

Quinoxaline-Based Dual Donor, Dual Acceptor Organic Dyes for Dye-Sensitized Solar Cells

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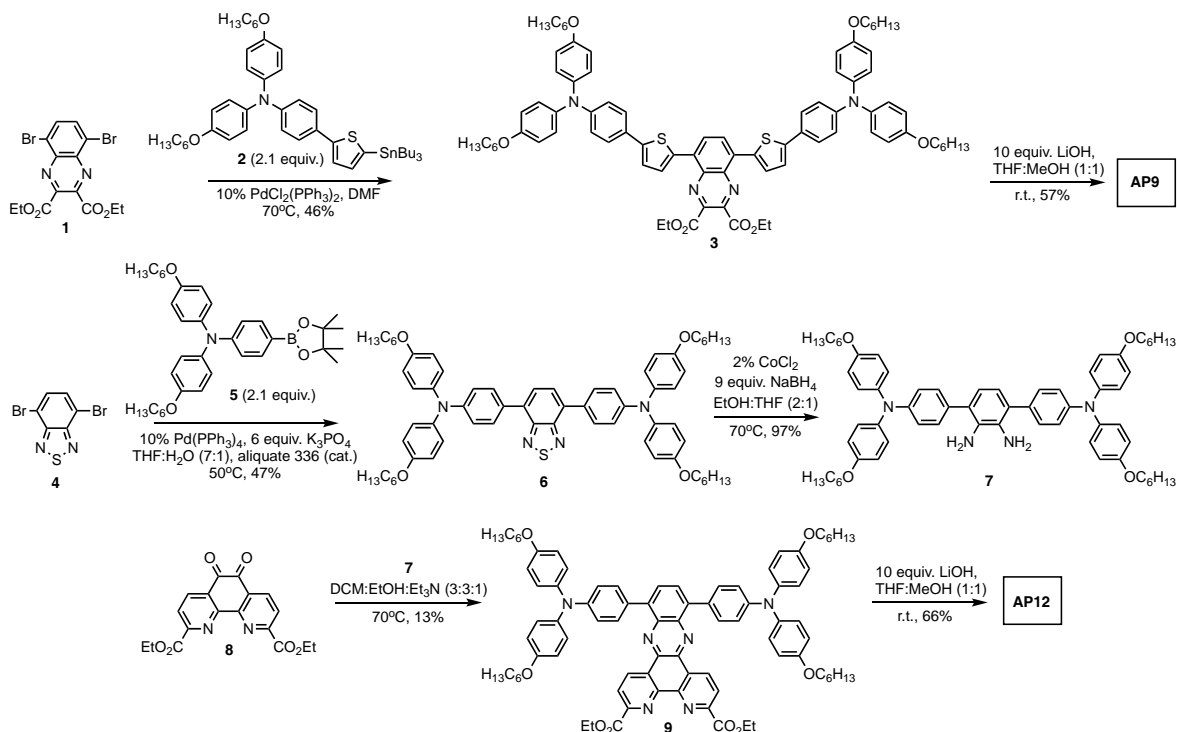
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Synthetic Details for AP9 and AP12

General Synthetic and Characterization Information: Reagents were purchased and used as received without further purification. Thin-layer chromatography (TLC) was conducted with Sorbtech silica XHL TLC plates and visualized with UV light. Flash column chromatography was performed with Silicycle ultrapure silica gel P60, 40-63 μm (230-400 mesh). ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance-500 (500 MHz) or a Bruker Avance-300 (300 MHz) spectrometer. Data reported as: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, br = broad, ap = apparent, dd = doublet of doublets, coupling constant(s) in Hz, integration. UV-Vis Spectra were measured with a Cary 5000 UV-Vis spectrometer. All samples were measured in a 1 cm cell at room temperature with dichloromethane as a solvent. Cyclic voltammetry was measured with a CH Instruments electrochemical analyzer. Voltammetry measurements were carried out in CH_2Cl_2 using 0.1 M Bu_4NPF_6 electrolyte in a three-electrode system under N_2 using a glassy carbon working electrode (or FTO/ TiO_2 /dye glass plate for film studies), platinum reference electrode, and platinum counter electrode with ferrocene as an internal standard. Values are reported versus NHE.



Synthesis of diethyl 5,8-bis(5-(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)thiophen-2-yl)quinoxaline-2,3-dicarboxylate (3): To a flame dry flask was added diethyl 5,8-dibromo-4a,8a-dihydroquinoxaline-2,3-dicarboxylate (**1**) (50 mg, 0.11 mmol, 1.0 equiv.), 4-(hexyloxy)-*N*-(4-(hexyloxy)phenyl)-*N*-(4-(5-(tributylstannyl)thiophen-2-yl)phenyl)aniline (**2**) (197 mg, 0.24 mmol, 2.1 equiv.), and *N,N*-dimethylformamide (0.6 mL, 0.2 M). The mixture was sparged with N_2 for 30 minutes, then $\text{PdCl}_2(\text{PPh}_3)_2$ (8 mg, 10 mol%) was added. The flask was sealed under N_2 with a plastic cap and electrical tape and stirred at 70 $^\circ\text{C}$ for 4 hours. The reaction mixture was quenched with water, and extracted with diethyl ether. The organic layer was separated and solvent was evaporated under reduced pressure. The crude mixture purified by silica gel column chromatography with 6% ethyl acetate:hexanes as eluent. The final product was concentrated to a green solid (67 mg, 0.050 mmol, 46% yield). ^1H NMR (500 MHz, CDCl_3): δ 8.22 (s, 2H), 7.93 (d, J = 3.9 Hz, 2H), 7.49 (d, J = 8.7 Hz, 4H), 7.26 (ap s, 2H), 7.08 (d, J = 8.9 Hz, 8H), 6.93 (d, J = 8.8 Hz, 4H), 6.84 (d, J = 8.9 Hz, 8H), 4.56 (q, J = 7.1 Hz, 4H), 3.94 (t, J = 6.5 Hz, 8H), 1.80-1.75 (m, 8H), 1.52-1.46 (m, 8H), 1.35-1.33 (m, 16H), 1.25 (m, 6H), 0.91 (t, J = 7.0 Hz, 12H) ppm. ^{13}C NMR (75 MHz, CDCl_3): δ 164.6, 155.8, 149.2, 148.0, 142.2, 140.5, 137.8, 135.9, 131.5, 129.1, 128.6, 126.9, 126.5, 122.2, 122.0, 120.4, 115.4, 68.4, 62.9, 31.8, 29.5, 29.4, 25.9, 22.2, 14.3 ppm. IR (neat): 3047,

2922, 2854, 1724, 1601 cm^{-1} . MS (ESI-TOF) m/z : calc'd $[\text{M} + \text{Cs}]^+$ for $\text{C}_{82}\text{H}_{92}\text{N}_4\text{O}_8\text{S}_2\text{Cs}$: 1457.5411; found 1457.6111 with an isotopic pattern identical to the predicted pattern.

Synthesis of 5,8-bis(5-(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)thiophen-2-yl)quinoxaline-2,3-dicarboxylic acid (AP9): In a round bottom flask, diethyl 5,8-bis(5-(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)thiophen-2-yl)quinoxaline-2,3-dicarboxylate (**3**) (10 mg, 0.0068 mmol) was dissolved in THF (10 mL, 0.68 mM) and mixed with methanol (10 mL, 0.68 mM). Lithium hydroxide (1.0 g, 41.7 mmol) was added, and the mixture was allowed to stir for 2 hours at room temperature. The reaction mixture was acidified with acetic acid, then extracted with water and diethyl ether. The organic layer was evaporated under reduced pressure. A green solid was centrifuged with 3 mL of methanol for 10 minutes, then methanol was decanted and the solid was left under high vacuum to evaporate the remaining solvent to give a green solid (5.0 mg, 0.0039 mmol, 57% yield). ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.39 (s, 2H), 8.17 (ap s, 2H), 7.54 (d, $J = 8.4$ Hz, 4H), 7.44 (d, $J = 3.6$ Hz, 2H), 7.05 (d, $J = 8.7$ Hz, 8H), 6.92 (d, $J = 8.9$ Hz, 8H), 6.82 (d, $J = 8.6$ Hz, 4H), 3.94 (t, $J = 6.2$ Hz, 8H), 1.72-1.69 (m, 8H), 1.50-1.40 (m, 8H), 1.42-1.29 (m, 16H), 0.89 ppm (ap s, 12H). ^{13}C NMR data is not available due to limited solubility of the compound. IR (neat, cm^{-1}): 2923, 2854, 1600. HRMS (ESI-TOF) m/z : calc'd $[\text{M}-\text{H}]^-$ for $\text{C}_{78}\text{H}_{84}\text{N}_4\text{O}_8\text{S}_2$ 1267.5652; found 1267.5712 with an isotopic pattern identical to the predicted pattern.

