Electronic Supplementary Information

Single- and double-helices of α,α'-dibenzylaminotripyrrin: solution and solid state studies.

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Contents

1. Experimental Procedure

General information

Commercially available solvents and reagents were used without further purification, unless otherwise noted. The spectroscopic grade solvents were used for all the spectroscopic studies. Silica gel column chromatography was performed on Wakogel C-300. UV/Vis absorption spectra were recorded on a Shimadzu UV-3600 spectrometer. ^{1}H and ^{19}F NMR spectra were recorded on a JEOL ECA-600 spectrometer (operating as 600 MHz for ^{1}H, 151 MHz for ^{13}C and 565 MHz for ^{19}F) using the residual solvent as the internal reference for ^{1}H (δ = 7.26 ppm in $CDCl_3$, δ = 2.50 ppm in DMSO-d_6) for ^{13}C (δ = 77.16 ppm in $CDCl_3$) and hexafluorobenzene as an external reference for ^{19}F (δ = –162.9 ppm). High-resolution atmospheric-pressure-chemical-ionization time-of-flight mass-spectrometry (HR-APCI-TOF-MS) was recorded on a BRUKER micrOTOF model using positive ion mode. Single-crystal X-ray diffraction analysis data were collected at –180 °C with a Rigaku XtaLAB P200 by using graphite monochromated Cu-K_α radiation (λ = 1.54187 Å). The structures were solved by direct methods (SHELXT-2014/5)[S1] and refined with full-matrix least-square technique (SHELXL-2014/7).[S2] All calculations were carried out using the *Gaussian 09* program.[S3]

1-benzylamino-14-bromo-5,10-diphenyltripyrrin 3

The geometry was obtained from X-ray structures.A mixture of 1,14-dibromo-5,10-diphenyltripyrrane **2** (16.1 mg, 30 μmol),[S4] dry THF (3 mL) was added benzylamine (26 μL, 0.24 mmol), and the resulting solution was stirred at room temperature for 24 h under N_2. After quenching with water, the aqueous layer was extracted with ethyl acetate. The organic fraction was washed by water and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness. The crude product was purified by silica-gel column chromatography using dichloromethane as eluent to afford amorphous solid of **3** (16.7 mg, 30 μmol) in 99% yield.

^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 14.40 (s, 1H, NH), 7.25-7.5 (15H, Ph-H), 6.81 (d, J = 4.6 Hz, 1H, β-H), 6.62 (d, J = 4.6 Hz, 1H, β-H), 6.86 (br, 1H, β-H), 6.37 (d, J = 4.1 Hz, 1H, β-H), 6.27 (br, 2H, β-H), 6.09 (br, 1H, β-H) and 4.67 (s, 2H, benzyl-H). (The signals assigned to amine-NH protons were not observed because of their broadness.)

^{13}C-NMR (151 MHz, $CDCl_3$, 25 °C) δ / ppm = 169.80, 152.73, 147.69, 143.78, 140.42,

139.26, 138.33, 137.65, 137.22, 136.04, 135.46, 131.28, 131.17, 129.04, 128.95, 128.00, 127.87, 127.70, 125.51, 125.45, 124.53, 118.09 and 48.08. (Some signals were not observed because of their broadness or overlapping with the major signals.)
HR APCI-TOF-MS (positive): *m*/*z* calcd for $[C_{33}H_{26}N_4{}^{79}Br]^+$: 557.1335 $[M+H]^+$; found: 557.1313.

5,10-bis(*p*-trifluoromethylphenyl)tripyrrane

The synthetic procedure is based on the previously reported method albeit with slight modifications.[S5]
Pyrrole (0.22 mL, 3.2 mmol) was added to an aqueous HCl solution (0.12 M, 2 L) under dark conditions. After 5 min, *p*-trifluoromethylbenzaldehyde (0.27 mL, 2.0 mmol) was added to the reaction mixture and the solution was stirred for 6 h. Then, reaction was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with ethyl acetate, washed with brine and dried over anhydrous Na_2SO_4. The crude product was purified with silica gel column chromatography using *n*-hexane/ethyl acetate/dichloromethane (*v*/*v* = 8:1.5:0.5) as an eluent. Evaporation in vacuo afforded amorphous solid (162 mg, 0.32 mmol) in 32% yield. For the compound data, see ref S5.

1,14-dibromo-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin 4

5,10-Bis(*p*-trifluoromethylphenyl)tripyrrane (375 mg, 0.73 mmol) was dissolved in dry THF (15 mL, 50 mM) and was cooled down to –78°C under dark conditions. To the solution was added NBS (140 mg, 1.1 eq.) and the mixture was stirred for 1 h. Another 1.1 eq. of NBS was added to the solution and the mixture was stirred for an additional 1.5 h. Reaction was quenched with saturated aqueous $Na_2S_2O_3$. The mixture was extracted with dichloromethane, washed with with brine and dried over anhydrous Na_2SO_4. The crude product was purified with silica gel column chromatography using *n*-hexane/dichloromethane (*v*/*v* = 1:1) as an eluent. The product is unstable under ambient conditions and used in the next step immediately. The residue was dissolved in dichloromethane (200 mL, ~3.5 mM). To the solution was added DDQ (340 mg, 1.5 mmol, 2 eq.) and the reaction mixture was stirred for 5 min, and then passed through alumina short pad using dichloromethane as an eluent. After the solvent was removed under reduced pressure, recrystallization from dichloromethane/methanol afforded 1,14-dibromo-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **4** (195 mg, 0.29 mmol) as red solids in 40% yield.

^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 7.73 (d, *J* = 8.2 Hz, 4H, Ar-H), 7.58 (d, *J* = 8.2 Hz, 4H, Ar-H), 6.68 (d, *J* = 4.6 Hz, 2H, *β*), 6.57 (d, *J* = 4.6 Hz, 2H, *β*) and 6.24 (s, 2H, *β*); ^{13}C-NMR (151 MHz, $CDCl_3$, 25 °C) δ / ppm = 152.3, 150.6, 140.0, 138.9, 136.6, 136.2, 131.4, 130.0, 125.1, 124.9, 123.1 and 122.5; ^{19}F-NMR (585 MHz, $CDCl_3$, 25°C) δ = –62.60 ppm.

HR APCI-TOF-MS: *m*/*z* = 664.9536 (calcd. for $[C_{28}H_{15}{}^{79}Br_2F_6N_3]^+$; $[M]^+$, *m*/*z* = 664.9531)

*$[M+H]^+$ species were observed simultaneously.

1,14-di(benzylamino)-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin 5

To a THF solution (3 mL, 10 mM) of dibromotripyrrin **4** (18.4 mg, 30 μmol) was added benzylamine (12 μL, 0.12 mmol, 4 eq.) at 80 °C under N_2. After 12 h, the reaction was quenched with triethylamine. The reaction mixture was purified with silica gel column chromatography using dichloromethane/*n*-hexane (*v*/*v* = 9:1) as an eluent. After blue-green colored impurities were eluted, then gradient elution was conducted using dichloromethane/ethyl acetate (*v*/*v* = 10:1 to 1:1) as an eluent. Evaporation afforded 1,14-dibenzylamino-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **5** (17.9 mg, 25 μmol) as red solids in 83% yield.

^{1}H-NMR (600 MHz, $CDCl_3$, 10 mM, 25 °C) δ / ppm = 7.63 (d, *J* = 7.7 Hz, 4H, Ar-H), 7.56 (d, *J* = 8.2 Hz, 4H, Ar-H), 7.30 (t, *J* = 6.9 Hz, 4H, Ph), 7.27 (brs, 6H, Ph), 6.66 (d, *J* = 4.6 Hz, 4H, β), 6.23 (d, *J* = 4.2 Hz, 2H, β), 6.15 (d, *J* = 4.1 Hz, 2H, β) and 4.54 (brs, 4H, $C\underline{H}_2Ph$); ^{13}C-NMR (151 MHz, $CDCl_3$, 25 °C) δ / ppm = 142.4, 138.9, 137.8, 136.7, 131.8, 130.0(q, $J_{C\text{-}F}$ = 32.3 Hz), 128.9, 127.7, 125.3, 124.9, 124.7, 123.4, 117.9 and 47.5; ^{19}F-NMR (585 MHz, $CDCl_3$, 25 °C) δ = –62.3 ppm.

HR APCI-TOF-MS: *m*/*z* = 720.2553 (calcd. for $[C_{42}H_{32}F_6N_5]^+$; $[M+H]^+$, *m*/*z* = 720.2556)

1,14-di(1-phenylethylamino)-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin 6-(*R*) and 6-(*S*)

To a THF solution (0.8 mL, 40 mM) of dibromotripyrrin **4** (20 mg, 30 μmol) was added (*R*)/(*S*)-1-phenylethylamine (50 μL, 0.39 mmol, 13 eq.) at 80 °C under N_2. After 12 h, the reaction was quenched with triethylamine. The reaction mixture was purified with silica gel column chromatography using dichloromethane/*n*-hexane (*v*/*v* = 9:1) as an eluent. After blue-green colored impurities were eluted, then gradient elution was conducted using dichloromethane/ethyl acetate (*v*/*v* = 10:1 to 1:1) as an eluent. Evaporation afforded 1,14-di(1-phenylethylamino)-5,10-bis(*p*-

trifluoromethylphenyl)tripyrrin as red solids. Yields: **6-(*R*)** (13 mg, 17 μmol, 58%) and **6-(*S*)** (14 mg, 19 μmol, 62%).

^{1}H-NMR (600 MHz, $CDCl_3$, 4 mM, monomer, 25 °C) δ / ppm = 7.65 (d, *J* = 8.3 Hz, 4H, Ar-H), 7.55 (d, *J* = 7.8 Hz, 4H, Ar-H), 7.32-7.28 (m, 8H, Ph-H), 7.23 (t, *J* = 7.6 Hz, 2H, Ph-H), 6.63 (d, *J* = 4.6 Hz, 2H, *β*), 6.19 (d, *J* = 4.1 Hz, 4H, *β*+*β*), 4.94 (brs, 2H, C<u>H</u>(Me)Ph) and 1.48 (d, *J* = 6.4 Hz, 6H, CH(<u>Me</u>)Ph); ^{13}C-NMR (151 MHz, $CDCl_3$) δ / ppm = 167.9, 149.8, 144.3, 142.5, 137.7, 136.6, 131.8, 131.4, 130.0 (q, $J_{C\text{-}F}$ = 32.3 Hz), 128.8, 127.5, 126.2, 125.2, 124.7, 123.4, 118.0, 53.2 and 23.4; ^{19}F-NMR (585 MHz, $CDCl_3$, 25 °C) δ = –62.3 ppm.
HR APCI-TOF-MS: *m*/*z* = 747.2806 (calcd. for $[C_{44}H_{35}F_6N_5]^+$; $[M]^+$, *m*/*z* = 747.2791).
*$[M+H]^+$ species were observed simultaneously.

