

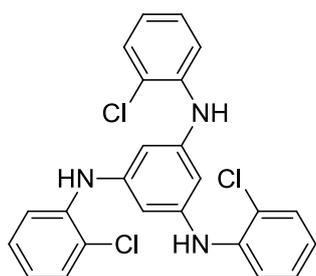
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1. General Remarks

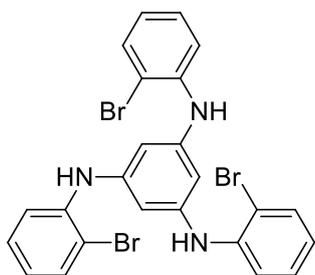
All reagents and solvents were commercially available and were used without further purification unless otherwise noted. For thin layer chromatography Silica gel 60 F254 plates from Merck were used and examined under UV-light irradiation (254 nm and 365 nm). Flash column chromatography was performed on silica gel (particle size: 200-300 mesh). IR-Spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. NMR spectra were taken on Bruker AVANCE III HD (600MHz) and AVANCE NEO (400MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to traces of CHCl_3 , benzene, CH_2Cl_2 and DMSO in the corresponding deuterated solvent. HRMS experiments were carried out on a ThermoFisher LTQ Orbitrap XL. Absorption spectra were recorded on a Shimadzu UV2600. Emission spectra, absolute quantum yields, as well as fluorescence lifetimes were measured on FluoroMax-4 spectrometer equipped with an integral sphere and a time-correlated single photon counting system with a NanoLED laser. Electrochemical data were obtained in dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) and ferrocene was used as an internal standard. CV and DPV were measured using a glassy carbon working electrode, a platinum counter electrode, and a Ag reference electrode tested on CHI660E station. Crystal structure analysis was accomplished with a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer at 150 K. 2-Bromo-4-*tert*-butylaniline^[S1] and 2-bromo-4-*tert*-butylpyridine^[S2] were synthesized according to the reported method.

2. Experimental part

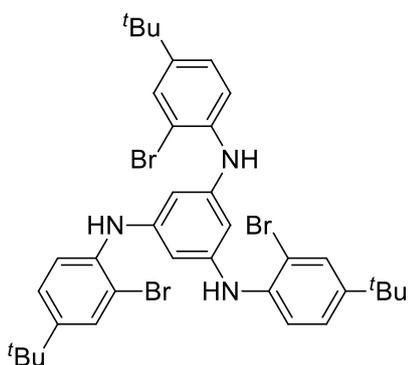


Method a: A 38 mL screw capped glass vial was charged with 1,3,5-tribromobenzene (629 mg, 2 mmol), 2-chloroaniline (918 mg, 7.2 mmol), $\text{Pd}_2(\text{dba})_3$ (110 mg, 0.12 mmol) and $^t\text{BuONa}$ (769 mg, 8 mmol). Under the protection of argon, dry toluene (2 mL) and $^t\text{Bu}_3\text{P}(\text{HfBF}_4$ (110 mg, 0.38 mmol) were added to the vial and the mixture was bubbled with argon for 2 minute. The vial was quickly sealed and heated in an oil bath at 120 °C for 12 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na_2SO_4 . The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 1:2) to give the product **2aCl** as colourless solid (260 mg, 0.57 mmol, 29%).

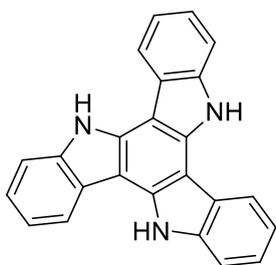
Method b: 2-Chloroaniline (2.55 g, 20 mmol), phloroglucinol (631 mg, 5 mmol) and hydrochloric acid (37%, 0.4 mL) were added in a 100 mL flask. The flask was heated in an oil bath at 120°C for 5 hours. After cooling down to room temperature, ethanol (50 mL) was added to the flask and the solid was crashed. The suspension was filter off and the solid was further washed with ethanol (100 mL) to give compound **2aCl** as colourless powder (1.85 g, 4.07 mmol, 81%). m.p. 170°C. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ (ppm) = 7.49 (s, 3H), 7.39 (dd, J = 7.9, 1.5 Hz, 3H), 7.34 (dd, J = 8.2, 1.5 Hz, 3H), 7.21 (td, J = 8.1, 7.7, 1.5 Hz, 3H), 6.88 (td, J = 7.6, 1.5 Hz, 3H), 6.34 (s, 3H). ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) δ (ppm) = 144.45, 140.12, 129.82, 127.54, 123.43, 121.59, 119.96, 100.49. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3405, 1589, 1513, 1479, 1311, 1171, 1126, 1042, 825, 742, 686. HRMS (ESI) (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{24}\text{H}_{19}\text{N}_3\text{Cl}_3$, 454.0645; found, 454.0650.



2-Bromoaniline (10.91 g, 63.4 mmol), phloroglucinol (2 g, 15.8 mmol) and hydrochloric acid (37%, 0.8 mL) were added in a 100 mL flask. The flask was heated in an oil bath at 120°C for 4 hours. After cooling down to room temperature, ethanol (50 mL) was added to the flask and the solid was crashed. The suspension was filter off and the solid was further washed with ethanol (100 mL) to give compound **2aBr** as grayish powder (7.21 g, 12.3 mmol, 77%). m.p. 180°C. ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm) = 7.56 (d, *J* = 8.0 Hz, 3H), 7.40–7.30 (m, 6H), 7.26 (t, *J* = 7.8 Hz, 3H), 6.83 (t, *J* = 7.7 Hz, 3H), 6.27 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ (ppm) = 144.84, 141.37, 133.13, 128.25, 122.53, 120.91, 114.81, 99.74. IR (KBr) $\tilde{\nu}$ (cm⁻¹) = 3395, 3063, 1586, 1511, 1476, 1307, 1170, 1120, 1023, 824, 742, 663. HRMS (ESI) (*m/z*): [M+H]⁺ calculated. for C₂₄H₁₉N₃Br₃, 585.9129; found, 585.9128.

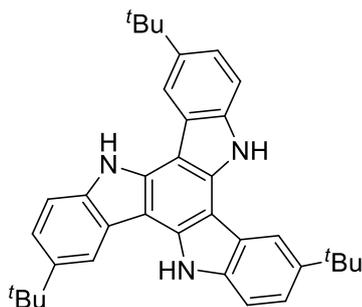


2-Bromo-4-*tert*-butylaniline (7.41 g, 32.5 mmol), phloroglucinol (1.07 g, 8.5 mmol) and hydrochloric acid (37%, 0.5 mL) were added in a 100 mL flask. The flask was heated in an oil bath at 120°C for 4 hours. After cooling down to room temperature, ethanol (20 mL) was added to the flask and the solid was crashed. The suspension was filter off and the solid was further washed with ethanol (40 mL) to give compound **2b** as colourless powder (5.46 g, 7.2 mmol, 85%). m.p. 230°C. ¹H NMR (600 MHz, DMSO-*d*₆) δ (ppm) = 7.50 (d, *J* = 2.2 Hz, 3H), 7.30 (dd, *J* = 8.5, 2.2 Hz, 3H), 7.26 (d, *J* = 8.5 Hz, 3H), 7.22 (s, 3H), 6.12 (s, 3H), 1.24 (s, 27H). ¹³C NMR (150 MHz, DMSO-*d*₆) δ (ppm) = 145.53, 145.35, 138.67, 129.53, 125.09, 121.56, 115.34, 97.60, 33.96, 31.03. IR (KBr) $\tilde{\nu}$ (cm⁻¹) = 3397, 2962, 2903, 2867, 1597, 1512, 1491, 1389, 1362, 1307, 1266, 1176, 1117, 1041, 876, 855, 816, 731, 690, 599, 421. HRMS (ESI) (*m/z*): [M+H]⁺ calculated. for C₃₆H₄₃N₃Br₃, 754.1007; found, 754.1005.

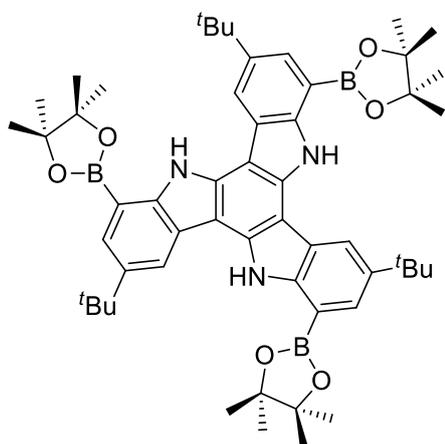


Method a: A 38 mL screw capped glass vial was charged with compound **2aCl** (114 mg, 0.25 mmol), Pd(OAc)₂ (3.5 mg, 0.015 mmol), anhydrous K₂CO₃ (69 mg, 0.5 mmol). Under the protection of argon, dry DMAc (2 mL) and ^tBu₃PHBF₄ (9 mg, 0.03 mmol) were added to the vial and the mixture was bubbled with argon for 2 minute. The vial was quickly sealed and heated in an oil bath at 130 °C for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na₂SO₄. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:4) to give the product **3a** as grayish yellow powder (63 mg, 0.18 mmol, 73%).

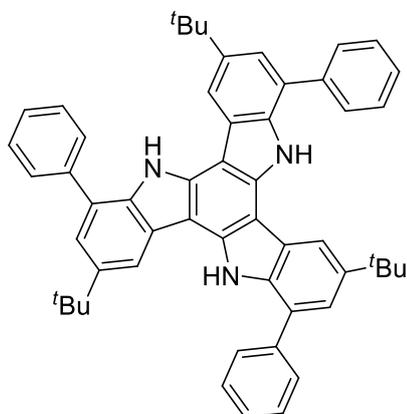
Method b: A 120 mL screw capped glass vial was charged with compound **2aBr** (2.00 g, 3.4 mmol), Pd(OAc)₂ (22 mg, 0.1 mmol), anhydrous K₂CO₃ (0.94 g, 6.80 mmol). Under the protection of argon, dry DMAc (15 mL) and Cy₃PHBF₄ (74 mg, 0.2 mmol) were added to the vial and the mixture was bubbled with argon for 2 minute. The vial was quickly sealed and heated in an oil bath at 130 °C for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (250 mL) and washed with water (200 mL) and dried over Na₂SO₄. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:4) to give the product **3a** as grayish yellow powder (0.97 g, 2.8 mmol, 83%). ¹H NMR (600 MHz, DMSO-*d*₆) δ (ppm) = 11.87 (s, 3H), 8.68 (d, *J* = 7.7 Hz, 3H), 7.74 (d, *J* = 7.9 Hz, 3H), 7.40 (t, *J* = 7.4 Hz, 3H), 7.34 (t, *J* = 7.3 Hz, 3H). The characterization matches well with the reported data.^[S3]



A 120 mL screw capped glass vial was charged with compound **2b** (3.03 g, 4.0 mmol), Pd(OAc)₂ (90 mg, 0.4 mmol), anhydrous K₂CO₃ (1.66 g, 12.0 mmol). Under the protection of argon, dry DMAc (20 mL) and Cy₃PHBF₄ (295 mg, 0.8 mmol) were added to the vial and the mixture was bubbled with argon for 2 minute. The vial was quickly sealed and heated in an oil bath at 130 °C for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (250 mL) and washed with water (200 mL) and dried over Na₂SO₄. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:10) to give the product **3b** as colourless powder (1.68 g, 3.3 mmol, 82%). m.p. >400°C (dec.). ¹H NMR (600 MHz, DMSO-*d*₆) δ (ppm) = 11.64 (s, 3H), 8.58 (d, *J* = 1.8 Hz, 3H), 7.66 (d, *J* = 8.4 Hz, 3H), 7.44 (dd, *J* = 8.4, 1.8 Hz, 3H), 1.54 (s, 27H). ¹³C NMR (150 MHz, DMSO-*d*₆) δ (ppm) = 141.81, 136.74, 134.15, 122.39, 119.79, 116.45, 110.00, 100.71, 34.79, 32.31. IR (KBr) $\tilde{\nu}$ (cm⁻¹) = 3479, 3057, 2960, 2902, 2864, 1639, 1616, 1485, 1461, 1391, 1368, 1303, 1283, 1256, 1202, 1107, 1067, 935, 858, 635, 435. HRMS (ESI) (*m/z*): [M+Na]⁺calculated. for C₃₆H₃₉N₃Na, 536.3042; found, 536.3026.

