
H	8.41691	48.83158	26.62107
C	8.31076	56.83843	26.96976
H	7.9058	56.84799	27.80688
C	7.31689	50.88323	28.87865
H	6.9057	50.89545	29.71269
C	8.58191	50.83675	26.36804
C	8.26663	52.05382	26.99283
C	7.61224	49.672	28.25974
H	7.39227	48.87142	28.68117

Total electronic energy: -6027.75600241

Dimer (2):





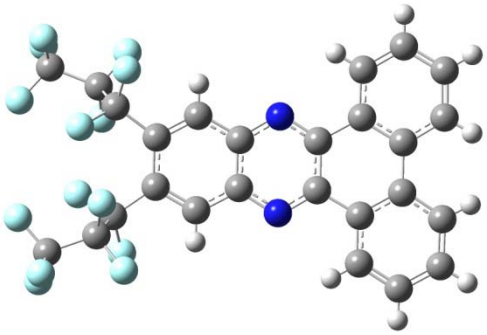
Coordinates of crystal structure geometry

Br	5.76734	59.62502	24.17569
C	5.36117	58.01141	25.06954
C	5.37995	55.60648	25.08217
N	5.70731	54.45237	24.46018
C	5.38814	53.32268	25.07409
C	6.34169	52.05913	23.18121
H	6.5437	52.86901	22.77272
C	5.74904	49.64969	24.40434
H	5.56262	48.83158	24.80784
C	5.66877	56.83843	24.45915
H	6.07372	56.84799	23.62203
C	6.66263	50.88323	22.55025
H	7.07383	50.89545	21.71623
C	5.39762	50.83675	25.06087
C	5.7129	52.05382	24.43608
C	6.36729	49.672	23.16916
H	6.58725	48.87142	22.74774
Br	4.34809	59.62502	27.25322
C	4.75426	58.01141	26.35937
C	4.73548	55.60648	26.34674
N	4.40812	54.45237	26.96873
C	4.72729	53.32268	26.35482
C	3.77374	52.05913	28.2477
H	3.57173	52.86901	28.65619
C	4.36639	49.64969	27.02457
H	4.55281	48.83158	26.62107
C	4.44665	56.83843	26.96976
H	4.0417	56.84799	27.80688
C	3.4528	50.88323	28.87865
H	3.0416	50.89545	29.71269
C	4.71781	50.83675	26.36804
C	4.40253	52.05382	26.99283
C	3.74814	49.672	28.25974
H	3.52818	48.87142	28.68117
Br	9.63144	59.62502	24.17569
C	9.22527	58.01141	25.06954
C	9.24405	55.60648	25.08217
N	9.57141	54.45237	24.46018
C	9.25224	53.32268	25.07409
C	10.20579	52.05913	23.18121
H	10.4078	52.86901	22.77272
C	9.61314	49.64969	24.40434
H	9.42672	48.83158	24.80784
C	9.53287	56.83843	24.45915
H	9.93783	56.84799	23.62203
C	10.52673	50.88323	22.55025
H	10.93793	50.89545	21.71623
C	9.26172	50.83675	25.06087

C	9.577	52.05382	24.43608
C	10.23139	49.672	23.16916
H	10.45135	48.87142	22.74774
Br	8.21219	59.62502	27.25322
C	8.61836	58.01141	26.35937
C	8.59957	55.60648	26.34674
N	8.27222	54.45237	26.96873
C	8.59139	53.32268	26.35482
C	7.63784	52.05913	28.2477
H	7.43583	52.86901	28.65619
C	8.23049	49.64969	27.02457
H	8.41691	48.83158	26.62107
C	8.31076	56.83843	26.96976
H	7.9058	56.84799	27.80688
C	7.31689	50.88323	28.87865
H	6.9057	50.89545	29.71269
C	8.58191	50.83675	26.36804
C	8.26663	52.05382	26.99283
C	7.61224	49.672	28.25974
H	7.39227	48.87142	28.68117

Total electronic energy: -12055.54915230

Monomer (3):



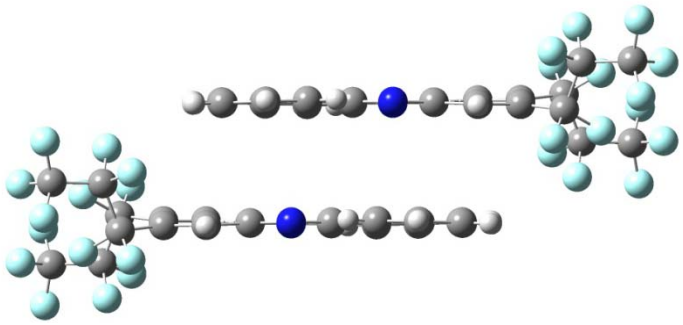
Coordinates of crystal structure geometry

F	-2.81737	13.37855	9.03046
F	-0.72411	12.72006	6.34599
F	-1.13248	12.0519	9.24644
F	-2.76563	13.4172	6.5136
F	-1.41208	10.29283	7.20078
F	-3.39727	10.94205	7.65589
F	-2.69726	10.98031	5.6264
C	-0.71122	21.50732	8.518
C	-1.38375	20.28887	8.31937
N	-1.36084	17.89256	8.32913

C	-1.34846	15.50513	8.41416
H	-2.25648	15.50397	8.21065
C	-0.68119	16.73981	8.53333
C	-0.68899	19.02096	8.50964
C	-2.72627	20.2939	7.93606
H	-3.16246	19.4843	7.7904
C	-1.85269	12.5964	7.07046
C	-2.76495	22.66857	7.98623
H	-3.23033	23.4685	7.88588
C	-1.59701	13.08409	8.50824
C	-1.43939	22.69408	8.34725
H	-1.01796	23.51101	8.48037
C	-3.41458	21.46636	7.77088
H	-4.30936	21.45515	7.5158
C	-0.71037	14.3091	8.5877
C	-2.35132	11.16928	6.89762
F	2.81737	13.37855	8.39304
F	0.72411	12.72006	11.07751
F	1.13248	12.0519	8.17706
F	2.76563	13.4172	10.9099
F	1.41208	10.29283	10.22272
F	3.39727	10.94205	9.76761
F	2.69726	10.98031	11.7971
C	0.71122	21.50732	8.9055
C	1.38375	20.28887	9.10413
N	1.36084	17.89256	9.09437
C	1.34846	15.50513	9.00934
H	2.25648	15.50397	9.21285
C	0.68119	16.73981	8.89017
C	0.68899	19.02096	8.91386
C	2.72627	20.2939	9.48744
H	3.16246	19.4843	9.63311
C	1.85269	12.5964	10.35304
C	2.76495	22.66857	9.43727
H	3.23033	23.4685	9.53762
C	1.59701	13.08409	8.91526
C	1.43939	22.69408	9.07625
H	1.01796	23.51101	8.94313
C	3.41458	21.46636	9.65262
H	4.30936	21.45515	9.9077
C	0.71037	14.3091	8.83581
C	2.35132	11.16928	10.52589

Total electronic energy: -2502.67847973

Dimer (3):



Coordinates of crystal structure geometry

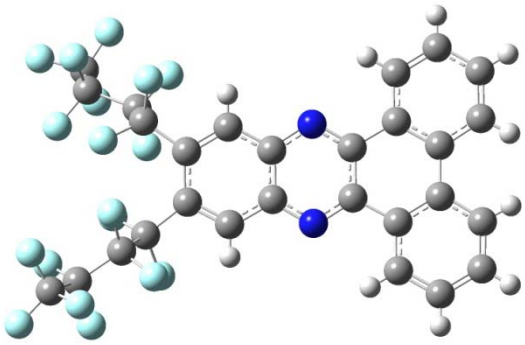
F	-2.81737	13.37855	9.03046
F	-0.72411	12.72006	6.34599
F	-1.13248	12.0519	9.24644
F	-2.76563	13.4172	6.5136
F	-1.41208	10.29283	7.20078
F	-3.39727	10.94205	7.65589
F	-2.69726	10.98031	5.6264
C	-0.71122	21.50732	8.518
C	-1.38375	20.28887	8.31937
N	-1.36084	17.89256	8.32913
C	-1.34846	15.50513	8.41416
H	-2.25648	15.50397	8.21065
C	-0.68119	16.73981	8.53333
C	-0.68899	19.02096	8.50964
C	-2.72627	20.2939	7.93606
H	-3.16246	19.4843	7.7904
C	-1.85269	12.5964	7.07046
C	-2.76495	22.66857	7.98623
H	-3.23033	23.4685	7.88588
C	-1.59701	13.08409	8.50824
C	-1.43939	22.69408	8.34725
H	-1.01796	23.51101	8.48037
C	-3.41458	21.46636	7.77088
H	-4.30936	21.45515	7.5158
C	-0.71037	14.3091	8.5877
C	-2.35132	11.16928	6.89762
F	2.81737	13.37855	8.39304
F	0.72411	12.72006	11.07751
F	1.13248	12.0519	8.17706
F	2.76563	13.4172	10.9099
F	1.41208	10.29283	10.22272
F	3.39727	10.94205	9.76761
F	2.69726	10.98031	11.7971

C	0.71122	21.50732	8.9055
C	1.38375	20.28887	9.10413
N	1.36084	17.89256	9.09437
C	1.34846	15.50513	9.00934
H	2.25648	15.50397	9.21285
C	0.68119	16.73981	8.89017
C	0.68899	19.02096	8.91386
C	2.72627	20.2939	9.48744
H	3.16246	19.4843	9.63311
C	1.85269	12.5964	10.35304
C	2.76495	22.66857	9.43727
H	3.23033	23.4685	9.53762
C	1.59701	13.08409	8.91526
C	1.43939	22.69408	9.07625
H	1.01796	23.51101	8.94313
C	3.41458	21.46636	9.65262
H	4.30936	21.45515	9.9077
C	0.71037	14.3091	8.83581
C	2.35132	11.16928	10.52589
F	2.81737	25.26545	4.90834
F	0.72411	25.92394	7.59281
F	1.13248	26.5921	4.69236
F	2.76563	25.2268	7.4252
F	1.41208	28.35117	6.73802
F	3.39727	27.70195	6.28291
F	2.69726	27.66369	8.3124
C	0.71122	17.13668	5.4208
C	1.38375	18.35513	5.61943
N	1.36084	20.75144	5.60967
C	1.34846	23.13887	5.52464
H	2.25648	23.14003	5.72815
C	0.68119	21.90419	5.40547
C	0.68899	19.62304	5.42916
C	2.72627	18.3501	6.00274
H	3.16246	19.15969	6.14841
C	1.85269	26.0476	6.86834
C	2.76495	15.97543	5.95256
H	3.23033	15.1755	6.05292
C	1.59701	25.55991	5.43056
C	1.43939	15.94993	5.59155
H	1.01796	15.13299	5.45843
C	3.41458	17.17764	6.16792
H	4.30936	17.18885	6.423
C	0.71037	24.3349	5.3511
C	2.35132	27.47472	7.04118
F	-2.81737	25.26545	5.54576
F	-0.72411	25.92394	2.86129
F	-1.13248	26.5921	5.76174