2. NMR Spectra

1-benzylamino-14-bromo-5,10-diphenyltripyrrin **3**

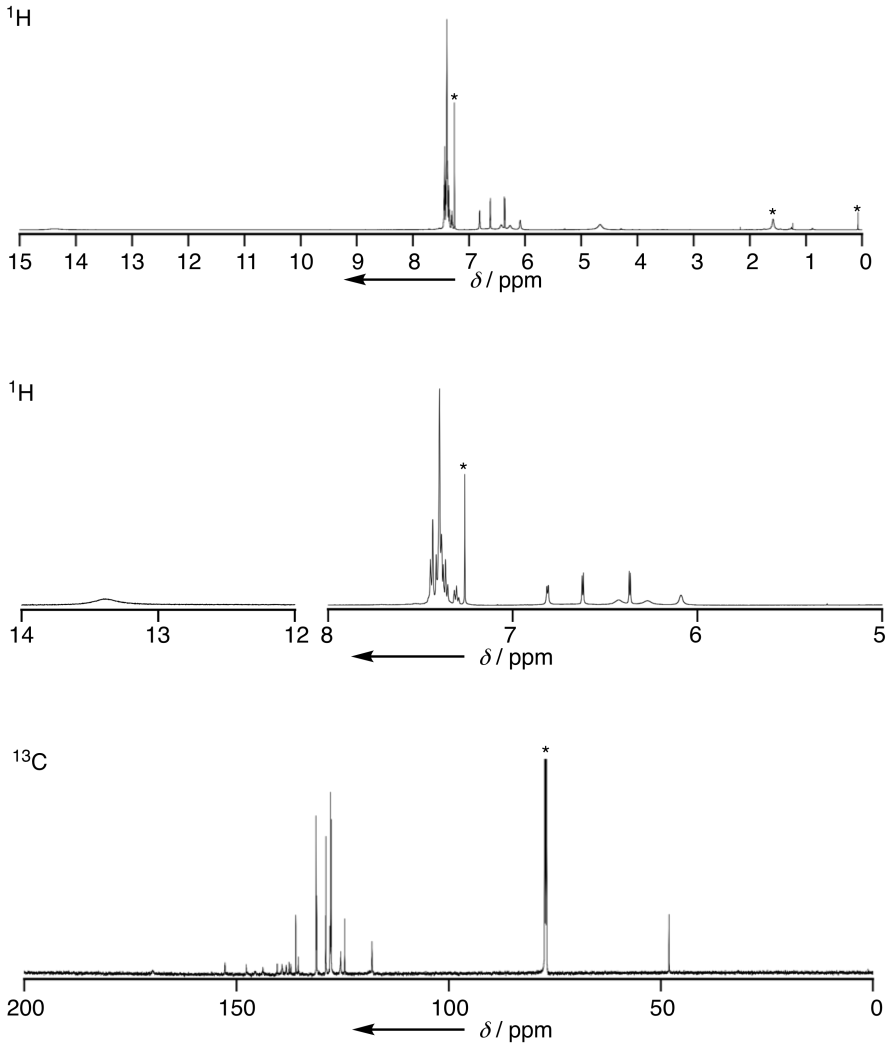


Figure S2-1. ^{1}H and ^{13}C NMR spectra of **3** at 25 °C in $CDCl_3$. *Solvent and impurities.

1,14-dibromo-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **4**

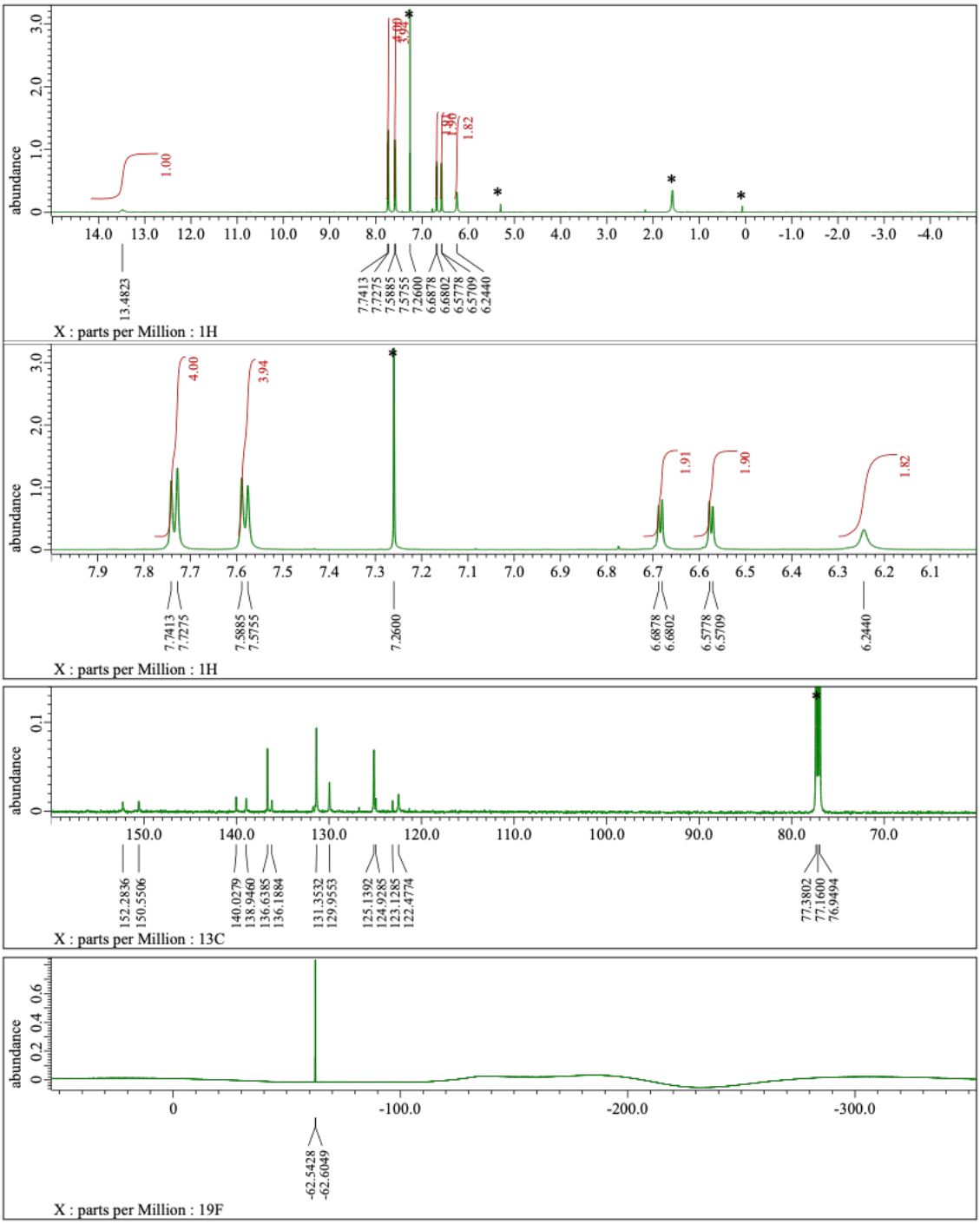


Figure S2-2. ^{1}H, ^{13}C and ^{19}F NMR spectra of **4** at 25 °C in $CDCl_3$. *Solvent and impurities.

1,14-dibenzylamino-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **5**

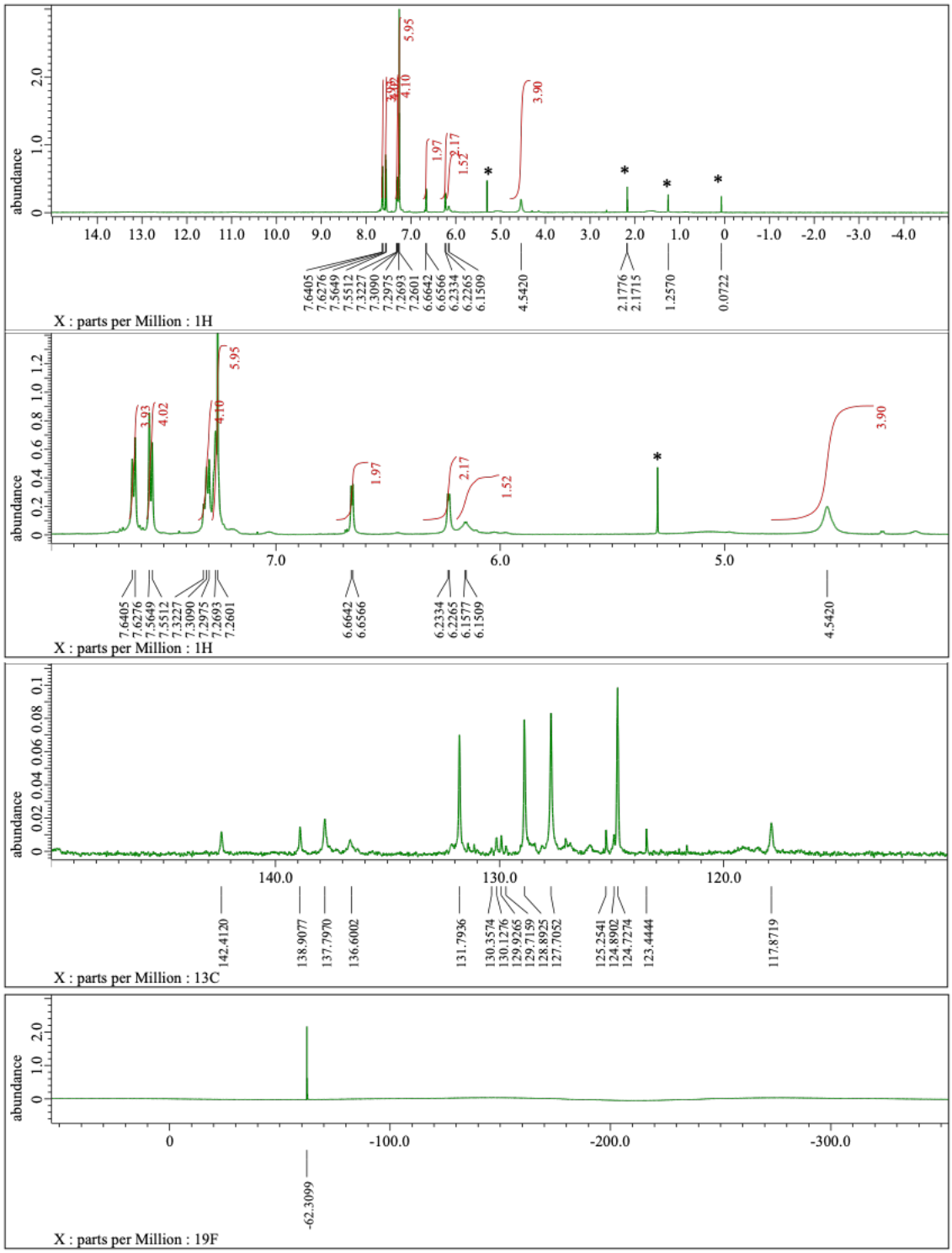


Figure S2-3. ^{1}H, ^{13}C and ^{19}F NMR spectra of **5** at 25 °C in $CDCl_3$. *Solvent and impurities.

