Electronic Supporting Information

Aza-benzannulated-perylenebisimide-porphyrin dyad as an intensely absorbing donor in bulk-heterojunction organic solar cell

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Abbreviations used-

Al	**Aluminium**
APCI	**Atmospheric pressure chemical ionization**
CHL	**Chloroform**
COSY	**Correlation spectroscopy (homonuclear)**
CV	**Cyclic voltammetry**
d (NMR)	**Doublet**
DCM	**Dichloromethane**
DFT	**Density functional theory**
DMF	**Dimethylformamide**
DPV	**Differential pulse voltammetry**
Equiv.	**Equivalents**
ESI	**Electron spray ionization**
HMBC	**Heteronuclear multiple-bond correlation spectroscopy**
HOMO	**Highest occupied molecular orbital**
HRMS	**High resolution mass spectrometry**
HSQC	**Heteronuclear single-quantum correlation spectroscopy**
IR	**Infrared spectroscopy**
ITO	**Indium-doped tin oxide**
LUMO	**Lowest unoccupied molecular orbital**
m (NMR)	**Multiplet**
m/z	**Mass to charge ratio**
NMR	**Nuclear magnetic resonance**
NOESY	**Nuclear Overhauser Effect Spectroscopy**
PBI	**Perylenebisimide**
$PC_{71}BM$	**[6,6]-phenyl-C_{71}-butyric acid methyl ester.**
PDI	**Perylenediimide**
PEDOT	**Poly(3,4-ethylenedioxythiophene)**
PFN	**Poly[(9, 9-bis (3′-(N,N-dimethylamino) propyl)-2, 7-fluorene)-alt-2, 7-(9, 9-dioctylfluorene)]**
PS	**Pictet-Spengler**
PSS	**Poly(styrene sulfonate)**
PTCDA or PDA	**Perylene tetracarboxylic dianhydride**
s (NMR)	**Singlet**
SCE	**Standard calomel electrode**
SPS	**Solvent purification system**
t (NMR)	**Triplet**
TA	**Transient absorption (spectroscopy)**
TFSA	**Trifluoromethanesulphonic acid**
THF	**Tetrahydrofuran**
TLC	**Thin-layer chromatography**
TMS	**Tetramethylsilane**
TOL	**Toluene**
VT	**Variable temperature**

Symbols used-

λ denotes wavelength

Δ denotes heat

CS or δ stands for chemical shift

Materials and Methods

The reactions were carried out under an argon atmosphere wherever required. The chemicals were received from Sigma Aldrich and Spectrochem. Spectroscopic grade (UV grade) solvents were used for all the spectroscopic and electrochemical measurements. Silica gel mesh 100-120 was used for column chromatography, and silica gel 60 F_{254} TLCs were used for monitoring reaction progress. Bruker Avance 500 MHz and 700 MHz spectrometer instruments were used for recording ^{1}H and ^{13}C NMR spectra in solvent $CDCl_3$. Chemical shifts were calibrated in parts per million (ppm) relative to the residual solvent signals and TMS signals. HRMS (APCI and ESI) were recorded on a Bruker micro TOF-QII mass spectrometer. Matrix-assisted-LASER desorption/ionization (MALDI) were recorded using the Bruker Ultra Flextreme MALDI-TOF mass spectrometer. Steady-state absorptions were recorded on a Perkin Elmer LAMBDA 950 UV/VIS/NIR spectrophotometer with a 1 cm path length quartz cuvette, and steady-state fluorescence emission measurements were recorded on a Horiba Scientific spectrophotometer. Cyclic voltammetry (CV) experiments using CH potentiostat were performed on the CH instrument. CV and DPV experiments were done using a conventional three-electrode system consisting of a glassy-carbon electrode as the working electrode, a saturated calomel electrode (SCE) as a reference electrode, and Pt-wire as the counter electrode, and all the data were recorded using 0.1 M solutions of tetrabutylammonium hexafluorophosphate (TBAP) as supporting electrolyte in dichloromethane. All the voltammograms were recorded at a scan rate of 100 mV/s at room temperature. Single crystal X-ray diffraction (SCXRD) measurements were done at 100 K on a Bruker D8 Venture diffractometer with a CCD detector with Mo-Kα radiation. Density functional theory (DFT) calculations were performed using the Gaussian 09 program with the B3LYP exchange-correlation function.[1]

Device fabrication and characterization: We have fabricated the polymer solar cells (PSCs) with the conventional configuration ITO/ PEDOT:PSS / **PDPP or Zn-PDPP**: $PC_{71}BM$ /PFN-Br/Al. The ITO coated glass substrates were cleaned in detergent, and subsequently ultra-sonicated in deionized water, acetone, and isopropyl alcohol and dried in vacuum oven to remove all the traces of residues. For each molecule, the photovoltaic performance optimization process was started with identifying the donor (**PDPP or Zn-PDPP**) to acceptor ($PC_{71}BM$) ratio (weight ratio varying from 1:0.4 to 1:6) with 16 mg/mL concentration in chloroform solution. We have added 5 % pyridine as solvent additive and after that solvent vapor annealing was applied to maximize the performance of the PSCs. The devices were fabricated by depositing PEDOT:PSS as hole transport layer having thickness of 35-40 nm. The BHJ active layer was deposited by spin coating (2500 rpm, 60 s) on the top of PEDOT:PSS layer under ambient conditions. For the solvent vapor annealing (SVA), the optimized active layer was exposed to the THF vapours for 40s. A thin layer of PFN-Br was spin coated on the top of the active layer from the methanol solution. The aluminium (Al) electrode was deposited onto the top of PFN layer *via* thermal evaporation at the pressure less than 10^{-5} Torr. The current-voltage characteristics of the OSCs were measured under illumination intensity of 100 mW/cm^2 (AM1.5 G) using a solar simulator and a Keithley 2400 source meter unit. The incident photon to current conversion efficiency (IPCE) measurements were performed using Bentham IPCE system.

The hole only (ITO/PEDOT:PSS/active layer/Au and electron only (ITO/ZnO/active layer/Al) were fabricated as in a same manner as employed for OSCs. Dark J-V characteristics were measured and fitted with space charge limited current model to estimate the hole and electron mobilities.

For transient photocurrent (TPC) and transient photovoltage (TPV) measurements, the device was mounted on a conductive clip and under steady-state illumination from a focused quartz tungsten halogen lamp light source. An optical perturbation is applied to the device with 1kHz femtosecond pulse laser under 500 nm excitation. The TPV signal was acquired by a digital oscilloscope at open circuit condition. The TPC signal was measured under short circuit condition by applying a 50 Ω resistor.

Formulas used:

LUMO and HOMO energies are calculated using the following formulae for electrochemical data:

$E_{LUMO} = E_{LUMO}$ vs SCE = $-(E_{1/2}^{red} + 4.41)$ eV

E_{LUMO} = energy of lowest unoccupied molecular orbital

$E_{HOMO} = E_{HOMO}$ vs SCE = $-(E_{1/2}^{oxid} + 4.41)$ eV

E_{HOMO} = energy of highest occupied molecular orbital

$E_{1/2}^{red}$ = electrochemical potential of 1st reduction

$E_{1/2}^{oxid}$ = electrochemical potential of 1st oxidation

$E_{opt} = 1240/\lambda_{onset}$

Where, E_{opt} is the optical band gap and λ_{onset} is the onset of absorption.