F	-2.76563	25.2268	3.0289
F	-1.41208	28.35117	3.71608
F	-3.39727	27.70195	4.17119
F	-2.69726	27.66369	2.1417
C	-0.71122	17.13668	5.0333
C	-1.38375	18.35513	4.83467
N	-1.36084	20.75144	4.84443
C	-1.34846	23.13887	4.92946
H	-2.25648	23.14003	4.72595
C	-0.68119	21.90419	5.04863
C	-0.68899	19.62304	5.02494
C	-2.72627	18.3501	4.45136
H	-3.16246	19.15969	4.3057
C	-1.85269	26.0476	3.58576
C	-2.76495	15.97543	4.50153
H	-3.23033	15.1755	4.40118
C	-1.59701	25.55991	5.02354
C	-1.43939	15.94993	4.86255
H	-1.01796	15.13299	4.99567
C	-3.41458	17.17764	4.28618
H	-4.30936	17.18885	4.0311
C	-0.71037	24.3349	5.10299
C	-2.35132	27.47472	3.41291

Total electronic energy: -5005.40670572

Monomer (4):



Coordinates of crystal structure geometry

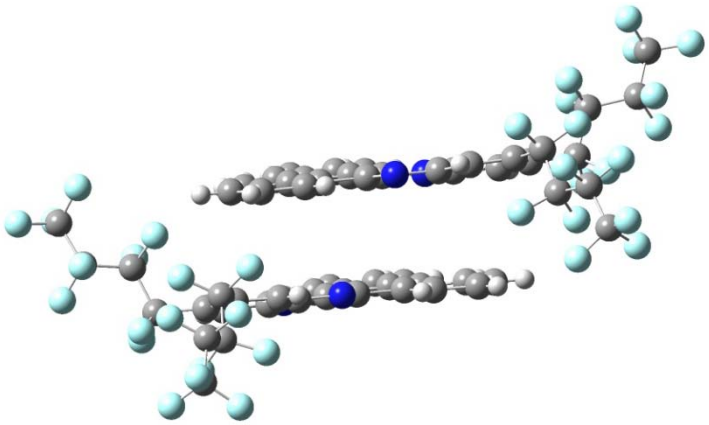
F	4.61796	1.78043	2.35735
F	2.79051	-0.60163	5.61697
F	2.74593	0.50019	3.74962
F	5.50721	-0.3045	3.42334
F	7.49542	1.45597	3.15321
F	6.59594	1.00542	0.71459

F	7.54949	3.5981	2.84107
F	5.02642	3.86843	2.72446
F	5.34061	-1.15344	5.41083
F	8.47016	2.04141	-0.83748
F	1.17422	-1.22664	2.355
F	6.25982	3.10438	0.34944
F	3.34583	-2.85438	4.51446
F	3.71994	-1.96047	2.58194
N	6.03038	4.65837	7.36731
F	9.26076	1.49104	1.04597
F	0.75407	-1.79141	4.33542
F	1.33351	-3.28065	2.91214
C	5.66285	3.38856	9.38543
C	6.07423	4.5019	11.56649
N	5.30773	2.28962	8.72856
F	8.92611	3.54684	0.56774
C	5.32235	2.35437	7.37556
C	6.5331	5.74113	9.4455
C	5.64531	3.37777	10.8519
C	6.064	4.58283	8.68929
C	6.98832	6.88144	8.76821
H	6.98613	6.89763	7.8369
C	7.00074	6.83828	11.52683
H	7.00659	6.84187	12.45815
C	7.43696	7.97319	9.4616
H	7.7402	8.72501	9.00693
C	6.54552	5.70336	10.8574
C	5.1879	2.24285	11.52722
H	4.90147	1.50363	11.04076
C	4.85324	-0.16727	4.58906
C	7.43623	7.94442	10.8574
H	7.73508	8.68544	11.33523
C	3.34875	-0.5144	4.38254
C	5.61974	3.55403	5.28833
H	5.78926	4.35261	4.84505
C	5.34719	2.42991	4.55372
C	5.04176	1.19427	6.60757
H	4.81671	0.40828	7.05164
C	5.59416	3.30942	13.60816
H	5.58101	3.28604	14.53909
C	5.43487	2.61157	3.04838
C	1.5571	-2.0504	3.28553
C	5.09072	1.19067	5.2369
C	5.15648	2.21048	12.89947
H	4.84374	1.45687	13.34549
C	6.04646	4.42636	12.97367
H	6.34166	5.14939	13.47506
C	5.65116	3.53425	6.69945

C	6.88383	2.47487	2.51951
C	7.03216	2.24106	0.991
C	8.46724	2.34717	0.45663
C	3.02433	-1.81479	3.65224

Total electronic energy: -2978.05519771

Dimer (4):



Coordinates of crystal structure geometry

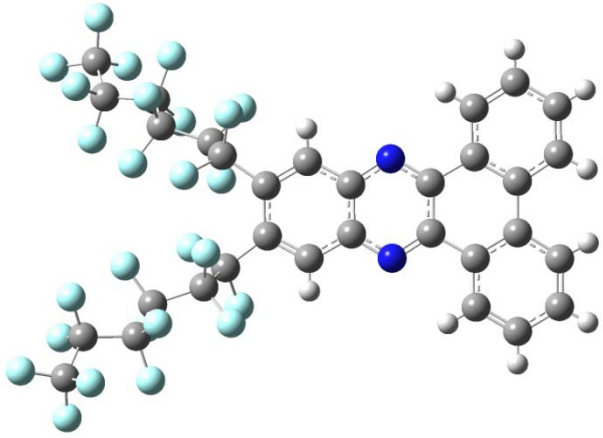
F	4.61796	1.78043	2.35735
F	2.79051	-0.60163	5.61697
F	2.74593	0.50019	3.74962
F	5.50721	-0.3045	3.42334
F	7.49542	1.45597	3.15321
F	6.59594	1.00542	0.71459
F	7.54949	3.5981	2.84107
F	5.02642	3.86843	2.72446
F	5.34061	-1.15344	5.41083
F	8.47016	2.04141	-0.83748
F	1.17422	-1.22664	2.355
F	6.25982	3.10438	0.34944
F	3.34583	-2.85438	4.51446
F	3.71994	-1.96047	2.58194
N	6.03038	4.65837	7.36731
F	9.26076	1.49104	1.04597
F	0.75407	-1.79141	4.33542
F	1.33351	-3.28065	2.91214
C	5.66285	3.38856	9.38543
C	6.07423	4.5019	11.56649
N	5.30773	2.28962	8.72856
F	8.92611	3.54684	0.56774
C	5.32235	2.35437	7.37556
C	6.5331	5.74113	9.4455
C	5.64531	3.37777	10.8519

C	6.064	4.58283	8.68929
C	6.98832	6.88144	8.76821
H	6.98613	6.89763	7.8369
C	7.00074	6.83828	11.52683
H	7.00659	6.84187	12.45815
C	7.43696	7.97319	9.4616
H	7.7402	8.72501	9.00693
C	6.54552	5.70336	10.8574
C	5.1879	2.24285	11.52722
H	4.90147	1.50363	11.04076
C	4.85324	-0.16727	4.58906
C	7.43623	7.94442	10.8574
H	7.73508	8.68544	11.33523
C	3.34875	-0.5144	4.38254
C	5.61974	3.55403	5.28833
H	5.78926	4.35261	4.84505
C	5.34719	2.42991	4.55372
C	5.04176	1.19427	6.60757
H	4.81671	0.40828	7.05164
C	5.59416	3.30942	13.60816
H	5.58101	3.28604	14.53909
C	5.43487	2.61157	3.04838
C	1.5571	-2.0504	3.28553
C	5.09072	1.19067	5.2369
C	5.15648	2.21048	12.89947
H	4.84374	1.45687	13.34549
C	6.04646	4.42636	12.97367
H	6.34166	5.14939	13.47506
C	5.65116	3.53425	6.69945
C	6.88383	2.47487	2.51951
C	7.03216	2.24106	0.991
C	8.46724	2.34717	0.45663
C	3.02433	-1.81479	3.65224
F	0.96451	1.78043	17.27415
F	-0.86294	-0.60163	14.01454
F	-0.90752	0.50019	15.88188
F	1.85376	-0.3045	16.20816
F	3.84197	1.45597	16.47829
F	2.94249	1.00542	18.91691
F	3.89604	3.5981	16.79043
F	1.37297	3.86843	16.90704
F	1.68716	-1.15344	14.22067
F	4.81671	2.04141	20.46898
F	-2.47923	-1.22664	17.27651
F	2.60637	3.10438	19.28206
F	-0.30762	-2.85438	15.11704
F	0.06649	-1.96047	17.04957
N	2.37694	4.65837	12.26419

F	5.60731	1.49104	18.58553
F	-2.89938	-1.79141	15.29608
F	-2.31994	-3.28065	16.71936
C	2.0094	3.38856	10.24607
C	2.42078	4.5019	8.06501
N	1.65428	2.28962	10.90294
F	5.27266	3.54684	19.06376
C	1.6689	2.35437	12.25595
C	2.87965	5.74113	10.186
C	1.99186	3.37777	8.7796
C	2.41055	4.58283	10.9422
C	3.33487	6.88144	10.86329
H	3.33268	6.89763	11.79461
C	3.34729	6.83828	8.10467
H	3.35314	6.84187	7.17335
C	3.78351	7.97319	10.1699
H	4.08675	8.72501	10.62457
C	2.89207	5.70336	8.7741
C	1.53445	2.24285	8.10428
H	1.24802	1.50363	8.59074
C	1.19979	-0.16727	15.04244
C	3.78278	7.94442	8.7741
H	4.08163	8.68544	8.29627
C	-0.3047	-0.5144	15.24896
C	1.96629	3.55403	14.34317
H	2.13581	4.35261	14.78645
C	1.69374	2.42991	15.07778
C	1.38831	1.19427	13.02393
H	1.16326	0.40828	12.57986
C	1.94071	3.30942	6.02334
H	1.92756	3.28604	5.09241
C	1.78142	2.61157	16.58312
C	-2.09635	-2.0504	16.34597
C	1.43727	1.19067	14.3946
C	1.50303	2.21048	6.73203
H	1.19029	1.45687	6.28601
C	2.39301	4.42636	6.65783
H	2.68821	5.14939	6.15644
C	1.99771	3.53425	12.93205
C	3.23038	2.47487	17.11199
C	3.37871	2.24106	18.6405
C	4.81379	2.34717	19.17487
C	-0.62912	-1.81479	15.97926