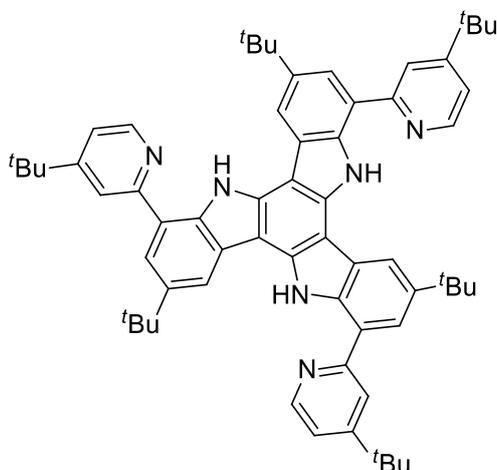


In a glovebox, [Ir(COD)OMe]₂ (30 mg, 0.09 mmol Ir), dtbpy (24 mg, 0.09 mmol) and a small amount of B₂pin₂ (69 mg, 0.3 mmol) were mixed in THF (2 mL) and the mixture was stirred vigorously until the solution became brownish-red. The catalyst solution was then added to a 38 mL vial containing a suspension of triazatruxene **3b** (514 mg, 1.0 mmol) and B₂pin₂ (1.07 mg, 4.2 mmol) in THF (4 mL). The vial was sealed and heated in an oil bath at 80 °C for 24 hours. After cooling to room temperature, solvent was removed by rotary evaporation and the crude product was washed with methanol (2x15 mL) to give boronic ester **4** (872 mg, 0.98 mmol, 98%) as a colorless powder. m.p. >400°C (dec.). ¹H NMR (400 MHz, C₆D₆) δ (ppm) = 10.34 (s, 3H), 8.61 (s, 3H), 8.49 (s, 3H), 1.64 (s, 27H), 1.29 (s, 36H). ¹³C NMR (100 MHz, C₆D₆) δ (ppm) = 143.52, 142.00, 135.46, 122.89, 119.99, 102.05, 84.03, 67.83, 35.07, 32.51, 25.30. IR (KBr) $\tilde{\nu}$ (cm⁻¹) = 3453, 2959, 1635, 1601, 1477, 1433, 1411, 1386, 1368, 1290, 1266, 1246, 1231, 1201, 1176, 1140, 1023, 978, 903, 871, 852, 781, 760, 681, 644, 594, 503. HRMS (ESI) (*m/z*): [M+H]⁺calculated. for C₅₄H₇₃N₃B₃O₆, 892.5779; found, 892.5789.



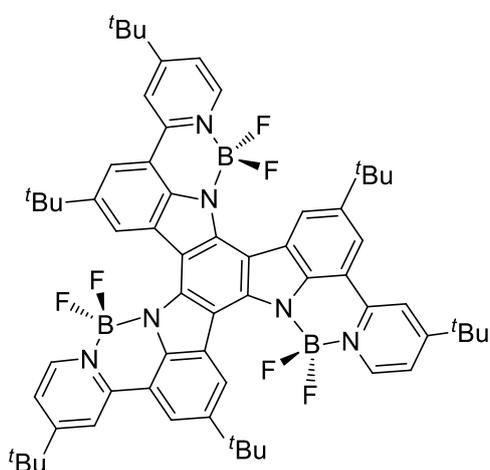
An 8 mL screw capped glass vial was charged with bromobenzene (275 mg, 1.75 mmol), boronic ester (446 mg, 0.5 mmol), Pd₂(dba)₃ (23 mg, 0.025 mmol) and K₂CO₃ (207 mg, 1.5 mmol). Under the protection of argon, THF (4 mL) and water (1 mL) were added to the vial and the mixture was bubbled with argon for 2 minutes, followed by adding *t*Bu₃PHBF₄ (23 mg, 0.079 mmol). The vial was quickly sealed and heated in a heating mantel at 80 °C for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na₂SO₄. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 1:3) to give the product **5** as colourless solid (335 mg, 0.45 mmol, 90%). m.p. 310°C (dec.). ¹H NMR (400 MHz, C₆D₆) δ (ppm) = 9.09 (s, 3H), 8.13 (s, 3H), 7.78 (d, *J* = 7.5 Hz, 6H), 7.74 (s, 3H), 7.40 (t,

$J = 7.5$ Hz, 6H), 7.27 (t, $J = 7.5$ Hz, 3H), 1.54 (s, 27H). ^{13}C NMR (100 MHz, C_6D_6) δ (ppm) = 143.99, 140.30, 135.46, 134.93, 129.57, 128.83, 125.40, 123.89, 121.53, 115.40, 103.28, 34.96, 32.15. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3477, 3062, 2956, 1636, 1482, 1401, 1365, 1326, 1274, 1150, 1073, 1031, 853, 766, 703, 644, 595, 452. HRMS (ESI) (m/z): $[\text{M}+\text{H}]^+$ calcd. for $\text{C}_{54}\text{H}_{52}\text{N}_3$, 742.4161; found, 742.4169.



An 8 mL screw capped glass vial was charged with 2-bromo-4-*tert*-butylpyridine **6** (75 mg, 0.35 mmol), boronic ester (89 mg, 0.1 mmol) and K_2CO_3 (83 mg, 0.6 mmol). Under the protection of argon, toluene (1 mL), ethanol (0.1 mL) and water (0.1 mL) were added to the vial and the mixture was bubbled with argon for 3 minutes, followed by adding $\text{Pd}(\text{PPh}_3)_4$ (12 mg, 0.01 mmol). The vial was quickly sealed and heated in a heating mantel at 100°C for 40 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na_2SO_4 . The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography

(dichloromethane/petroleum ether 1:2) to give the product **7** as light yellow solid (68 mg, 0.075 mmol, 75%). m.p. 320°C (dec.). ^1H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 12.49 (s, 3H), 8.90 (d, $J = 5.2$ Hz, 3H), 8.49 (d, $J = 1.6$ Hz, 3H), 8.23–8.20 (m, 3H), 8.13 (d, $J = 1.6$ Hz, 3H), 7.42 (dd, $J = 5.2$, 1.7 Hz, 3H), 1.71 (s, 27H), 1.50 (s, 27H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 161.29, 158.39, 148.92, 142.94, 136.13, 135.23, 124.55, 120.25, 119.52, 118.10, 117.49, 117.28, 101.53, 35.41, 35.31, 32.38, 30.81. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3435, 2961, 2868, 1637, 1603, 1543, 1481, 1396, 1365, 1324, 1283, 1267, 1248, 1111, 1072, 914, 858, 833, 642, 583, 546. HRMS (ESI) (m/z): $[\text{M}+\text{H}]^+$ calculated. for $\text{C}_{63}\text{H}_{73}\text{N}_6$, 913.5897; found, 913.5897.



A 38 mL screw capped glass vial was charged with compound **7** (31 mg, 0.034 mmol). Under the protection of argon, dry toluene (2.5 mL), dry Et_3N (0.2 mL) and $\text{BF}_3\cdot\text{Et}_2\text{O}$ (0.2 mL) were added to the vial. The vial was quickly sealed and heated in an oil bath at 120°C for 40 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na_2SO_4 . The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 2:1) to give the product **8** as orange solid (7 mg, 0.007 mmol, 20%). m.p. $>400^\circ\text{C}$ (dec.); ^1H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 9.82 (s, 3H), 8.95 (d, $J = 6.5$ Hz, 3H), 8.43 (d, $J = 1.9$ Hz, 3H), 8.18 (s, 3H), 7.66 (dd, $J = 6.6$, 1.9 Hz, 3H), 1.69 (s, 27H), 1.55 (s, 27H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ (ppm) = 166.84, 150.64, 141.95 (d, $J = 5.1$ Hz), 140.15, 137.88, 128.38, 125.55, 120.42, 116.21 (d, $J = 7.3$ Hz), 110.19, 108.08, 36.32, 35.78, 32.29, 30.30. ^{11}B NMR (128 MHz, CD_2Cl_2) δ (ppm) = 3.53. ^{19}F NMR (377 MHz, CD_2Cl_2) δ (ppm) = -123.90. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2961, 1629, 1393, 1272, 1059. HRMS (ESI) (m/z): $[\text{M}+\text{H}]^+$ calculated. for $\text{C}_{63}\text{H}_{70}\text{B}_3\text{F}_6\text{N}_6$, 1057.5845; found, 1057.5847.

3. NMR spectra

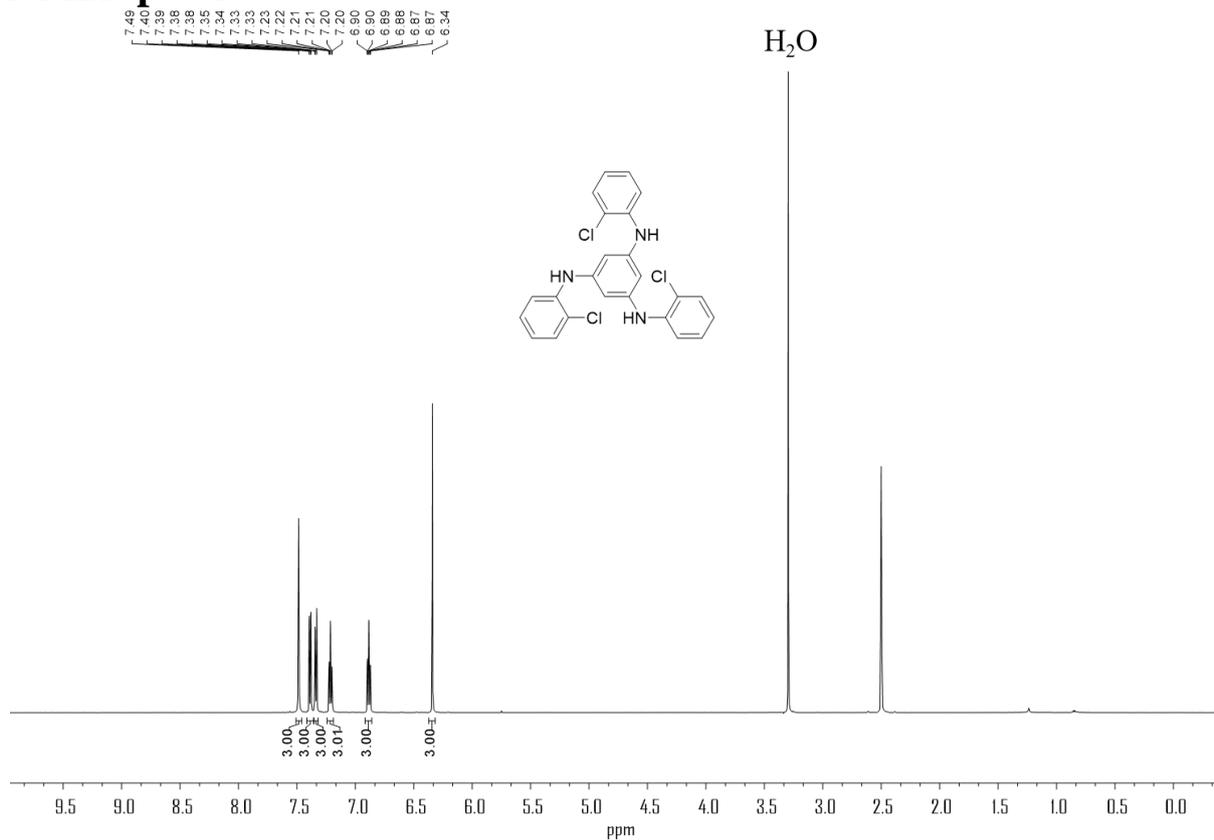


Figure S1. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound 2aCl.