Syntheses and Procedures

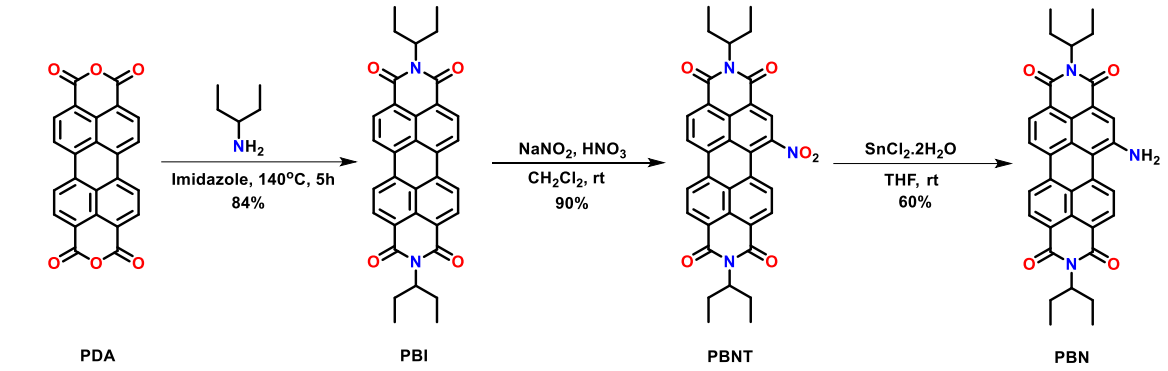


Figure S1. Synthetic scheme for PBI precursors

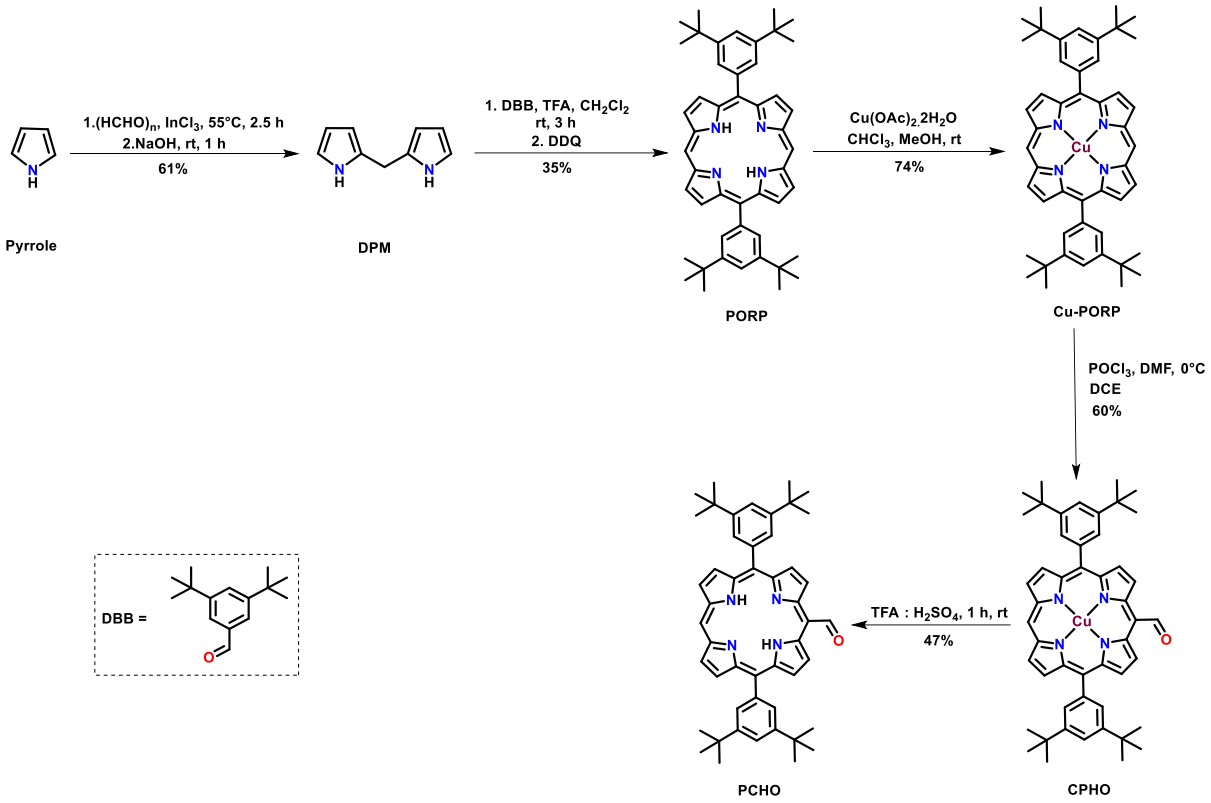


Figure S2. Synthetic scheme for porphyrin precursors

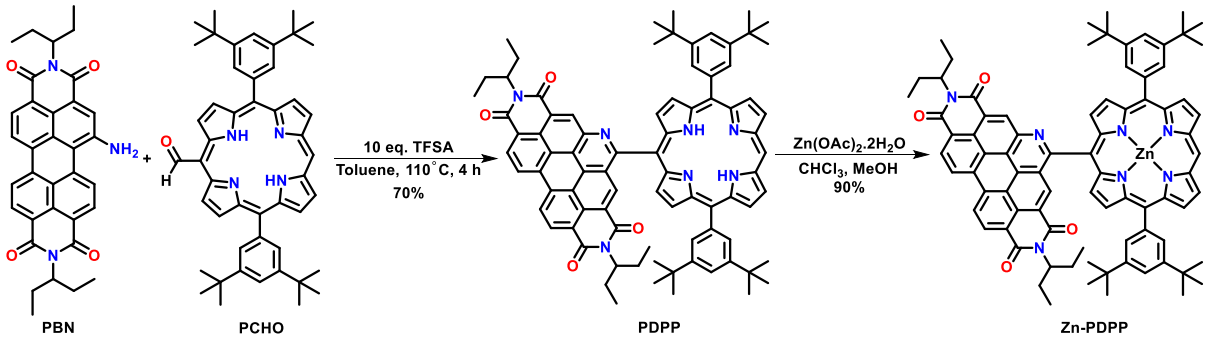


Figure S3. Synthetic scheme for **PDPP** and **Zn-PDPP**

Synthetic Procedures

Synthesis of N, N'-Di(3-pentyl)-perylene-3,4:9,10-tetracarboxylic acid bisimide (PBI)

A mixture of perylene-3,4,9,10-tetracarboxylic acid bisanhydride (**PTCDA** or **PDA**) (2.8g, 7 mmol), 3-pentylamine (2 ml, 17 mmol) and imidazole (40 g) was stirred at 140°C for 5h, and then the mixture was diluted with ethanol. This was followed by the addition of 2M HCl. The reaction mixture was allowed to settle down. The precipitates formed were collected by vacuum filtration and washed with water until the filtrate was pH neutral; it was then oven-dried and purified by repetitive silica gel column chromatography (chloroform-hexane) to get the desired product in 84% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 8.68 (d, *J* = 8 Hz, 4H), 8.63 (d, *J* = 8.0 Hz, 4H), 5.07 (m, 2H), 2.27 (m, 4H), 1.95 (m, 4H), 0.93 (t, *J* = 7.5 Hz, 12H). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{34}H_{30}N_2O_4$: 531.2278; found: 531.2249.

Synthesis of N, N'-Di(3-pentyl)-1-nitro-perylene-3,4:9,10-tetracarboxylic acid bisimide (PBNT)

PBI (2.6 g, 4.9 mmol) was added to a 250 mL round-bottom flask, and 150 mL of anhydrous dichloromethane was then added as a solvent. While stirring, concentrated nitric acid (6.0 g, 4.0 mL) was added drop-wise in the air. After the complete addition of HNO_3, the reaction mixture was allowed to stir under air for 2 h while being monitored by TLC. After 2 h, TLC analysis indicated the complete conversion to the desired product. Work-up for the reaction mixture was done with sodium hydroxide and water; the organic product was extracted with dichloromethane (DCM). The organic phase was collected, and the solvent was removed in a vacuum. This was purified by column chromatography (neutral alumina) with DCM being the mobile phase to obtain a bright red solid in 90% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 8.80 (d, 2H), 8.71 (m, 4H), 8.26 (d, J = 8 Hz, 1H), 5.05 (m, 2H), 2.25 (m, 4H), 1.94 (m, 4H), 0.92 (t, 12H). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{34}H_{29}N_3O_6$: 576.212; found: 576.215.

Synthesis of N, N'-Di(3-pentyl)-1-amino-perylene-3,4:9,10-tetracarboxylic acid bisimide (PBN)

PBNT (1.11 g, 1.93 mmol) and tin (II)chloride dihydrate (2.63 g, 11.58 mmol) were dissolved in 70 mL THF. Under an inert atmosphere, the reaction was stirred for 30 min at room temperature and then 2 h under reflux. The blue reaction mixture was diluted with 200 mL ethyl acetate and after the addition of 100 mL saturated sodium hydrogen carbonate solution, a white precipitate occurred, which was filtered off. The organic solution was washed with 100 mL brine and twice with 100 mL water. Column chromatography (Basic alumina, DCM/ethyl acetate) gave (0.63g) 60% of a blue solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 8.90 (d, J = 8 Hz, 1H), 8.70 (m, 2H), 8.66 (d, J = 8 Hz, 1H), 8.59 (d, 1H), 8.49 (d, 1H), 8.17 (s, 1H), 5.15 (s, 2H), 5.06 (m, 2H), 2.27 (m, 4H), 1.94 (m, 4H), 0.93 (m, 12H). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{34}H_{31}N_3O_4$: 546.238; found: 546.238.

Synthesis of meso-free dipyrromethane (DPM): The synthesis of dipyrromethane involved taking paraformaldehyde (0.15 g, 5 mmol) and pyrrole (17 mL) in a 250 mL round bottomed flask. The flask was covered by aluminium foil and fitted with a septum. The flask and its contents were de-gassed using argon and the setup was placed in an oil bath at 60°C. After half an hour, indium chloride (0.111 g, 0.5 mmol) was added, and the reaction was continued with for three hours. Upon completion, sodium hydroxide pellets (0.6 g) were added. The separation

techniques involved the use of separating funnel and column chromatography to isolate the desired product from other by-products (namely, polypyrroles). Further purification was done by column chromatography, affording white crystals (yield: 61%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ (ppm): 7.82 (br s, 2H), 6.65 (s, 2H), 6.15 (d, 2H), 6.04 (s, 2H), 3.97 (s, 2H). **MALDI (Q-TOF) m/z:** calculated for $C_9H_{10}N_2$:146.08; found: 146.06.