Total electronic energy: -5956.15336376

Monomer (5):



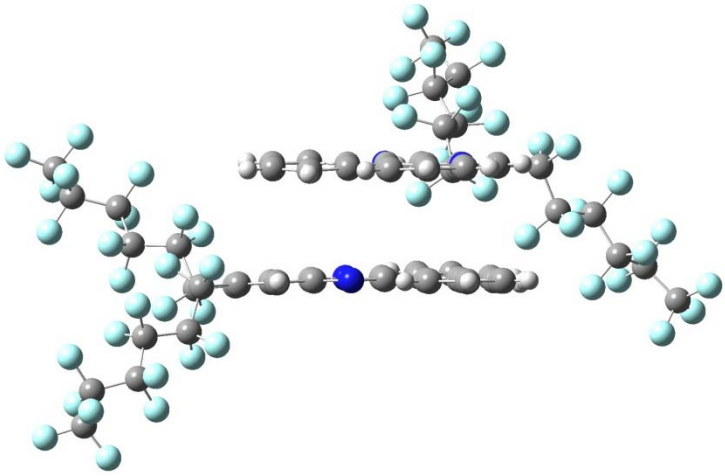
Coordinates of crystal structure geometry

F	8.09195	8.32684	5.64125
F	6.18229	7.20519	3.92824
F	3.29371	7.77736	4.6609
F	5.34268	9.32465	4.92769
F	4.59568	6.15922	1.858
F	3.09416	5.6579	4.27775
F	6.918	11.53039	4.94587
F	5.4481	10.18337	6.91204
F	7.9406	9.89049	7.14928
F	5.53244	5.17239	4.24639
F	9.16576	12.12375	5.91214
F	10.06637	10.20233	5.46809
F	8.79678	12.35842	3.03652
F	7.69285	9.9301	3.6819
F	4.24553	8.27143	2.27659
F	1.47667	7.41996	2.73745
F	10.59198	13.79712	4.36229
F	11.86383	12.10702	4.65135
F	2.08737	5.59375	1.72165
F	2.11448	8.91314	0.71856
F	10.17255	10.66925	2.91789
F	3.25832	7.34596	-0.25043
F	1.05046	5.94594	-0.7222
F	11.51066	12.88671	2.66746
N	5.53545	6.73325	10.25443
F	-0.14609	7.25428	0.50131
N	4.79674	4.35681	8.90093
F	0.77034	7.99492	-1.28033
C	4.44884	3.25227	11.0089
C	3.74552	0.93347	11.0498
H	3.51058	0.15248	10.60348
C	5.35849	6.61796	6.08894

C	4.07911	2.13657	13.09414
H	4.06028	2.144	14.02587
C	5.2124	5.63243	10.90982
C	5.24252	5.67705	12.37149
C	5.12129	5.49296	8.23418
C	5.65443	6.82622	13.03915
H	5.94133	7.56259	12.54875
C	4.4383	3.30805	12.41376
C	4.78318	4.66735	14.5031
H	4.47068	3.95516	15.01214
C	5.65669	7.84337	6.77887
C	5.48048	6.67375	8.90502
C	4.81933	4.54834	13.0996
C	7.45339	9.47229	5.95122
C	5.0859	5.4911	6.82614
H	4.87204	4.70268	6.38118
C	5.19433	5.79978	15.13394
H	5.17249	5.84069	16.06203
C	4.09342	2.07706	10.35215
H	4.0904	2.06033	9.42178
C	3.75757	0.98925	12.44057
H	3.54221	0.22872	12.93052
C	5.64614	6.89689	14.40811
H	5.93756	7.66486	14.84397
C	3.85019	6.74255	4.00369
C	7.81108	10.52477	4.88315
C	2.36448	6.89503	1.88708
C	5.94509	9.17291	6.12484
C	5.26286	6.45804	4.57136
C	5.74178	7.82664	8.14055
H	5.98274	8.60948	8.58096
C	3.78844	7.03077	2.49293
C	4.83213	4.42933	10.22761
C	9.21621	11.12911	4.99814
C	9.78098	11.69068	3.68645
C	2.1815	7.59234	0.52358
C	10.95343	12.6353	3.84871
C	0.92546	7.19255	-0.25725

Total electronic energy: -3928.85828137

Dimer (5):



Coordinates of crystal structure geometry

F	4.32685	8.32684	17.08375
F	2.41719	7.20519	18.79676
F	-0.47139	7.77736	18.0641
F	1.57758	9.32465	17.79731
F	0.83058	6.15922	20.867
F	-0.67094	5.6579	18.44725
F	3.1529	11.53039	17.77913
F	1.683	10.18337	15.81296
F	4.1755	9.89049	15.57572
F	1.76734	5.17239	18.47861
F	5.40066	12.12375	16.81286
F	6.30127	10.20233	17.25691
F	5.03168	12.35842	19.68849
F	3.92775	9.9301	19.0431
F	0.48043	8.27143	20.44841
F	-2.28843	7.41996	19.98755
F	6.82688	13.79712	18.36271
F	8.09873	12.10702	18.07365
F	-1.67773	5.59375	21.00335
F	-1.65062	8.91314	22.00644
F	6.40745	10.66925	19.80711
F	-0.50678	7.34596	22.97543
F	-2.71464	5.94594	23.4472
F	7.74556	12.88671	20.05754
N	1.77035	6.73325	12.47057
F	-3.91119	7.25428	22.22369
N	1.03164	4.35681	13.82407
F	-2.99476	7.99492	24.00533

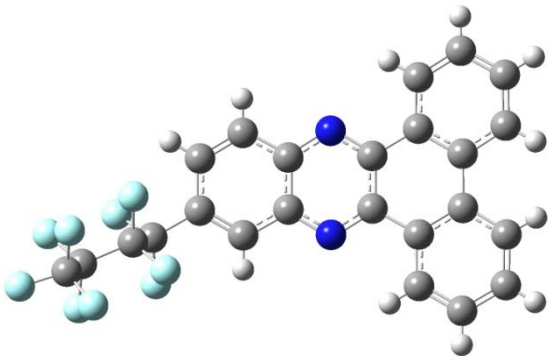
C	0.68374	3.25227	11.7161
C	-0.01958	0.93347	11.6752
H	-0.25452	0.15248	12.12152
C	1.59339	6.61796	16.63606
C	0.31401	2.13657	9.63086
H	0.29518	2.144	8.69913
C	1.4473	5.63243	11.81518
C	1.47742	5.67705	10.35351
C	1.35619	5.49296	14.49082
C	1.88933	6.82622	9.68585
H	2.17623	7.56259	10.17625
C	0.6732	3.30805	10.31124
C	1.01808	4.66735	8.2219
H	0.70558	3.95516	7.71286
C	1.89159	7.84337	15.94613
C	1.71538	6.67375	13.81998
C	1.05423	4.54834	9.6254
C	3.68829	9.47229	16.77378
C	1.3208	5.4911	15.89886
H	1.10694	4.70268	16.34382
C	1.42923	5.79978	7.59106
H	1.40739	5.84069	6.66297
C	0.32832	2.07706	12.37285
H	0.32531	2.06033	13.30321
C	-0.00753	0.98925	10.28443
H	-0.22289	0.22872	9.79448
C	1.88104	6.89689	8.3169
H	2.17246	7.66486	7.88103
C	0.08509	6.74255	18.72131
C	4.04598	10.52477	17.84185
C	-1.40062	6.89503	20.83792
C	2.17999	9.17291	16.60016
C	1.49776	6.45804	18.15364
C	1.97668	7.82664	14.58445
H	2.21764	8.60948	14.14404
C	0.02334	7.03077	20.23207
C	1.06703	4.42933	12.49739
C	5.45111	11.12911	17.72686
C	6.01588	11.69068	19.03855
C	-1.5836	7.59234	22.20142
C	7.18833	12.6353	18.87629
C	-2.83964	7.19255	22.98225
F	8.09195	8.32684	5.64125
F	6.18229	7.20519	3.92824
F	3.29371	7.77736	4.6609
F	5.34268	9.32465	4.92769
F	4.59568	6.15922	1.858
F	3.09416	5.6579	4.27775

F	6.918	11.53039	4.94587
F	5.4481	10.18337	6.91204
F	7.9406	9.89049	7.14928
F	5.53244	5.17239	4.24639
F	9.16576	12.12375	5.91214
F	10.06637	10.20233	5.46809
F	8.79678	12.35842	3.03652
F	7.69285	9.9301	3.6819
F	4.24553	8.27143	2.27659
F	1.47667	7.41996	2.73745
F	10.59198	13.79712	4.36229
F	11.86383	12.10702	4.65135
F	2.08737	5.59375	1.72165
F	2.11448	8.91314	0.71856
F	10.17255	10.66925	2.91789
F	3.25832	7.34596	-0.25043
F	1.05046	5.94594	-0.7222
F	11.51066	12.88671	2.66746
N	5.53545	6.73325	10.25443
F	-0.14609	7.25428	0.50131
N	4.79674	4.35681	8.90093
F	0.77034	7.99492	-1.28033
C	4.44884	3.25227	11.0089
C	3.74552	0.93347	11.0498
H	3.51058	0.15248	10.60348
C	5.35849	6.61796	6.08894
C	4.07911	2.13657	13.09414
H	4.06028	2.144	14.02587
C	5.2124	5.63243	10.90982
C	5.24252	5.67705	12.37149
C	5.12129	5.49296	8.23418
C	5.65443	6.82622	13.03915
H	5.94133	7.56259	12.54875
C	4.4383	3.30805	12.41376
C	4.78318	4.66735	14.5031
H	4.47068	3.95516	15.01214
C	5.65669	7.84337	6.77887
C	5.48048	6.67375	8.90502
C	4.81933	4.54834	13.0996
C	7.45339	9.47229	5.95122
C	5.0859	5.4911	6.82614
H	4.87204	4.70268	6.38118
C	5.19433	5.79978	15.13394
H	5.17249	5.84069	16.06203
C	4.09342	2.07706	10.35215
H	4.0904	2.06033	9.42178
C	3.75757	0.98925	12.44057
H	3.54221	0.22872	12.93052