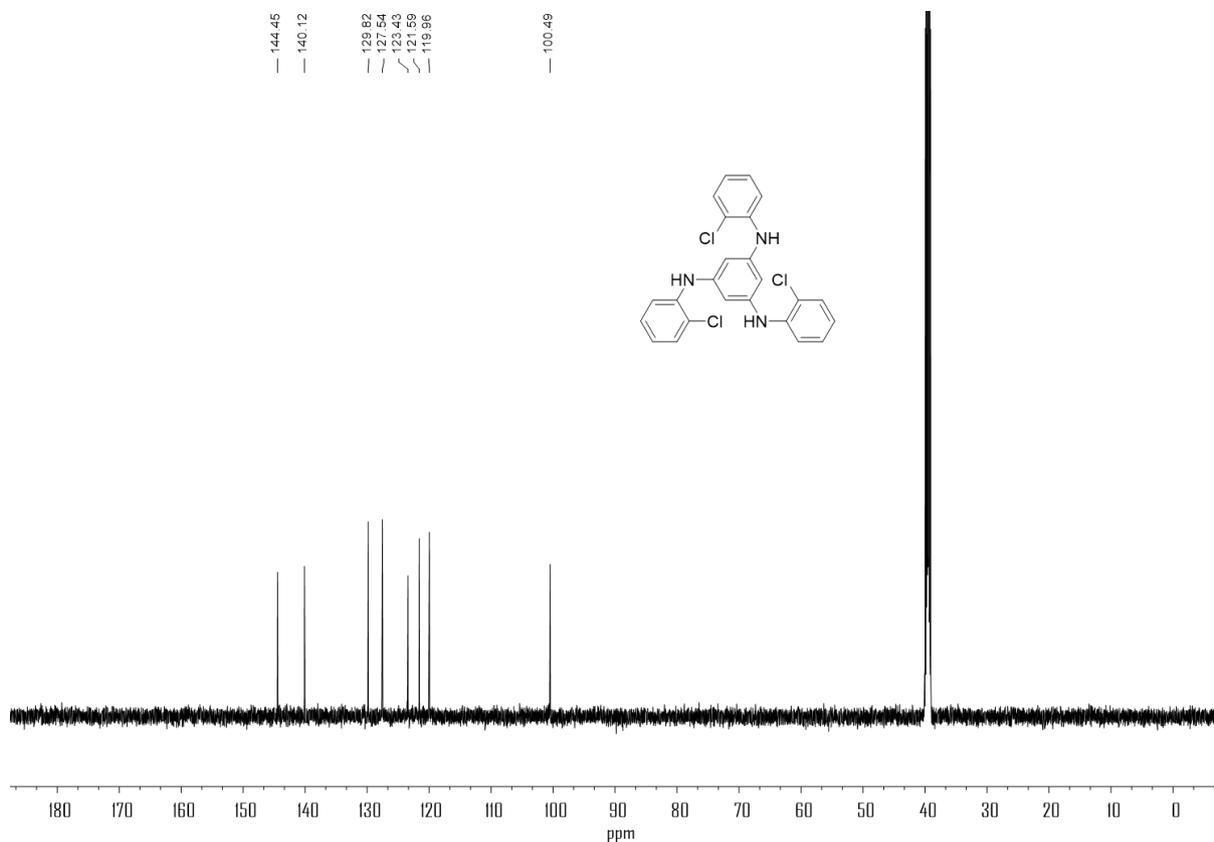


Figure S2. ^{13}C NMR spectrum (DMSO- d_6 , 100 MHz) of compound 2aCl.

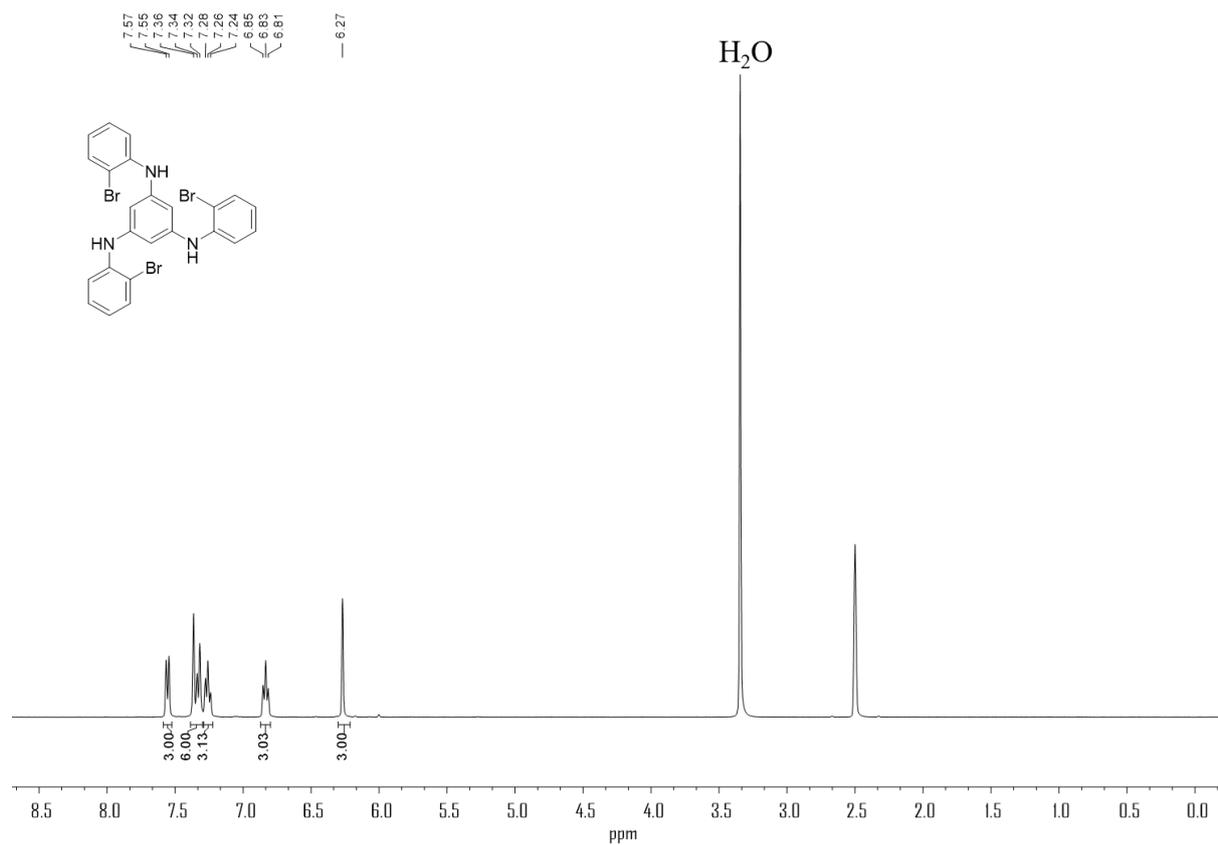


Figure S3. ¹H NMR spectrum (DMSO-*d*₆, 400 MHz) of compound **2aBr**.

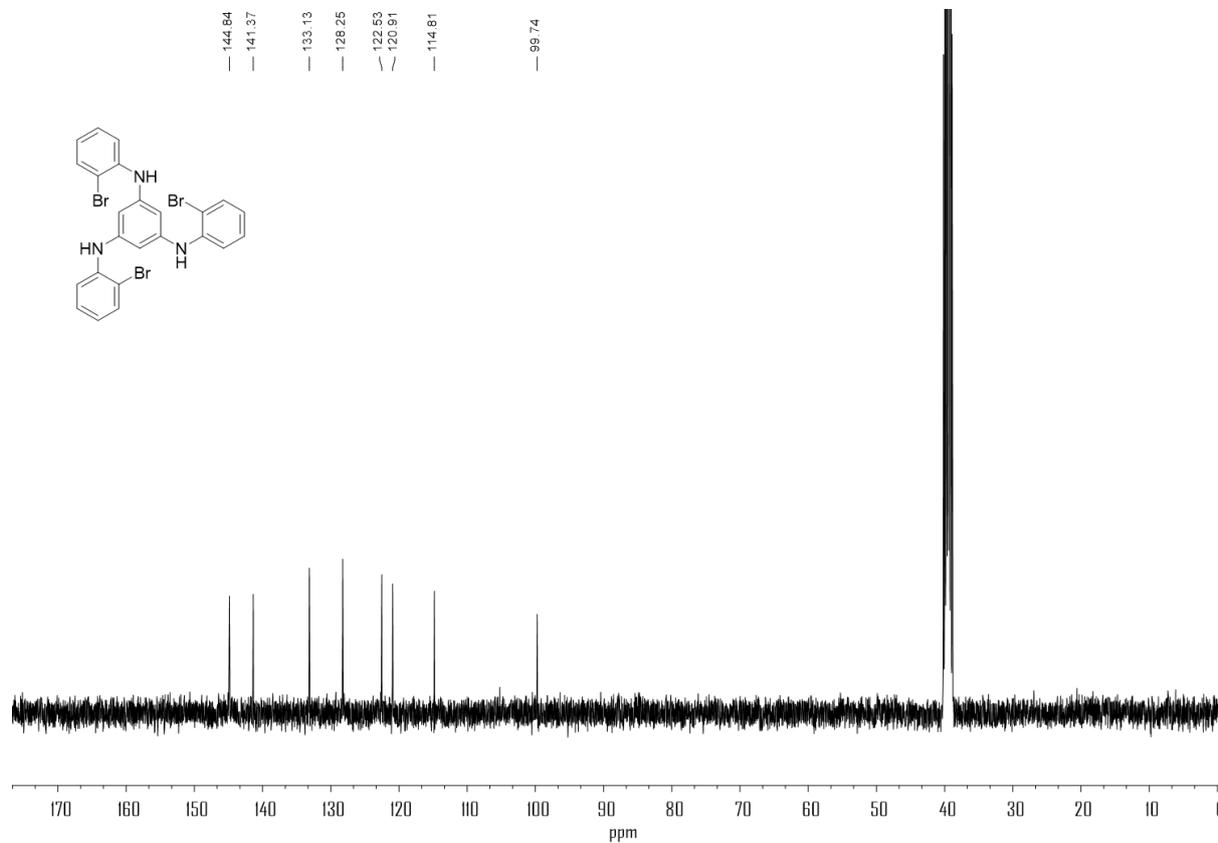


Figure S4. ¹³C NMR spectrum (DMSO-*d*₆, 100 MHz) of compound **2aBr**.

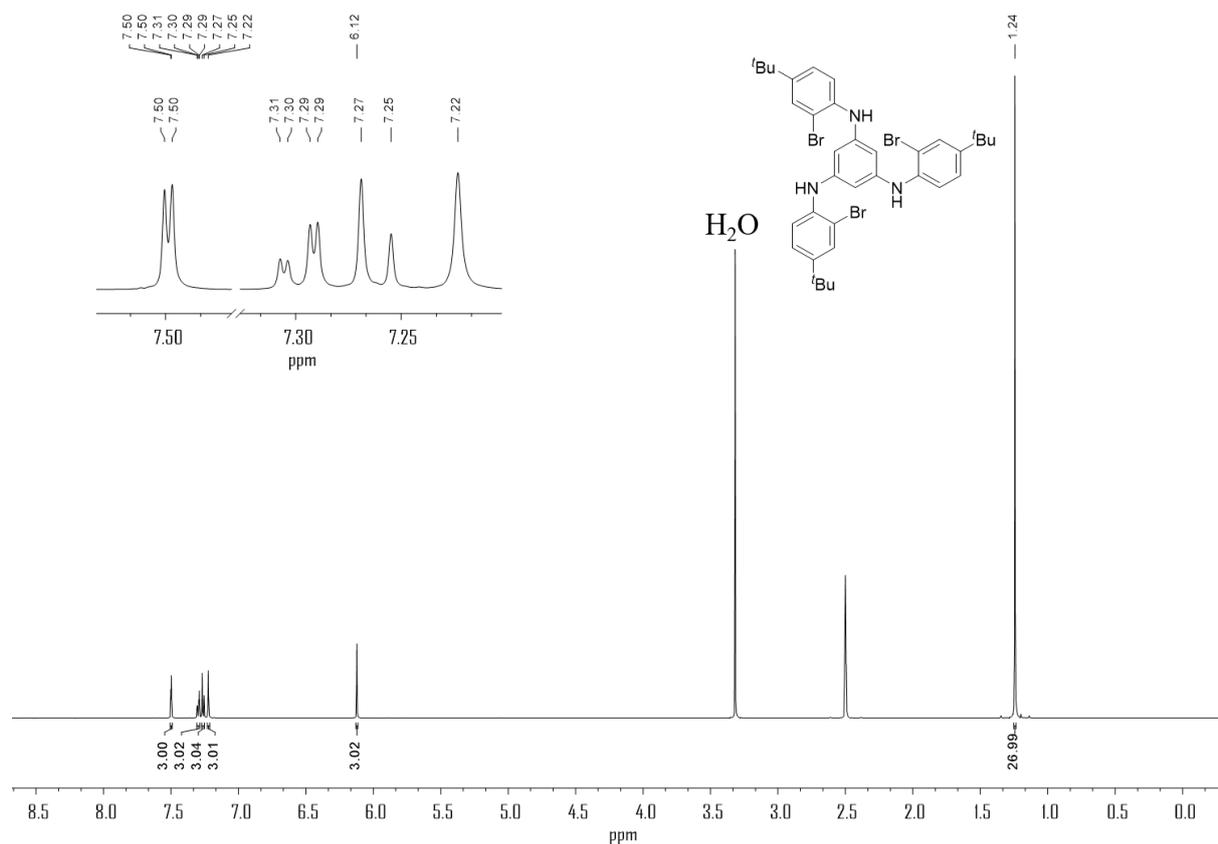


Figure S5. ¹H NMR spectrum (DMSO-*d*₆, 600 MHz) of compound **2b**.