Synthesis of 5,15-Bis(3,5-di-tert-butylphenyl) porphyrin (PORP): This particular step involved synthesizing the porphyrin, using 3,5-di-tert-butylbenzaldehyde (1.88 g, 8.65 mmol), **DPM** (1.26 g, 8.65 mmol) and dissolving it in dichloromethane (1.5 L). The solution was degassed and trifluoroacetic acid (300 μL) was added. The reaction proceeded for three hours. The penultimate addition was that of dichlorodicyanoquinone (2.60 g, 11.24 mmol) followed by addition of triethylamine (11 mL) for quenching the acidic residue. Finally, after evaporation of the solvent and putting the remains through a round of column chromatography, the synthesis of 5, 15-bis(3, 5-di-tert-butylphenyl)porphyrin was completed. (yield: 35%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 10.32 (s, 2H, H-meso), 9.41 (d, *J*=4.5 Hz, 4H, H-β), 9.15 (d, *J* =4.5 Hz, 4H, H-β), 8.16 (d, 4H, Ar-H), 7.85 (s, 2H, Ar-H), 1.58 (s, 36H, CH_3), -3.00 (s, 2H, NH). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{48}H_{54}N_4$: 687.442; found: 687.442

Synthesis of 5, 15-bis(3,5-di-tertbutylphenyl) porphinato copper (Cu-PORP): Metallation on the already synthesized **PORP** (1 g, 1.455 mmol) was done. In a 250 mL round bottomed flask, porphyrin was dissolved in 30 mL chloroform and 25 mL methanol was added to it. Cupric acetate(monohydrate) was added in excess (3 g) and the contents were stirred on a magnetic stirrer, overnight. This was followed by extraction using dichloromethane. This functionalization is necessary because the subsequent formylation reaction has reactants like $POCl_3$, that can decompose the free-base porphyrin moiety. The mixture was further purified by recrystallization to get pure **Cu-PORP** in 74% yield. **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{48}H_{52}CuN_4$: 748.35; found: 748.35

Synthesis of 5-formyl-10,20-bis(3,5-ditertbutylphenyl) porphinato copper (CPHO):
In a 1L two-neck round-bottommed flask equipped with a reflux condenser and a dropping funnel, anhydrous dimethylformamide (60 mL) was added. Phosphorous oxychloride (50 mL) was added dropwise using the dropping funnel and the setup was maintained in an ice bath. After the orange-coloured DMF-$POCl_3$ complex was formed and started solidifying, the ice bath was replaced by an oil bath, and it was heated to about 50°C. The funnel was covered by aluminium foil and a solution of copper porphyrin in 250 mL 1, 2-dichloroethane was added dropwise to the complex. The mixture was heated at 50°C, overnight. After cooling in an ice bath, a saturated solution of sodium acetate was added to the mixture and stirred overnight. This completed the hydrolysis. The extraction was done in dichloromethane and water and subsequently in a saturated solution of sodium bicarbonate and in brine (10% NaCl). The solution was passed through sodium sulphate and finally the monoformylated product was purified using column chromatography with dichloromethane and hexane (yield: 60%). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{49}H_{52}CuN_4O$: 776.351; found: 776.349.

Synthesis of 10,20-Bis(3,5-ditertbutylphenyl)-porphyrin-5-carboxaldehyde (PCHO): In a 100 mL round bottomed flask, 5-formyl-10,20-bis(3,5-ditertbutylphenyl) porphinato copper **CPHO** (100 mg) was taken and a 1:1 mixture (40 mL) of trifluoroacetic acid and concentrated sulphuric acid was added to the flask. The contents were subjected to stirring for an hour. This was followed by extraction into a flask filled with ice and dichloromethane was used for transferring it. The separation was done using a separating funnel and aqueous sodium

hydrogen carbonate solution was used after washing it thoroughly with dichloromethane and water. Purification was done using column chromatography. (yield: 47%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 12.62 (s, 1H), 10.25 (s, 1H), 10.09 (d, 2H), 9.29 (d, 2H), 9.11 (d, 2H), 8.93 (d, 2H), 8.08 (s, 4H), 7.86 (s, 2H), 1.57 (s, 36H), -2.34 (s, 2H, NH). **HRMS (ESI/Q-TOF) m/z:** $[M+H]^+$ calculated for $C_{49}H_{54}N_4O$: 715.437; found: 715.439.

Synthesis of PDPP: 1-aminoperylenebisimide (**PBN**) (48 mg, 0.089 mmol), 10,20-bis(3,5-ditertbutylphenyl)-porphyrin-5-carboxaldehyde (**PCHO**) (127 mg, 0.178 mmol) and trifluoromethanesulphonic acid (TFSA) (78 μL, 0.89 mmol) were dissolved in 10-15 mL dry toluene, heated for 3 h at 110°C under an argon atmosphere and a color change to reddish-brown was observed. The heating was then stopped, and the reaction mixture was allowed to cool down to room temperature. The reaction was then quenched by addition of 30 mL water and thereafter neutralized with 15% sodium hydroxide solution. Then 50 mL of ethyl acetate and 25 ml brine were added, the organic phase was separated and washed with 100 mL of water. The crude product was further purified by column chromatography (basic alumina, chloroform) and recrystallization to give 76 mg (70%) of a dark purple solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 10.33(s, 1H), 9.85(s, 1H), 9.52(d, J = 8.5 Hz, 1H), 9.48(d, J = 8 Hz, 1H), 9.41(d, J = 4.5 Hz, 2H), 9.26(d, J = 8 Hz, 1H), 9.16(d, J = 8 Hz, 1H), 9.11(d, J = 4.5 Hz, 2H), 8.89(d, J = 5 Hz, 2H), 8.65(s, 1H), 8.32(d, J = 4.5 Hz, 2H), 8.21(m, 2H), 8.07(m, 2H), 7.78(m, 2H), 5.23(m, 2H), 2.37(m, 4H), 2.04(m, 4H), 1.53(m, 25H), 1.25(m, 6H), 1.02(m, 7H), 0.88(m, 3H), 0.66(m, 7H), -2.61(s, 2H). **^{13}C{^{1}H} (175 MHz, $CDCl_3$)** δ (ppm): 163.33, 149.01, 148.98, 142.91, 140.48, 133.30, 130.21, 130.16, 127.77, 127.24, 124.20, 123.93, 123.58, 122.96, 121.77, 121.08, 113.37, 106.09, 58.13, 57.74, 35.10, 35.06, 31.75, 31.72, 31.61, 26.93, 25.13, 24.76, 22.67, 14.14, 11.45, 11.13. **HRMS-APCI (m/z):** calculated for $C_{83}H_{81}N_7O_4$: 1240.6423; found: 1240.6409.

Synthesis of Zn-PDPP: PDPP (20 mg, 0.016 mmol) was dissolved in 20 mL of chloroform and zinc acetate dihydrate (added in excess) and 5 mL of methanol was added. The solution was stirred for 4 h at room temperature. The reaction mixture was extracted with water and chloroform and then dried over anhydrous sodium sulphate. Recrystallization was done using DCM-MeOH to obtain pure product as a reddish-brown solid in 90% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ (ppm): 10.39(s, 1H), 9.83(s, 1H), 9.53(d, J = 8.5 Hz, 1H), 9.49(d, J = 8.5Hz, 1H), 9.48(d, J = 4.5 Hz, 2H), 9.23(d, J = 8 Hz, 1H), 9.20(d, J = 4.5 Hz, 2H), 9.19 (d, J = 8.5Hz, 1H), 8.99(d, J = 4.5 Hz, 2H), 8.66(s, 1H), 8.42(m, 2H), 8.20 (m, 2H, Ar), 8.08(m, 2H, Ar), 7.78(m, 2H, Ar), 5.19-4.74(m, 2H), 2.37 (m, 2H), 2.02 (m, 3H), 1.72-1.65 (m, 3H), 1.51 (s, 36H), 1.00 (t, 6H), 0.64 (t, 6H). **^{13}C{^{1}H} (175 MHz, $CDCl_3$)** δ (ppm): 163.76, 151.22, 150.42, 149.97, 149.82, 148.69, 148.67, 141.46, 133.71, 133.17, 132.11, 130.46, 130.03, 129.96, 122.80, 120.86, 107.15, 58.10, 57.72, 35.08, 35.04, 31.76, 31.73, 25.11, 24.75, 11.42, 11.10. **HRMS-ESI (m/z):** calculated for $C_{83}H_{79}N_7O_4Zn$: 1302.5558; found: 1302.5531.