C	5.64614	6.89689	14.40811
H	5.93756	7.66486	14.84397
C	3.85019	6.74255	4.00369
C	7.81108	10.52477	4.88315
C	2.36448	6.89503	1.88708
C	5.94509	9.17291	6.12484
C	5.26286	6.45804	4.57136
C	5.74178	7.82664	8.14055
H	5.98274	8.60948	8.58096
C	3.78844	7.03077	2.49293
C	4.83213	4.42933	10.22761
C	9.21621	11.12911	4.99814
C	9.78098	11.69068	3.68645
C	2.1815	7.59234	0.52358
C	10.95343	12.6353	3.84871
C	0.92546	7.19255	-0.25725

Total electronic energy: -7857.75805773

Monomer (7):



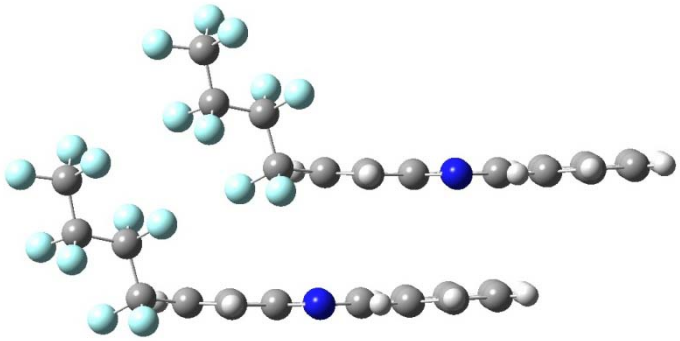
Coordinates of crystal structure geometry

F	10.54544	1.06031	18.9127
F	10.01938	2.36617	20.58586
F	12.18636	3.87213	20.17355
F	12.91414	2.52235	18.6263
F	12.81534	0.31683	20.12902
F	12.47216	1.72019	21.75576
F	10.21451	0.40608	22.421
F	11.90097	-0.88454	22.25653
F	10.40002	-0.88228	20.74239
N	8.33052	5.3423	15.3846
N	8.372	6.29279	18.04697
C	9.19536	4.83913	16.30554
C	10.9144	3.25146	16.84831
H	11.48252	2.5608	16.59314

C	5.62882	7.8218	15.25476
C	6.57686	7.81029	17.5576
C	7.52073	6.77979	17.14393
C	5.63801	8.31415	16.64844
C	4.69446	7.81297	13.02178
H	4.07206	8.13701	12.41143
C	10.93309	3.71329	18.18833
C	10.08342	3.80046	15.93798
H	10.0944	3.4932	15.06027
C	6.54491	6.84179	14.84889
C	5.60805	6.85233	12.63125
H	5.60205	6.52782	11.7597
C	6.51993	6.38241	13.53327
H	7.13776	5.74177	13.26351
C	10.11189	4.73144	18.56163
H	10.14026	5.04795	19.43564
C	4.7356	9.2898	17.10299
H	4.11028	9.64464	16.51312
C	11.77863	3.02507	19.19737
C	9.21675	5.31342	17.6373
C	7.50143	6.29859	15.79513
C	6.58915	8.27495	18.88124
H	7.21647	7.94109	19.48116
C	11.8647	0.96812	20.8237
C	4.76154	9.72945	18.40733
H	4.15459	10.37482	18.69018
C	4.70415	8.29143	14.3137
H	4.08518	8.93823	14.56551
C	11.06116	1.85426	19.88791
C	11.08079	-0.08901	21.55893
C	5.68457	9.21679	19.29807
H	5.69227	9.5106	20.1804

Total electronic energy: -1928.04379296

Dimer (7):



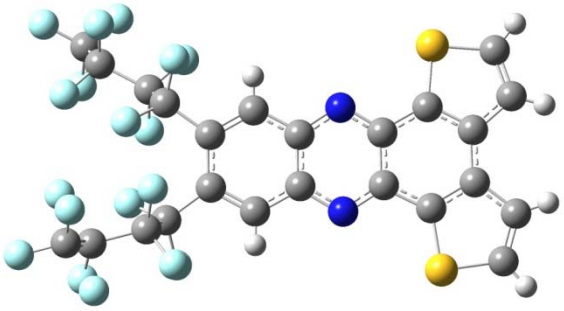
Coordinates of crystal structure geometry

F	5.42794	1.06031	18.9127
F	4.90188	2.36617	20.58586
F	7.06886	3.87213	20.17355
F	7.79664	2.52235	18.6263
F	7.69784	0.31683	20.12902
F	7.35466	1.72019	21.75576
F	5.09701	0.40608	22.421
F	6.78347	-0.88454	22.25653
F	5.28252	-0.88228	20.74239
N	3.21302	5.3423	15.3846
N	3.2545	6.29279	18.04697
C	4.07786	4.83913	16.30554
C	5.7969	3.25146	16.84831
H	6.36502	2.5608	16.59314
C	0.51132	7.8218	15.25476
C	1.45936	7.81029	17.5576
C	2.40323	6.77979	17.14393
C	0.52051	8.31415	16.64844
C	-0.42304	7.81297	13.02178
H	-1.04544	8.13701	12.41143
C	5.81559	3.71329	18.18833
C	4.96592	3.80046	15.93798
H	4.9769	3.4932	15.06027
C	1.42741	6.84179	14.84889
C	0.49055	6.85233	12.63125
H	0.48455	6.52782	11.7597
C	1.40243	6.38241	13.53327
H	2.02026	5.74177	13.26351
C	4.99439	4.73144	18.56163
H	5.02276	5.04795	19.43564
C	-0.3819	9.2898	17.10299
H	-1.00722	9.64464	16.51312
C	6.66113	3.02507	19.19737
C	4.09925	5.31342	17.6373
C	2.38393	6.29859	15.79513
C	1.47165	8.27495	18.88124
H	2.09897	7.94109	19.48116
C	6.7472	0.96812	20.8237
C	-0.35596	9.72945	18.40733
H	-0.96291	10.37482	18.69018
C	-0.41335	8.29143	14.3137
H	-1.03232	8.93823	14.56551
C	5.94366	1.85426	19.88791
C	5.96328	-0.08901	21.55893
C	0.56707	9.21679	19.29807

H	0.57477	9.5106	20.1804
F	10.54544	1.06031	18.9127
F	10.01938	2.36617	20.58586
F	12.18636	3.87213	20.17355
F	12.91414	2.52235	18.6263
F	12.81534	0.31683	20.12902
F	12.47216	1.72019	21.75576
F	10.21451	0.40608	22.421
F	11.90097	-0.88454	22.25653
F	10.40002	-0.88228	20.74239
N	8.33052	5.3423	15.3846
N	8.372	6.29279	18.04697
C	9.19536	4.83913	16.30554
C	10.9144	3.25146	16.84831
H	11.48252	2.5608	16.59314
C	5.62882	7.8218	15.25476
C	6.57686	7.81029	17.5576
C	7.52073	6.77979	17.14393
C	5.63801	8.31415	16.64844
C	4.69446	7.81297	13.02178
H	4.07206	8.13701	12.41143
C	10.93309	3.71329	18.18833
C	10.08342	3.80046	15.93798
H	10.0944	3.4932	15.06027
C	6.54491	6.84179	14.84889
C	5.60805	6.85233	12.63125
H	5.60205	6.52782	11.7597
C	6.51993	6.38241	13.53327
H	7.13776	5.74177	13.26351
C	10.11189	4.73144	18.56163
H	10.14026	5.04795	19.43564
C	4.7356	9.2898	17.10299
H	4.11028	9.64464	16.51312
C	11.77863	3.02507	19.19737
C	9.21675	5.31342	17.6373
C	7.50143	6.29859	15.79513
C	6.58915	8.27495	18.88124
H	7.21647	7.94109	19.48116
C	11.8647	0.96812	20.8237
C	4.76154	9.72945	18.40733
H	4.15459	10.37482	18.69018
C	4.70415	8.29143	14.3137
H	4.08518	8.93823	14.56551
C	11.06116	1.85426	19.88791
C	11.08079	-0.08901	21.55893
C	5.68457	9.21679	19.29807
H	5.69227	9.5106	20.1804

Total electronic energy: -3856.12390381

Monomer (10):



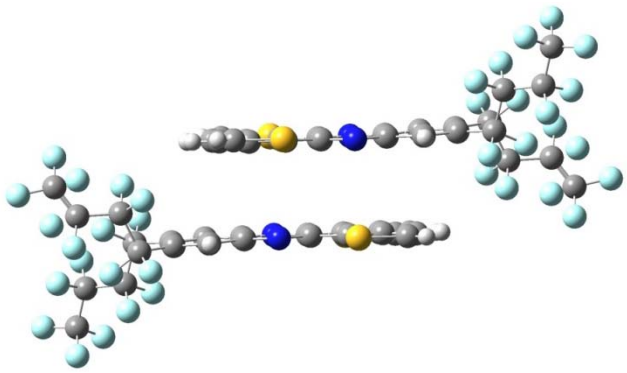
Coordinates of crystal structure geometry

S	2.73497	-0.38616	22.01375
S	2.12843	-5.68981	18.86364
F	0.52999	-0.04655	13.09347
F	3.43444	-1.97396	12.88372
F	0.85369	-2.18421	13.0324
F	5.07681	1.49351	14.0984
F	3.39617	0.15668	12.53262
F	2.26346	2.90092	15.56881
F	2.10925	2.01952	13.61227
F	4.75699	3.02362	15.58188
F	3.96088	2.79186	11.89385
F	3.40511	4.50165	13.52996
F	-1.0002	-0.30825	10.84915
N	2.80107	-0.51614	18.89196
N	2.58118	-2.98836	17.47304
C	2.81618	0.61711	15.4033
F	2.06271	-1.88078	10.57179
C	2.85651	0.61855	16.7747
H	2.92426	1.43143	17.2214
C	2.71226	-1.79607	15.42452
H	2.68056	-2.60781	14.97178
C	2.51735	-2.93686	21.66905
F	1.59709	0.22304	10.63465
F	5.32933	4.82652	11.745
C	2.7619	-0.82904	13.19716
F	-0.09641	-1.26168	9.17119
F	6.37	3.12413	12.41839
C	2.39109	-4.13878	19.55269
C	1.33918	-0.99986	12.59891
C	2.68503	-1.68344	19.52406
C	2.6957	-1.80451	16.84192
F	-0.65041	-2.38686	10.87171