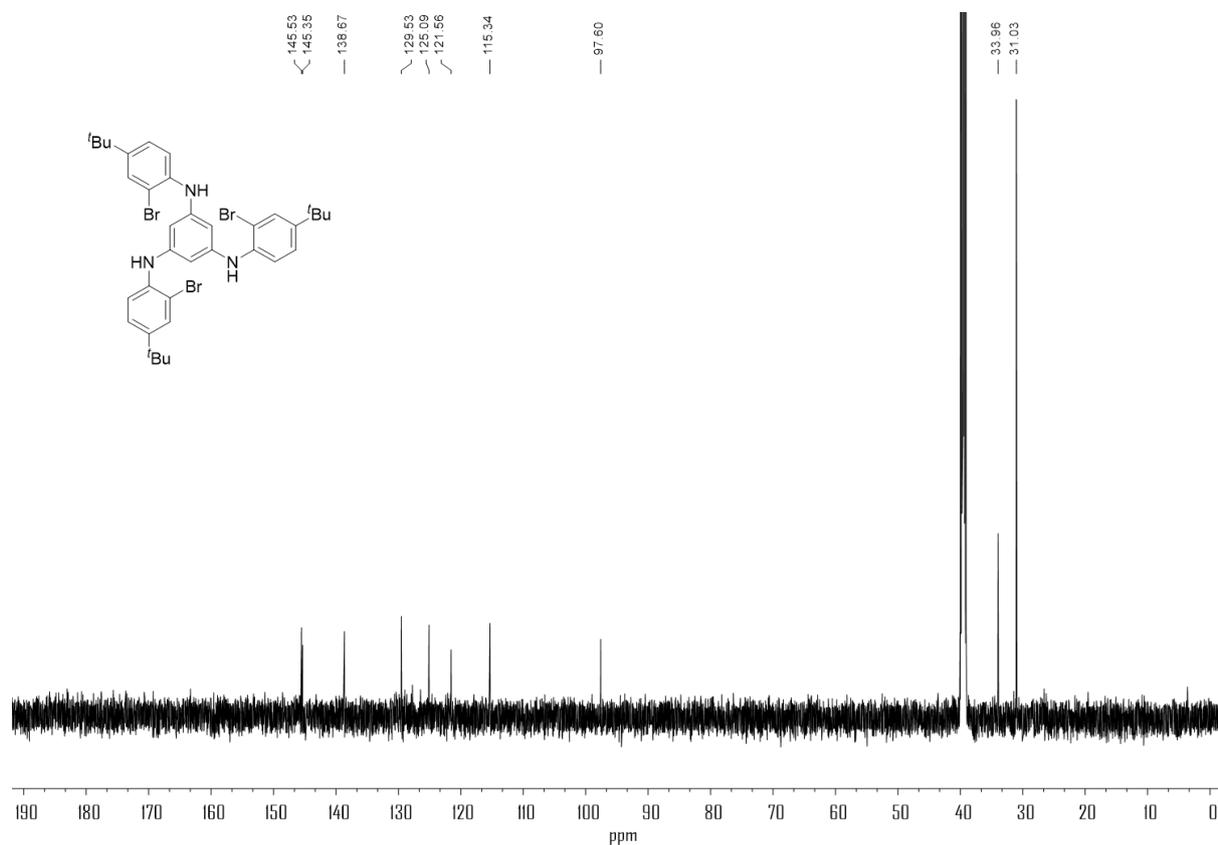


Figure S6. ¹³C NMR spectrum (DMSO-*d*₆, 150 MHz) of compound **2b**.

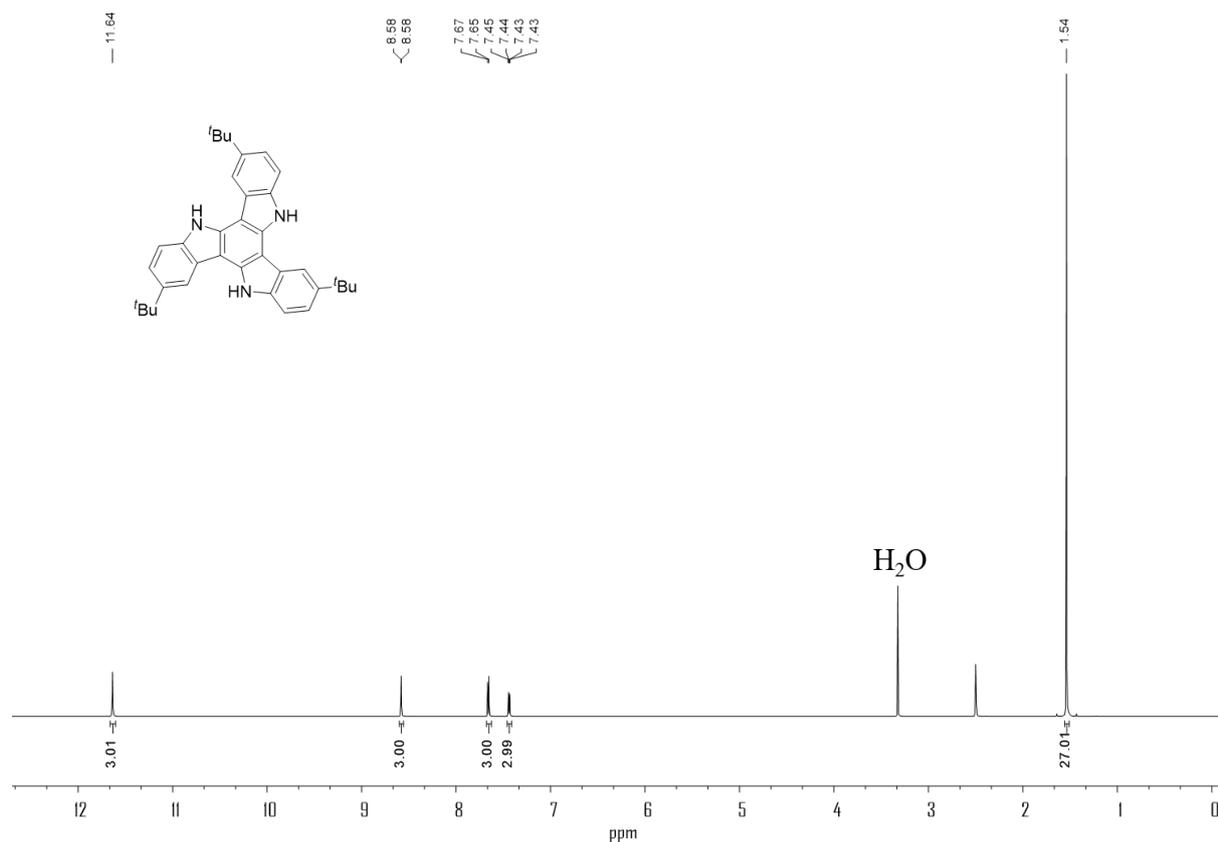


Figure S7. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of compound **3b**.

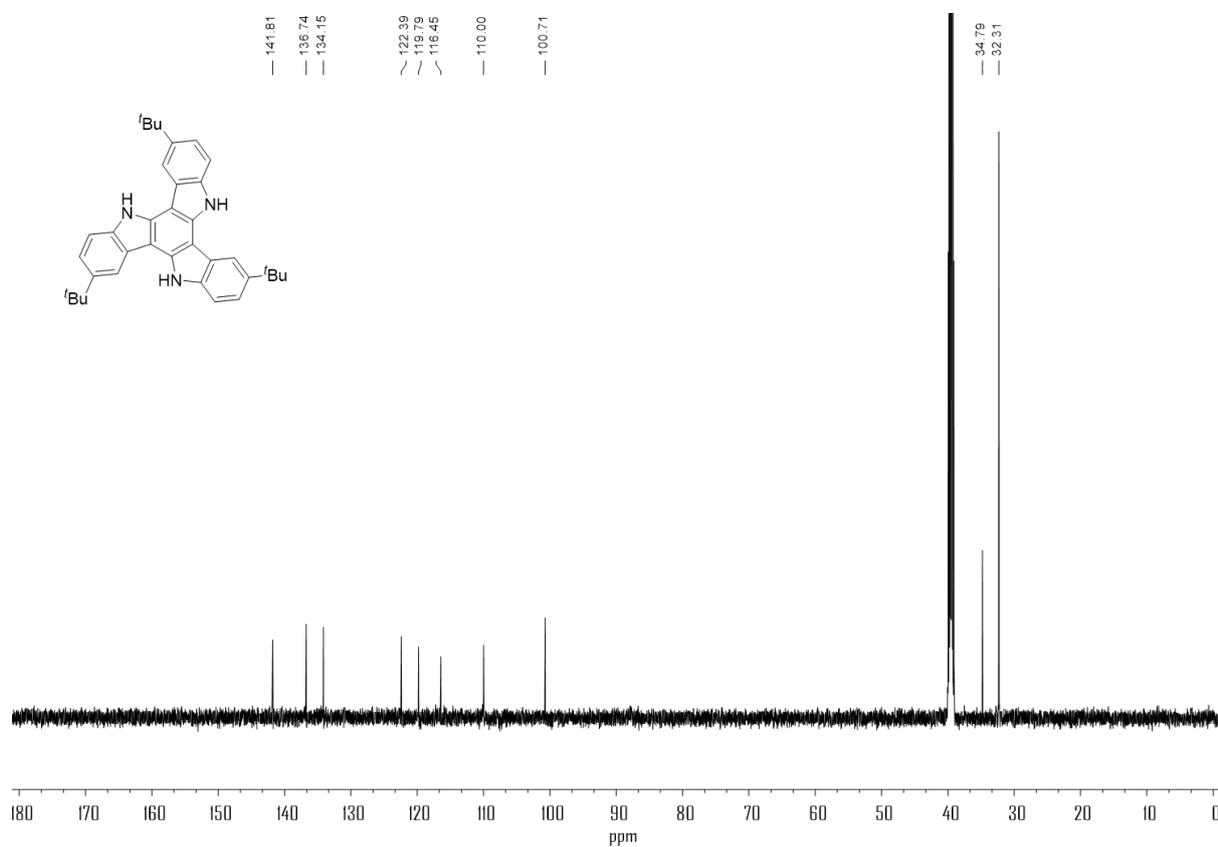


Figure S8. ^{13}C NMR spectrum (DMSO- d_6 , 150 MHz) of compound **3b**.