NMR Spectra

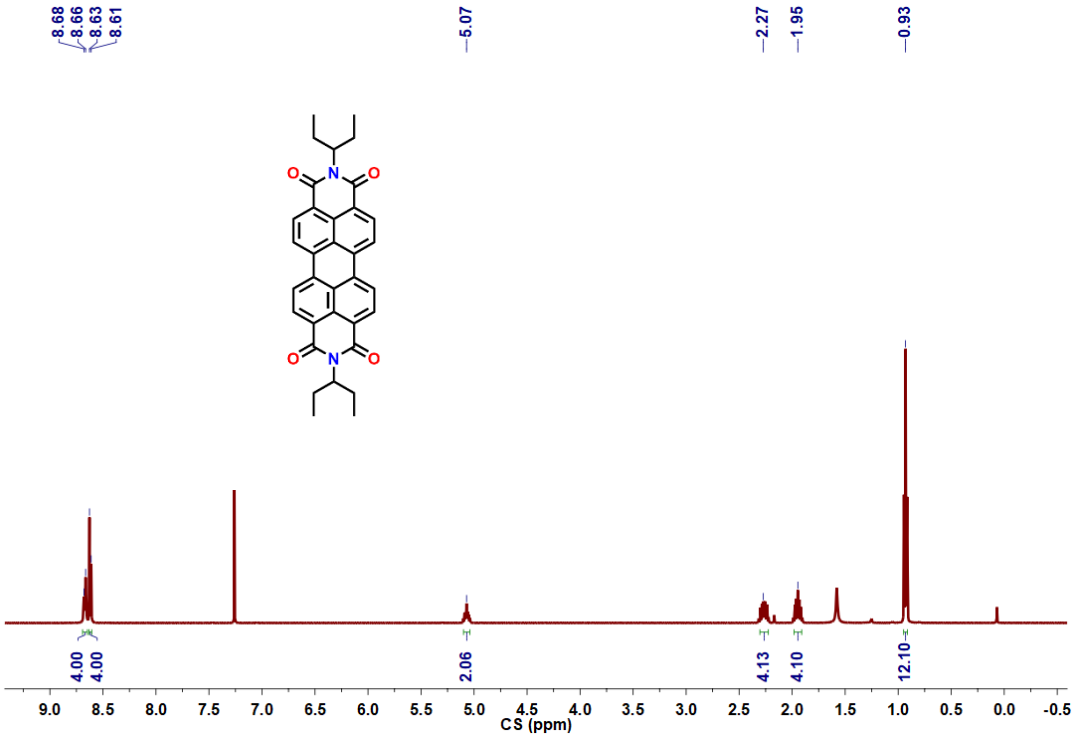


Figure S4. ^{1}H NMR spectra of **PBI** in $CDCl_3$ (500 MHz) at 298K

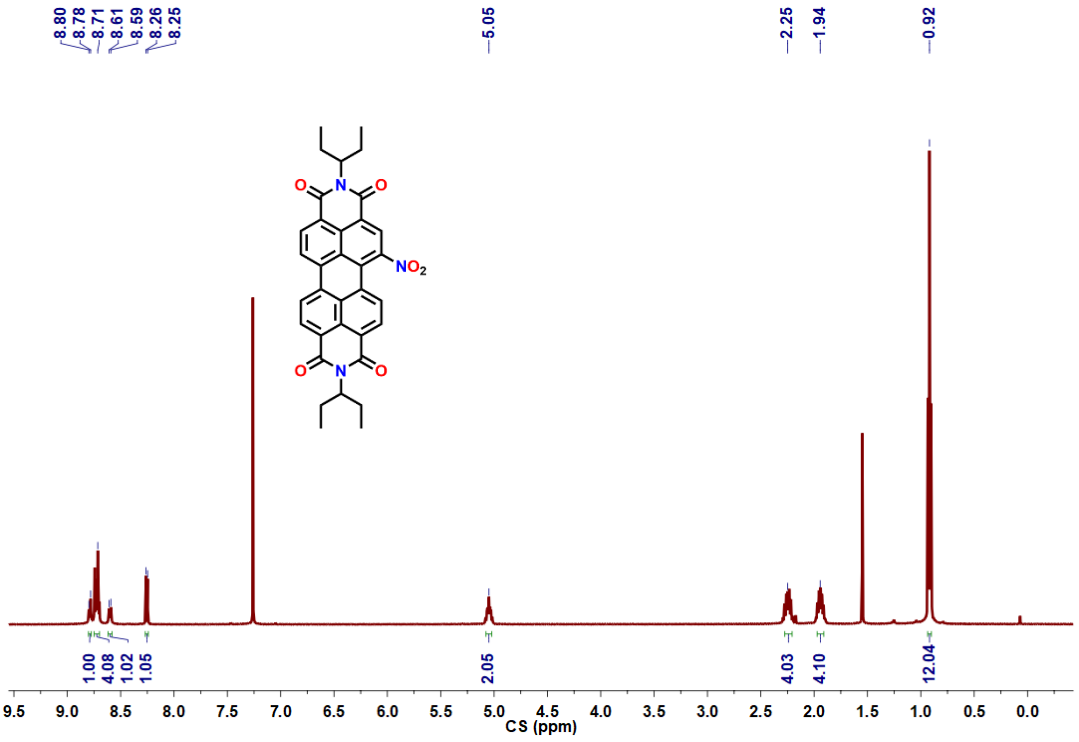


Figure S5. ^{1}H NMR spectra of **PBNT** in $CDCl_3$ (500 MHz) at 298K

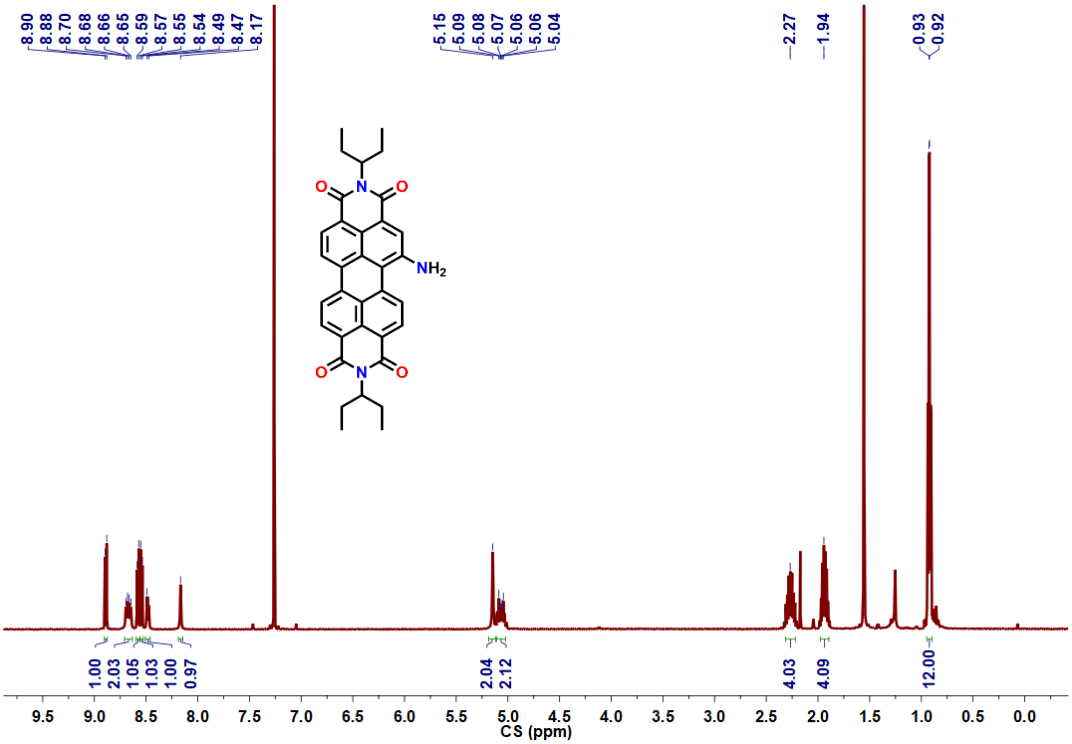


Figure S6. ^{1}H NMR spectra of **PBN** in $CDCl_3$ (500 MHz) at 298K

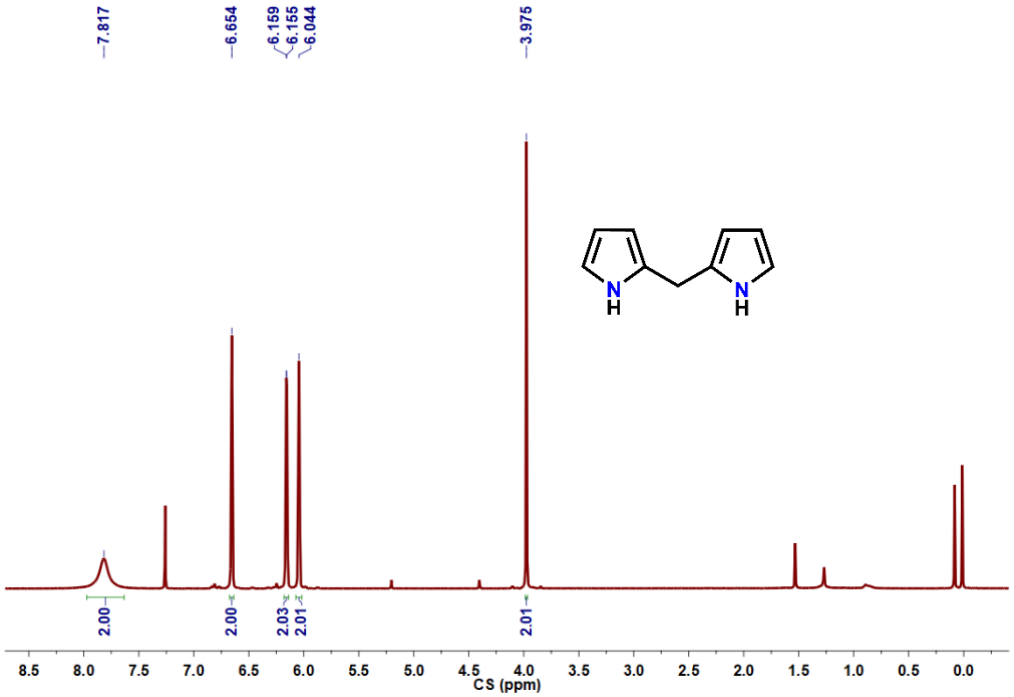


Figure S7. ^{1}H NMR spectra of **DPM** in $CDCl_3$ (500 MHz) at 298K