C	2.55853	-2.93164	18.80202
C	2.79848	-0.57506	17.53223
F	5.77774	4.73639	14.03298
C	2.49637	-2.7173	23.06701
H	2.42252	-3.39755	23.69686
C	2.15312	-5.49721	21.42181
H	2.10777	-5.71913	22.32381
C	2.84243	1.98238	14.75245
C	2.37947	-4.17731	20.94028
C	2.01187	-6.38957	20.42017
H	1.86536	-7.29694	20.56204
C	4.26278	2.51349	14.44316
C	2.65021	-1.74512	20.96038
C	2.59591	-1.40598	23.38316
H	2.58949	-1.08929	24.25755
C	2.77291	-0.64284	14.70008
C	1.23557	-0.98618	11.0733
C	4.36372	3.57389	13.30663
C	-0.13965	-1.26868	10.46299
C	5.44843	3.93705	12.72242

Total electronic energy: -3619.64965498

Dimer (10):



Coordinates of crystal structure geometry

S	2.73497	-0.38616	22.01375
S	2.12843	-5.68981	18.86364
F	0.52999	-0.04655	13.09347
F	3.43444	-1.97396	12.88372
F	0.85369	-2.18421	13.0324
F	5.07681	1.49351	14.0984
F	3.39617	0.15668	12.53262
F	2.26346	2.90092	15.56881
F	2.10925	2.01952	13.61227
F	4.75699	3.02362	15.58188
F	3.96088	2.79186	11.89385

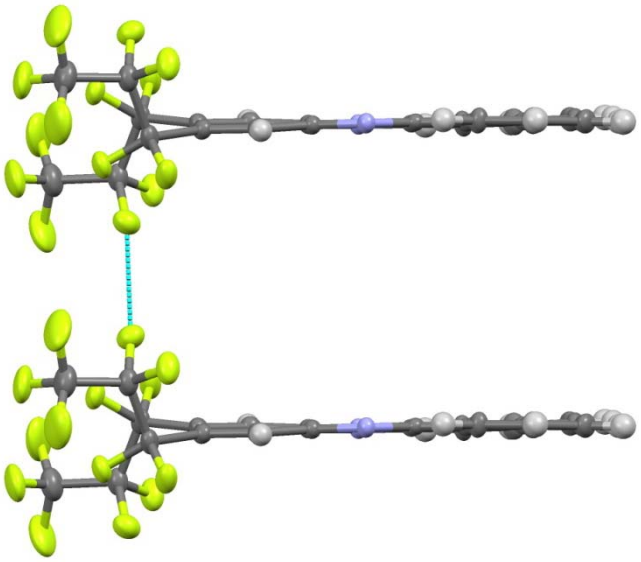
F	3.40511	4.50165	13.52996
F	-1.0002	-0.30825	10.84915
N	2.80107	-0.51614	18.89196
N	2.58118	-2.98836	17.47304
C	2.81618	0.61711	15.4033
F	2.06271	-1.88078	10.57179
C	2.85651	0.61855	16.7747
H	2.92426	1.43143	17.2214
C	2.71226	-1.79607	15.42452
H	2.68056	-2.60781	14.97178
C	2.51735	-2.93686	21.66905
F	1.59709	0.22304	10.63465
F	5.32933	4.82652	11.745
C	2.7619	-0.82904	13.19716
F	-0.09641	-1.26168	9.17119
F	6.37	3.12413	12.41839
C	2.39109	-4.13878	19.55269
C	1.33918	-0.99986	12.59891
C	2.68503	-1.68344	19.52406
C	2.6957	-1.80451	16.84192
F	-0.65041	-2.38686	10.87171
C	2.55853	-2.93164	18.80202
C	2.79848	-0.57506	17.53223
F	5.77774	4.73639	14.03298
C	2.49637	-2.7173	23.06701
H	2.42252	-3.39755	23.69686
C	2.15312	-5.49721	21.42181
H	2.10777	-5.71913	22.32381
C	2.84243	1.98238	14.75245
C	2.37947	-4.17731	20.94028
C	2.01187	-6.38957	20.42017
H	1.86536	-7.29694	20.56204
C	4.26278	2.51349	14.44316
C	2.65021	-1.74512	20.96038
C	2.59591	-1.40598	23.38316
H	2.58949	-1.08929	24.25755
C	2.77291	-0.64284	14.70008
C	1.23557	-0.98618	11.0733
C	4.36372	3.57389	13.30663
C	-0.13965	-1.26868	10.46299
C	5.44843	3.93705	12.72242
S	5.89251	-3.79785	17.28645
S	6.49905	1.50581	20.43655
F	8.0975	-4.13745	26.20673
F	5.19304	-2.21004	26.41647
F	7.7738	-1.99979	26.2678
F	3.55067	-5.67751	25.2018
F	5.23132	-4.34069	26.76758

F	6.36403	-7.08492	23.73138
F	6.51823	-6.20352	25.68792
F	3.87049	-7.20763	23.71832
F	4.6666	-6.97586	27.40634
F	5.22237	-8.68565	25.77024
F	9.62769	-3.87575	28.45104
N	5.82642	-3.66786	20.40824
N	6.04631	-1.19564	21.82715
C	5.8113	-4.80111	23.8969
F	6.56478	-2.30322	28.7284
C	5.77097	-4.80255	22.5255
H	5.70322	-5.61543	22.07879
C	5.91523	-2.38793	23.87567
H	5.94693	-1.57619	24.32841
C	6.11014	-1.24714	17.63115
F	7.03039	-4.40704	28.66554
F	3.29815	-9.01052	27.55519
C	5.86558	-3.35496	26.10303
F	8.72389	-2.92232	30.129
F	2.25748	-7.30814	26.8818
C	6.2364	-0.04522	19.7475
C	7.2883	-3.18414	26.70128
C	5.94246	-2.50056	19.77613
C	5.93178	-2.37949	22.45827
F	9.27789	-1.79714	28.42848
C	6.06895	-1.25236	20.49818
C	5.829	-3.60894	21.76797
F	2.84974	-8.92039	25.26722
C	6.13112	-1.4667	16.23318
H	6.20497	-0.78645	15.60334
C	6.47437	1.31321	17.87839
H	6.51971	1.53513	16.97639
C	5.78506	-6.16638	24.54775
C	6.24801	-0.00669	18.35991
C	6.61562	2.20557	18.88003
H	6.76212	3.11293	18.73816
C	4.36471	-6.69749	24.85704
C	5.97727	-2.43888	18.33981
C	6.03158	-2.77802	15.91703
H	6.03799	-3.09471	15.04264
C	5.85458	-3.54116	24.60011
C	7.39191	-3.19782	28.22689
C	4.26376	-7.75789	25.99356
C	8.76713	-2.91532	28.83721
C	3.17906	-8.12105	26.57778

Total electronic energy: -7239.34431404

5.2 Rf-Rf chain interactions

Compound (3): Middle molecule has been removed to calculate only Rf-Rf interactions



Coordinates of crystal structure geometry

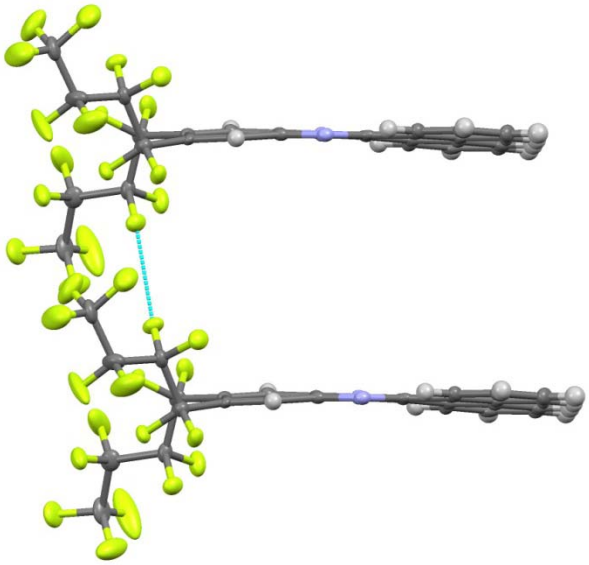
F	19.78337	25.26545	4.90834
F	17.69011	25.92394	7.59281
F	18.09848	26.5921	4.69236
F	19.73163	25.2268	7.4252
F	18.37808	28.35117	6.73802
F	20.36327	27.70195	6.28291
F	19.66325	27.66369	8.3124
C	17.67722	17.13668	5.4208
C	18.34975	18.35513	5.61943
N	18.32684	20.75144	5.60967
C	18.31446	23.13887	5.52464
H	19.22248	23.14003	5.72815
C	17.64719	21.90419	5.40547
C	17.65499	19.62304	5.42916
C	19.69227	18.3501	6.00274
H	20.12846	19.15969	6.14841
C	18.81869	26.0476	6.86834
C	19.73095	15.97543	5.95256
H	20.19633	15.1755	6.05292
C	18.56301	25.55991	5.43056
C	18.40539	15.94993	5.59155
H	17.98396	15.13299	5.45843
C	20.38058	17.17764	6.16792
H	21.27536	17.18885	6.423
C	17.67637	24.3349	5.3511
C	19.31732	27.47472	7.04118
F	14.14863	25.26545	5.54576
F	16.24189	25.92394	2.86129

F	15.83352	26.5921	5.76174
F	14.20037	25.2268	3.0289
F	15.55392	28.35117	3.71608
F	13.56873	27.70195	4.17119
F	14.26874	27.66369	2.1417
C	16.25478	17.13668	5.0333
C	15.58225	18.35513	4.83467
N	15.60516	20.75144	4.84443
C	15.61754	23.13887	4.92946
H	14.70952	23.14003	4.72595
C	16.28481	21.90419	5.04863
C	16.27701	19.62304	5.02494
C	14.23973	18.3501	4.45136
H	13.80354	19.15969	4.3057
C	15.11331	26.0476	3.58576
C	14.20105	15.97543	4.50153
H	13.73567	15.1755	4.40118
C	15.36899	25.55991	5.02354
C	15.5266	15.94993	4.86255
H	15.94804	15.13299	4.99567
C	13.55142	17.17764	4.28618
H	12.65664	17.18885	4.0311
C	16.25563	24.3349	5.10299
C	14.61468	27.47472	3.41291
F	17.69011	25.92394	0.62341
F	19.78337	25.26545	-2.06106
F	18.09848	26.5921	-2.27704
F	19.73163	25.2268	0.4558
F	18.37808	28.35117	-0.23138
F	20.36327	27.70195	-0.68649
F	19.66325	27.66369	1.343
C	17.67722	17.13668	-1.5486
C	18.34975	18.35513	-1.34997
N	18.32684	20.75144	-1.35973
C	18.31446	23.13887	-1.44476
H	19.22248	23.14003	-1.24125
C	17.64719	21.90419	-1.56393
C	17.65499	19.62304	-1.54024
C	19.69227	18.3501	-0.96666
H	20.12846	19.15969	-0.821
C	18.81869	26.0476	-0.10106
C	19.73095	15.97543	-1.01683
H	20.19633	15.1755	-0.91648
C	18.56301	25.55991	-1.53884
C	18.40539	15.94993	-1.37785
H	17.98396	15.13299	-1.51097
C	20.38058	17.17764	-0.80148
H	21.27536	17.18885	-0.5464
C	17.67637	24.3349	-1.6183
C	19.31732	27.47472	0.07179
F	14.14863	25.26545	-1.42364