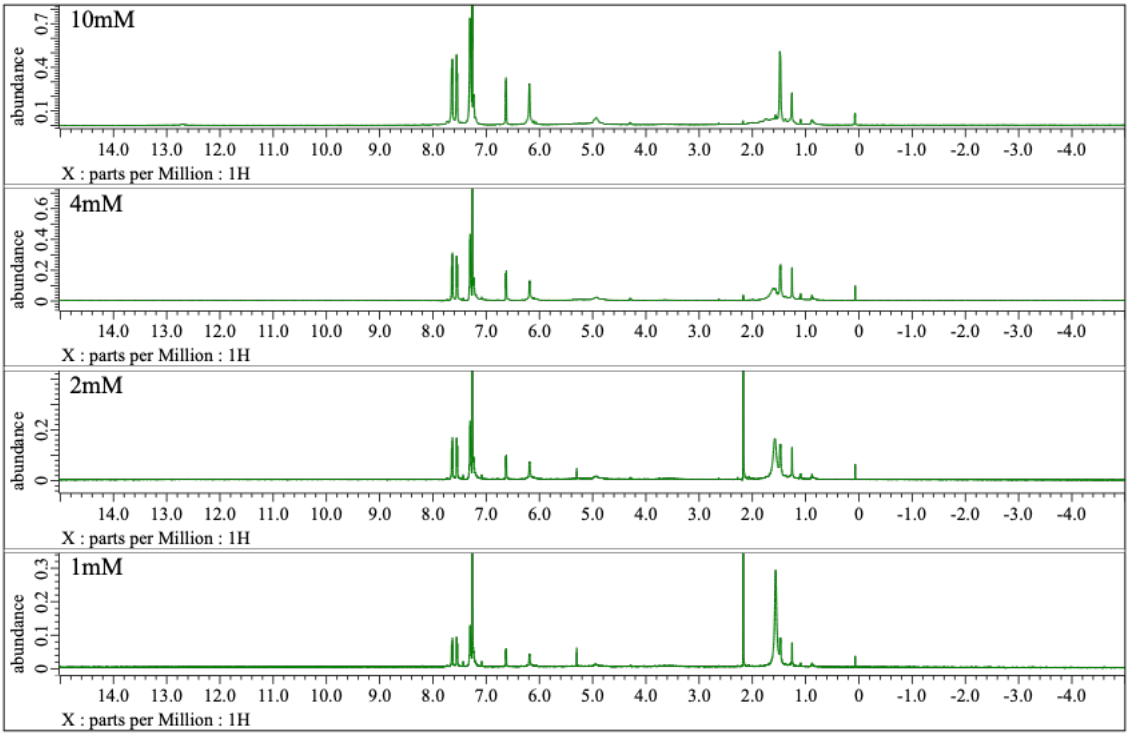
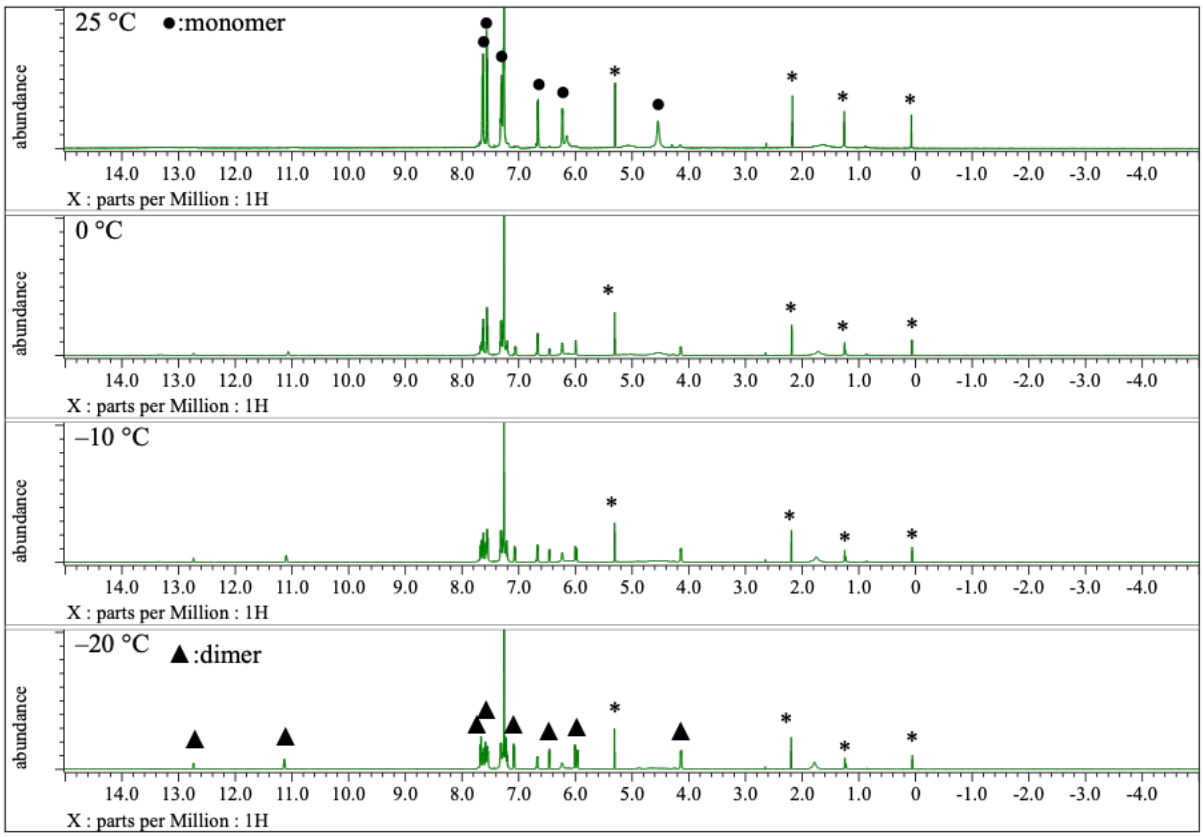
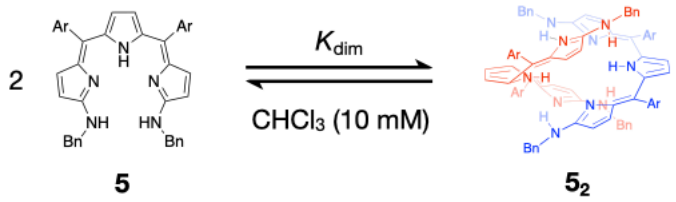


Figure S2-4. ^{1}H NMR spectra of several concentration of $CDCl_3$ solution of **5** at 25 °C. *Solvent and impurities. (No dimerization was observed.)





$$K_{dim} = \frac{[5_2]}{[5]^2}$$

van't Hoff equation

$$\ln K_{dim} = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}$$

T / K	[**5**] / mM	[$\mathbf{5}_2$] / mM	K_{dim} / M^{-1}	lnK_{dim}
298	8.96	0.52	6.47	1.87
273	7.25	1.38	26.2	3.27
263	6.41	1.79	43.7	3.78
253	5.26	2.37	85.5	4.45

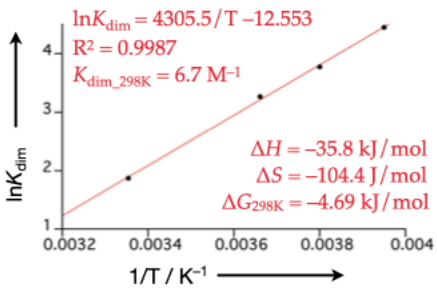


Figure S2-5. ^{1}H NMR spectra of **5** at different temperatures in $CDCl_3$ and a van't Hoff plot for **5**. *Solvent and impurities.

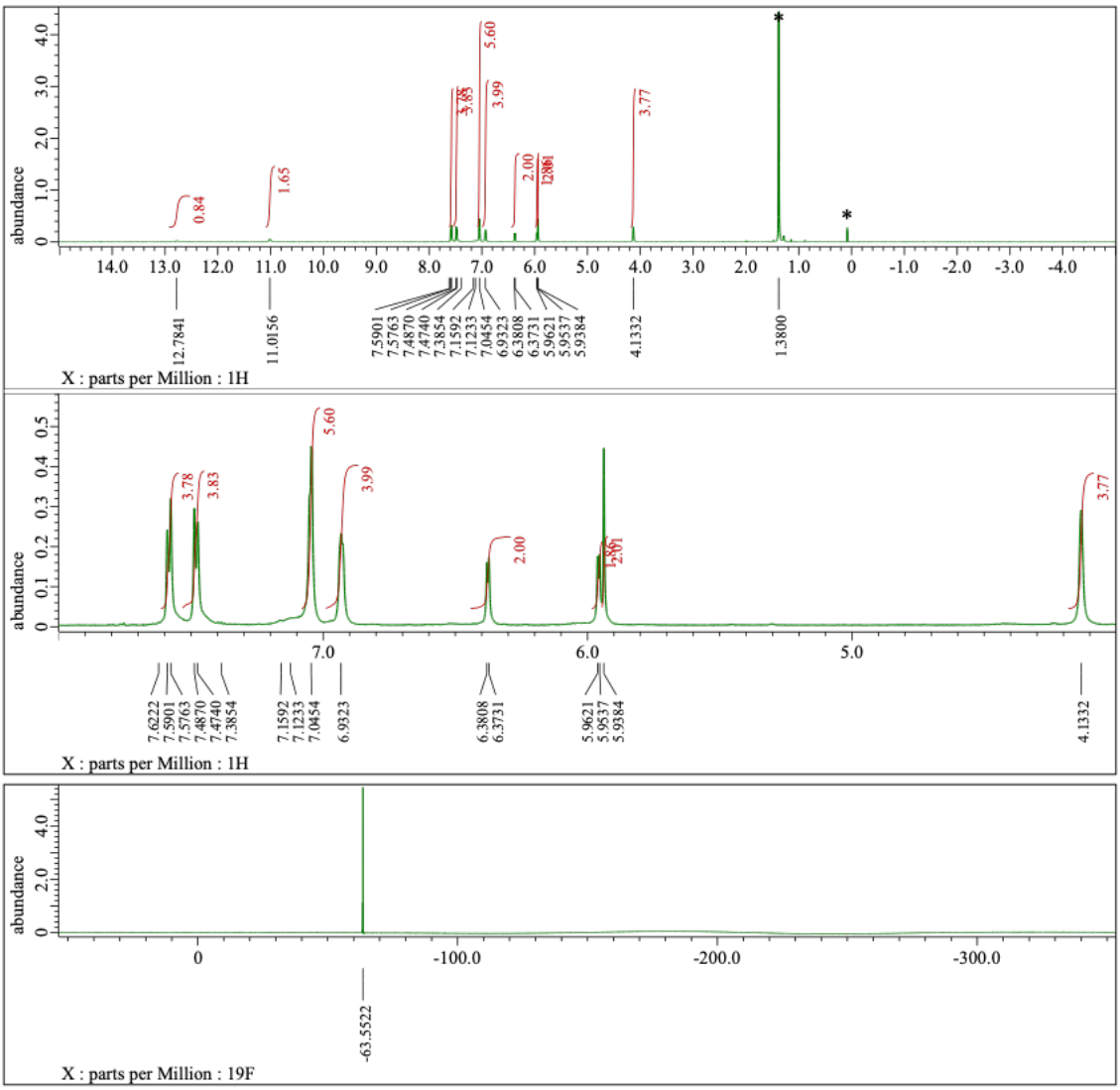


Figure S2-6. ^{1}H and ^{19}F NMR spectra of **5** at 25 °C in cyclohexane-d_{12}. *Solvent and impurities.

^{1}H-NMR (600 MHz, cyclohexane-d_{12}, 10 mM) δ / ppm = 12.78 (s, 1H, NH), 11.02 (s, 2H, NH), 7.58 (d, J = 8.3 Hz, 4H, Ar-H), 7.48 (d, J = 7.8 Hz, 4H, Ar-H), 7.05 (brs, 6H, Ph-H), 6.93 (brs, 4H, Ph-H), 6.38 (d, J = 4.6 Hz, 2H, β), 5.96 (d, *J* = 5.0 Hz, 2H, β), 5.94 (s, 2H, β) and 4.13 (s, 4H, C$\underline{H}_2$Ph); ^{19}F-NMR (565 MHz, cyclohexane-d_{12}) δ = –63.6 ppm.