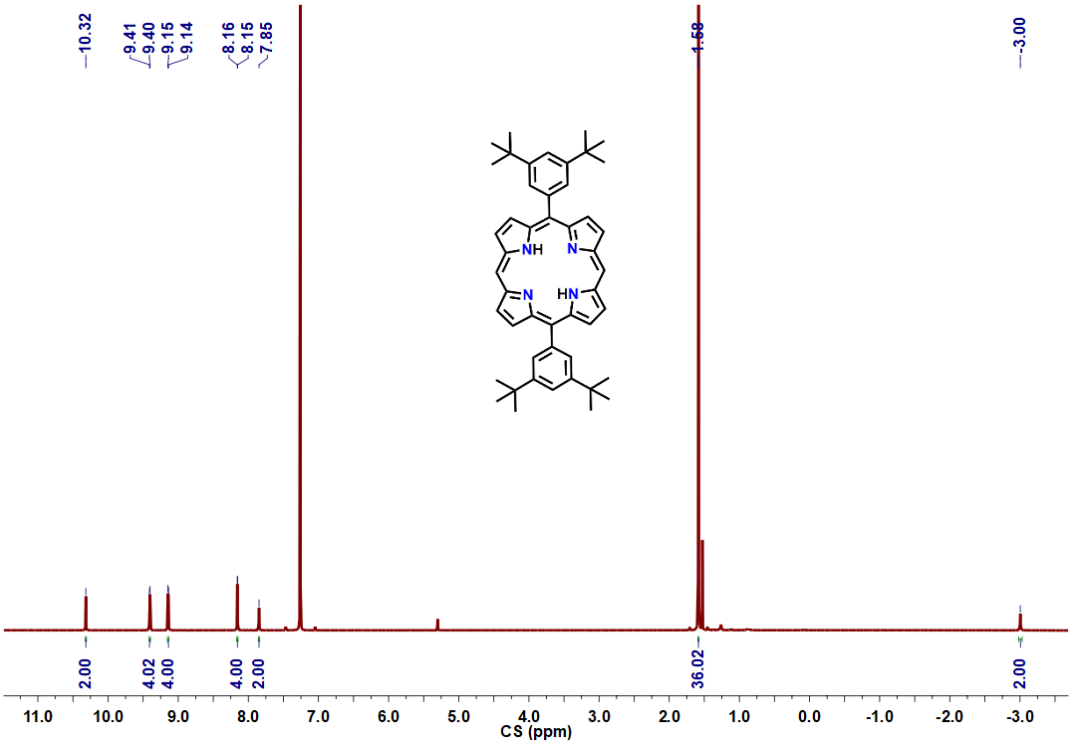


Figure S8. ^{1}H NMR spectra of **PORP** in $CDCl_3$ (500 MHz) at 298K

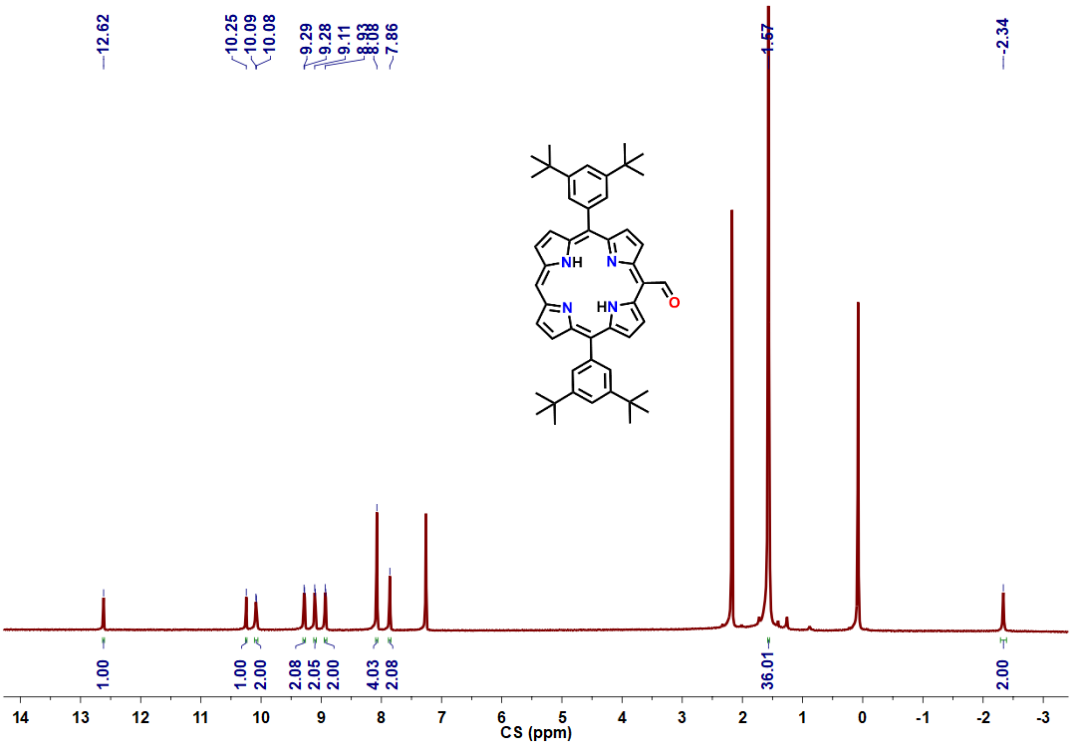


Figure S9. ^{1}H NMR spectra of **PCHO** in $CDCl_3$ (500 MHz) at 298K

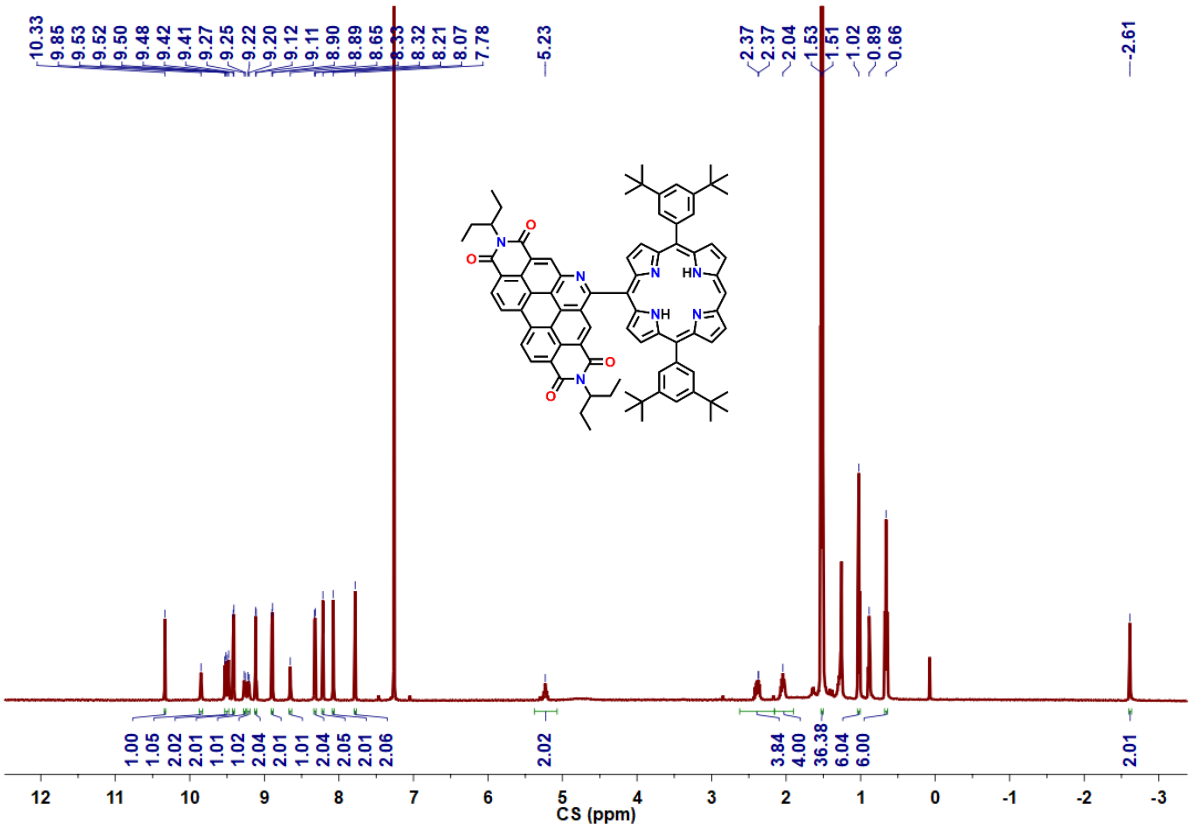


Figure S10. ^{1}H NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

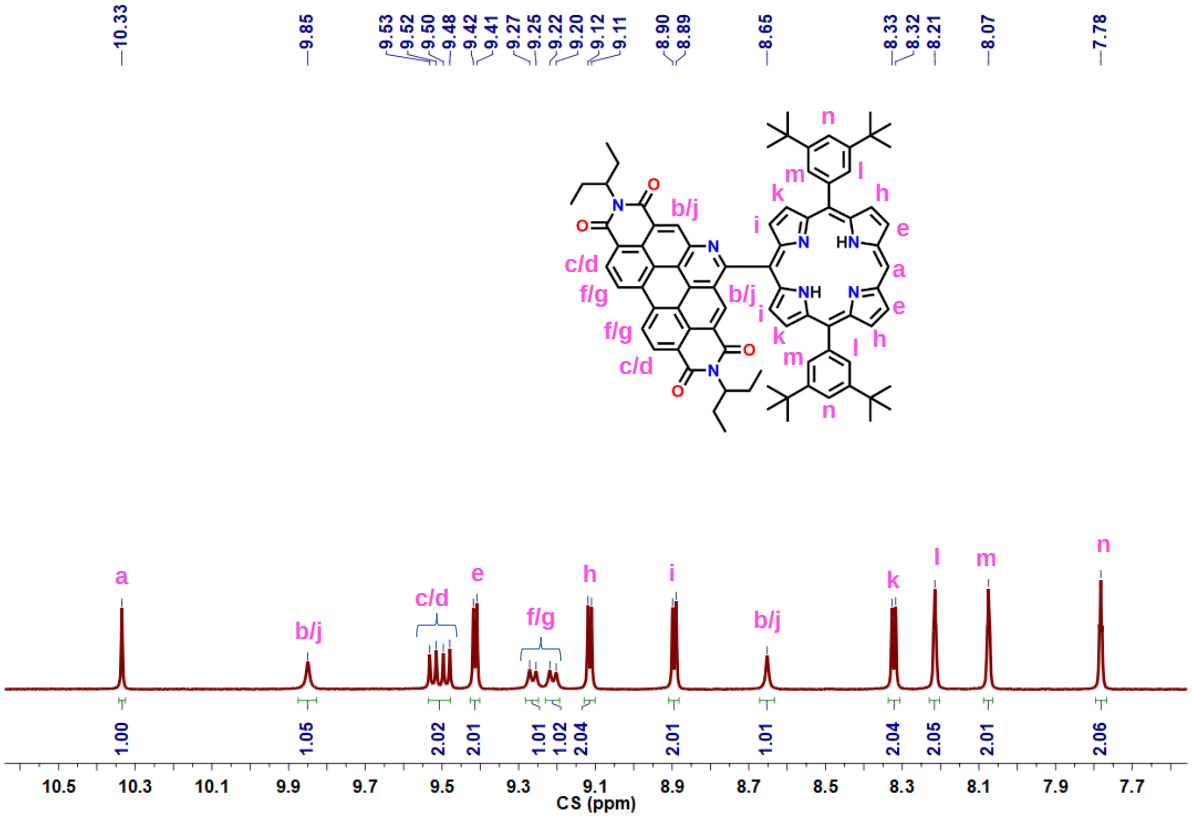