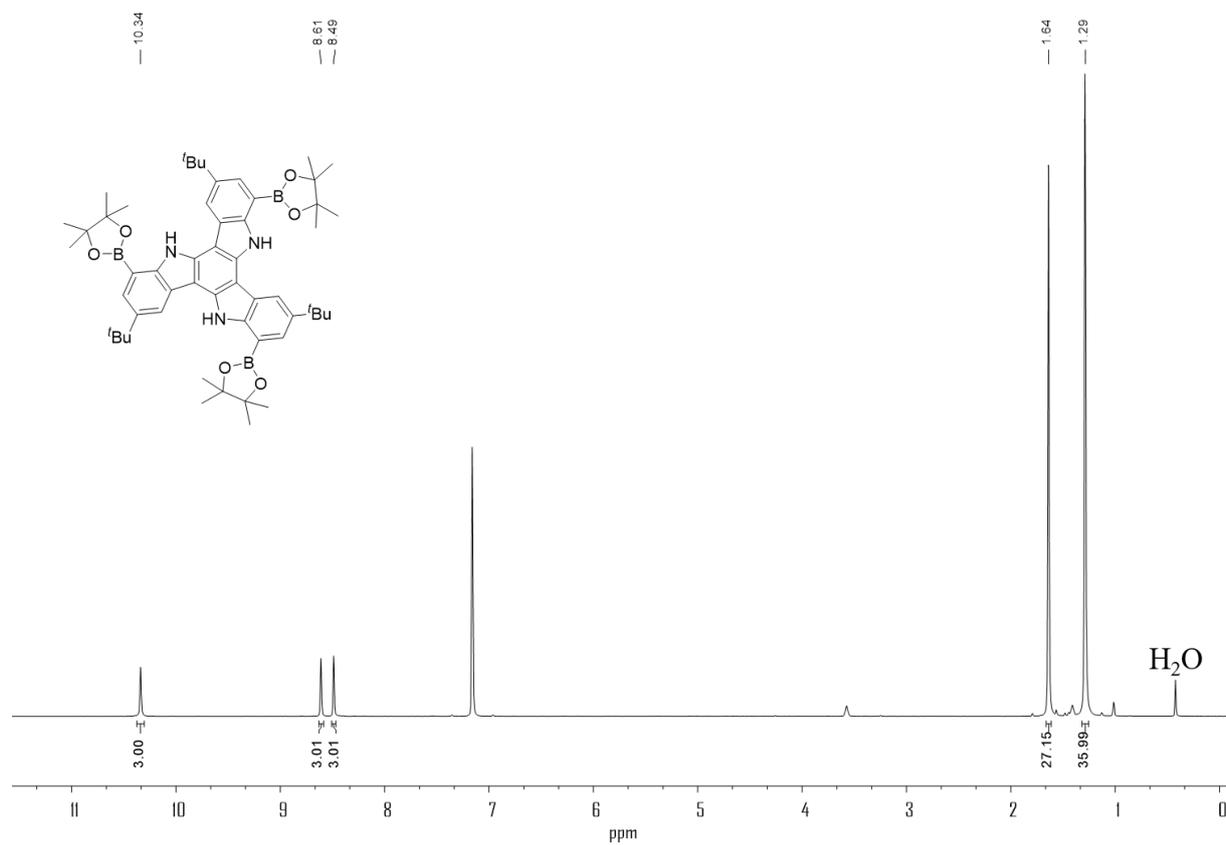


Figure S9. ¹H NMR spectrum (C₆D₆, 400 MHz) of compound 4.

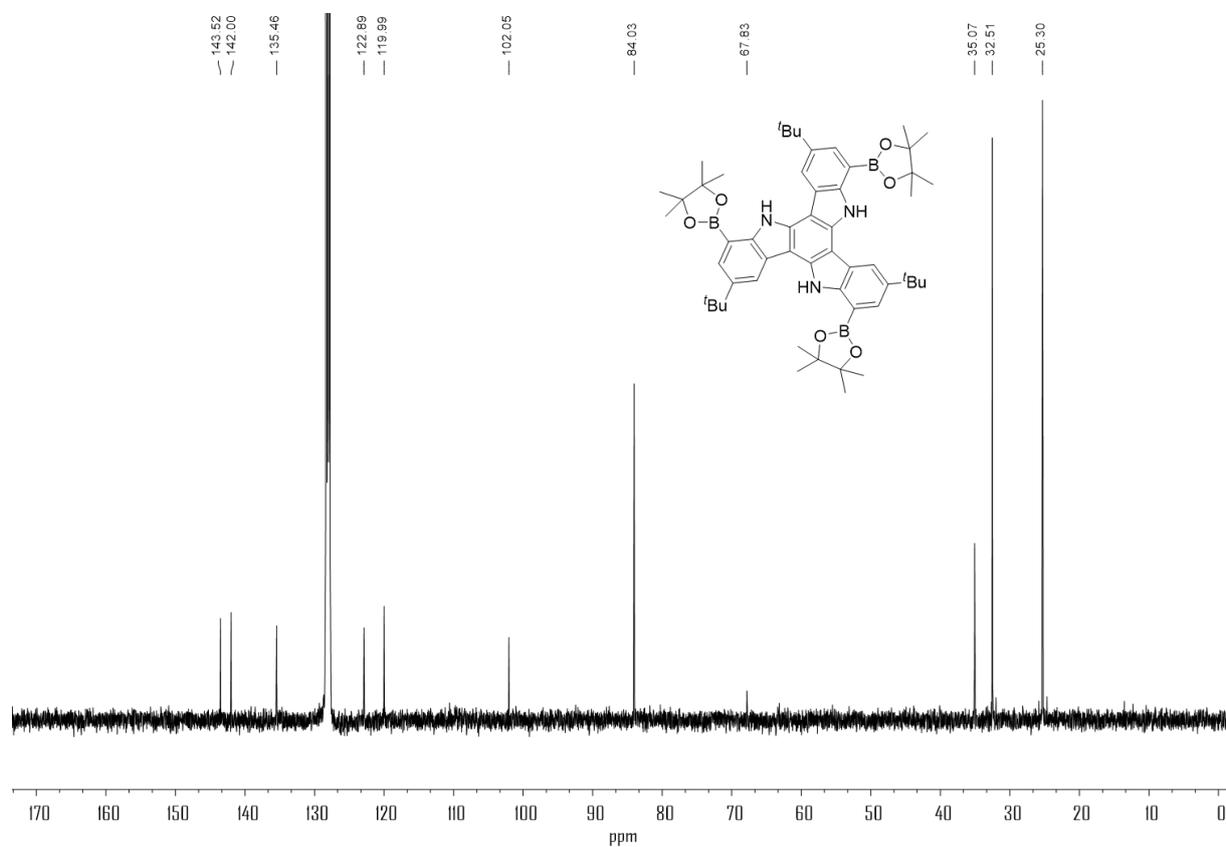


Figure S10. ¹³C NMR spectrum (C₆D₆, 100 MHz) of compound 4.

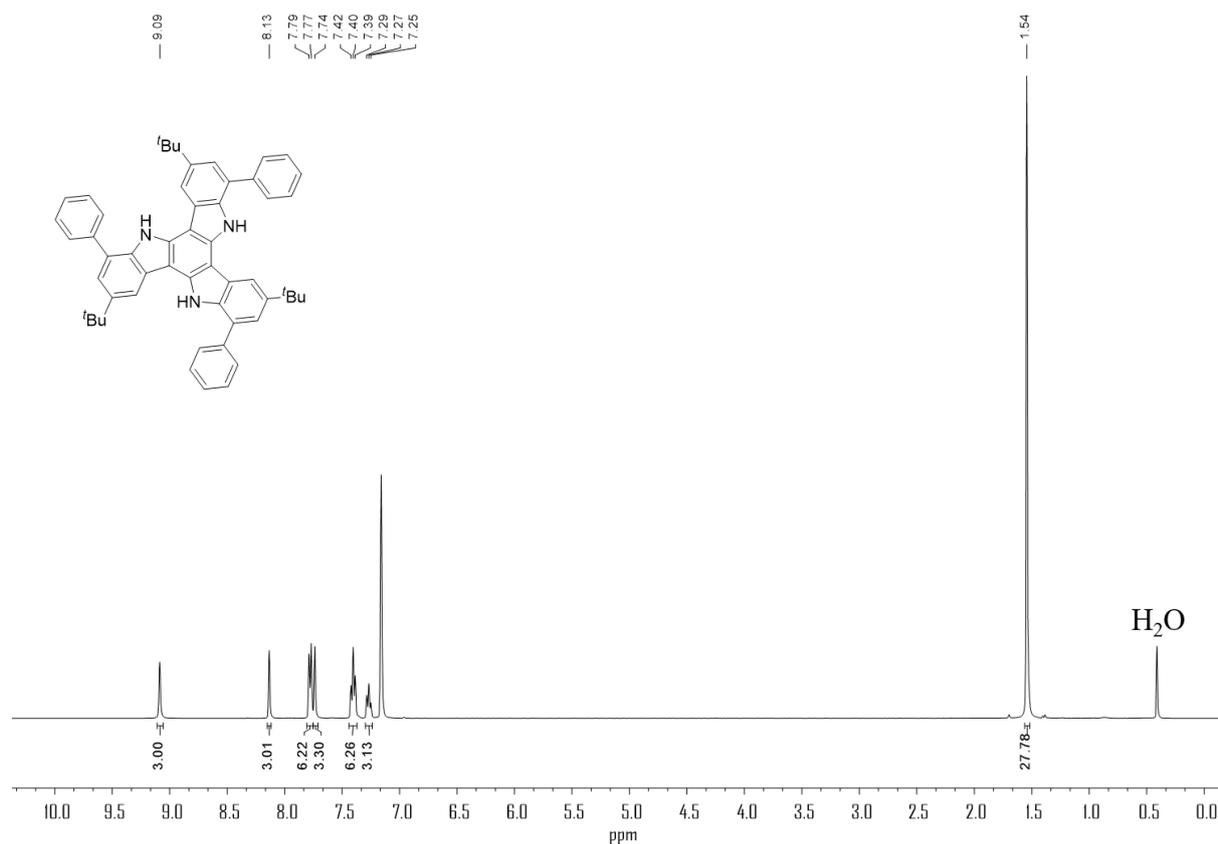


Figure S11. ^1H NMR spectrum (C_6D_6 , 400 MHz) of compound 5.

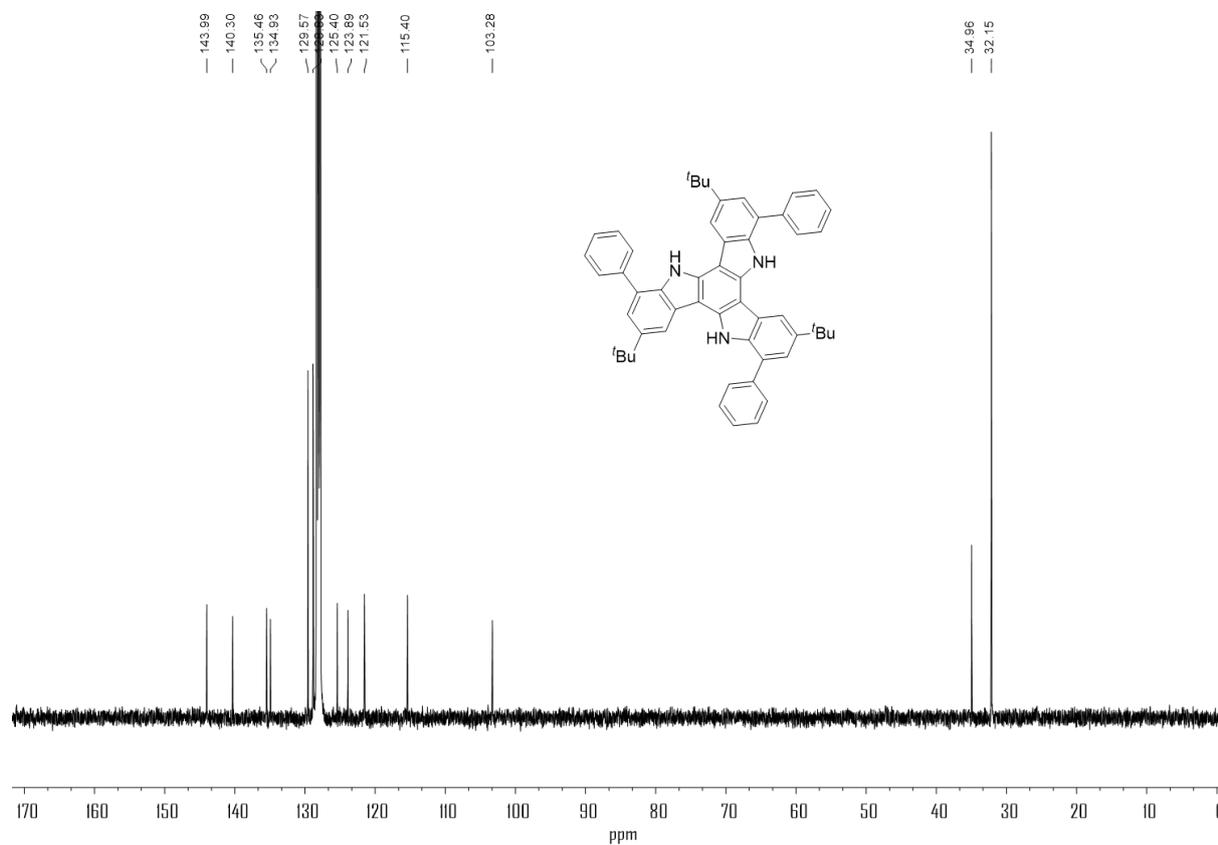


Figure S12. ^{13}C NMR spectrum (C_6D_6 , 100 MHz) of compound 5.