*Synthesis of 4,4'-(benzo[*c*][1,2,5]thiadiazole-4,7-diyl)bis(*N,N*-bis(4-(hexyloxy)phenyl)aniline) (6)*: To a round bottom flask was added 4,7-dibromobenzo[*c*][1,2,5]thiadiazole (**4**) (0.120g, 0.41 mmol, 1.0 equiv.), 4-(hexyloxy)-*N*-(4-(hexyloxy)phenyl)-*N*-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline (**5**) (494 mg, 0.86 mmol, 2.1 equiv.), and K_3PO_4 (341 mg, 2.4 mmol, 6.0 equiv.). The solids were dissolved in a mixture of THF (8.0 mL, 0.017 M) and water (1.2 mL, 0.34 M). The mixture was sparged with N_2 for 30 minutes, then $\text{Pd}(\text{PPh}_3)_4$ (47 mg, 0.041 mmol, 10 mol%) was added. The mixture was stirred under N_2 for 24 hours at 50 $^\circ\text{C}$. The reaction was quenched with water and extracted with diethyl ether. The organic layer was separated, and solvent was removed under reduced pressure. The crude residue was loaded onto a silica gel column for purification with 50% dichloromethane:hexane as eluent to afford a dark red thick oil (200 mg, 0.19 mmol, 47% yield). ^1H NMR (500 MHz, CDCl_3): δ 7.80 (d, $J = 8.8$ Hz, 4H), 7.68 (s, 2H), 7.12 (d, $J = 8.9$ Hz, 8H), 7.05 (d, $J = 8.8$, 4H), 6.85 (d, $J = 8.9$ Hz, 8H), 3.94 (t, $J = 6.5$ Hz, 8H), 1.81-1.75 (m, 8H), 1.50-1.40 (m, 8H), 1.40-1.29 (m, 16H), 0.91 (m, 12H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 155.9, 154.4, 149.0, 140.5, 132.2, 129.8, 129.1, 127.2, 127.1, 119.9, 115.5, 68.4, 31.8, 29.5, 25.9, 22.8, 14.2 ppm; IR (neat, cm^{-1}): 2928, 2861, 1603. HRMS (ESI-TOF) m/z : calc'd for $\text{C}_{66}\text{H}_{78}\text{N}_4\text{O}_4\text{SCs}$ $[\text{M} + \text{Cs}]^+$: 1155.4799; found 1155.4745 with an isotopic pattern identical to the predicted pattern.

*Synthesis of *N,N,N',N'*-tetrakis(4-(hexyloxy)phenyl)-[1,1':4',1''-terphenyl]-2',3',4,4''-tetraamine (7)*: To a round bottom flask was added 4,4'-(benzo[*c*][1,2,5]thiadiazole-4,7-diyl)bis(*N,N*-bis(4-(hexyloxy)phenyl)aniline) (**6**) (190 mg, 0.185 mmol, 1.0 equiv.) was dissolved in ethanol (13 mL, 0.13 M) and THF (6 mL, 0.03 M). NaBH_4 (63 mg, 1.62 mmol, 9.0 equiv.) and $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.88 mg, 0.0036 mmol, 2 mol%) were added. The reaction was stirred at 70 $^\circ\text{C}$ for 2 hours. The reaction mixture was then cooled to room temperature and filtered through a pad of silica with diethyl ether. Solvent was removed under reduced pressure to give a white solid (180 mg, 0.181 mmol, 97% yield) which was used without further purification. ^1H NMR (300 MHz, CDCl_3): δ 7.26 (d, $J = 8.7$ Hz, 4H), 7.09 (d, $J = 8.9$ Hz, 8H), 6.98 (d, $J = 8.5$ Hz, 4H), 6.83 (d, $J = 8.9$ Hz, 8H), 6.75 (s, 2H), 3.93 (t, $J = 6.5$ Hz, 8H), 1.80-1.73 (m, 8H), 1.48-1.43 (m, 8H), 1.40-1.30 (m, 16H), 0.91 (t, $J = 6.9$ Hz, 12H) ppm. No further characterized was attempted due to the limited stability of the compound.

*Synthesis of diethyl 10,13-bis(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)dipyrido[3,2-*a*:2',3'-*c*]phenazine-3,6-dicarboxylate (9)*: To a flame dried flask was added diethyl 5,6-dioxo-5,6-dihydro-1,10-phenanthroline-2,9-dicarboxylate (**8**) (64 mg, 0.18 mmol, 1.0 equiv.) and *N,N,N',N'*-tetrakis(4-(hexyloxy)phenyl)-[1,1':4',1''-terphenyl]-2',3',4,4''-tetraamine (**7**) (180 mg, 0.18 mmol, 1.0 equiv.) were mixed in triethylamine (0.5 mL, 0.2 M), dichloromethane (1.6 mL, 0.11 M), and ethanol (1.6 mL, 0.1 M). The mixture was stirred at 80 $^\circ\text{C}$ overnight. Then, solvent was removed under reduced pressure. The crude product mixture was subjected to silica gel column

chromatography and eluted with 5% methanol:dichloromethane. Solvent was evaporated under reduced pressure to yield a purple solid (30 mg, 0.022 mmol, 13% yield). ^1H NMR (300 MHz, CDCl_3): δ 9.59 (d, J = 8.1 Hz, 2H), 8.56 (d, J = 8.3 Hz, 2H), 8.09 (s, 2H), 7.79 (d, J = 8.7 Hz, 4H), 7.21 (d, J = 8.8 Hz, 8H), 7.15 (d, J = 8.6 Hz, 4H), 6.90 (d, J = 8.7 Hz, 8H), 4.35 (br m, 4H), 3.97 (t, J = 6.5 Hz, 8H), 1.84-1.77 (m, 8H), 1.50-1.45 (m, 8H), 1.40-1.27 (m, 22H), 0.90 (t, J = 6.9 Hz, 12H) ppm. ^{13}C (75 MHz, CDCl_3): δ 165.5, 156.0, 150.3, 148.9, 147.6, 141.2, 140.6, 139.5, 139.2, 135.6, 131.7, 130.9, 130.6, 129.5, 127.2, 125.2, 119.4, 115.5, 68.4, 62.6, 31.8, 29.5, 25.9, 22.8, 14.4, 14.2 ppm. IR (neat, cm^{-1}): 2930, 2862, 1719, 1602. MS (ESI-TOF) m/z : calc'd for $\text{C}_{84}\text{H}_{92}\text{N}_6\text{O}_8\text{Cs}$ [$\text{M} + \text{Cs}$] $^+$: 1445.6031, found 1445.5500. The isotopic pattern is identical to the predicted pattern.

*Synthesis of 10,13-bis(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)dipyrido[3,2-*a*:2',3'-*c*]phenazine-3,6-dicarboxylic acid (API2):* In a round bottom flask diethyl 10,13-bis(4-(bis(4-(hexyloxy)phenyl)amino)phenyl)dipyrido[3,2-*a*:2',3'-*c*]phenazine-3,6-dicarboxylate (**9**) (25 mg, 0.019 mmol, 1.0 equiv.) was dissolved in THF (15 mL, 0.0012 M) and methanol (15 mL, 0.0012 M). Lithium hydroxide (1.0 g, 43 mmol) was added and the mixture was allowed to stir overnight at room temperature. The reaction mixture was acidified with acetic acid and extracted with water and diethyl ether. The solvent was removed under reduced pressure to yield a green solid (16 mg, 0.0127 mmol, 66% yield). ^1H VT-NMR recorded at 80 °C (500 MHz, $\text{DMSO}-d_6$): δ 9.39 (ap s, 2H), 8.49 (ap s, 2H), 8.11 (ap s, 2H), 7.82 (ap s, 4H), 7.17 (d, J = 8.2 Hz, 8H), 7.05 (d, J = 7.1 Hz, 4H), 6.97 (d, J = 7.8 Hz, 8H), 4.02 (t, J = 5.7 Hz, 8H), 1.76-1.73 (m, 8H), 1.47-1.45 (m, 8H), 1.41-1.27 (m, 16H), 0.91 (ap s, 12H) ppm. ^{13}C NMR data is not available due to limited solubility of the compound. IR (neat, cm^{-1}): 3424, 2952, 2924, 2856, 1727, 1600. HRMS (ESI-TOF) m/z : calc'd for $\text{C}_{80}\text{H}_{84}\text{N}_6\text{O}_8$ [$\text{M}-\text{H}$] $^-$: 1255.6272, found 1255.6553 with an isotopic pattern identical to the predicted pattern.