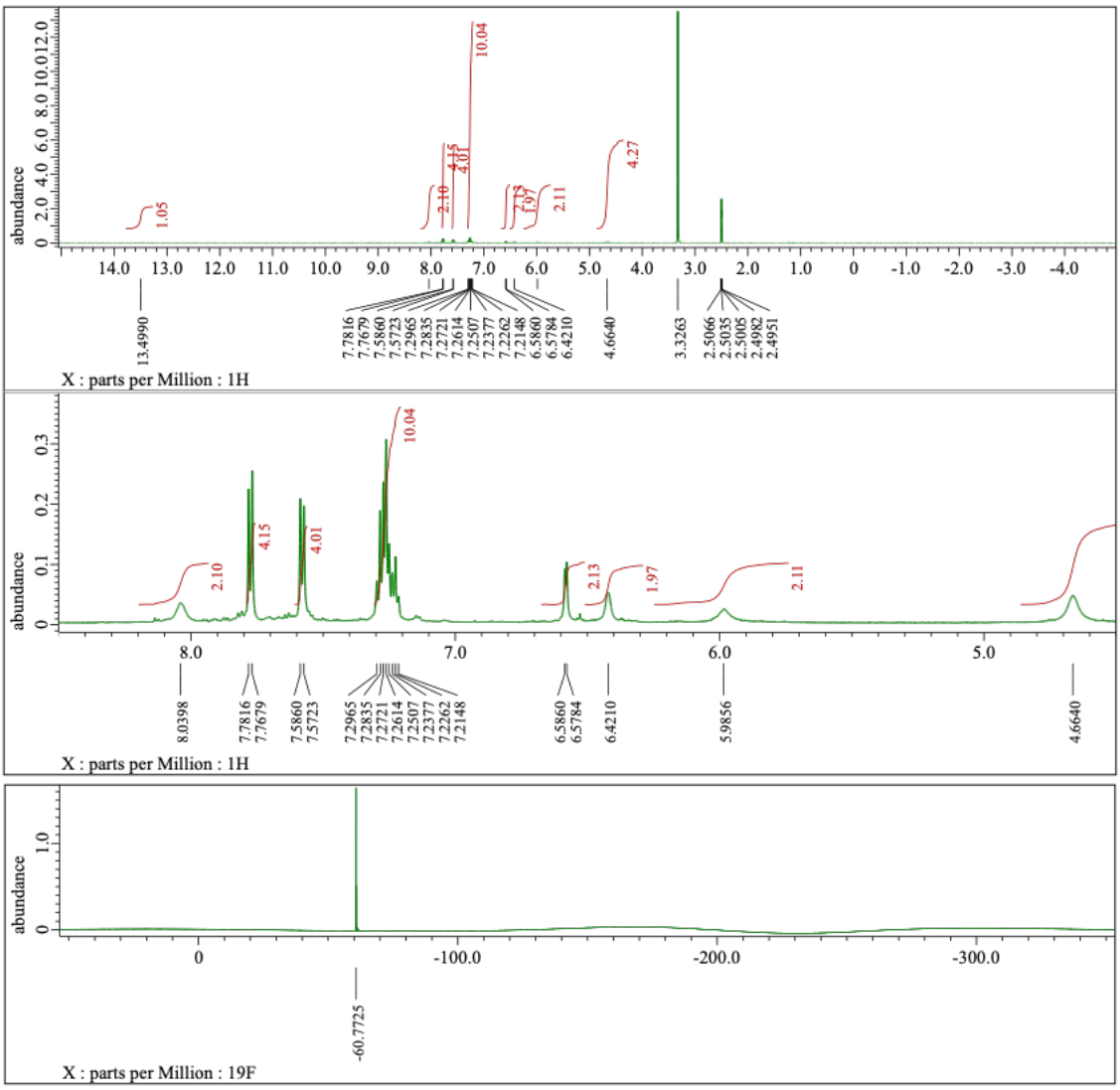


Figure S2-7. ^{1}H and ^{19}F NMR spectra of **5** at 25 °C in DMSO-*d*$_6$. *Solvent and impurities. ^{1}H-NMR (600 MHz, DMSO-*d*$_6$, 10 mM) δ / ppm = 13.50 (s, 1H, NH), 8.04 (s, 2H, NH), 7.77 (d, *J* = 8.3 Hz, 4H, Ar-H), 7.58 (d, *J* = 8.3 Hz, 4H, Ar-H), 7.26 (m, 10H, Ph-H), 6.58 (d, *J* = 4.6 Hz, 2H, β), 6.42 (brs, 2H, β), 5.99 (brs, 2H, β) and 4.66 (brs, 4H, C$\underline{H_2}$Ph), ^{19}F-NMR (565 MHz, DMSO-*d*$_6$) δ = –60.8 ppm

1,14-bis(1-phenylethylamino)-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **6**

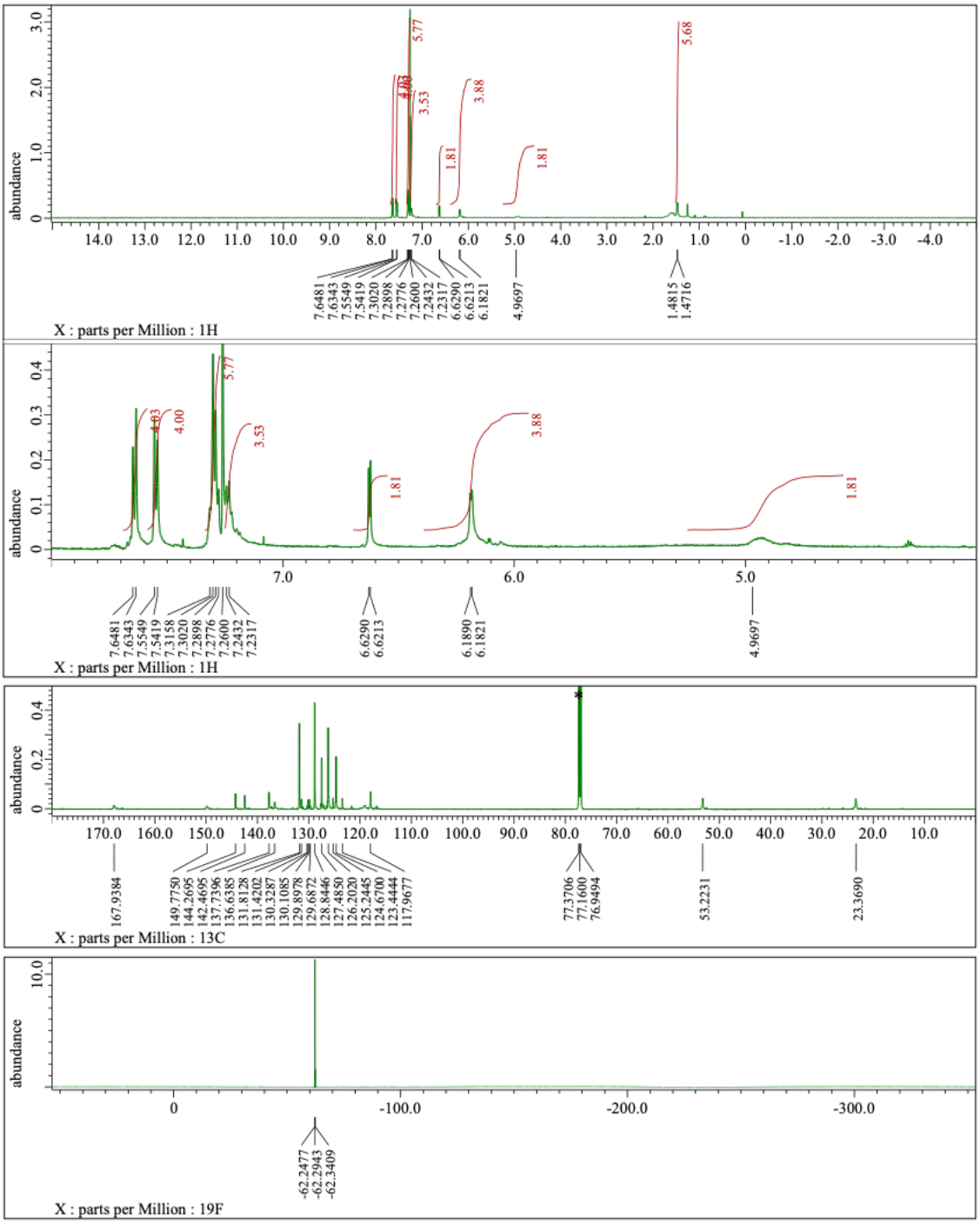


Figure S2-8. ^{1}H, ^{13}C and ^{19}F NMR spectra of **6** at 25 °C in $CDCl_3$. *Solvent and impurities.

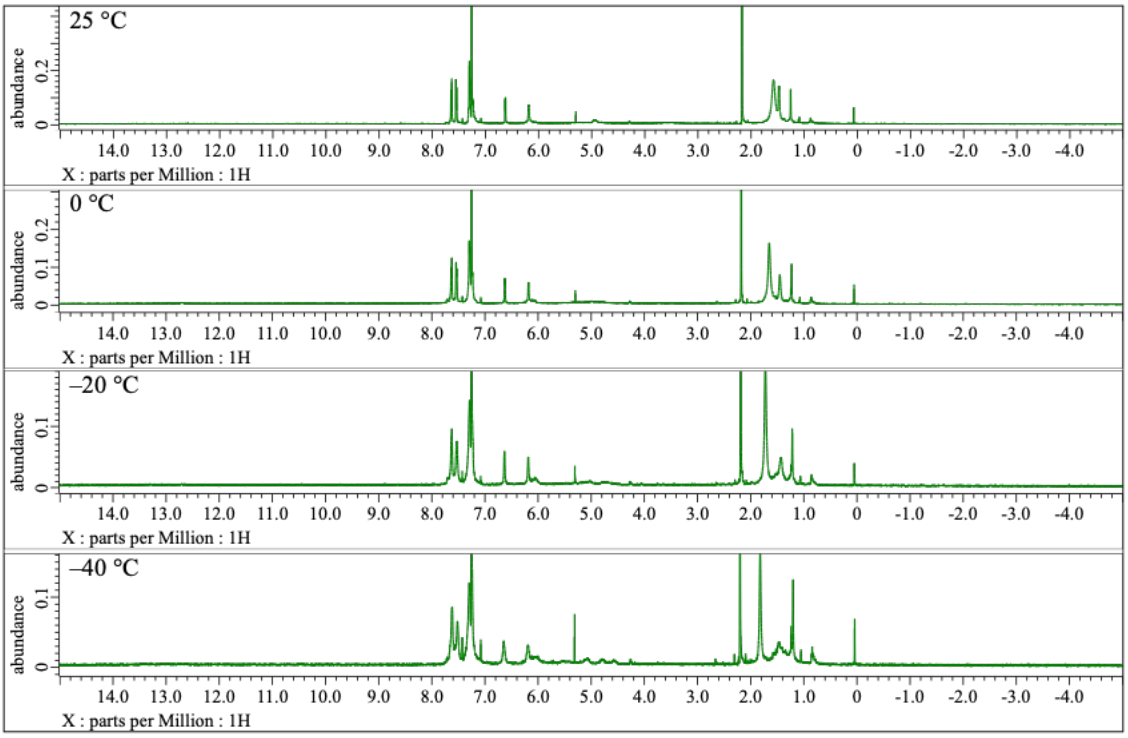


Figure S2-9. ^{1}H NMR spectra of **6** in $CDCl_3$ at different temperature. *Solvent and impurities. (No dimerization was observed.)

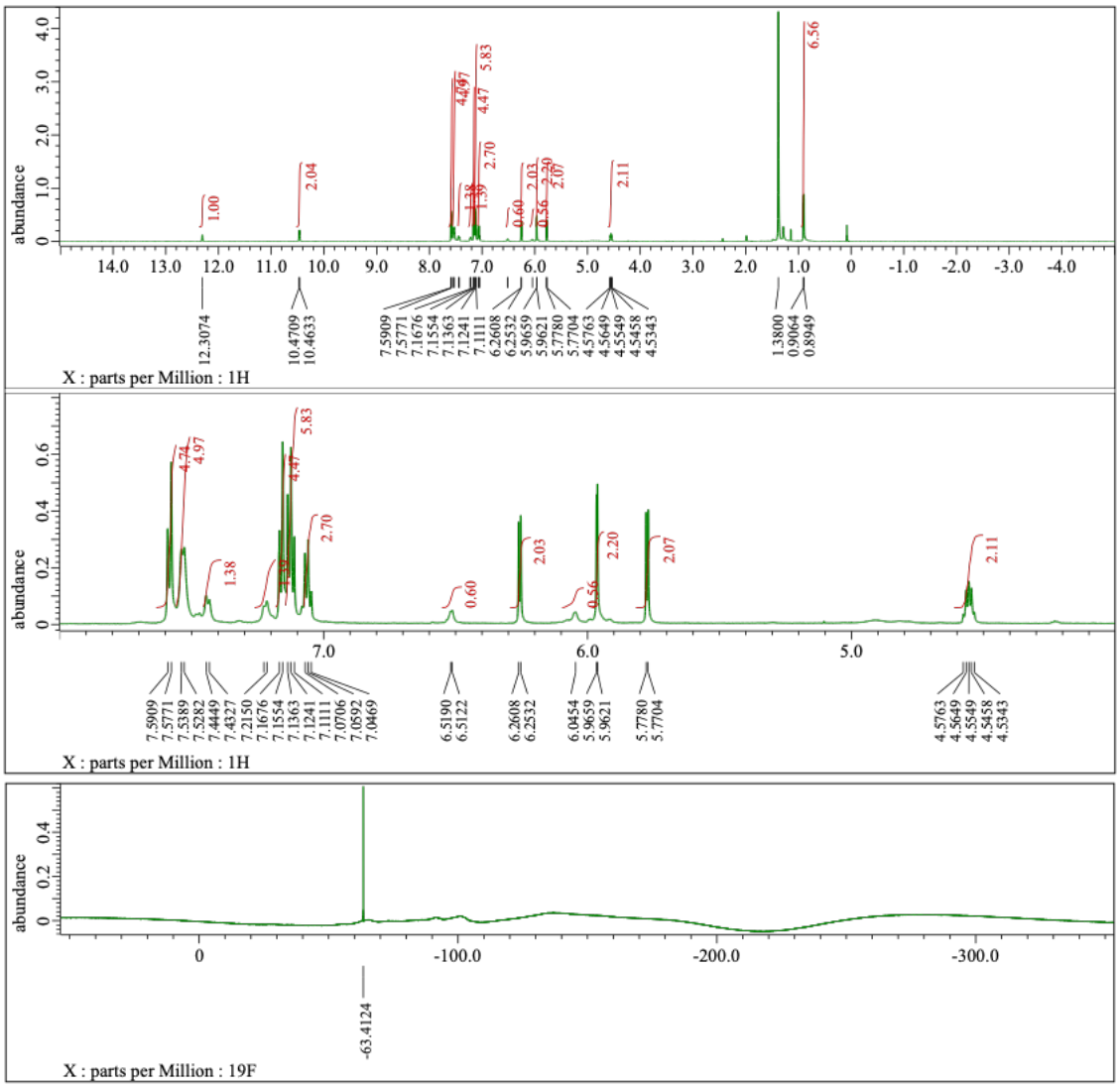


Figure S2-10. ^{1}H and ^{19}F NMR spectra of **6** at 25 °C in cyclohexane-d_{12}.