Figure S11. Partial ^{1}H NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

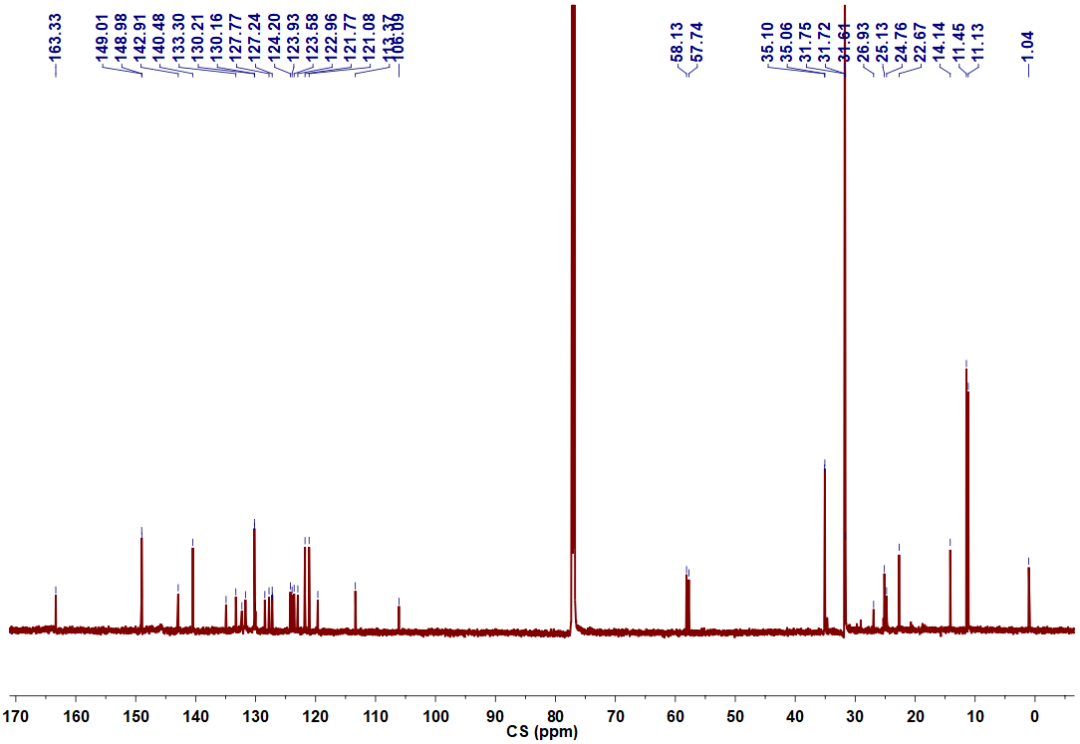


Figure S12. $^{13}C\{^{1}H\}$ NMR spectra of **PDPP** in $CDCl_3$ (175MHz) at 298K

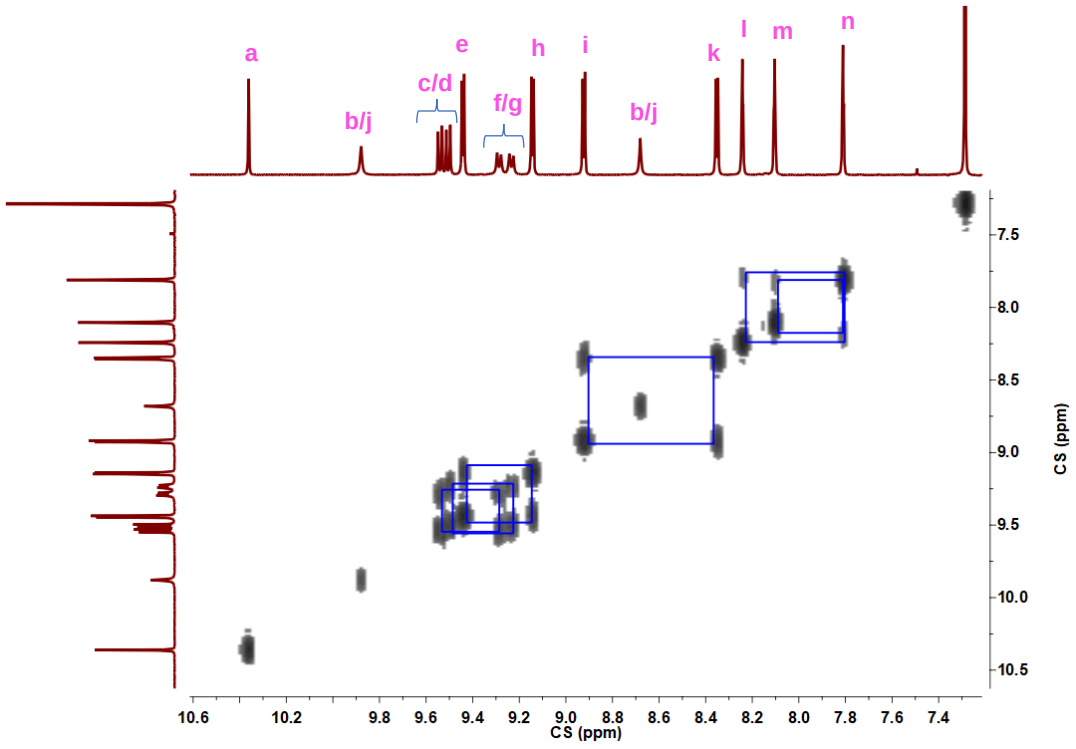


Figure S13. ^{1}H-^{1}H COSY NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

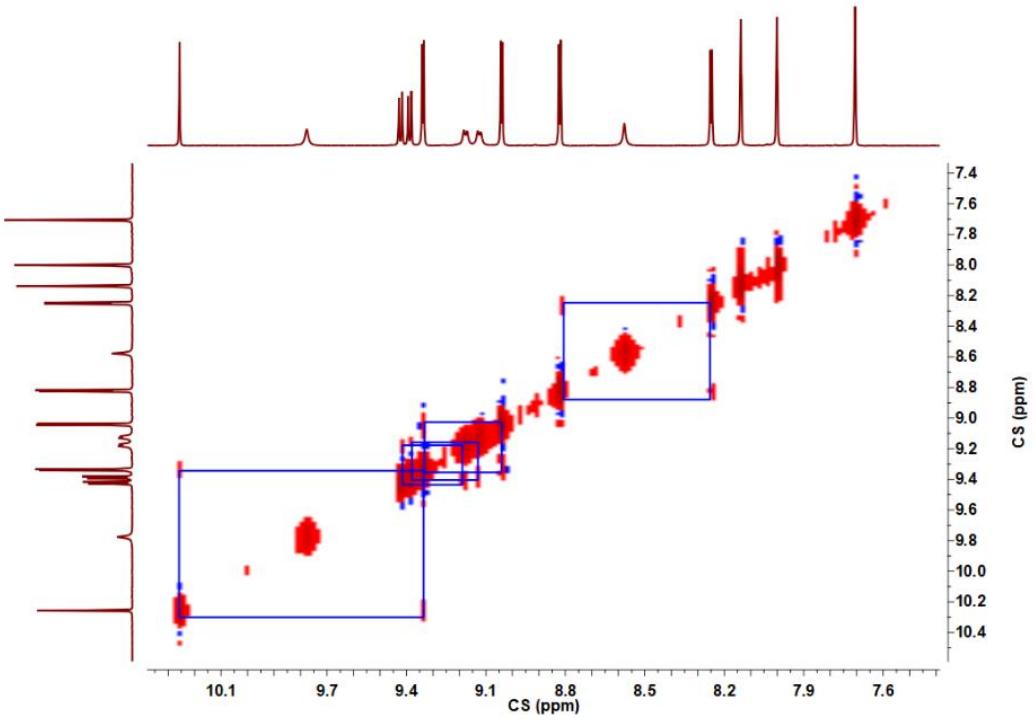


Figure S14. ^{1}H-^{1}H NOESY NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