General Information for Computational Studies: MM2 energy minimization in ChemBio3D Ultra (version:13.0.2.3021) was used for the initial energy minimization of the target dyes. All extended alkyl chains were truncated to methyl groups. Dihedral angles for the relevant groups were set to values between the global minimum and the next local minimum on the conformational energy diagram as calculated by ChemBio3D. Higher level geometry optimizations were performed sequentially by density functional theory (DFT) using Gaussian09 with the B3LYP functional with the following basis sets: first 3-21G, second 6-31G(*d,p*), and finally 6-311G(*d,p*).

General Information for Photovoltaic Measurements: Current-Voltage curves photovoltaic characteristics were measured using a 150 W xenon lamp (Model SF150B, SCIENCETECH Inc., Class ABA) solar simulator equipped with an AM 1.5 G filter for a less than 2% spectral mismatch. Prior to each measurement, the solar simulator output was calibrated with a KG5 filtered mono-crystalline silicon NREL calibrated reference cell from ABET Technologies (Model 15150-KG5). The current density-voltage characteristic of each cell was obtained with a Keithley digital sourcemeter (Model 2400). The incident photon-to-current conversion efficiency was measured with an IPCE instrument manufactured by Dyanamo comprised of a 175 W xenon lamp (CERMAX, Model LX175F), monochromator (Spectral Products, Model CM110, Czerny-Turner, dual-grating), filter wheel (Spectral Products, Model AB301T, fitted with filter AB3044 [440 nm high pass] and filter AB3051 [510 nm high pass]), a calibrated UV-enhanced silicon photodiode reference, and Dyanamo issued software.

DSC Device Fabrication Protocol: For the photoanode, TEC 10 glass was purchased from Hartford Glass. Once cut into 2x2 cm squares, the substrate was submerged in a 0.2% Deconex 21 aqueous solution and sonicated for 15 minutes at room temperature. The electrodes were rinsed with water and sonicated in acetone 10 minutes followed by sonication in ethanol for 10 minutes. Finally, the electrodes were placed under UV/ozone for 15 minutes (UV-Ozone Cleaning System, Model ProCleaner by UVFAB Systems). A compact TiO_2 underlayer is then applied by pretreatment of the substrate submerged in a 40 mM TiCl_4 solution in water (prepared from 99.9% TiCl_4 between 0-5 °C). The submerged substrates (conductive side up) were heated for 30 minutes at 70 °C in the TiCl_4 solution. After heating, the substrates were rinsed first with water while warm and then with ethanol. The photoanode consists of a thin TiO_2 film comprised of a 10 μm mesoporous TiO_2 layer (particle size, 20 nm,

Dyesol, DSL 18NR-T) and a 5.0 μm TiO_2 scattering layer (particle size >100 nm, Solaronix R/SP). Both layers were screen printed from a Sefar screen (54/137–64W). Between each print, the substrate was heated for 7 minutes at 125 $^\circ\text{C}$, and the thickness was measured with a profilometer (Alpha-Step D-500 KLA Tencor). The substrate was then sintered with progressive heating from 125 $^\circ\text{C}$ (5 minute ramp from r.t., 5 minute hold) to 325 $^\circ\text{C}$ (15 minute ramp from 125 $^\circ\text{C}$, 5 minute hold) to 375 $^\circ\text{C}$ (5 minute ramp from 325 $^\circ\text{C}$, 5 minute hold) to 450 $^\circ\text{C}$ (5 minute ramp from 375 $^\circ\text{C}$, 15 minute hold) to 500 $^\circ\text{C}$ (5 minute ramp from 450 $^\circ\text{C}$, 15 minute hold) using a programmable furnace (Vulcan® 3-Series Model 3-550). The cooled sintered photoanode was soaked 30 minutes at 70 $^\circ\text{C}$ in a 40 mM TiCl_4 water solution. The electrode was removed while warm and rinsed with water before heating again at 500 $^\circ\text{C}$ for 30 minutes prior to sensitization. The complete working electrode was prepared by immersing the TiO_2 film overnight in a 0.3 mM dye solution with added chenodeoxycholic acid (CDCA) in 1:4 THF:EtOH. The dye:CDCA molar ratio was 1:20 for the optimized devices. For preparing counter electrodes, 2x2 cm squares of TEC 7 FTO glass were drilled using a Dremel-4000 with Dremel 7134 Diamond Taper Point Bit from the glass side through to a taped FTO side. The electrodes were washed with water after tape removal, followed by a wash using 0.1 M HCl in EtOH and sonication in acetone for 10 minutes. The electrodes were then dried at 400 $^\circ\text{C}$ for 15 minutes. A thin layer of Pt-paste (Solaronix, Platisol T/SP) was slot printed on the FTO, and the printed electrodes were then heated at 450 $^\circ\text{C}$ for 10 minutes. After allowing them to cool to room temperature, the working electrodes were then sealed to the counter electrodes with a 25 μm thick hot melt ring shaped film (Surlyn, Dupont) by heating the system at 130 $^\circ\text{C}$ under 0.2 psi from a piston for 1 minute. Devices were completed by filling the electrolyte through pre-drilled holes in the counter electrodes. The holes were sealed with a Surlyn pre-cut circle and a thin glass cover by heating at 130 $^\circ\text{C}$ under 0.1 psi for 25 seconds. Finally, soldered contacts were added with a MBR Ultrasonic soldering machine (model USS-9210) with solder alloy (Cerasolzer wire dia 1.6 mm item # CS186-150). A circular black mask (active area 0.15 cm^2) was punched from black tape used in the subsequent photovoltaic studies. Reported DSC device PCE values are the average of multiple cells with PCE values varying in standard deviation by less than 0.2%.

Time-Correlated Single Photon Counting (TCSPC) General Information: Fluorescence lifetime curves were obtained using the 485 nm line of an LDH series 485B pulsed diode laser (pulse width approx. 100 ps) as the excitation source and emission was detected using a PicoQuant PDM series single photon avalanche diode (time resolution approx. 50ps) and TimeHarp 260 time correlated single photon counter (25 ps resolution).

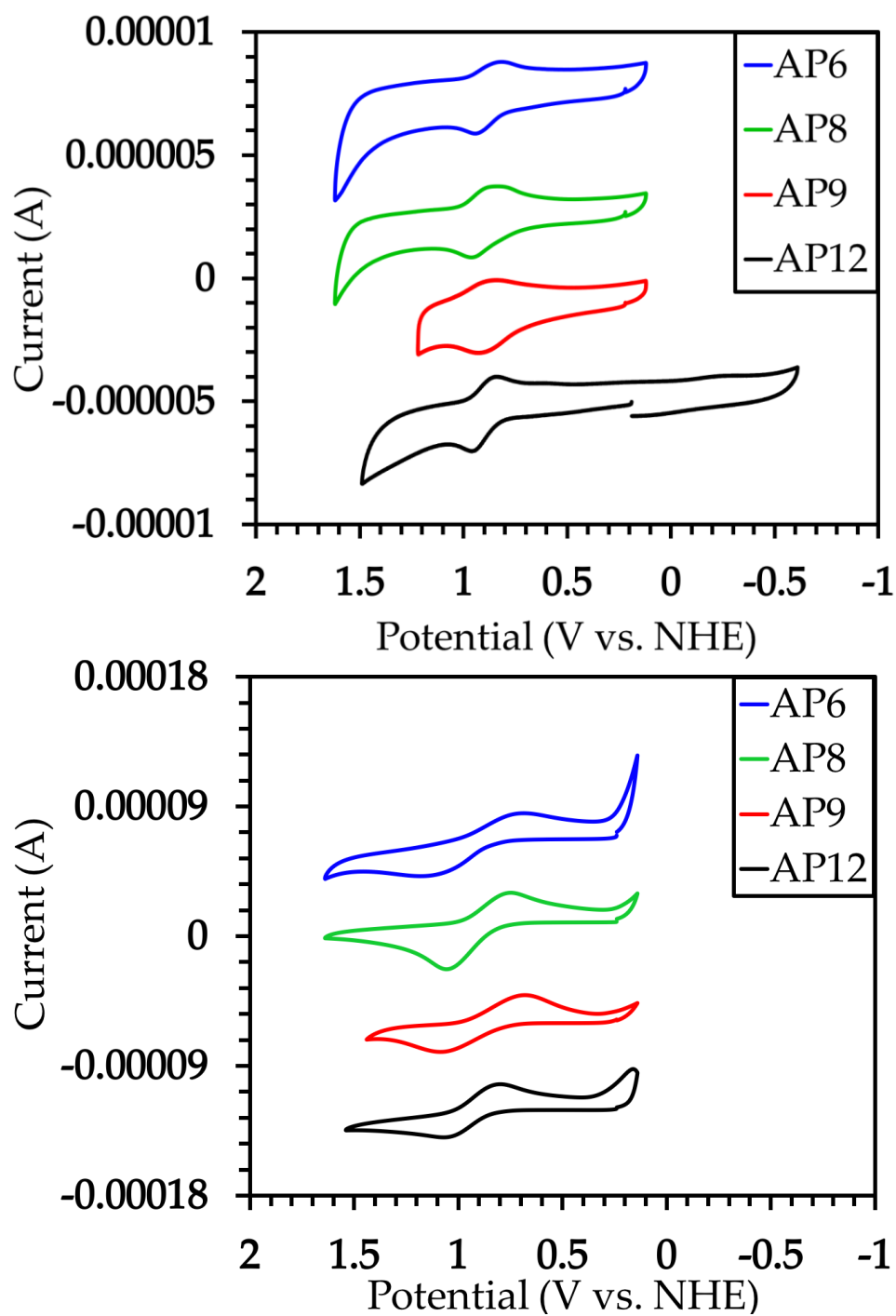


Figure S1. Cyclic voltammetry plots of **AP** dyes in DCM solution (top) and on TiO₂ (bottom).