^{1}H-NMR (600 MHz) (cyclohexane-d_{12}, 10 mM, dimer) δ / ppm = 12.31 (brs, 2H, NH), 10.47 (d, 4H, J = 4.6 Hz, NH), 7.58 (d, 8H, J = 8.2 Hz, Ar-H), 7.53 (d, 8H, J = 6.4 Hz, Ar-H), 7.16 (d, 8H, J = 7.3 Hz, Ph *o*-H), 7.12 (t, 8H, J = 7.6 Hz, Ph *m*-H), 7.06 (t, 4H, J = 7.4 Hz, Ph *p*-H), 6.26 (d, 4H, J = 4.6 Hz, β), 5.96 (d, 4H, J = 2.3 Hz, β), 5.77 (d, 4H, J = 4.6 Hz, β), 4.55 (dq, 4H, J_1 = 5.8 Hz, J_2 = 6.8 Hz, C<u>H</u>(Me)Ph) and 0.90 (d, 12H, J = 6.8 Hz, CH(<u>Me</u>)Ph).

Monomeric peaks (25% in intensity) were observed. ^{1}H-NMR (600 MHz) (cyclohexane-d_{12}, 10 mM, monomer) δ / ppm = 7.44 (d, 4H, J = 7.3 Hz), 7.22 (d, 4H, J = 6.8 Hz), 7.12 (brs, 4H), 7.06 (brs, 4H), 6.51, (brs, 2H) and 6.04 (brs, 2H) (the aliphatic proton signals were not observed presumably due to the broadening). ^{19}F-NMR (585 MHz, cyclohexane-d_{12}) δ = –63.4 ppm.

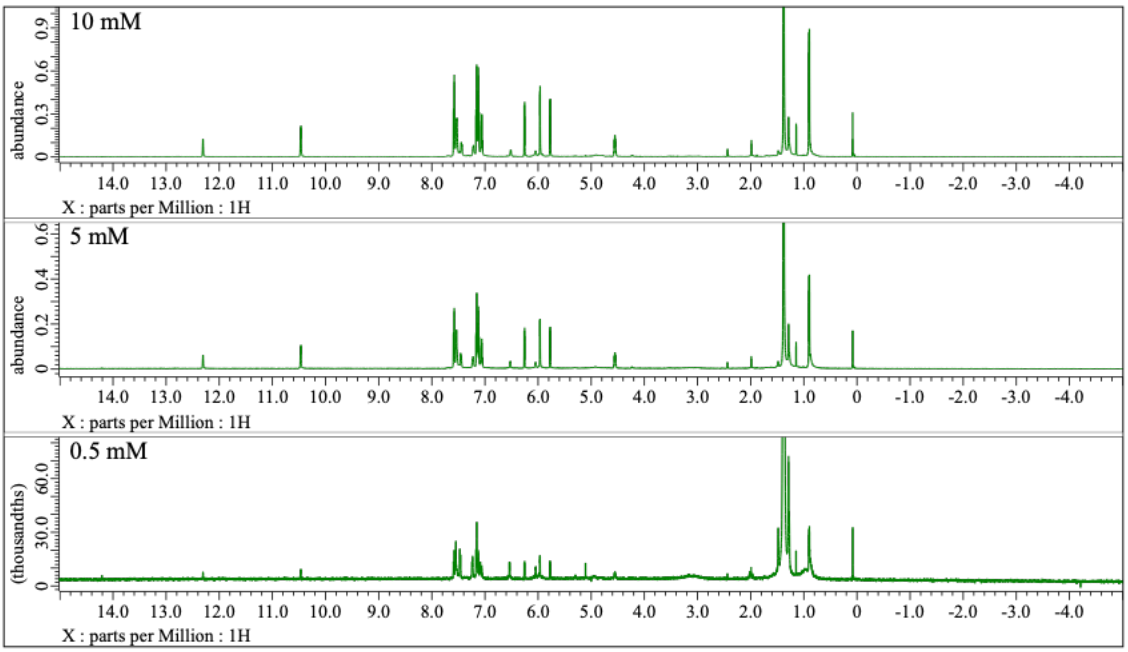


Figure S2-11. ^{1}H NMR spectra of several concentration of cyclohexane-d_{12} solution of **6** at 25 °C.

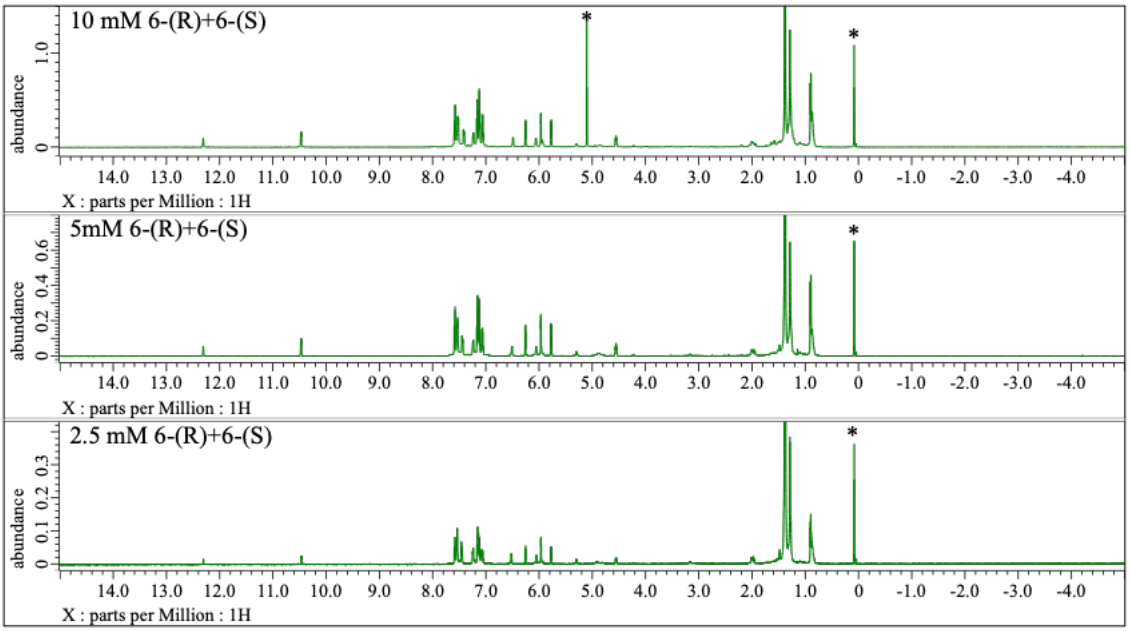


Figure S2-12. ^{1}H NMR spectra of several concentration of cyclohexane-d_{12} solution of a mixture of **6-(*R*)** and **6-(*S*)** at 25 °C.

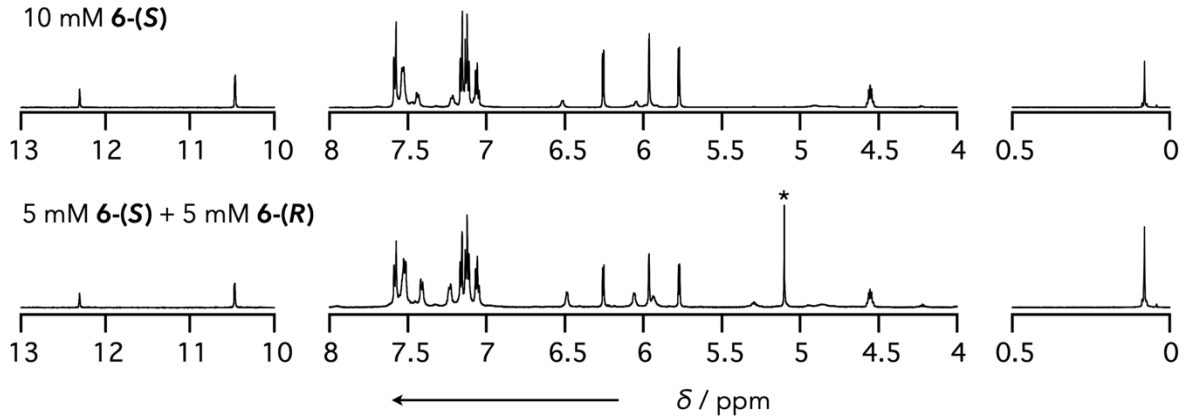


Figure S2-13. Comparison of the ^{1}H NMR spectra of **6-(*S*)** (10 mM) and a mixture of **6-(*R*)** and **6-(*S*)** (each 5 mM) in cyclohexane-d_{12} at 25 °C. New peaks assignable to the formation of the diastereomer (heterodimer) are not observed.