F	16.24189	25.92394	-4.10811
F	15.83352	26.5921	-1.20766
F	14.20037	25.2268	-3.9405
F	15.55392	28.35117	-3.25332
F	13.56873	27.70195	-2.79821
F	14.26874	27.66369	-4.8277
C	16.25478	17.13668	-1.9361
C	15.58225	18.35513	-2.13473
N	15.60516	20.75144	-2.12497
C	15.61754	23.13887	-2.03994
H	14.70952	23.14003	-2.24345
C	16.28481	21.90419	-1.92077
C	16.27701	19.62304	-1.94446
C	14.23973	18.3501	-2.51804
H	13.80354	19.15969	-2.66371
C	15.11331	26.0476	-3.38364
C	14.20105	15.97543	-2.46787
H	13.73567	15.1755	-2.56822
C	15.36899	25.55991	-1.94586
C	15.5266	15.94993	-2.10685
H	15.94804	15.13299	-1.97373
C	13.55142	17.17764	-2.68322
H	12.65664	17.18885	-2.9383
C	16.25563	24.3349	-1.86641
C	14.61468	27.47472	-3.55648

Total electronic energy: -5005.36314144

Compound (4): Middle molecule has been removed to calculate only Rf-Rf interactions



Coordinates of crystal structure geometry

F	6.34239	10.77343	2.35735
F	8.16985	8.39137	5.61697

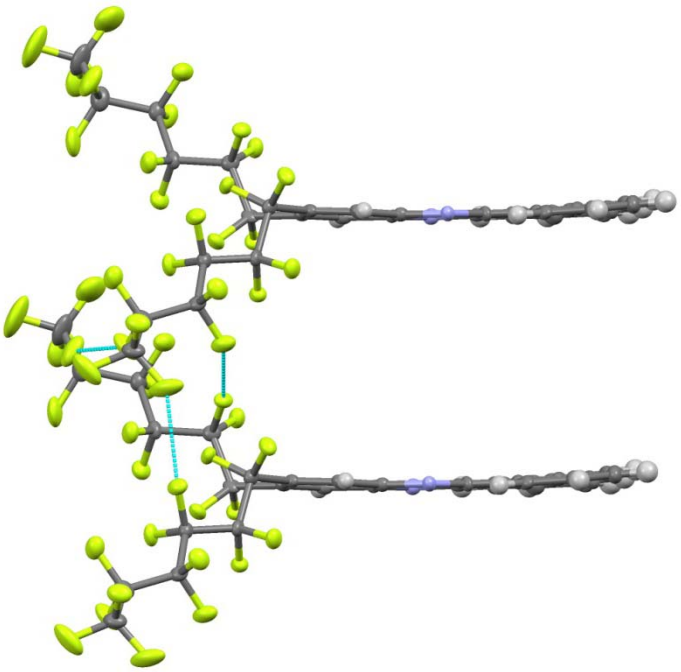
F	8.21442	9.49319	3.74962
F	5.45314	8.6885	3.42334
F	3.46493	10.44897	3.15321
F	4.36441	9.99842	0.71459
F	3.41086	12.5911	2.84107
F	5.93393	12.86143	2.72446
F	5.61974	7.83956	5.41083
F	2.49019	11.03441	-0.83748
F	9.78613	7.76635	2.355
F	4.70053	12.09738	0.34944
F	7.61452	6.13862	4.51446
F	7.24041	7.03253	2.58194
N	4.92997	13.65137	7.36731
F	1.69958	10.48404	1.04597
F	10.20628	7.20159	4.33542
F	9.62684	5.71235	2.91214
C	5.2975	12.38156	9.38543
C	4.88612	13.4949	11.56649
N	5.65262	11.28262	8.72856
F	2.03424	12.53984	0.56774
C	5.638	11.34737	7.37556
C	4.42725	14.73413	9.4455
C	5.31504	12.37077	10.8519
C	4.89635	13.57583	8.68929
C	3.97203	15.87444	8.76821
H	3.97422	15.89063	7.8369
C	3.95961	15.83128	11.52683
H	3.95376	15.83487	12.45815
C	3.52339	16.96619	9.4616
H	3.22015	17.71801	9.00693
C	4.41483	14.69636	10.8574
C	5.77245	11.23585	11.52722
H	6.05888	10.49663	11.04076
C	6.10711	8.82573	4.58906
C	3.52412	16.93742	10.8574
H	3.22527	17.67844	11.33523
C	7.6116	8.4786	4.38254
C	5.34061	12.54703	5.28833
H	5.17109	13.34561	4.84505
C	5.61316	11.42291	4.55372
C	5.91859	10.18727	6.60757
H	6.14364	9.40128	7.05164
C	5.36619	12.30242	13.60816
H	5.37934	12.27904	14.53909
C	5.52548	11.60457	3.04838
C	9.40325	6.9426	3.28553
C	5.86963	10.18367	5.2369
C	5.80387	11.20348	12.89947
H	6.11661	10.44987	13.34549
C	4.91389	13.41935	12.97367
H	4.61869	14.14239	13.47506

C	5.30919	12.52725	6.69945
C	4.07652	11.46787	2.51951
C	3.92819	11.23406	0.991
C	2.49311	11.34017	0.45663
C	7.93602	7.17821	3.65224
F	0.90752	9.49319	3.74962
C	-2.41055	13.57583	8.68929
C	-3.33487	15.87444	8.76821
C	-1.99771	12.52725	6.69945
F	-0.96451	10.77343	2.35735
F	0.86294	8.39137	5.61697
F	-1.85376	8.6885	3.42334
F	-3.84197	10.44897	3.15321
F	-2.94249	9.99842	0.71459
F	-3.89604	12.5911	2.84107
F	-1.37297	12.86143	2.72446
F	-1.68716	7.83956	5.41083
F	-4.81671	11.03441	-0.83748
F	2.47923	7.76635	2.355
F	-2.60637	12.09738	0.34944
F	0.30762	6.13862	4.51446
F	-0.06649	7.03253	2.58194
N	-2.37694	13.65137	7.36731
F	-5.60731	10.48404	1.04597
F	2.89938	7.20159	4.33542
F	2.31994	5.71235	2.91214
C	-2.0094	12.38156	9.38543
C	-2.42078	13.4949	11.56649
N	-1.65428	11.28262	8.72856
F	-5.27266	12.53984	0.56774
C	-1.6689	11.34737	7.37556
C	-2.87965	14.73413	9.4455
C	-1.99186	12.37077	10.8519
H	-3.33268	15.89063	7.8369
C	-3.34729	15.83128	11.52683
H	-3.35314	15.83487	12.45815
C	-3.78351	16.96619	9.4616
H	-4.08675	17.71801	9.00693
C	-2.89207	14.69636	10.8574
C	-1.53445	11.23585	11.52722
H	-1.24802	10.49663	11.04076
C	-1.19979	8.82573	4.58906
C	-3.78278	16.93742	10.8574
H	-4.08163	17.67844	11.33523
C	0.3047	8.4786	4.38254
C	-1.96629	12.54703	5.28833
H	-2.13581	13.34561	4.84505
C	-1.69374	11.42291	4.55372
C	-1.38831	10.18727	6.60757
H	-1.16326	9.40128	7.05164
C	-1.94071	12.30242	13.60816

H	-1.92756	12.27904	14.53909
C	-1.78142	11.60457	3.04838
C	2.09635	6.9426	3.28553
C	-1.43727	10.18367	5.2369
C	-1.50303	11.20348	12.89947
H	-1.19029	10.44987	13.34549
C	-2.39301	13.41935	12.97367
H	-2.68821	14.14239	13.47506
C	-3.23038	11.46787	2.51951
C	-3.37871	11.23406	0.991
C	-4.81379	11.34017	0.45663
C	0.62912	7.17821	3.65224

Total electronic energy: -5956.12096145

Compound (5): Middle molecule has been removed to calculate only Rf-Rf interactions



Coordinates of crystal structure geometry

F	-0.56175	17.62434	17.08375
F	1.34791	16.50269	18.79676
F	4.23649	17.07486	18.0641
F	2.18752	18.62215	17.79731
F	2.93452	15.45672	20.867
F	4.43604	14.9554	18.44725
F	0.6122	20.82789	17.77913
F	2.0821	19.48087	15.81296
F	-0.4104	19.188	15.57572
F	1.99776	14.46988	18.47861
F	-1.63556	21.42125	16.81286