Figure S2. ^1H NMR spectrum of compound **3** (CDCl_3 , 500 MHz).

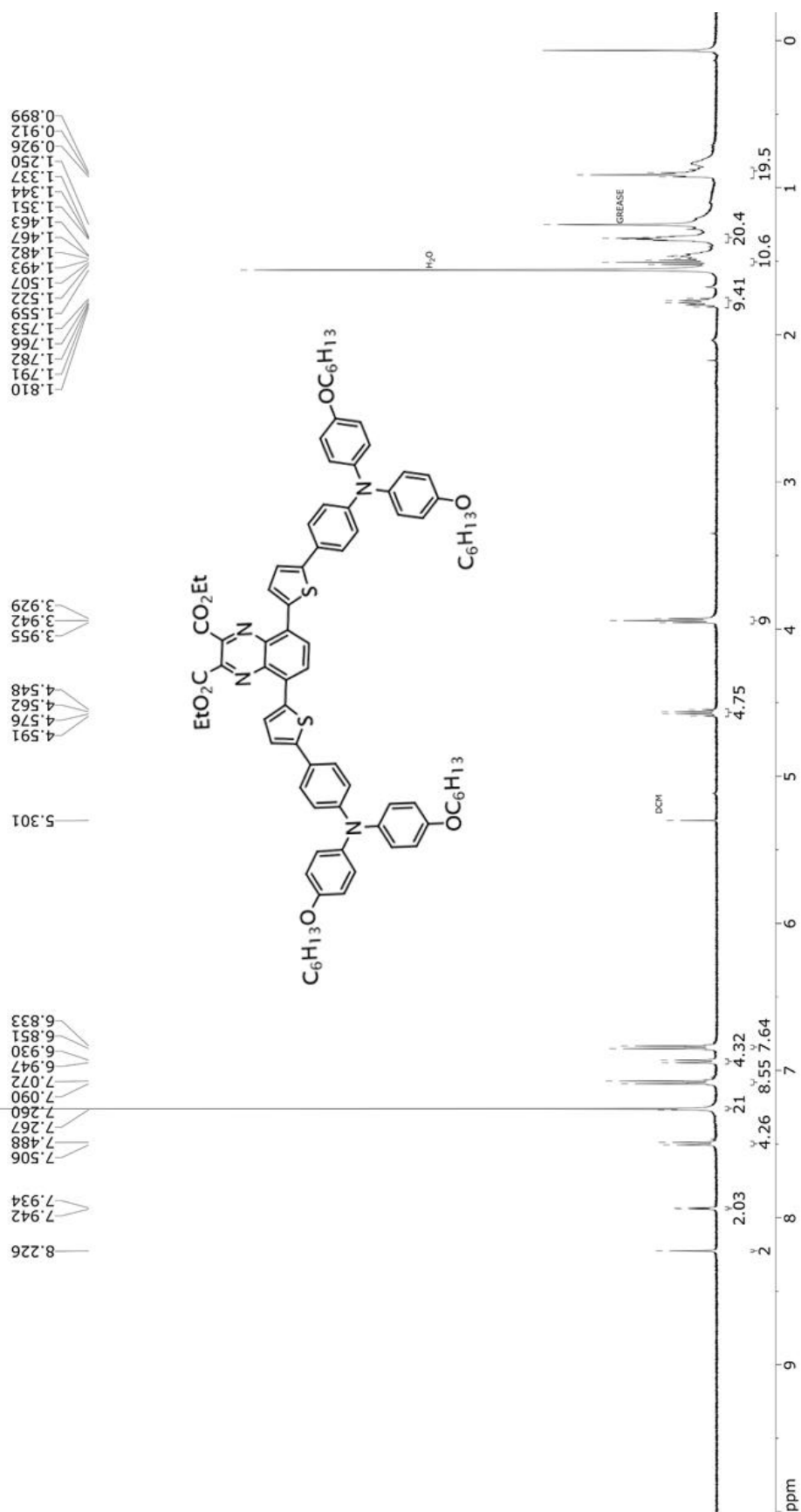


Figure S3. ^{13}C NMR spectrum of compound **3** (CDCl_3 , 75 MHz).

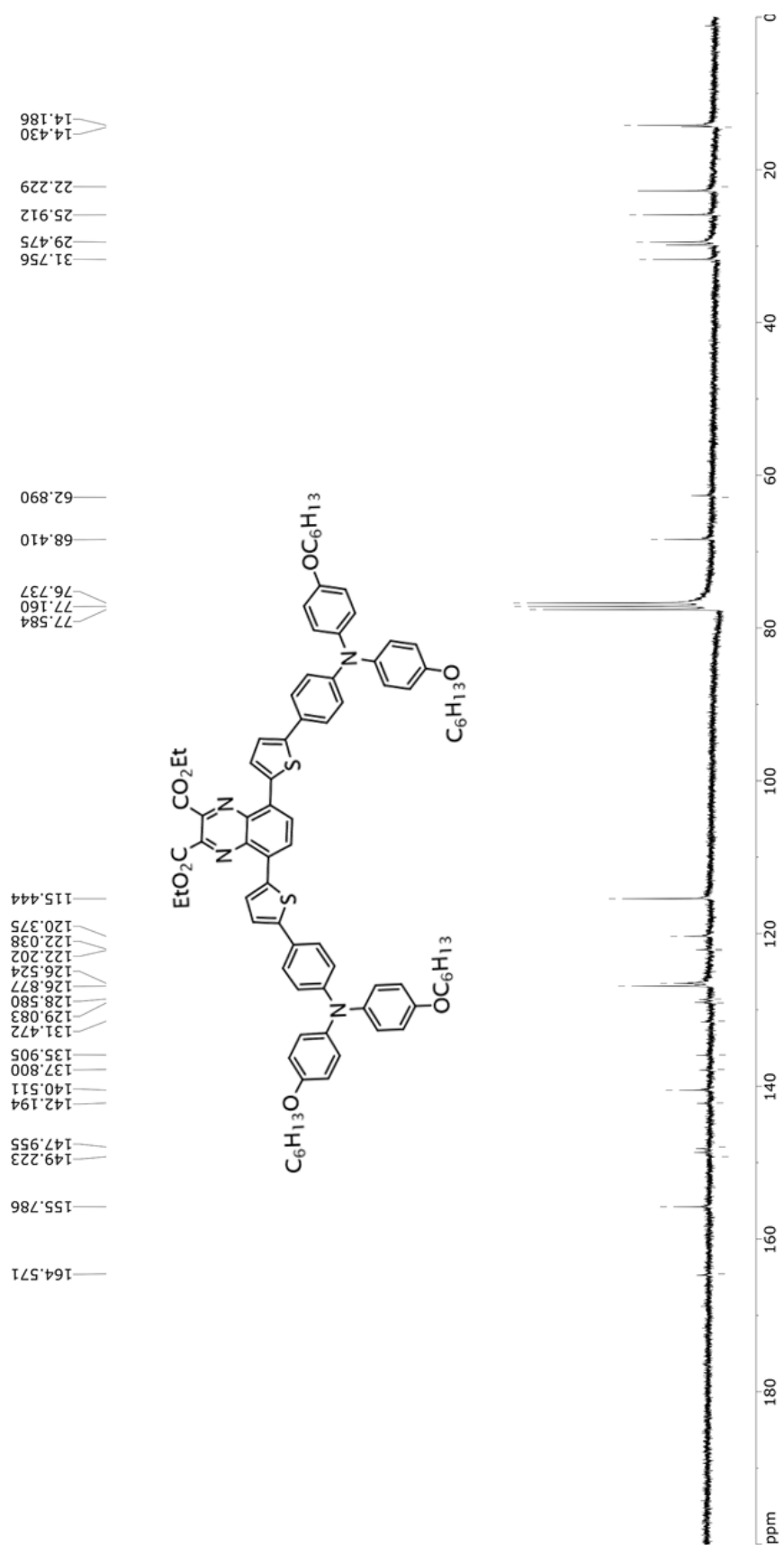


Figure S4. ^1H NMR spectrum of compound **AP9** (DMSO- d_6 , 500 MHz).