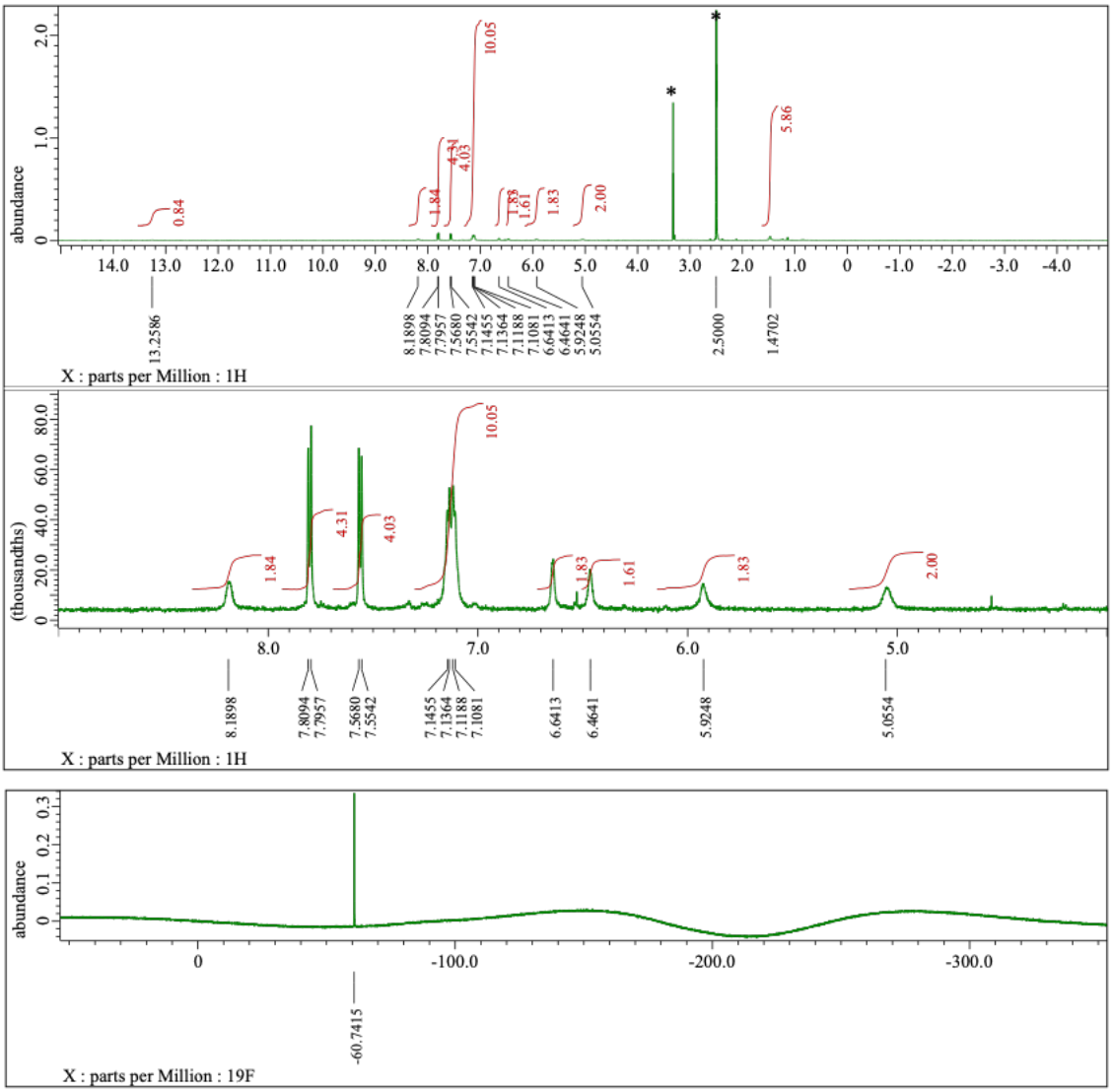


Figure S2-14. ^{1}H and ^{19}F NMR spectra of **6** at 25 °C in DMSO-d_6. *Solvent and impurities. ^{1}H-NMR (600 MHz, DMSO-d_6) δ / ppm = 13.26 (s, 1H, NH), 8.19 (s, 2H, NH), 7.80 (d, J = 8.3 Hz, 4H, Ar-H), 7.56 (d, J = 8.3 Hz, 4H, Ar-H), 7.12 (m, 10H, Ph-H), 6.64 (brs, 2H, β), 6.46 (brs, 2H, β), 5.92 (brs, 2H, β), 5.06 (brs, 2H, C<u>H</u>(Me)Ph) and 1.47 (brs, 6H, CH(<u>Me</u>)Ph); ^{19}F-NMR (565 MHz, DMSO-d_6) δ = –60.7 ppm.

3. Mass Spectra

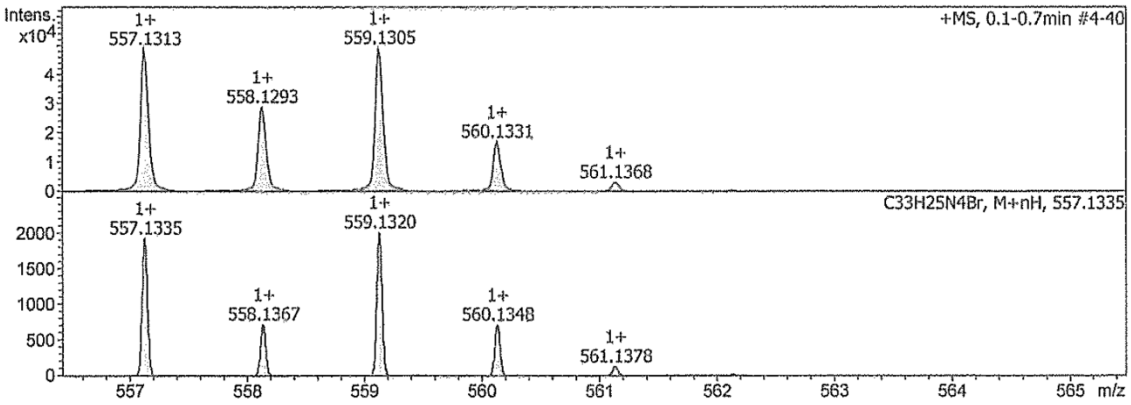


Figure S3-1. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **3**.

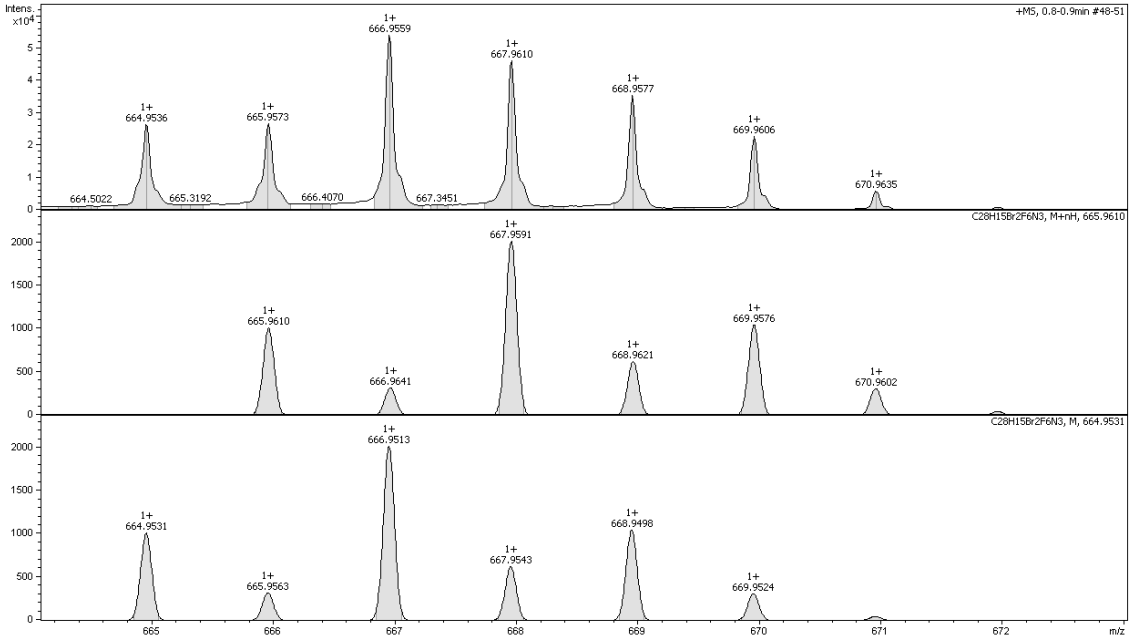


Figure S3-2. Observed (top) and simulated ((middle; $[M+H]^+$, bottom; $[M]^+$) HR-APCI-TOF-MS of **4**.

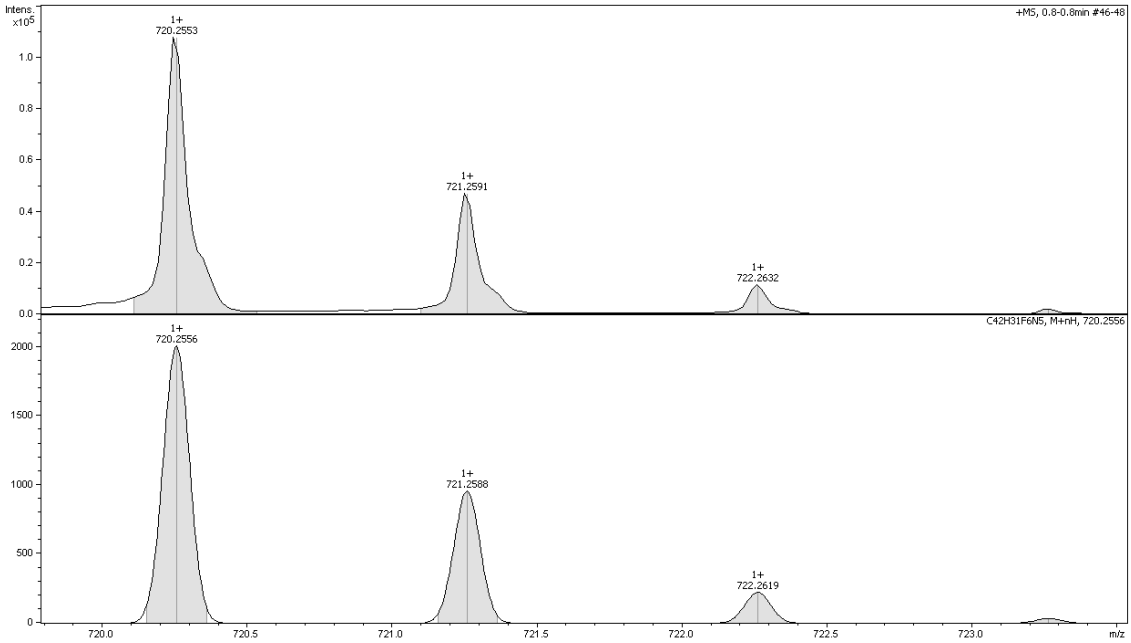


Figure S3-3. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **5**

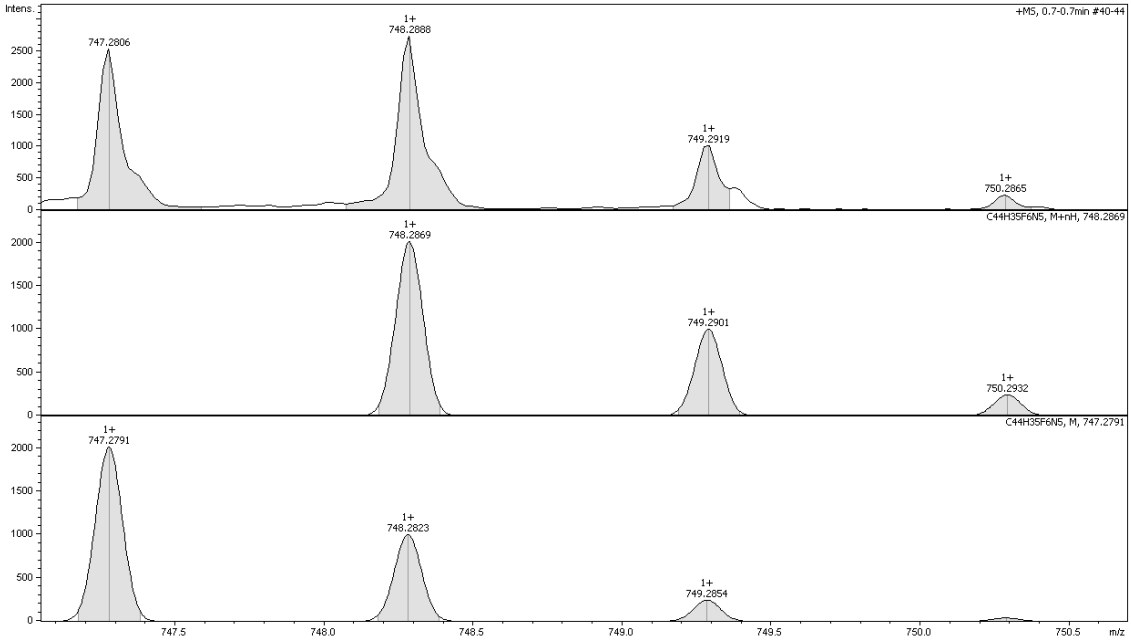


Figure S3-4. Observed (top), simulated (middle; $[M+H]^+$, bottom; $[M]^+$) HR-APCI-TOF-MS of **6**.

4. UV/Vis Absorption and CD spectra

1,14-dibromo-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **4**

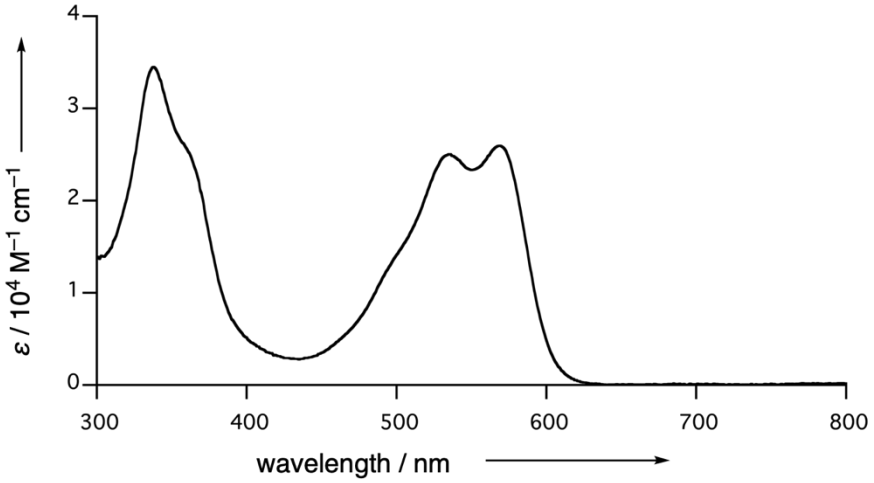


Figure S4-1. UV/Vis absorption spectrum of **4** in CH_2Cl_2.