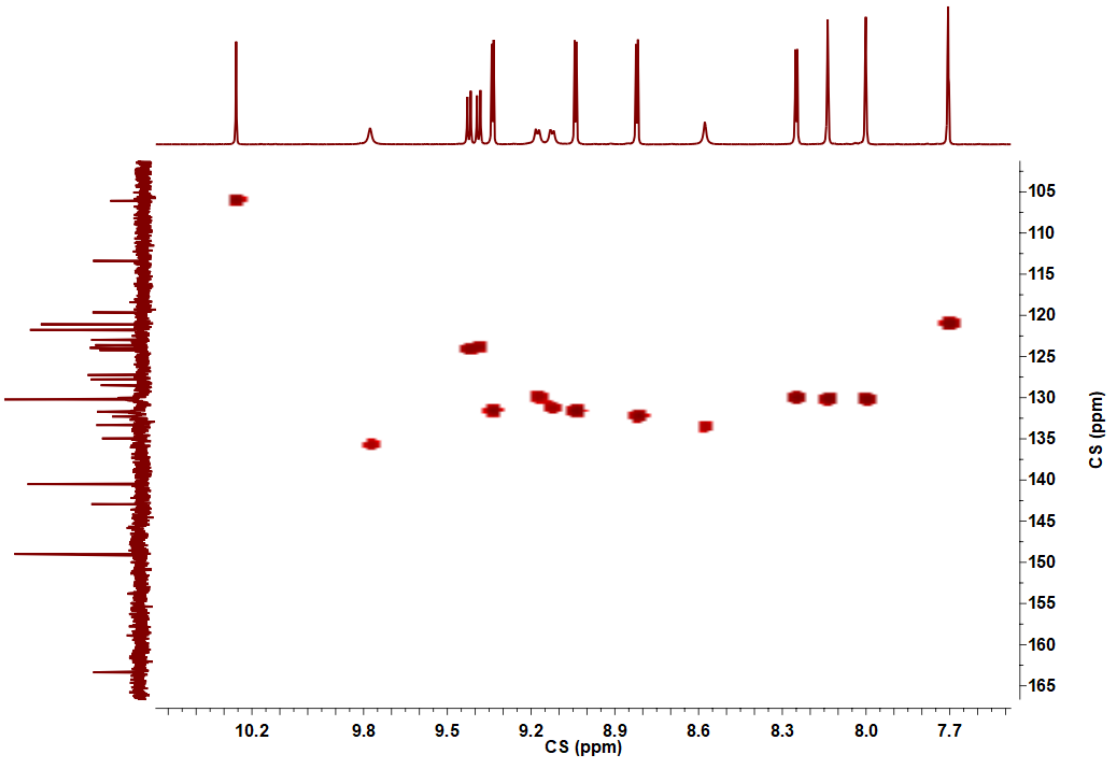


Figure S15. ^{1}H-^{13}C HSQC NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

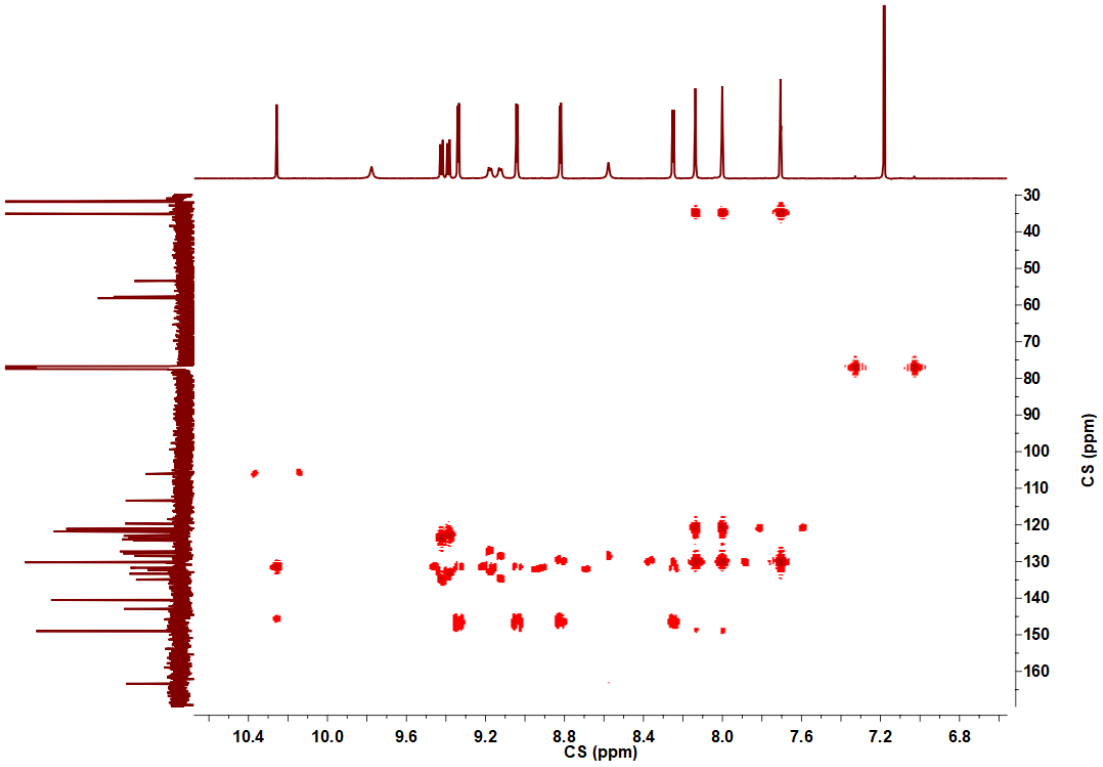


Figure S16. ^{1}H-^{13}C HMBC NMR spectra of **PDPP** in $CDCl_3$ (500 MHz) at 298K

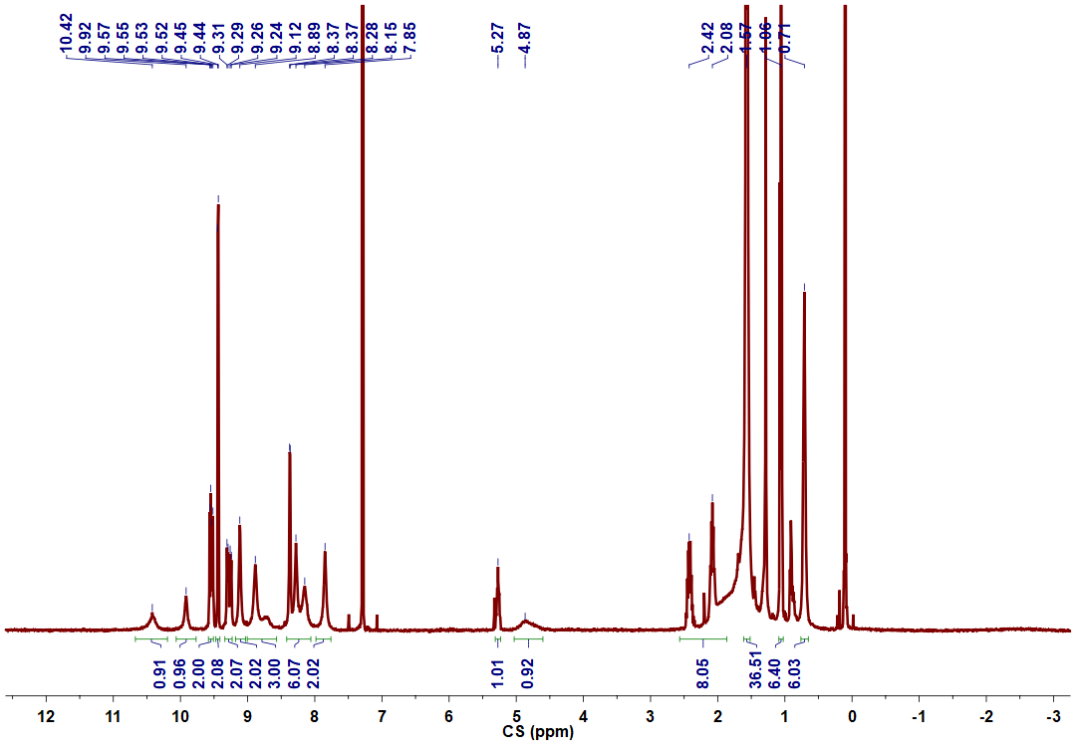


Figure S17. ^{1}H-NMR spectra of **PDPP** with TFA in $CDCl_3$ (500 MHz) at 298K

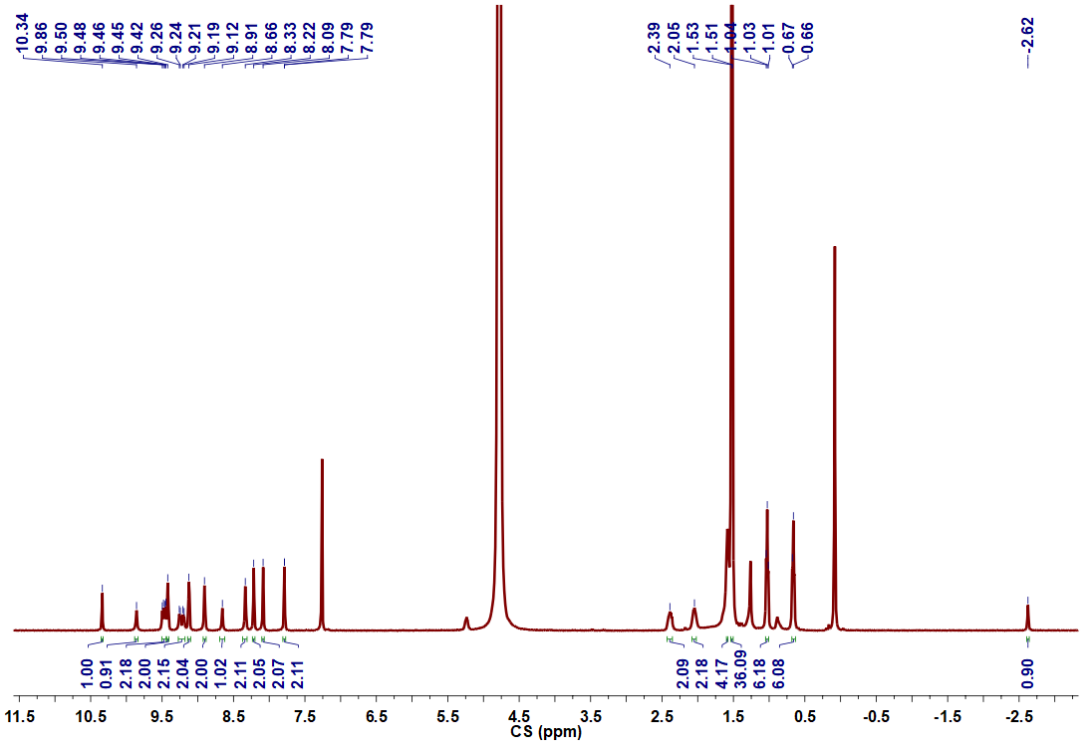


Figure S18. ^{1}H-NMR spectra of **PDPP** with D_2O in $CDCl_3$ (500 MHz) at 298K