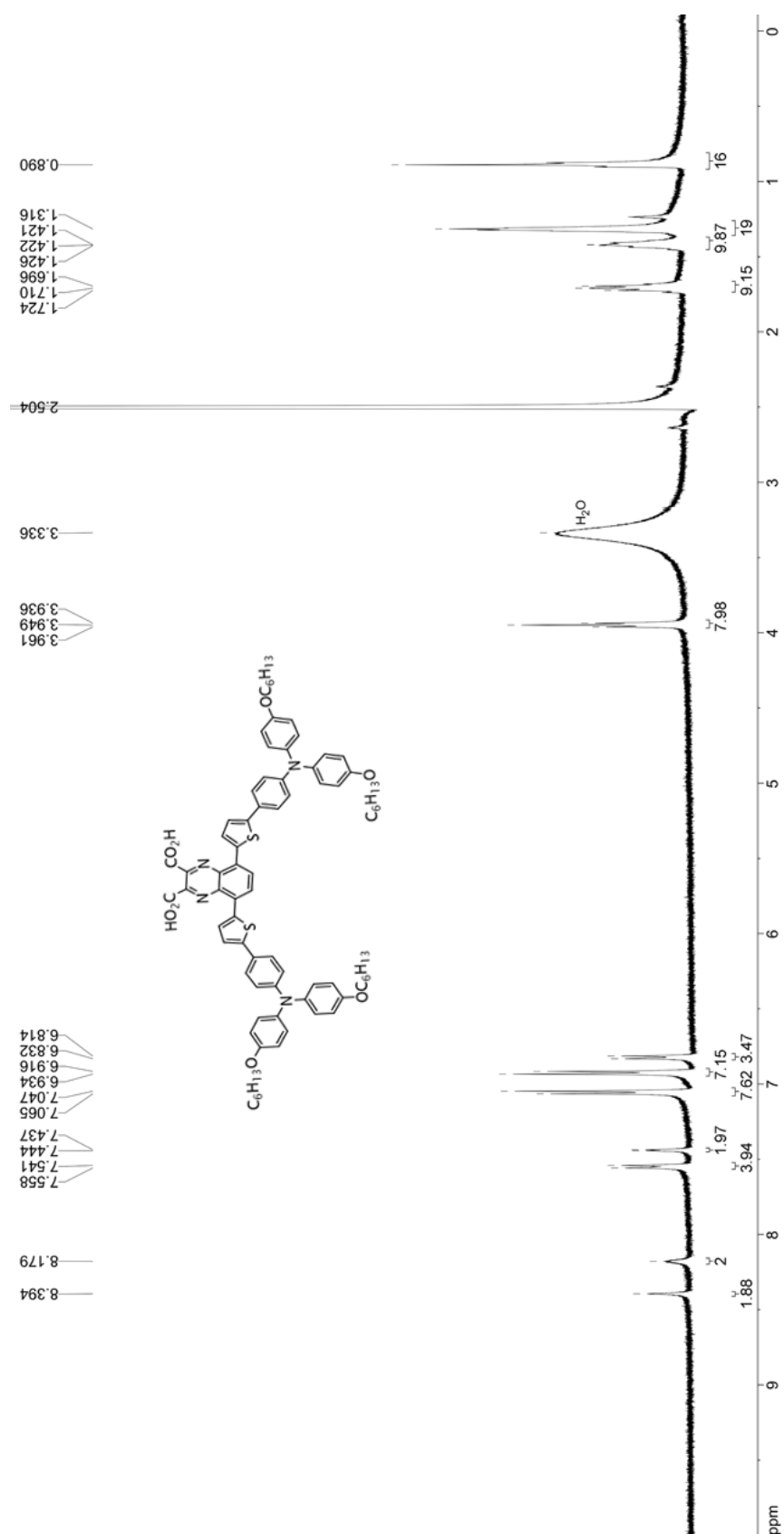


Figure S5. ^1H NMR spectrum of compound **6** (CDCl_3 , 500 MHz).



Figure S6. ^{13}C NMR spectrum of compound **6** (CDCl_3 , 125 MHz).

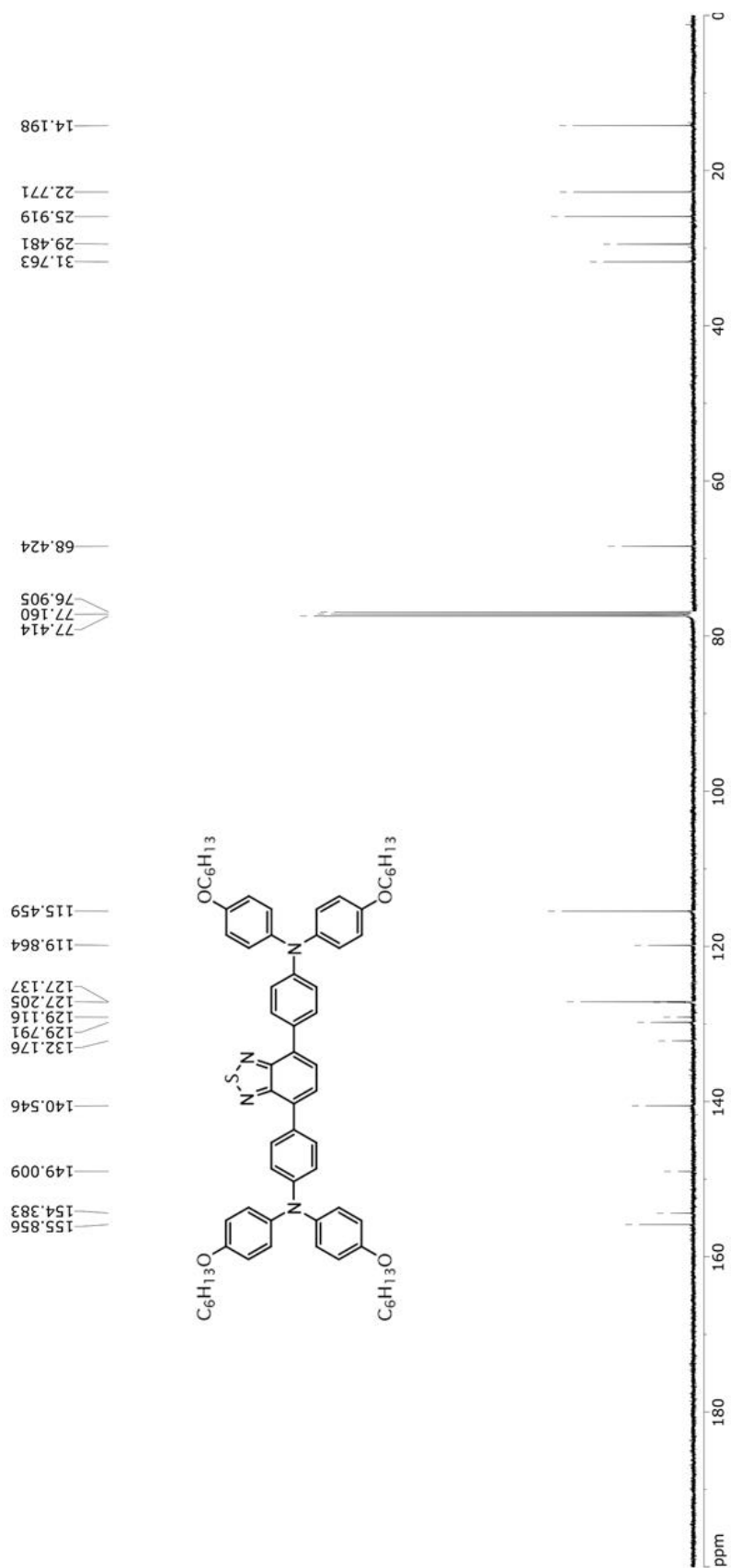


Figure S7. ^1H NMR spectrum of compound **7** (CDCl_3 , 300 MHz).