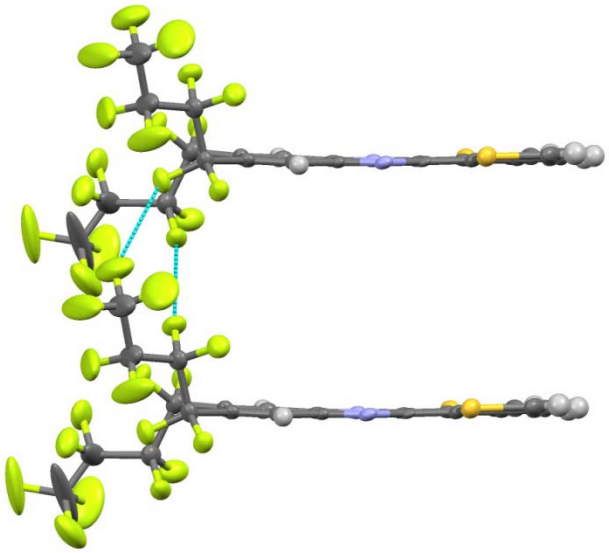
F	-2.53617	19.49983	17.25691
F	-1.26658	21.65592	19.68849
F	-0.16265	19.2276	19.0431
F	3.28467	17.56893	20.44841
F	6.05353	16.71746	19.98755
F	-3.06178	23.09462	18.36271
F	-4.33363	21.40452	18.07365
F	5.44283	14.89125	21.00335
F	5.41572	18.21064	22.00644
F	-2.64235	19.96675	19.80711
F	4.27188	16.64345	22.97543
F	6.47974	15.24344	23.4472
F	-3.98046	22.18421	20.05754
N	1.99475	16.03075	12.47057
F	7.67629	16.55178	22.22369
N	2.73346	13.65431	13.82407
F	6.75986	17.29242	24.00533
C	3.08136	12.54977	11.7161
C	3.78468	10.23097	11.6752
H	4.01962	9.44998	12.12152
C	2.17171	15.91546	16.63606
C	3.45109	11.43407	9.63086
H	3.46992	11.4415	8.69913
C	2.3178	14.92993	11.81518
C	2.28768	14.97455	10.35351
C	2.40891	14.79046	14.49082
C	1.87577	16.12372	9.68585
H	1.58887	16.86009	10.17625
C	3.0919	12.60555	10.31124
C	2.74702	13.96485	8.2219
H	3.05952	13.25266	7.71286
C	1.87351	17.14087	15.94613
C	2.04972	15.97124	13.81998
C	2.71087	13.84584	9.6254
C	0.07681	18.76979	16.77378
C	2.4443	14.7886	15.89886
H	2.65816	14.00018	16.34382
C	2.33587	15.09728	7.59106
H	2.35771	15.13819	6.66297
C	3.43678	11.37456	12.37285
H	3.4398	11.35783	13.30321
C	3.77263	10.28675	10.28443
H	3.98799	9.52622	9.79448
C	1.88406	16.19439	8.3169
H	1.59264	16.96236	7.88103
C	3.68001	16.04005	18.72131
C	-0.28088	19.82227	17.84185
C	5.16572	16.19253	20.83792
C	1.58511	18.47041	16.60016
C	2.26734	15.75554	18.15364
C	1.78842	17.12414	14.58445

H	1.54746	17.90698	14.14404
C	3.74176	16.32827	20.23207
C	2.69807	13.72683	12.49739
C	-1.68601	20.42661	17.72686
C	-2.25078	20.98818	19.03855
C	5.3487	16.88984	22.20142
C	-3.42323	21.9328	18.87629
C	6.60474	16.49005	22.98225
F	4.99403	19.49983	17.25691
F	3.19657	21.40452	18.07365
F	4.88785	19.96675	19.80711
F	6.96845	17.62434	17.08375
F	8.87811	16.50269	18.79676
F	11.76669	17.07486	18.0641
F	9.71772	18.62215	17.79731
F	10.46472	15.45672	20.867
F	11.96624	14.9554	18.44725
F	8.14241	20.82789	17.77913
F	9.6123	19.48087	15.81296
F	7.1198	19.188	15.57572
F	9.52796	14.46988	18.47861
F	5.89464	21.42125	16.81286
F	6.26362	21.65592	19.68849
F	7.36755	19.2276	19.0431
F	10.81487	17.56893	20.44841
F	13.58373	16.71746	19.98755
F	4.46842	23.09462	18.36271
F	12.97303	14.89125	21.00335
F	12.94592	18.21064	22.00644
F	11.80208	16.64345	22.97543
F	14.00994	15.24344	23.4472
F	3.54974	22.18421	20.05754
N	9.52495	16.03075	12.47057
F	15.20649	16.55178	22.22369
N	10.26366	13.65431	13.82407
F	14.29006	17.29242	24.00533
C	10.61156	12.54977	11.7161
C	11.31488	10.23097	11.6752
H	11.54982	9.44998	12.12152
C	9.70191	15.91546	16.63606
C	10.98129	11.43407	9.63086
H	11.00012	11.4415	8.69913
C	9.848	14.92993	11.81518
C	9.81788	14.97455	10.35351
C	9.93911	14.79046	14.49082
C	9.40597	16.12372	9.68585
H	9.11907	16.86009	10.17625
C	10.6221	12.60555	10.31124
C	10.27722	13.96485	8.2219
H	10.58972	13.25266	7.71286
C	9.40371	17.14087	15.94613

C	9.57992	15.97124	13.81998
C	10.24107	13.84584	9.6254
C	7.60701	18.76979	16.77378
C	9.9745	14.7886	15.89886
H	10.18836	14.00018	16.34382
C	9.86607	15.09728	7.59106
H	9.88791	15.13819	6.66297
C	10.96698	11.37456	12.37285
H	10.97	11.35783	13.30321
C	11.30283	10.28675	10.28443
H	11.51819	9.52622	9.79448
C	9.41426	16.19439	8.3169
H	9.12284	16.96236	7.88103
C	11.21021	16.04005	18.72131
C	7.24932	19.82227	17.84185
C	12.69592	16.19253	20.83792
C	9.11531	18.47041	16.60016
C	9.79754	15.75554	18.15364
C	9.31862	17.12414	14.58445
H	9.07766	17.90698	14.14404
C	11.27196	16.32827	20.23207
C	10.22827	13.72683	12.49739
C	5.84419	20.42661	17.72686
C	5.27942	20.98818	19.03855
C	12.8789	16.88984	22.20142
C	4.10697	21.9328	18.87629
C	14.13494	16.49005	22.98225

Total electronic energy: -7857.73248386

Compound (10): Middle molecule has been removed to calculate only Rf-Rf interactions



Coordinates of crystal structure geometry

S	5.59258	3.0199	-2.36365
S	6.19912	8.32356	0.78646

F	7.79757	2.6803	6.55663
F	4.89311	4.60771	6.76637
F	7.47387	4.81796	6.6177
F	3.25074	1.14024	5.5517
F	4.93138	2.47706	7.11748
F	6.0641	-0.26717	4.08129
F	6.21831	0.61422	6.03783
F	3.57056	-0.38988	4.06822
F	4.36667	-0.15812	7.75625
F	4.92244	-1.86791	6.12014
F	9.32776	2.94199	8.80095
N	5.52649	3.14988	0.75814
N	5.74638	5.62211	2.17705
C	5.51137	2.01664	4.2468
F	6.26485	4.51452	9.07831
C	5.47104	2.01519	2.8754
H	5.40329	1.20232	2.42869
C	5.6153	4.42981	4.22558
H	5.647	5.24156	4.67831
C	5.81021	5.57061	-2.01895
F	6.73046	2.4107	9.01544
F	2.99822	-2.19278	7.9051
C	5.56565	3.46279	6.45294
F	8.42396	3.89542	10.47891
F	1.95755	-0.49039	7.23171
C	5.93647	6.77253	0.09741
C	6.98837	3.63361	7.05118
C	5.64253	4.31719	0.12604
C	5.63185	4.43826	2.80818
F	8.97796	5.0206	8.77839
C	5.76902	5.56539	0.84808
C	5.52907	3.20881	2.11787
F	2.54981	-2.10264	5.61712
C	5.83118	5.35104	-3.41692
H	5.90504	6.0313	-4.04676
C	6.17444	8.13096	-1.77171
H	6.21978	8.35288	-2.67371
C	5.48513	0.65137	4.89765
C	5.94808	6.81106	-1.29019
C	6.31569	9.02332	-0.77007
H	6.46219	9.93068	-0.91194
C	4.06478	0.12026	5.20694
C	5.67734	4.37887	-1.31029
C	5.73165	4.03973	-3.73307
H	5.73806	3.72303	-4.60746
C	5.55465	3.27658	4.95002
C	7.09198	3.61992	8.5768
C	3.96383	-0.94014	6.34346
C	8.4672	3.90243	9.18711
C	2.87913	-1.3033	6.92768
F	9.96434	1.14024	5.5517

F	11.64499	2.47706	7.11748
C	12.24267	3.20881	2.11787
C	12.35613	4.31719	0.12604
C	12.52381	5.57061	-2.01895
S	12.30618	3.0199	-2.36365
S	12.91272	8.32356	0.78646
F	14.51117	2.6803	6.55663
F	11.60671	4.60771	6.76637
F	14.18747	4.81796	6.6177
F	12.7777	-0.26717	4.08129
F	12.93191	0.61422	6.03783
F	10.28416	-0.38988	4.06822
F	11.08027	-0.15812	7.75625
F	11.63604	-1.86791	6.12014
F	16.04136	2.94199	8.80095
N	12.24009	3.14988	0.75814
N	12.45998	5.62211	2.17705
C	12.22497	2.01664	4.2468
F	12.97845	4.51452	9.07831
C	12.18464	2.01519	2.8754
H	12.11689	1.20232	2.42869
C	12.3289	4.42981	4.22558
H	12.3606	5.24156	4.67831
F	13.44406	2.4107	9.01544
F	9.71182	-2.19278	7.9051
C	12.27925	3.46279	6.45294
F	15.13756	3.89542	10.47891
F	8.67115	-0.49039	7.23171
C	12.65007	6.77253	0.09741
C	13.70197	3.63361	7.05118
C	12.34545	4.43826	2.80818
F	15.69156	5.0206	8.77839
C	12.48262	5.56539	0.84808
F	9.26341	-2.10264	5.61712
C	12.54478	5.35104	-3.41692
H	12.61864	6.0313	-4.04676
C	12.88804	8.13096	-1.77171
H	12.93338	8.35288	-2.67371
C	12.19873	0.65137	4.89765
C	12.66168	6.81106	-1.29019
C	13.02929	9.02332	-0.77007
H	13.17579	9.93068	-0.91194
C	10.77838	0.12026	5.20694
C	12.39094	4.37887	-1.31029
C	12.44524	4.03973	-3.73307
H	12.45167	3.72303	-4.60746
C	12.26825	3.27658	4.95002
C	13.80558	3.61992	8.5768
C	10.67743	-0.94014	6.34346
C	15.1808	3.90243	9.18711
C	9.59273	-1.3033	6.92768

Total electronic energy: -7239.31067040

6. References:

(1) M. J. Frisch, G. W. T., H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.1, *Gaussian, Inc., Wallingford CT* 2009.