UV/Vis (CH_2Cl_2) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 338 (3.45), 535 (2.50), 571 (2.58).

1,14-dibenzylamino-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **5**

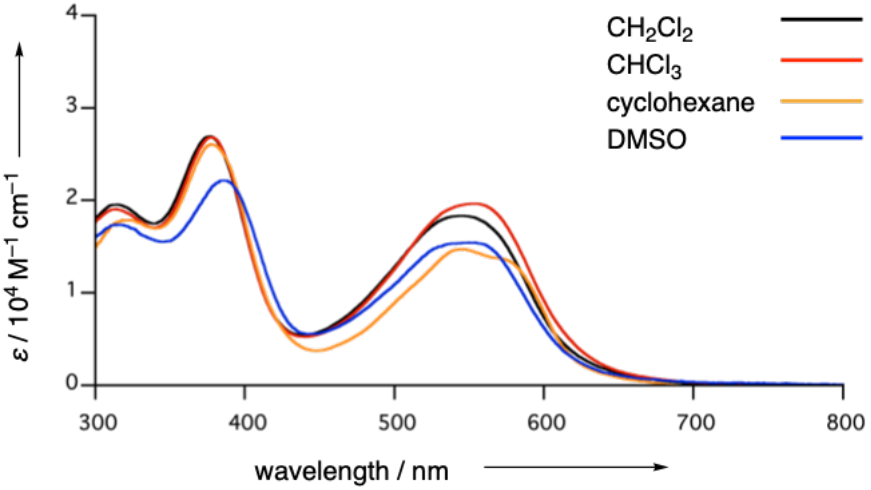


Figure S4-2. UV/Vis absorption spectrum of **5** in several solvents.

Absorption spectrum of **5** did not completely follow Lambert-Beer's law. Thus, the molar absorption coefficient ε was determined by a solution of a fixed concentrations.

UV/Vis (CH_2Cl_2, 2.5×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 315 (1.95), 377 (2.69), 543 (1.83); ($CHCl_3$, 2.5×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 312 (1.90), 377 (2.71), 555 (1.98); (cyclohexane, 2.6×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 323 (1.78), 377 (2.61), 544 (1.47); (DMSO, 2.6×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 318 (1.74), 387 (2.21), 554 (1.54).

1,14-bis(1-phenylethylamino)-5,10-bis(*p*-trifluoromethylphenyl)tripyrrin **6**

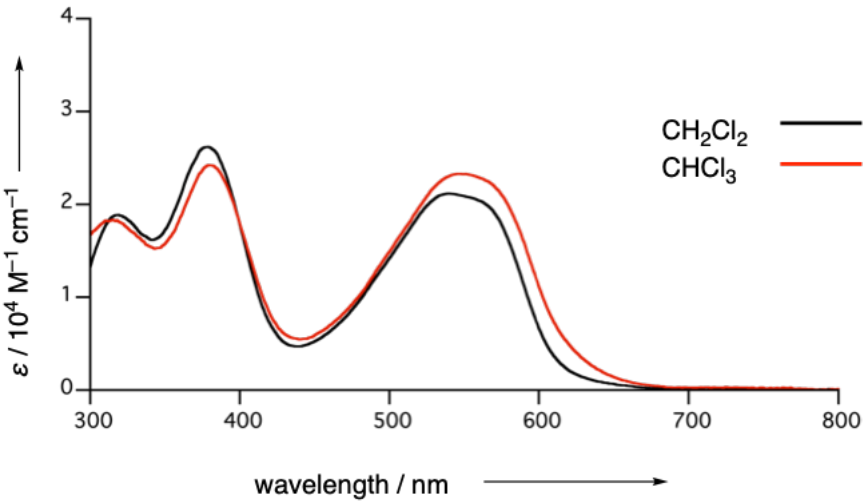


Figure S4-3. UV/Vis absorption spectra of **6** in CH_2Cl_2 (black) and $CHCl_3$ (red).

Absorption spectrum of **6** did not completely follow Lambert-Beer's law. Thus, the molar absorption coefficient ε was determined by a solution of a fixed concentration. UV/Vis (CH_2Cl_2, 1.3×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 319 (1.89), 379 (2.62). 540 (2.12) ($CHCl_3$, 1.6×10^{-5} M) λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1}) = 315 (1.84), 379 (2.43). 545 (2.34)

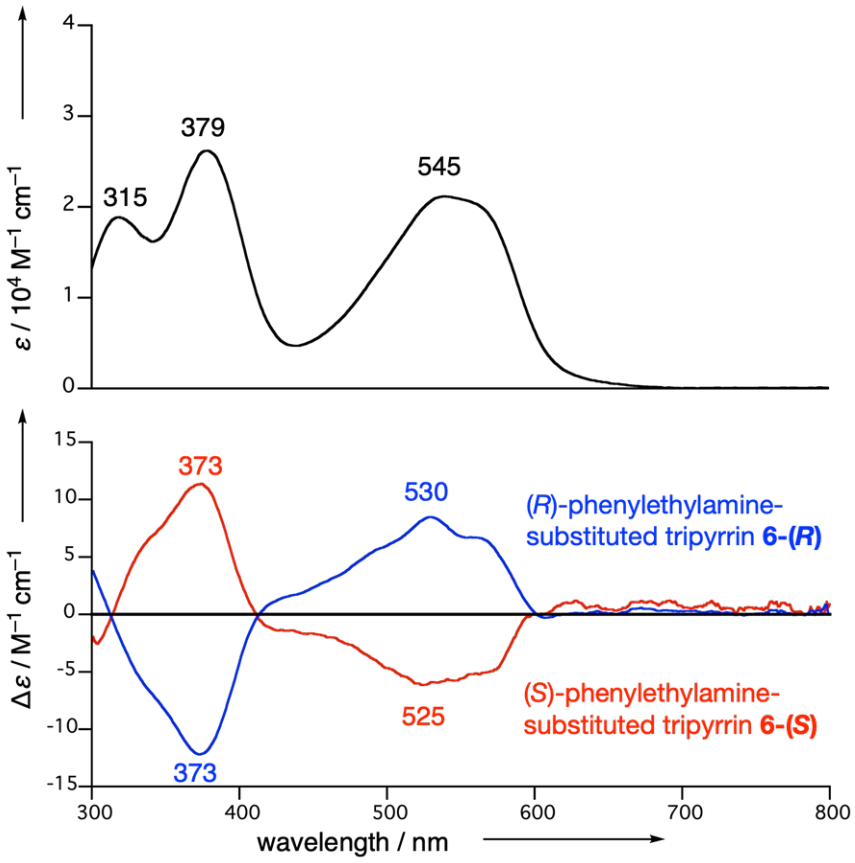


Figure S4-4. UV/Vis absorption and CD spectra of **6** in $CHCl_3$.

5. X-ray Crystallographic Details

Table S5-1. Crystallographic parameters.

Compound	**5**
Empirical Formula	$2(C_{42}H_{31}F_6N_5)$
Fw	1439.43
Crystal System	Monoclinic
Space Group	*C* 2/*c*
a	28.0551(4) Å
b	17.8120(2) Å
c	28.6373(4) Å
α	90°
β	104.597(2)°
γ	90°
Volume	13848.6(3) $Å^3$
Z	8
Density (calcd.)	1.381 $g \cdot cm^{-3}$
Completeness	0.964
Goodness-of-fit (all data)	1.047
$R_1(I>2\sigma(I))$	0.0544
wR_2 (all data)	0.1606
CCDC No.	2054819

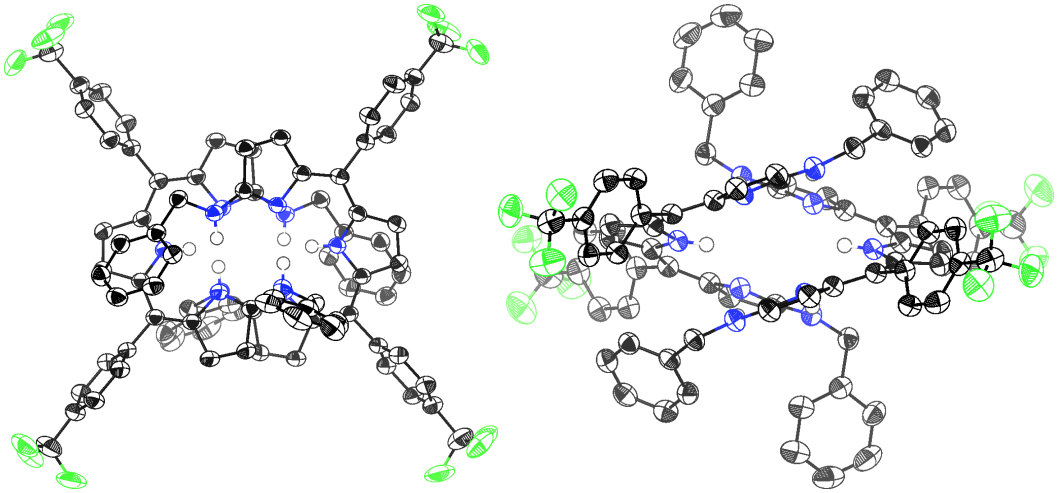


Figure S5-1. X-Ray structure of **5** (dimer) observed in the co-crystal. (left) Top view and (right) side view. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms except for NHs were omitted.

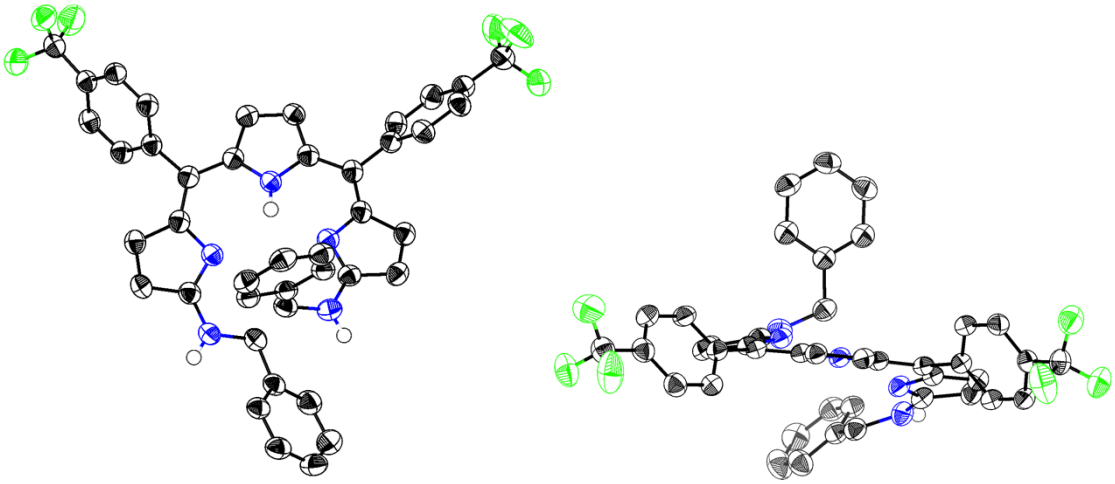


Figure S5-2. X-Ray structure of **5** (monomer) observed in the co-crystal. (left) Top view and (right) side view. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms except for NHs were omitted.