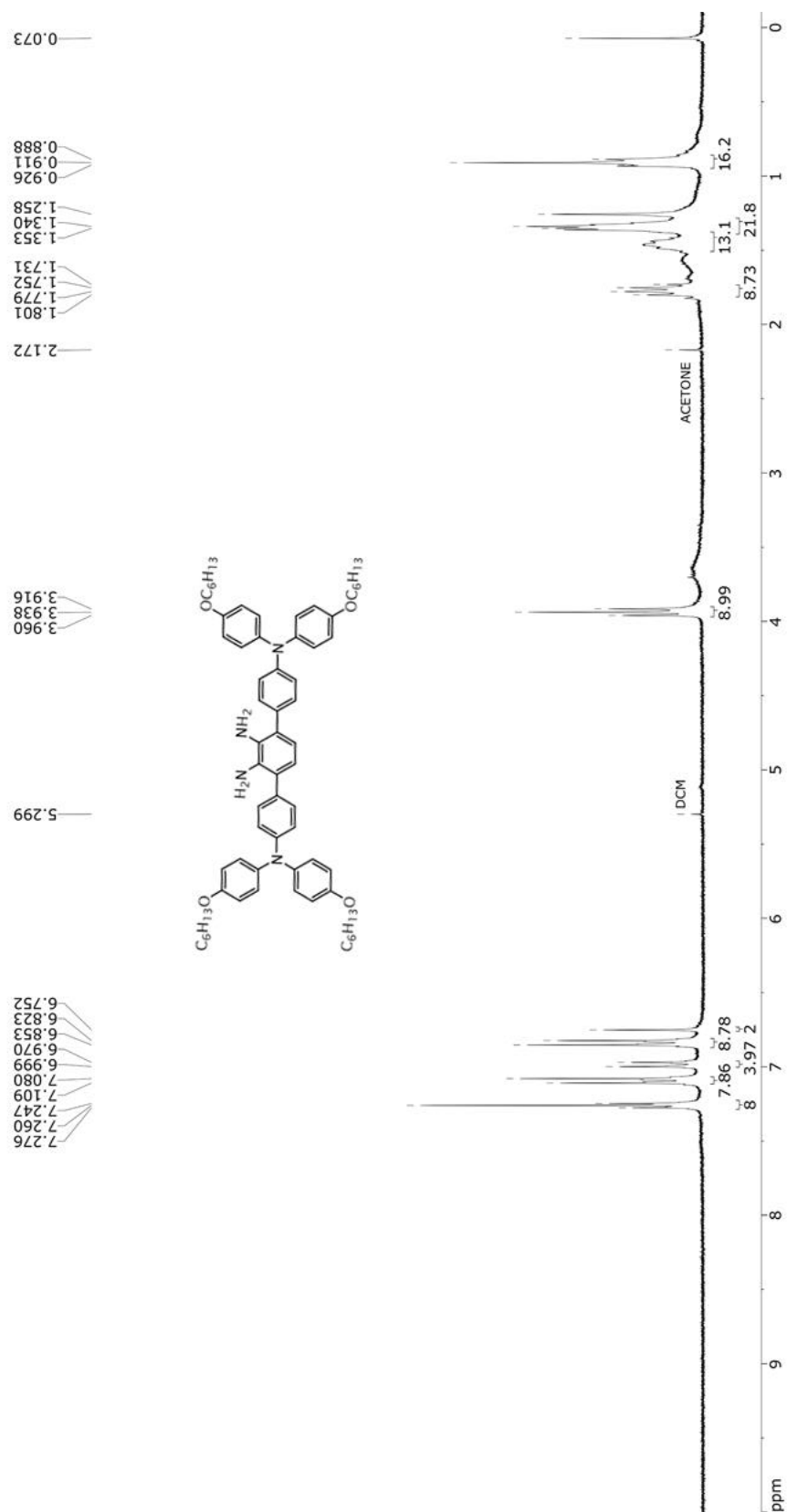


Figure S8. ^1H NMR spectrum of compound **9** (CDCl_3 , 300 MHz).

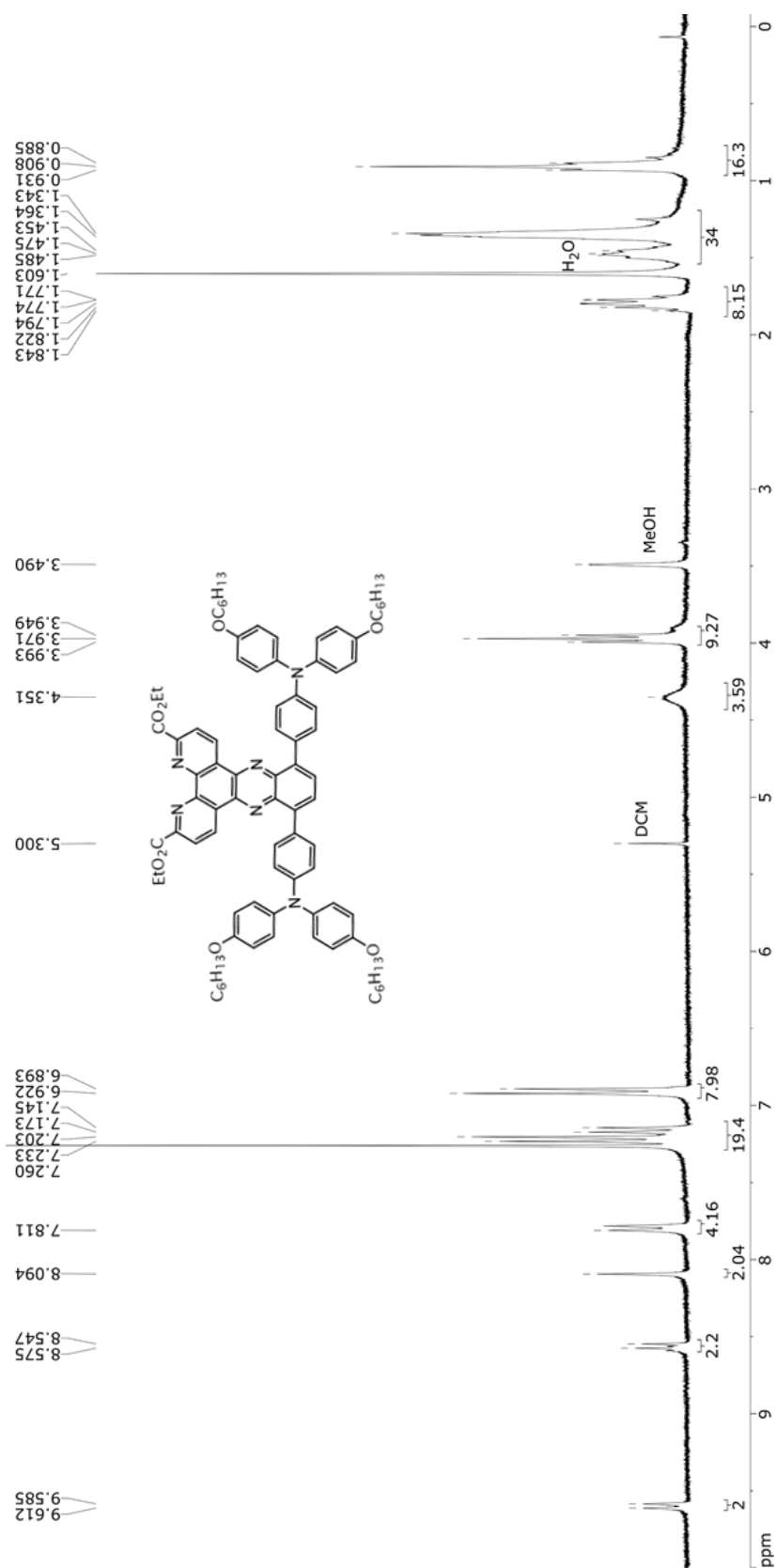


Figure S9. ^{13}C NMR spectrum of compound **9** (CDCl_3 , 75 MHz).