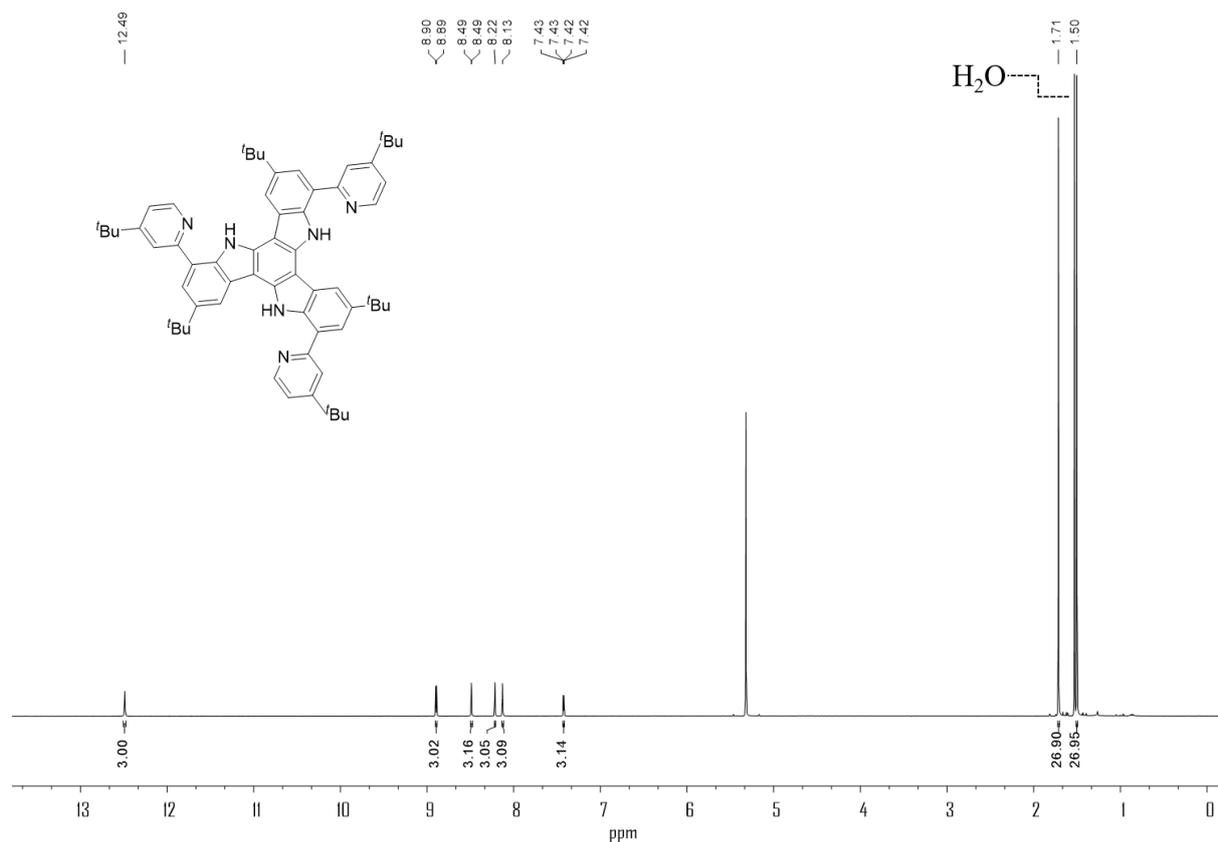


Figure S13. ¹H NMR spectrum (CD₂Cl₂, 600 MHz) of compound 7.

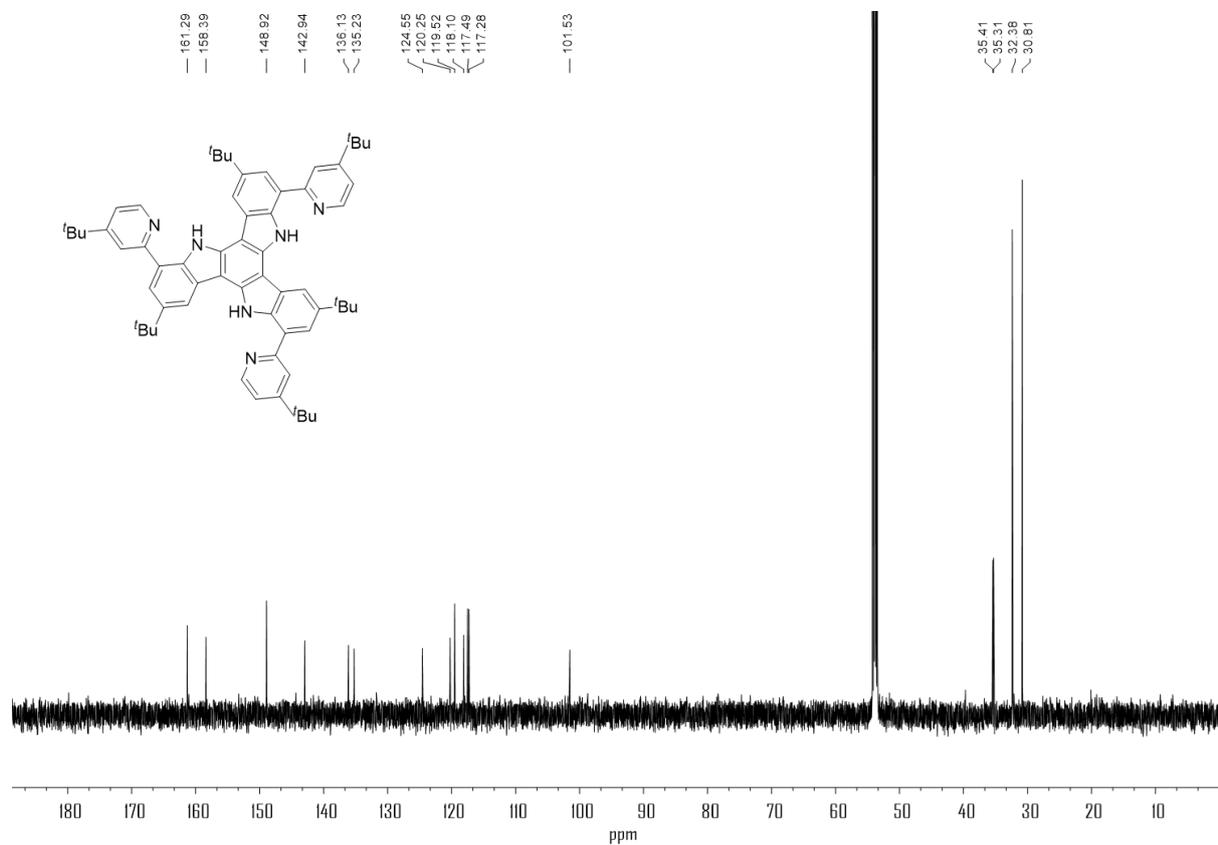


Figure S14. ¹³C NMR spectrum (CD₂Cl₂, 150 MHz) of compound 7.

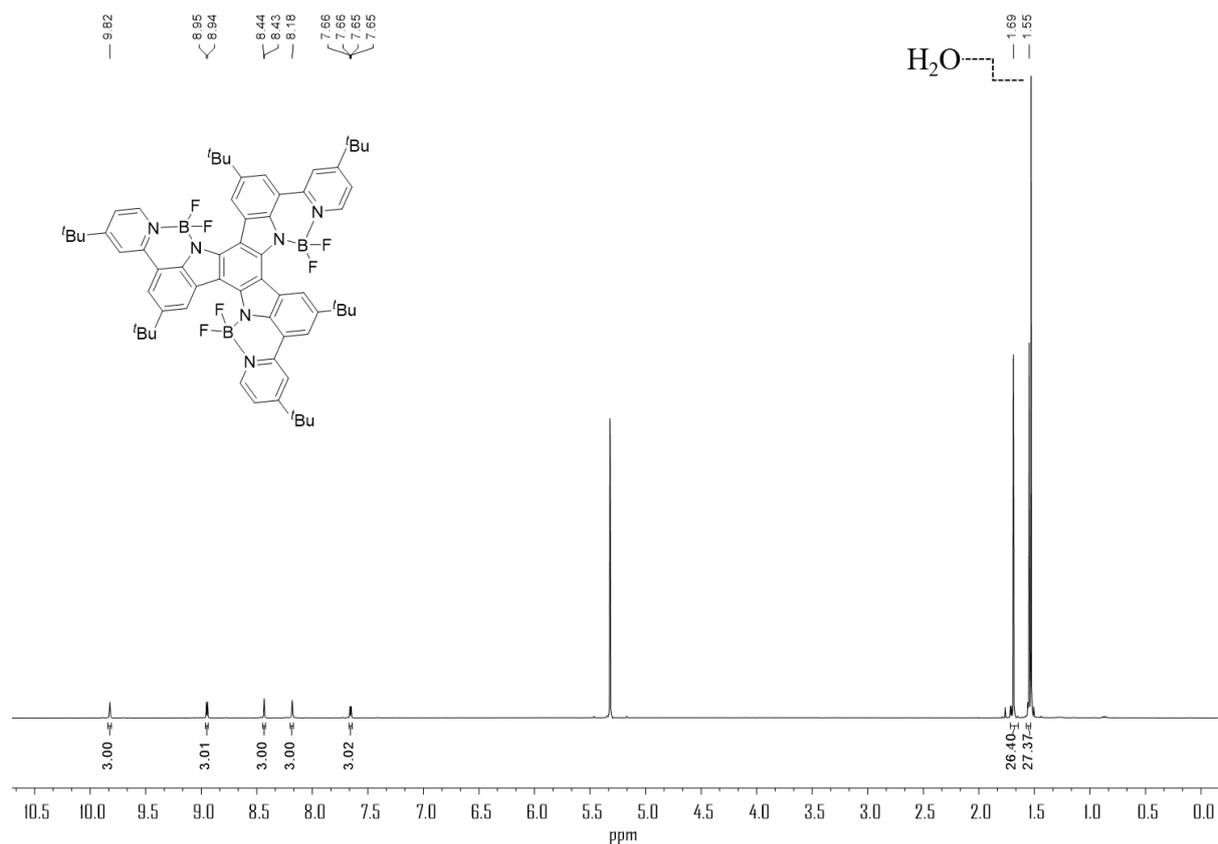


Figure S15. ¹H NMR spectrum (CD₂Cl₂, 600 MHz) of compound 8.