7. Powder XRD results for compounds 3,4,5, and 7:

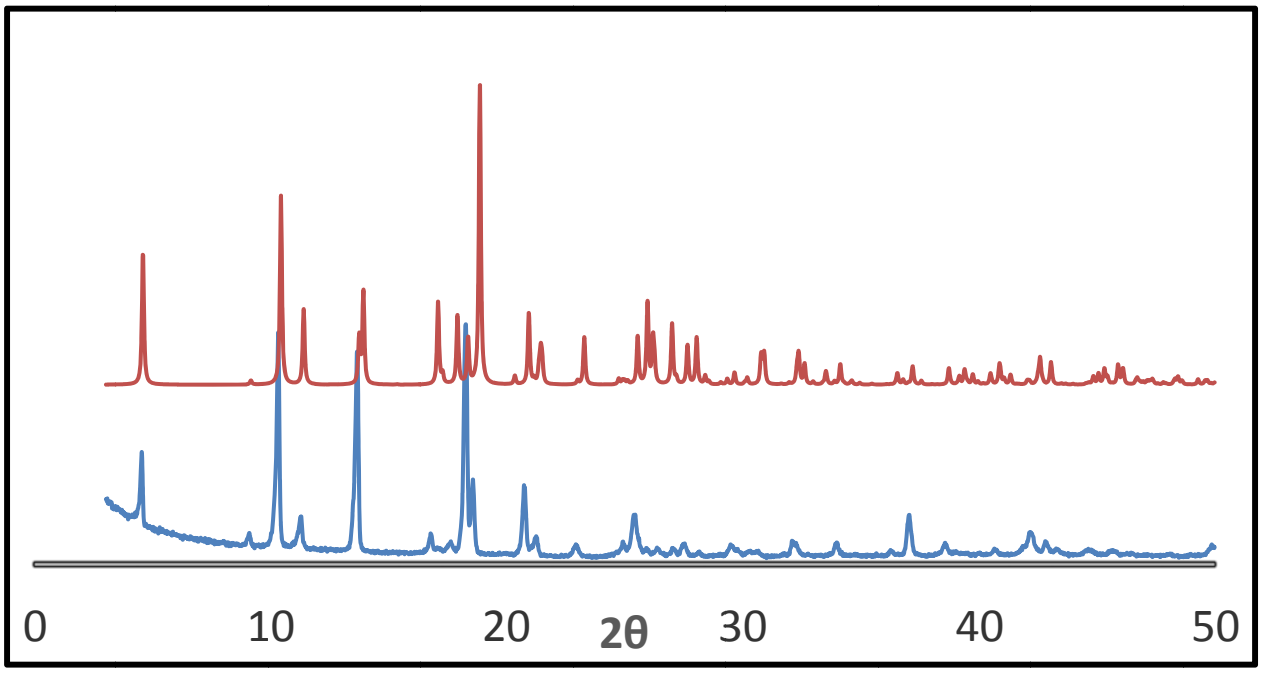


Figure S34: Powder XRD data of compound **3**. Experimental result (bottom, blue), simulated result from crystal structure (top, red).

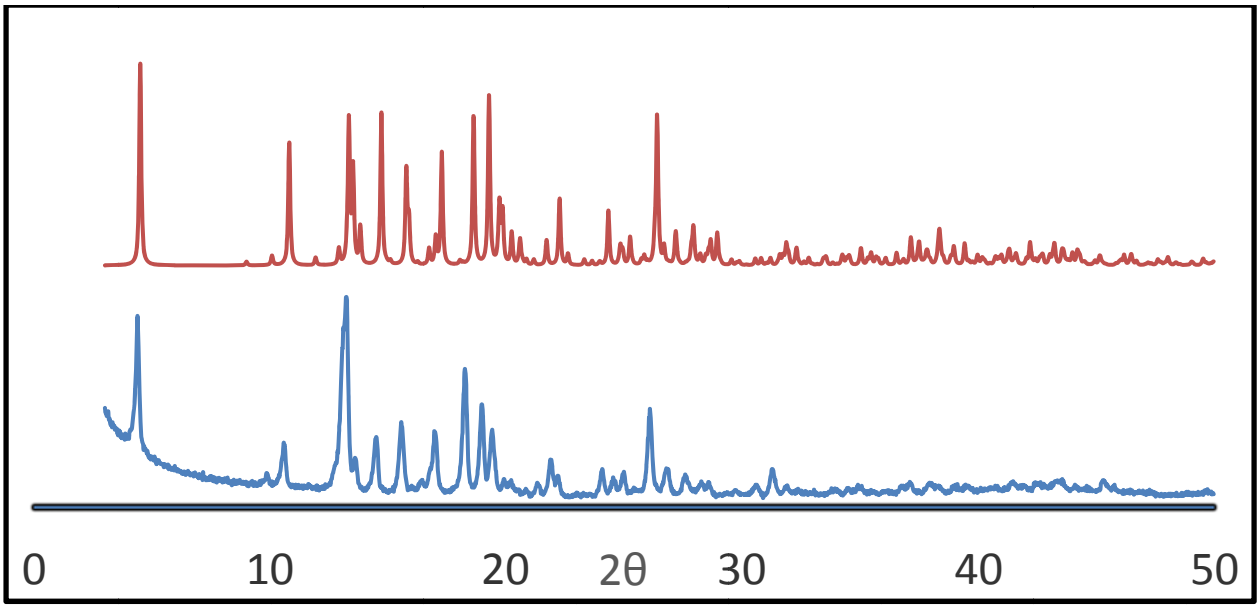


Figure S35: Powder XRD data of compound **4**. Experimental result (bottom, blue), simulated result from crystal structure (top, red).

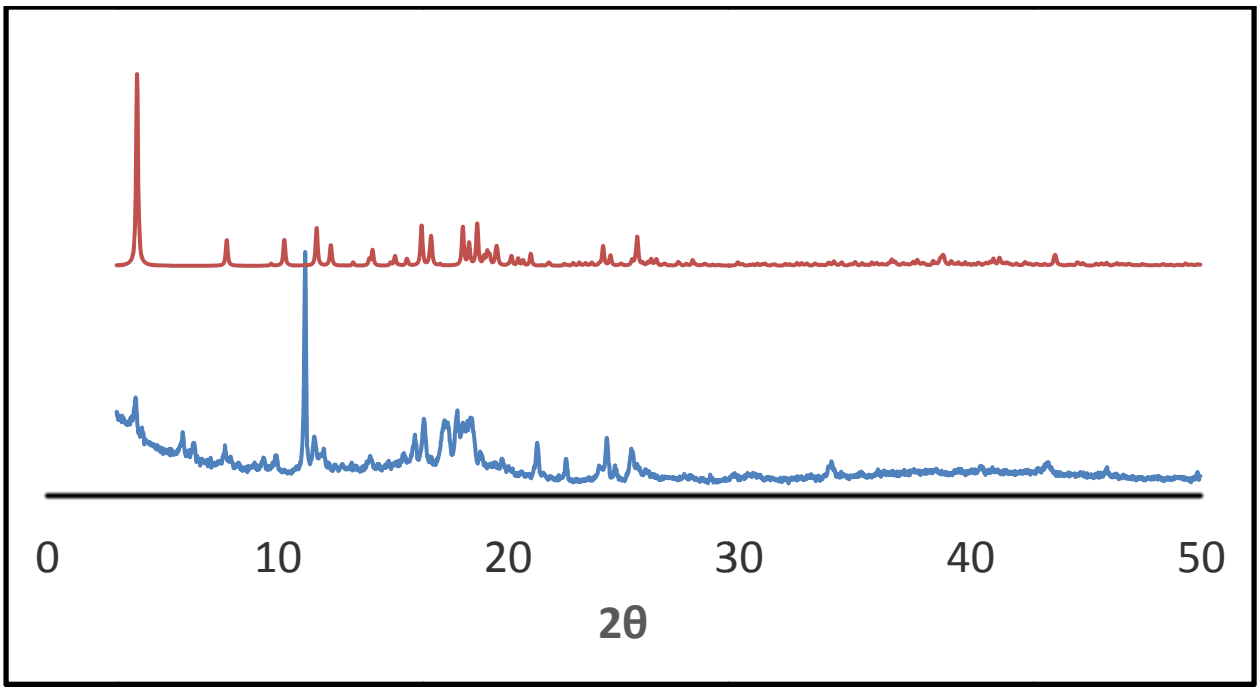


Figure S36: Powder XRD data of compound **5**. Experimental result (bottom, blue), simulated result from crystal structure (top, red).

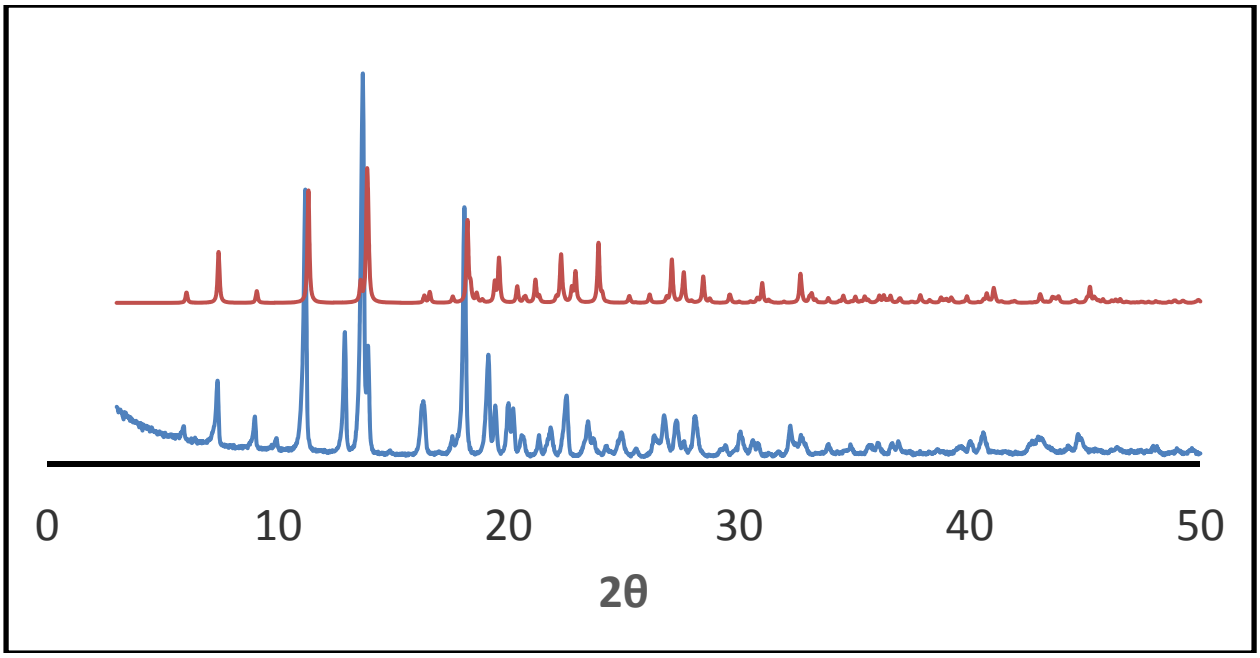


Figure S37: Powder XRD data of compound **7**. Experimental result (bottom, blue), simulated result from crystal structure (top, red).