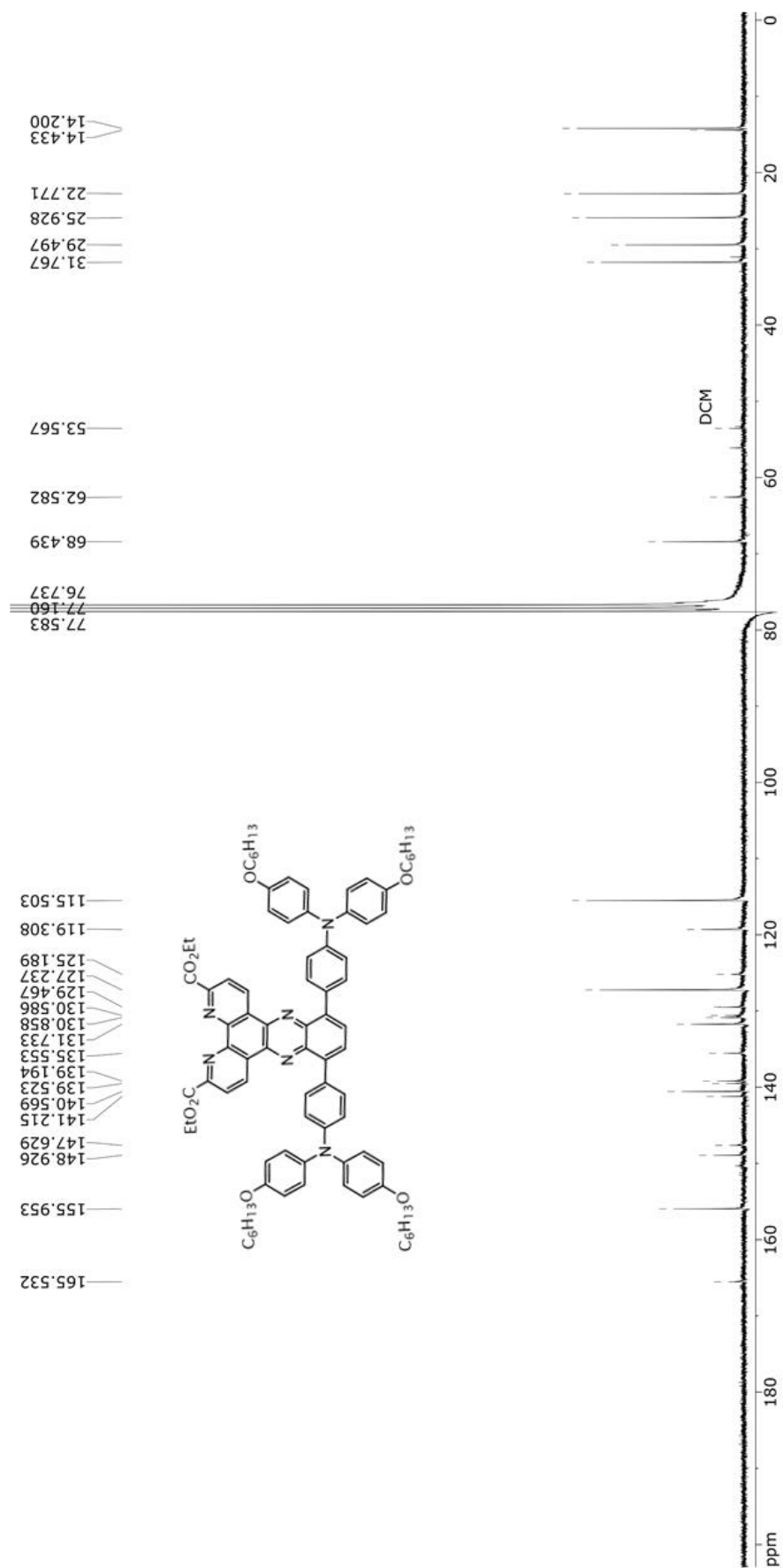
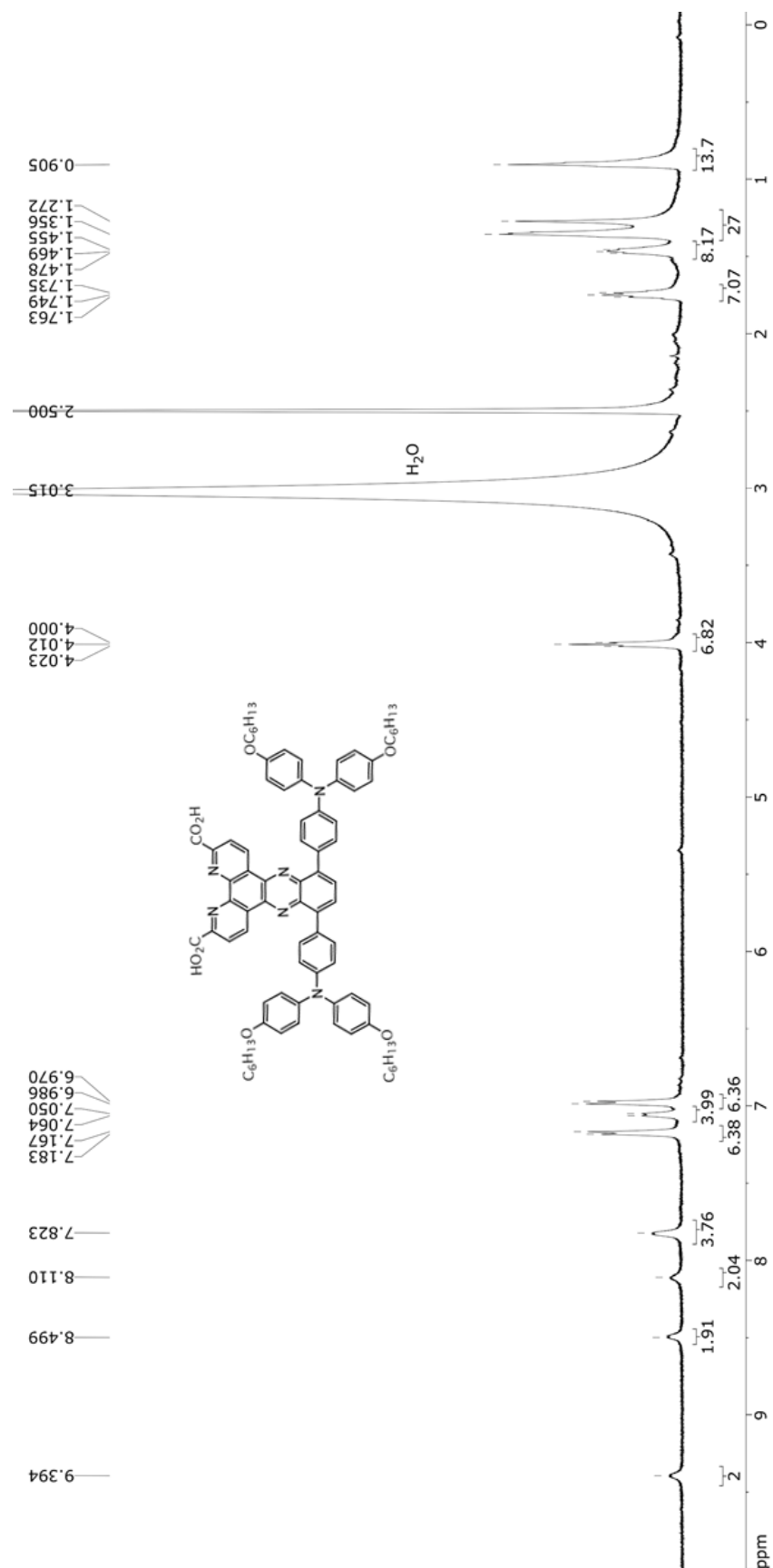


Figure S10. ^1H NMR spectrum of compound **AP12** (DMSO- d_6 , 500 MHz, 80°C).



XYZ Coordinates of Target Structures

AP9 XYZ coordinates

C	-12.69301	-0.17114	-2.35704
C	-11.52881	-0.68697	-1.78641
C	11.10074	-4.04101	0.06423
C	11.17475	-5.34593	-0.39717
C	-0.66954	0.75212	-0.24337
C	10.52335	-5.72476	-1.58093
C	-1.44145	1.91642	-0.19936
O	-10.803	-6.59762	2.80525
H	10.01503	0.93622	-0.40353
C	9.80673	-4.7622	-2.29789
C	9.11168	-1.00512	-0.15419
H	9.20279	-2.70281	-2.41087
H	-12.66786	0.16683	-3.38398
C	-6.619	0.4136	-0.19899
C	6.65048	0.43021	-0.09653
C	-6.66267	-0.9853	-0.03201
C	11.60888	-0.40045	1.4665
H	12.68185	-1.73066	-1.46301
H	14.80483	-0.6822	-0.68459
H	-14.46858	1.69845	-3.61788
H	-14.9131	0.05783	-4.17379
H	-10.49229	-7.83442	4.39079
H	-9.1446	-6.68904	4.13016
H	-10.66997	-6.12139	4.87096

C	9.74983	-3.44453	-1.84276
H	10.22891	-8.56009	-3.24608
H	8.90958	-7.36007	-3.11966
C	-9.09451	-0.97737	0.02363
H	10.38625	-6.971	-4.04988
H	16.32588	1.72296	2.73243
C	-9.05743	0.42461	-0.1341
H	7.90425	2.17171	-0.36708
H	-11.53621	-3.88723	-0.72131
C	-11.21022	-5.19832	0.9445
C	-5.36547	1.13438	-0.33006
H	-5.73593	-1.54803	-0.01636
H	-7.86701	-2.74198	0.18579
S	-3.79766	0.3874	0.21991
H	3.54408	3.98511	0.11468
H	-16.17907	1.17887	-3.59335
S	3.80613	0.31508	-0.1565
H	11.72356	-6.10392	0.14571
H	11.60039	-3.75916	0.982
C	9.08432	0.40049	-0.27531
O	15.18262	0.64241	1.4418
C	-7.86495	-1.66636	0.0734
C	5.4052	1.17339	-0.0654
C	5.1993	2.5305	0.03215
C	3.84471	2.94874	0.0411
C	-15.14807	0.8528	-3.45555
C	-10.23516	-6.80684	4.13333