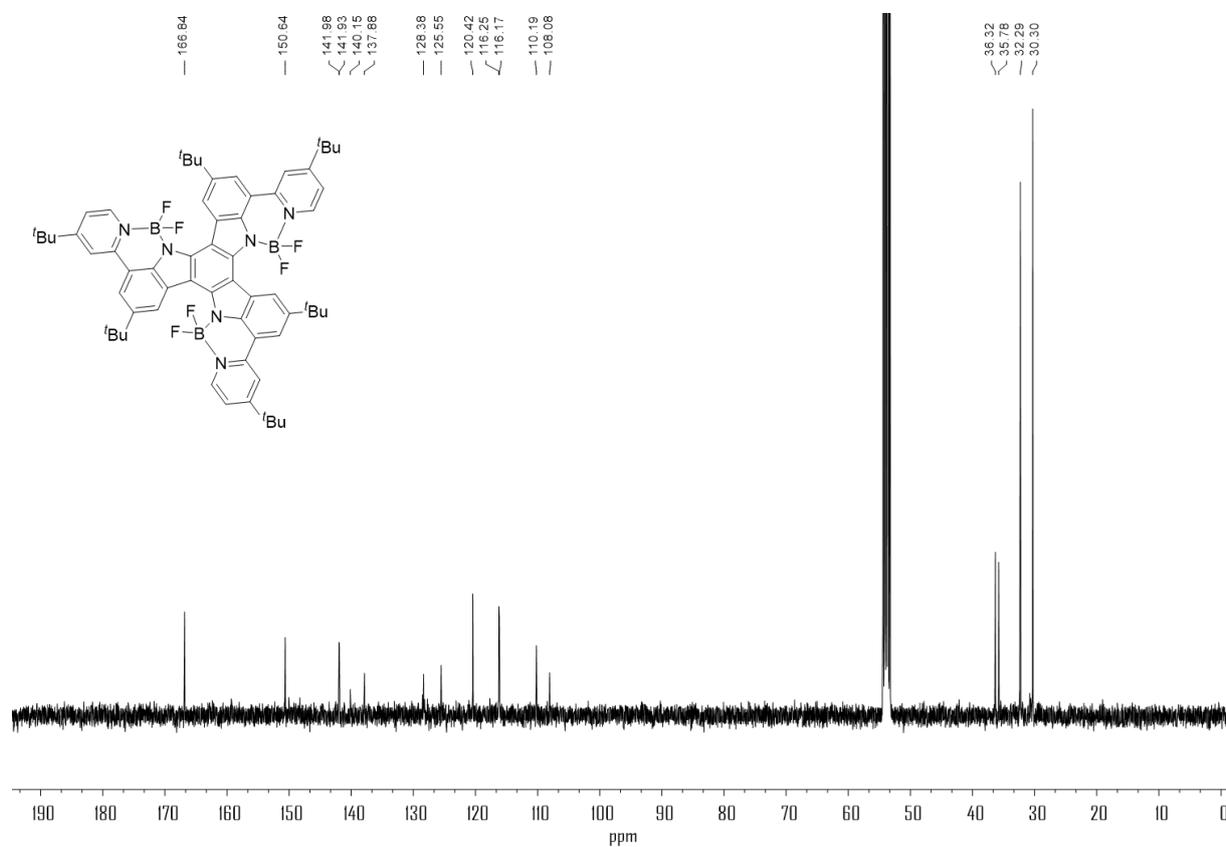


Figure S16. ¹³C NMR spectrum (CD₂Cl₂, 150 MHz) of compound 8.

4. X-ray crystallographic structure determination

Table S1. Crystal data and structure refinement for compound **4**.

Empirical formula	C ₅₇ H ₇₂ B ₃ N ₃ O ₆ S ₆
Formula weight	1119.96
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.2571(3)
b/Å	23.3294(7)
c/Å	23.0523(6)
α/°	90
β/°	96.593(3)
γ/°	90
Volume/Å ³	6014.0(3)
Z	4
ρ _{calc} /cm ³	1.237
μ/mm ⁻¹	2.491
F(000)	2376.0
Crystal size/mm ³	0.15 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.408 to 143.268
Index ranges	-13 ≤ h ≤ 10, -28 ≤ k ≤ 27, -28 ≤ l ≤ 28
Reflections collected	31856
Independent reflections	11485 [R _{int} = 0.0351, R _{sigma} = 0.0397]
Data/restraints/parameters	11485/216/790
Goodness-of-fit on F ²	1.060
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1059, wR ₂ = 0.3013
Final R indexes [all data]	R ₁ = 0.1199, wR ₂ = 0.3094
Largest diff. peak/hole / e Å ⁻³	1.00/-0.85

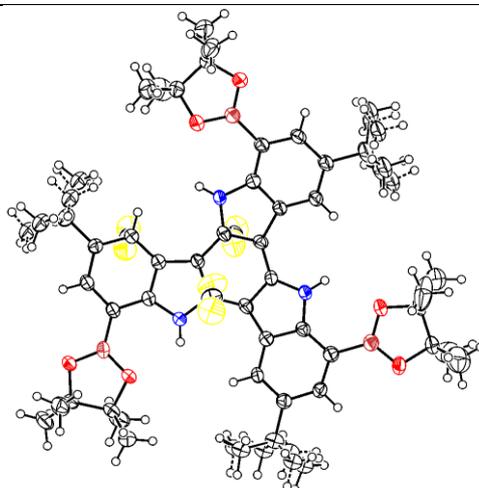


Figure S17. Crystal structure of **4** with an ellipsoid contour at the 50% probability level.

5. Optical characterization

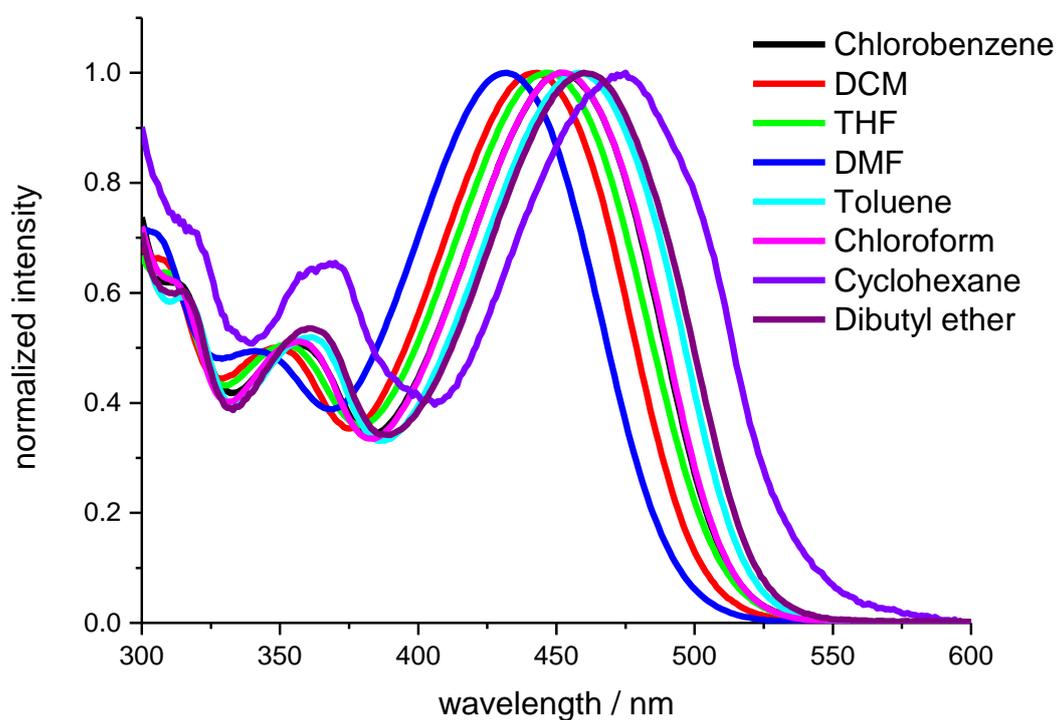


Figure S18. UV/vis absorption spectra of **8** in different solvents.

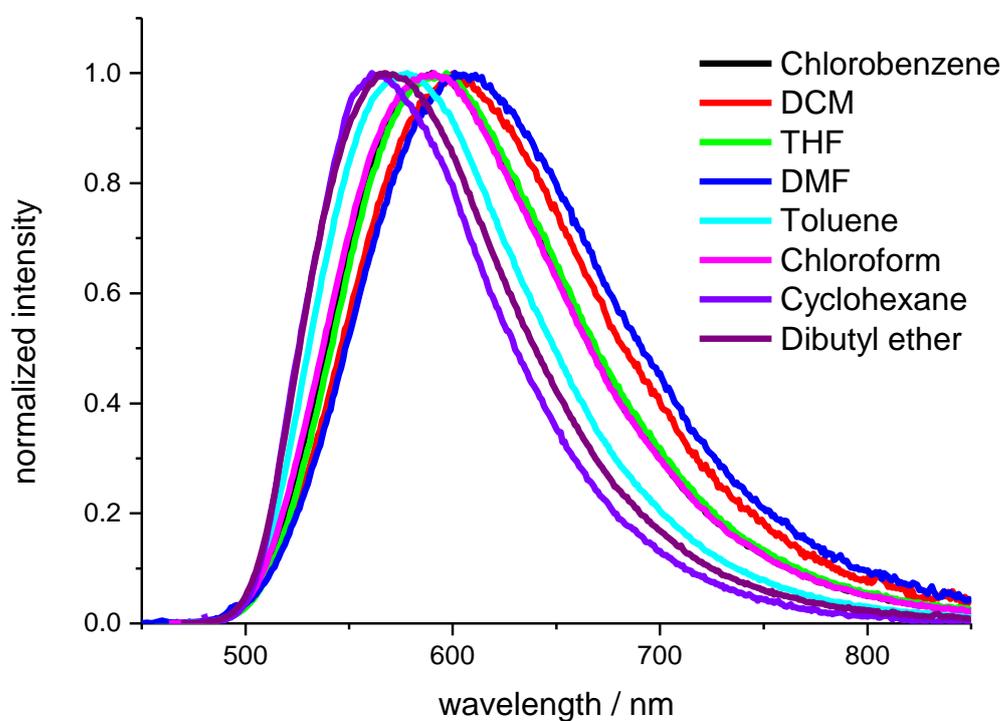


Figure S19. Fluorescence emission spectra of **8** in different solvents.

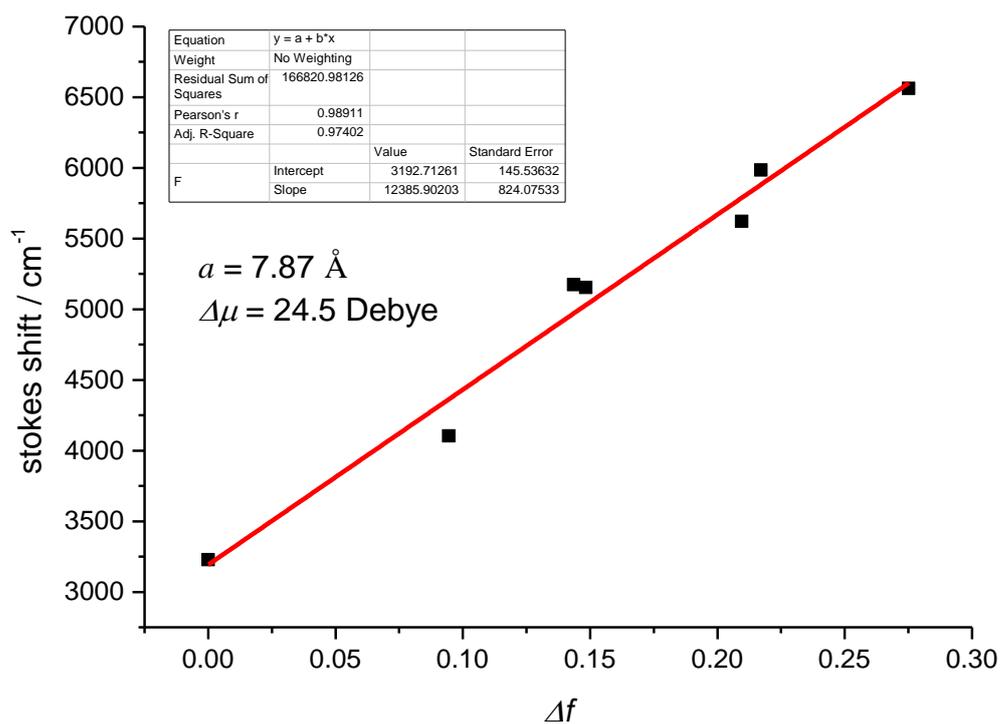


Figure S20. Lippert–Mataga plot, Onsager cavity radius and the calculated difference of dipole moment of the ground and excited states of **8**.