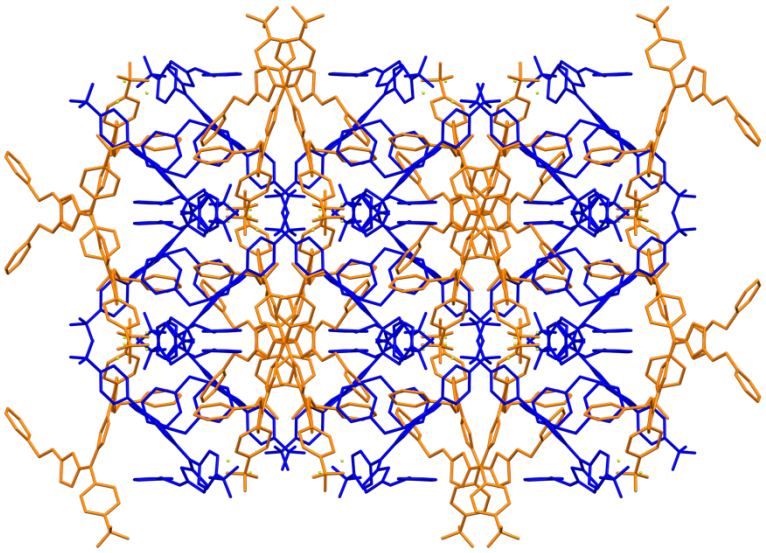


Figure S5-3. Packing structure of **5**. The monomeric helix is represented as blue and the dimeric helix as orange. Hydrogen atoms are omitted for clarity.

6. DFT Calculations

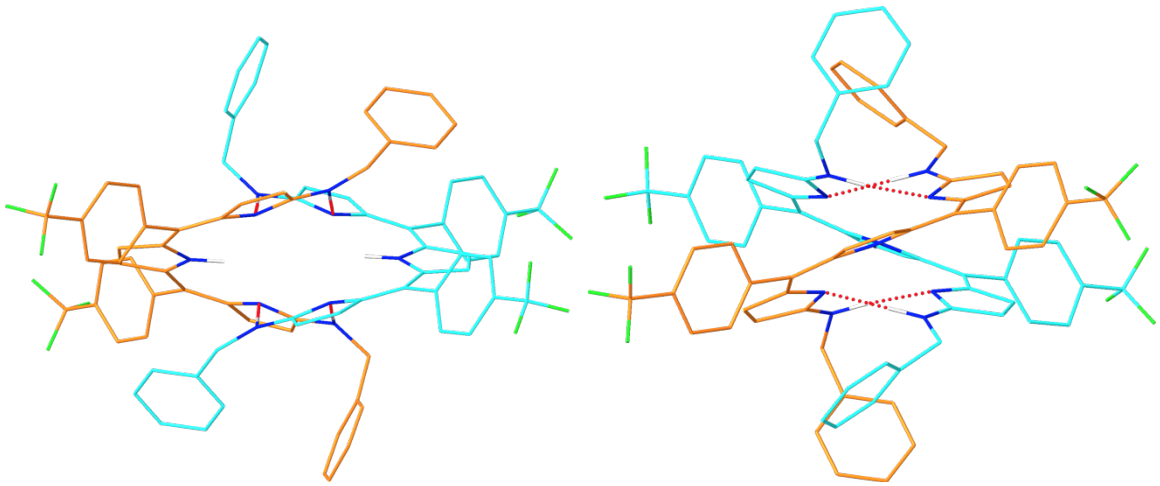


Figure S6-1. Optimized structure of **5** (dimer). Left: along x-axis. Right: along y-axis. The structure was calculated at B3LYP-D3(BJ)/6-311++G(d,p) level based on the crystal structure. Hydrogen atoms were omitted for clarity.

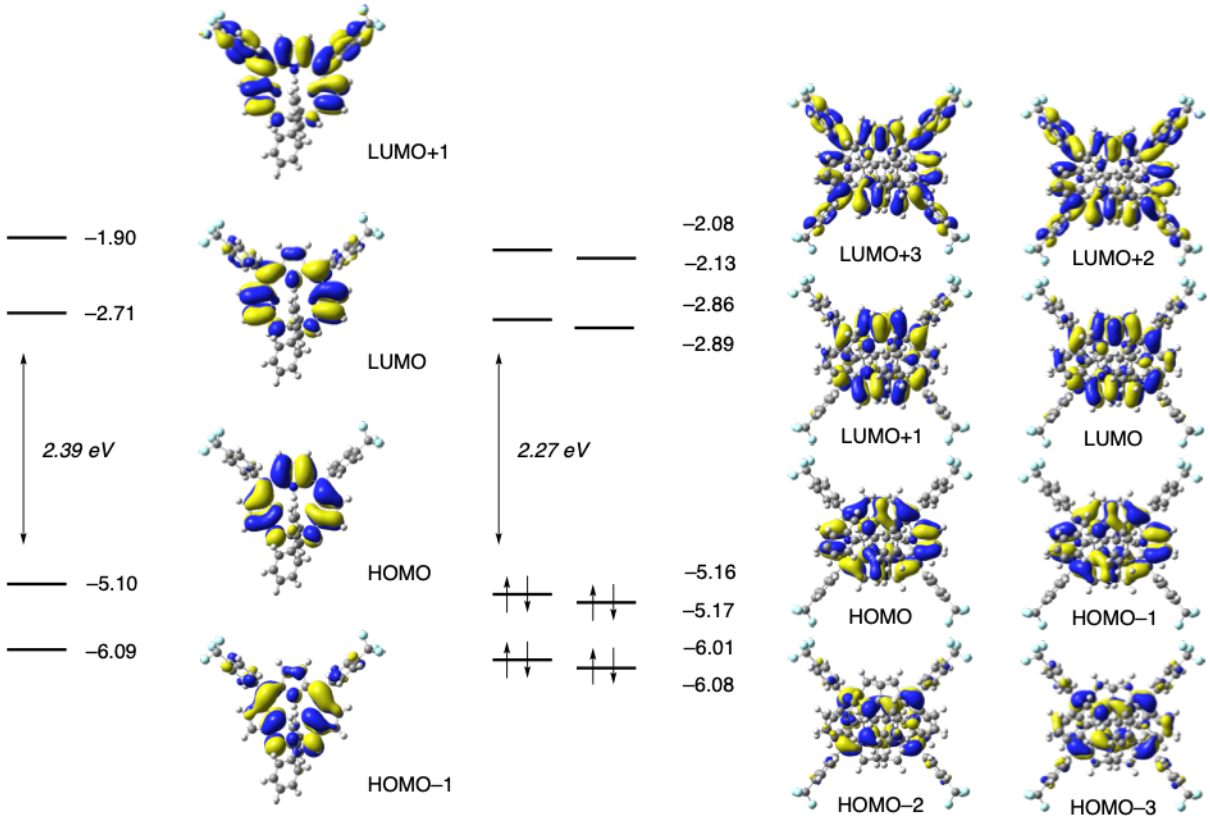


Figure S6-2. MO energy diagrams and Kohn-Sham orbital representations for **5** (left: monomer, right: dimer) calculated at B3LYP-D3(BJ)/6-311++G(d,p) level.

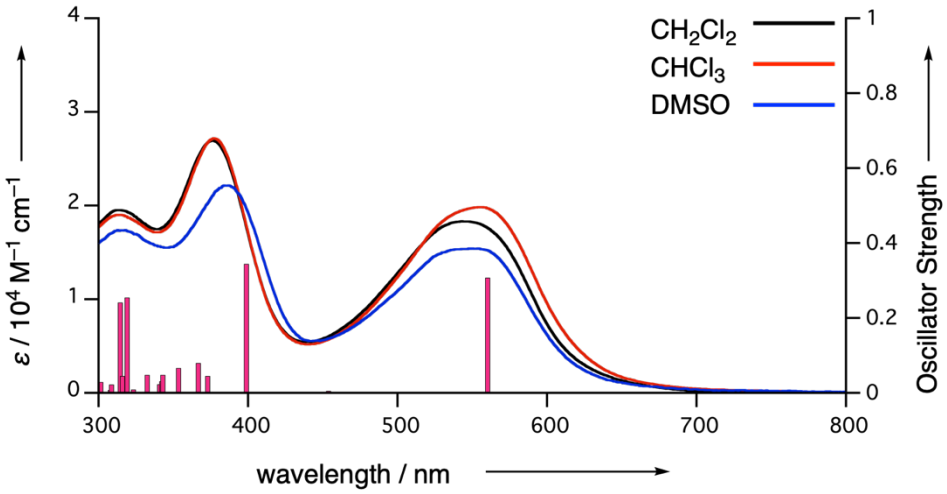


Figure S6-3. UV/Vis absorption spectrum of **5** in several solvents and TD-DFT simulation of **5** (monomer) calculated at B3LYP-D3(BJ)/6-311++G(d,p) level.

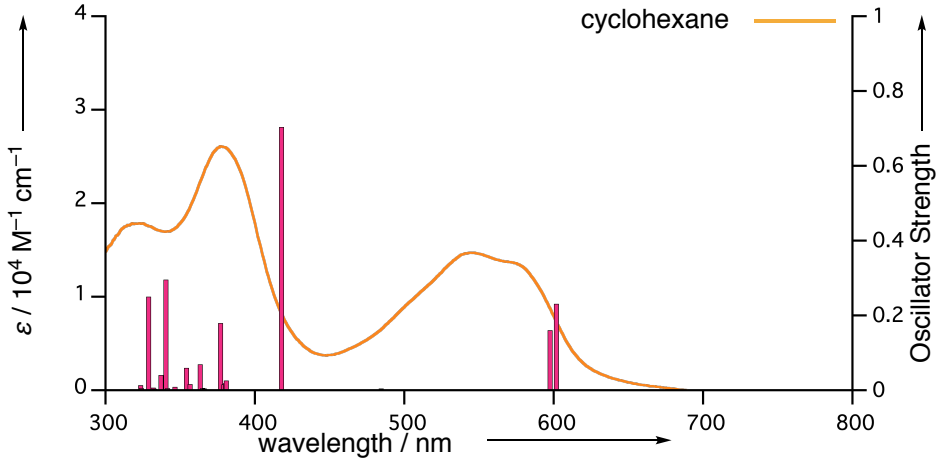


Figure S6-4. UV/Vis absorption spectrum of **5** in several solvents and TD-DFT simulation of **5** (dimer) calculated at B3LYP-D3(BJ)/6-311++G(d,p) level.

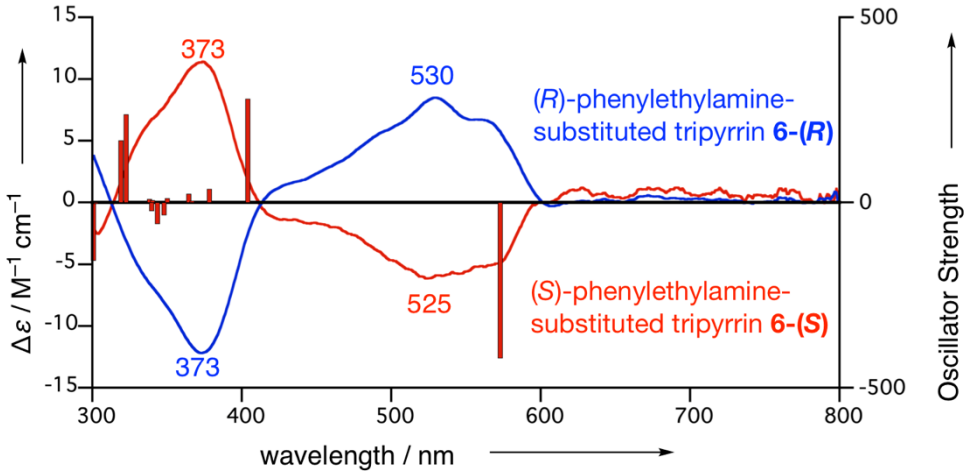


Figure S6-5. UV/Vis absorption and CD spectra of **6** in $CHCl_3$ and calculated CD spectra of **5** (monomer, *M*-configuration) calculated at B3LYP-D3(BJ)/6-311++G(d,p) level.

7. Supporting References

[S1] G. M. Sheldrick, *Acta Cryst*., 2015, **A71**, 3.
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[S3] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
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[S5] G. Cheng-Zhi, F. Ya-Qing, L. Peng-Peng and M. Shu-Xian, *J. Saudi Chem. Soc.*, 2015, **19**, 227.