C	9.9967	-7.49769	-3.17009
C	15.2897	1.38666	2.69274
H	9.30043	-5.02023	-3.21794
H	12.80409	0.73383	2.83046
H	10.71955	-0.32423	2.07936
C	-1.62492	6.63582	0.43752
O	-1.29045	7.82568	0.54224
O	-2.91055	6.25317	0.48628
C	1.73198	6.66567	0.30762
O	-15.08631	0.36982	-2.07964
N	10.33017	-1.71337	-0.18413
C	11.54896	-1.09466	0.25326
C	10.38476	-3.06743	-0.65427
C	-11.09434	-3.99855	0.26043
N	-10.32022	-1.66325	0.1303
C	-11.51564	-1.12969	-0.45949
C	-10.41162	-2.91129	0.83299
H	-10.62041	-0.74139	-2.3731
C	-0.71703	3.13994	-0.03917
C	0.72348	3.15118	-0.00006
H	15.07418	0.75151	3.56064
H	0.23169	7.99669	0.46996
N	-1.352	4.327	0.1113
N	1.36763	4.32794	0.11262
H	-2.89663	5.23559	0.39129
H	-9.98717	0.97673	-0.15642
H	-11.73528	-6.04159	0.51599

H	-9.50037	-4.36809	3.76686
H	-9.32952	-2.23505	2.56145
H	-12.70718	-1.40763	1.31128
H	14.61906	2.25455	2.70548
H	5.75983	-1.52099	0.15519
H	7.87571	-2.75291	0.099
H	-14.79144	-0.51404	0.27511
H	6.01406	3.23604	0.11463
H	-7.85979	2.17863	-0.3271
C	12.71577	-1.19242	-0.52454
C	13.89985	-0.61331	-0.09578
C	6.68635	-0.97481	0.01917
C	7.8807	-1.67634	-0.00482
C	13.95337	0.09525	1.11451
C	12.79493	0.19993	1.89002
O	10.65244	-7.05533	-1.94368
O	2.93556	6.42121	0.2668
C	-10.63461	-5.35649	2.21462
C	-9.94913	-4.28068	2.78678
C	-9.85063	-3.06724	2.10513
C	-12.70589	-1.063	0.28524
C	-13.86817	-0.56932	-0.28603
C	-13.87507	-0.11182	-1.61282
O	1.25767	7.91269	0.41812
H	-1.17545	-0.19859	-0.36113
H	1.24205	-0.19363	-0.23197
H	-3.438	3.73754	-1.24547

H	-5.91557	2.99847	-1.26014
C	7.88723	1.09566	-0.24543
C	2.92483	1.92212	-0.04749
C	-2.88497	1.88086	-0.30829
C	-7.85222	1.0985	-0.24209
C	0.72716	0.75723	-0.17733
C	1.48189	1.93175	-0.07361
C	-3.76655	2.79764	-0.829
C	-5.12843	2.38663	-0.84198
C	-0.68054	5.47635	0.24794
C	0.7366	5.49403	0.22135

AP12 XYZ coordinates

H	1.52105	7.50867	-0.05677
H	-4.91807	6.16528	-0.81973
C	-5.74709	-1.91615	-0.01906
H	-5.44807	-3.46953	1.44461
H	10.0423	-2.21831	-5.85669
H	-5.66288	-0.34168	-1.48736
C	0.71971	1.90378	-0.02596
H	-2.99939	-3.28916	1.45471
H	-3.21238	-0.16444	-1.47756
H	10.05297	-1.8777	5.88344
H	9.01882	-0.43253	6.08316
H	-9.94102	-2.30648	5.88513

H	10.77513	-0.32577	6.39925
C	-0.70405	1.89664	0.01442
H	10.53931	-3.83179	-6.44451
H	8.81319	-3.48765	-6.13138
C	1.43566	3.1719	-0.06231
C	0.72469	4.39338	-0.03217
H	9.1304	-3.81579	-0.05566
H	10.38766	-4.58511	-2.06636
H	3.24175	-0.14232	1.46018
H	-8.70874	-3.5784	6.13284
H	8.0928	-1.91523	-4.50922
H	6.87354	-1.13566	-2.52423
H	9.37311	-0.40467	0.01017
H	10.73145	0.2554	1.9923
H	8.0937	-1.97283	4.52902
H	6.77116	-2.6491	2.57251
H	-9.08292	-3.86308	0.06126
H	-10.32194	-4.64556	2.0778
H	-8.00972	-1.98727	4.51685
H	-6.80851	-1.19437	2.52638
H	-9.3419	-0.46886	0.00637
H	-10.71544	0.18781	-1.96665
H	-8.07131	-2.00806	-4.52481
H	-6.73364	-2.68061	-2.57766
H	-10.78728	-0.39285	-6.37358
H	-9.02695	-0.48887	-6.07712
H	-10.0513	-1.93781	-5.85643

H	-10.43113	-3.92575	6.46264
C	-7.59954	-2.04578	-2.43806
O	-10.3212	-0.42158	-4.3933
O	-9.9991	-3.89419	4.47469
O	10.08432	-3.81984	-4.4615
O	10.33173	-0.3689	4.41417
C	-10.01277	-0.8463	-5.75479
C	7.97032	-1.56913	1.15443
C	7.90755	-2.42486	-1.15222
C	8.90877	-3.40411	-1.03193
C	-9.74082	-3.38276	5.81689
C	10.01002	-0.78699	5.77453
C	9.84151	-3.29522	-5.8014
C	-3.3907	6.92603	0.19325
O	-2.86542	7.94658	0.59357
O	-4.72234	6.92963	-0.21634
C	3.35	6.94453	-0.15503
O	4.56229	7.11375	-0.2171
O	2.43274	7.94771	-0.10599
H	-3.36073	2.23448	0.18902
H	-4.56254	4.44568	0.28566
H	4.56455	4.52838	-0.21461
H	3.37516	2.26344	-0.15881
H	1.25633	-3.77885	0.02013
H	-1.19468	-3.78917	-0.05712
H	3.05947	-3.26079	-1.48202
H	5.50889	-3.42661	-1.46146

H	5.69197	-0.30639	1.48146
C	-4.96135	-2.74984	0.80056
C	-3.57618	-2.64801	0.79768
N	-7.15652	-2.00758	-0.00958
C	-7.85322	-2.47587	1.15512
C	-7.93383	-1.61549	-1.14921
N	7.20125	-1.96321	0.00928
N	-1.38666	5.57412	0.07433
N	1.37326	5.57556	-0.06296
C	2.70931	5.58517	-0.12479
C	9.6127	-3.83439	-2.14591
C	9.32854	-3.31298	-3.41739
C	8.3303	-2.34252	-3.54457
C	7.63659	-1.89657	-2.41891
C	9.09931	-0.74559	1.00023
C	9.86011	-0.37701	2.09848
C	9.50943	-0.80446	3.38814
C	8.38592	-1.62029	3.54923
C	7.63296	-2.00726	2.43965
C	-8.85402	-3.45599	1.03777
C	-9.54785	-3.89372	2.15513
C	-9.25351	-3.37963	3.42732
C	-8.2556	-2.40842	3.55158
C	-7.57237	-1.95467	2.42262
C	-9.06893	-0.80178	-0.98666
C	-9.83813	-0.43515	-2.07981
C	-9.4904	-0.85466	-3.37287

C	-8.36111	-1.66074	-3.54242
C	-1.43154	3.15715	0.05819
C	-0.7411	4.39033	0.03505
C	-2.83245	3.17802	0.14155
C	-3.48715	4.39752	0.17396
C	-2.72443	5.57786	0.12489
C	3.48931	4.42773	-0.16204
C	2.84129	3.20445	-0.13038
N	1.4053	0.7603	-0.02783
C	0.73923	-0.42537	-0.00804
C	-0.70524	-0.43183	-0.01342
N	-1.38097	0.74823	0.01153
C	1.47176	-1.65852	0.0034
C	0.7319	-2.83115	-0.00447
C	-0.67832	-2.83711	-0.02866
C	-1.42747	-1.67066	-0.0298
C	-2.90713	-1.71858	-0.01863
C	2.95138	-1.69537	-0.00376
C	3.62943	-2.61839	-0.82015
C	5.01498	-2.71212	-0.81709
C	5.7922	-1.87746	0.01008
C	5.1166	-0.95232	0.83205
C	3.7312	-0.86479	0.82301
C	-3.69544	-0.89056	-0.83964
C	-5.08059	-0.98519	-0.84166