6. CV and DPV curves

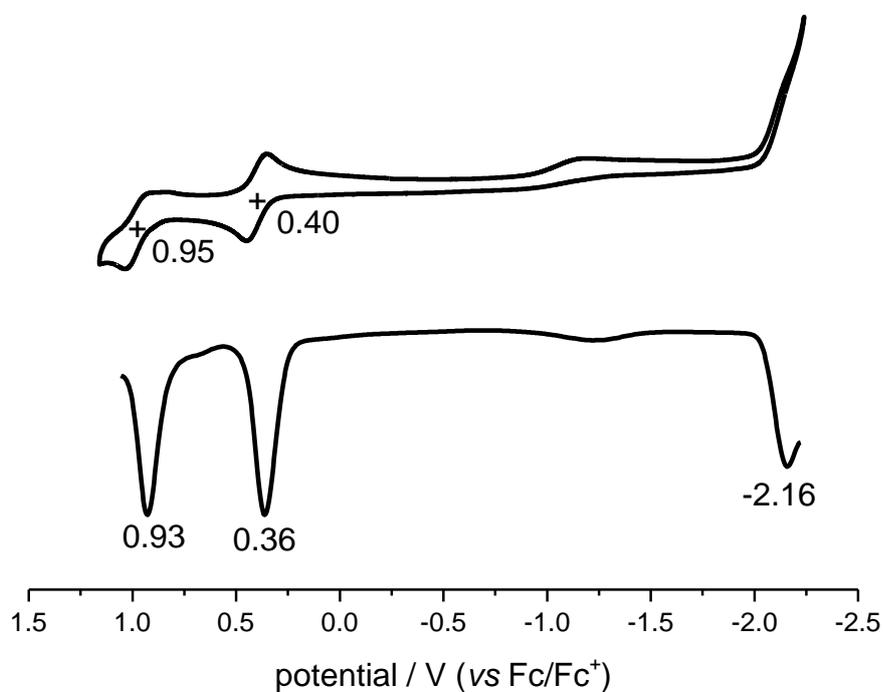


Figure S21. CV and DPV curves of **8** measured in dichloromethane at room temperature.

7. The theoretical calculations

All the theoretical calculations were carried out using a *Gaussian 16* software.^[S4] All the calculations were based on the optimized geometries at B3LYP/6-31G(d,p) level of theory. The frontier molecular orbitals are calculated at the B3LYP/6-311+G(d,p) level of theory. The calculations of excited state properties were performed using time-depended DFT methods at B3LYP /6-311+G(d,p) level of theory in the solvent dichloromethane.

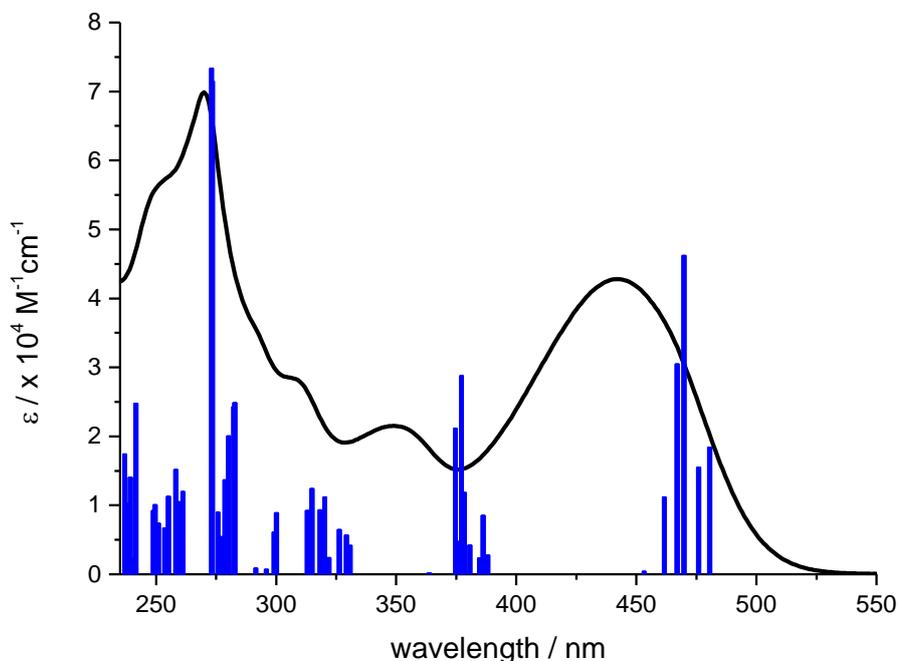


Figure S22. UV/Vis absorption spectrum of compound **8** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

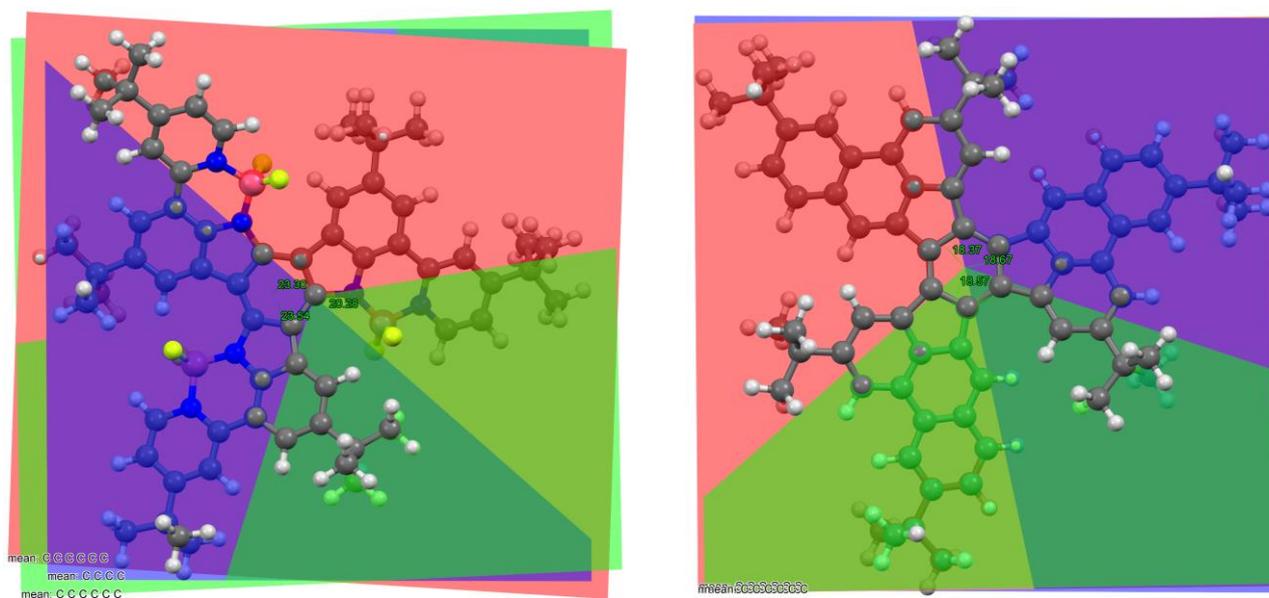


Figure S23. Comparison the dihedral angles of peripheral benzene rings of triazatruxene **8** with its all-carbon congener.

Table S2. TD-DFT calculated first-ten electron transitions of compound **8** in dichloromethane at B3LYP / 6-311+G(d,p) level.

Excited State 1:	Singlet-A	2.5656 eV	483.25 nm	f=0.1355	<S**2>=0.000
278 -> 280	2%				
278 -> 281	2%				
279 -> 280	87%				
279 -> 281	6%				
Excited State 2:	Singlet-A	2.5847 eV	479.69 nm	f=0.1194	<S**2>=0.000
278 -> 280	7%				
279 -> 280	7%				
279 -> 281	81%				
279 -> 282	3%				
Excited State 3:	Singlet-A	2.6237 eV	472.56 nm	f=0.3614	<S**2>=0.000
278 -> 280	67%				
278 -> 282	3%				
279 -> 281	3%				
279 -> 282	24%				
Excited State 4:	Singlet-A	2.6404 eV	469.56 nm	f=0.2219	<S**2>=0.000
278 -> 281	75%				
278 -> 282	6%				
279 -> 282	14%				
Excited State 5:	Singlet-A	2.6725 eV	463.93 nm	f=0.0970	<S**2>=0.000
278 -> 280	20%				
278 -> 281	14%				
279 -> 281	6%				
279 -> 282	57%				
Excited State 6:	Singlet-A	2.7205 eV	455.74 nm	f=0.0049	<S**2>=0.000
278 -> 281	6%				
278 -> 282	88%				
279 -> 280	2%				
Excited State 7:	Singlet-A	3.1373 eV	395.20 nm	f=0.0235	<S**2>=0.000
278 -> 283	9%				
278 -> 285	4%				
279 -> 283	16%				
279 -> 284	61%				

279 -> 285	6%
Excited State 8:	Singlet-A 3.1508 eV 393.51 nm f=0.0643 <S**2>=0.000
278 -> 283	4%
279 -> 283	54%
279 -> 284	9%
279 -> 285	31%
Excited State 9:	Singlet-A 3.1651 eV 391.72 nm f=0.0255 <S**2>=0.000
278 -> 284	6%
278 -> 285	7%
279 -> 283	16%
279 -> 284	13%
279 -> 285	54%
Excited State 10:	Singlet-A 3.1994 eV 387.52 nm f=0.0333 <S**2>=0.000
278 -> 283	83%
279 -> 283	9%
279 -> 284	4%

279 **HOMO**, 280 **LUMO**

Cartesian coordinates for theoretically optimized structures

Ground state **8** opt B3LYP/6-31G(d,p) Imaginary Frequency 0

C	1.34788900	-0.23364000	-0.33204500
C	0.48765800	-1.34611600	-0.07693900
C	-0.91873700	-1.17748600	0.02629300
C	-1.43503100	0.14921800	0.10645800
C	-0.56897600	1.27467800	0.13119300
C	0.80921700	1.07603100	-0.18900700
C	-0.72587400	2.68938300	0.42154500
C	0.53866000	3.27322700	0.17130900
N	1.45891200	2.32605500	-0.20441000
C	-2.07199700	-2.06343300	-0.02482300
C	-3.20892900	-1.21653400	0.02062200
N	-2.84017900	0.10142100	0.10532000
C	2.67077000	-0.79570400	-0.57107500
C	2.55145100	-2.18278300	-0.30551600
N	1.25564200	-2.52256500	-0.01504300

C	3.90060700	-0.32697400	-1.02519400
C	5.02284400	-1.17274600	-1.13432500
C	4.89641600	-2.50626500	-0.75308700
C	3.66579700	-3.04205900	-0.31855200
C	-2.28106200	-3.43098200	-0.17613600
C	-3.57718700	-3.98154900	-0.22287100
C	-4.67132200	-3.12131900	-0.18435700
C	-4.51761600	-1.72147000	-0.09427000
C	-1.73701700	3.49397800	0.95438600
C	-1.54560600	4.87221000	1.15187000
C	-0.30311700	5.42659900	0.83512900
C	0.76587900	4.65168800	0.35156700
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C	-5.18264900	-5.96522200	-0.44395000
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C	-2.93461300	-6.04615000	-1.53419200
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C	-4.00067800	5.03204700	1.85011800
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C	6.85733900	0.44108700	-0.55351300
C	6.13815000	0.17699200	-2.95949000
C	2.07086000	5.20524100	0.05060100
C	3.52714000	-4.37947500	0.22096000
C	-5.62467500	-0.79697900	-0.23551900
C	2.38784900	6.57403200	0.14270600
C	3.65096800	7.06919600	-0.15909000
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C	4.27498500	4.79880000	-0.65671200
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H	-2.08865700	5.42381900	3.81508000
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