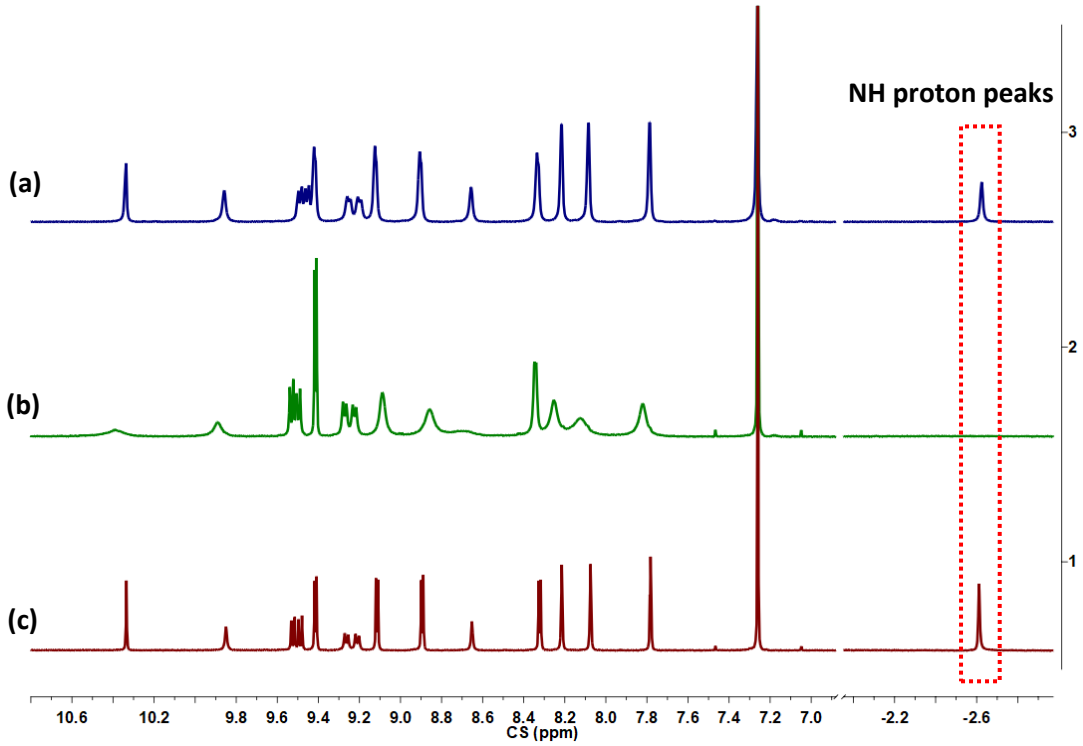


Figure S19. Partial ^{1}H-NMR spectra of **PDPP (c)** with D_2O **(a)** and TFA **(b)** in $CDCl_3$ (500 MHz) at 298K

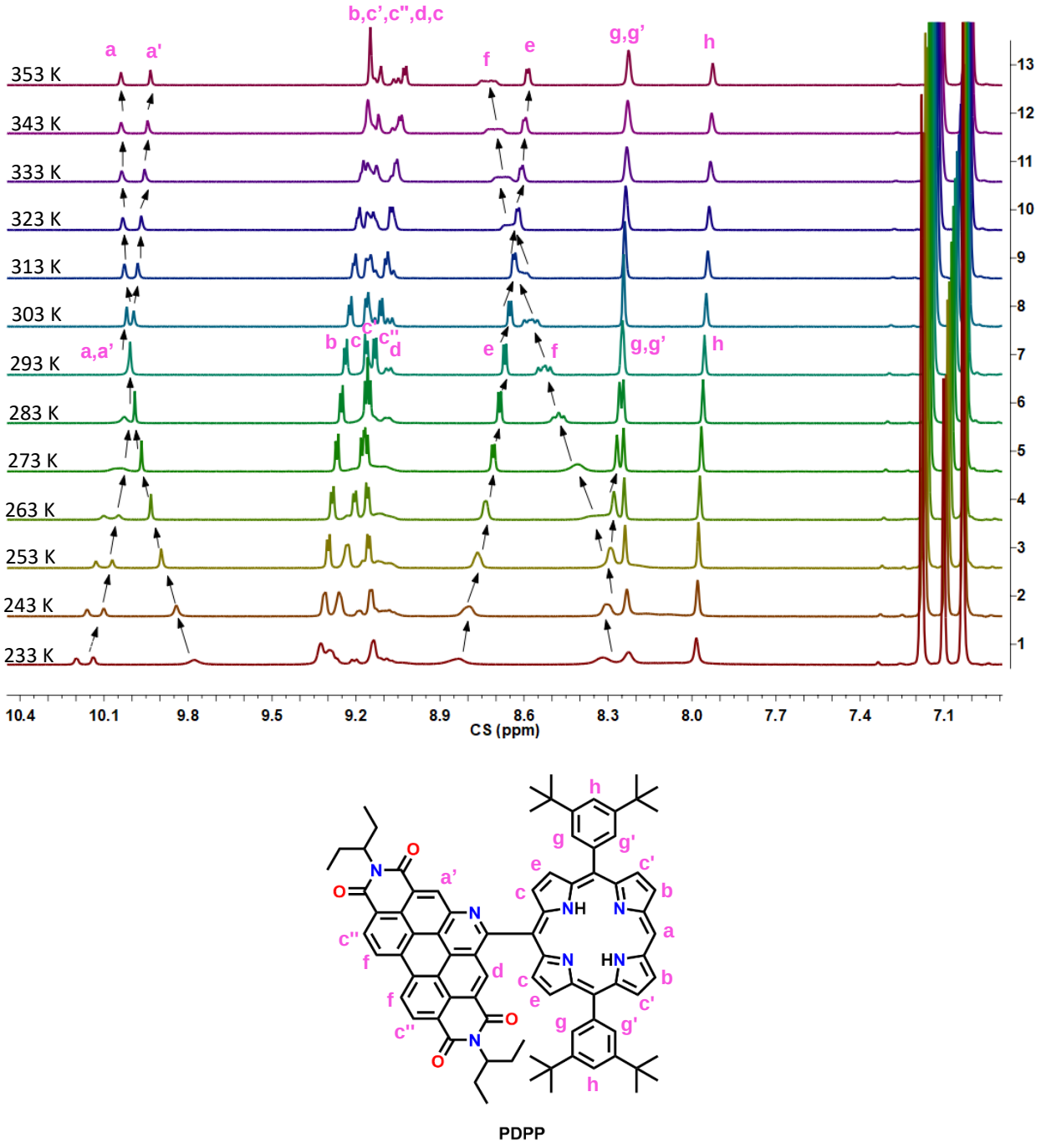


Figure S20. VT-^{1}H NMR spectra of **PDPP** in Toluene-D_8 (500 MHz) (arrows indicate the change in peak positions with temperature)

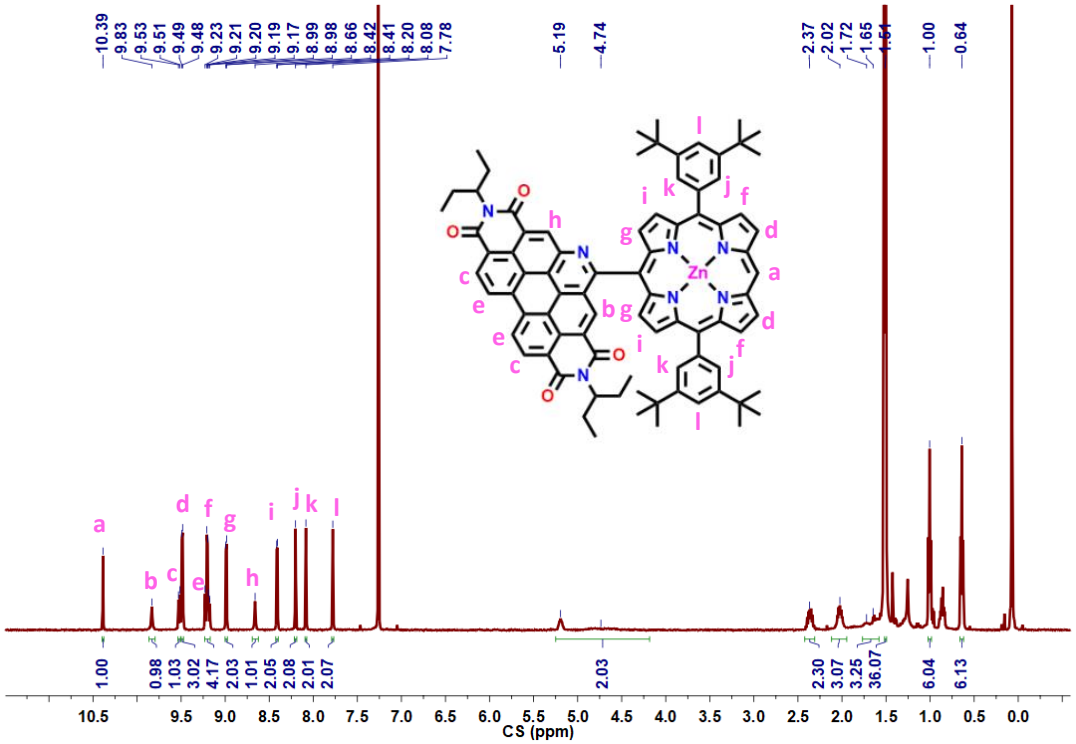


Figure S21. ^{1}H NMR spectra of **Zn-PDPP** in $CDCl_3$ (500 MHz) at 298K

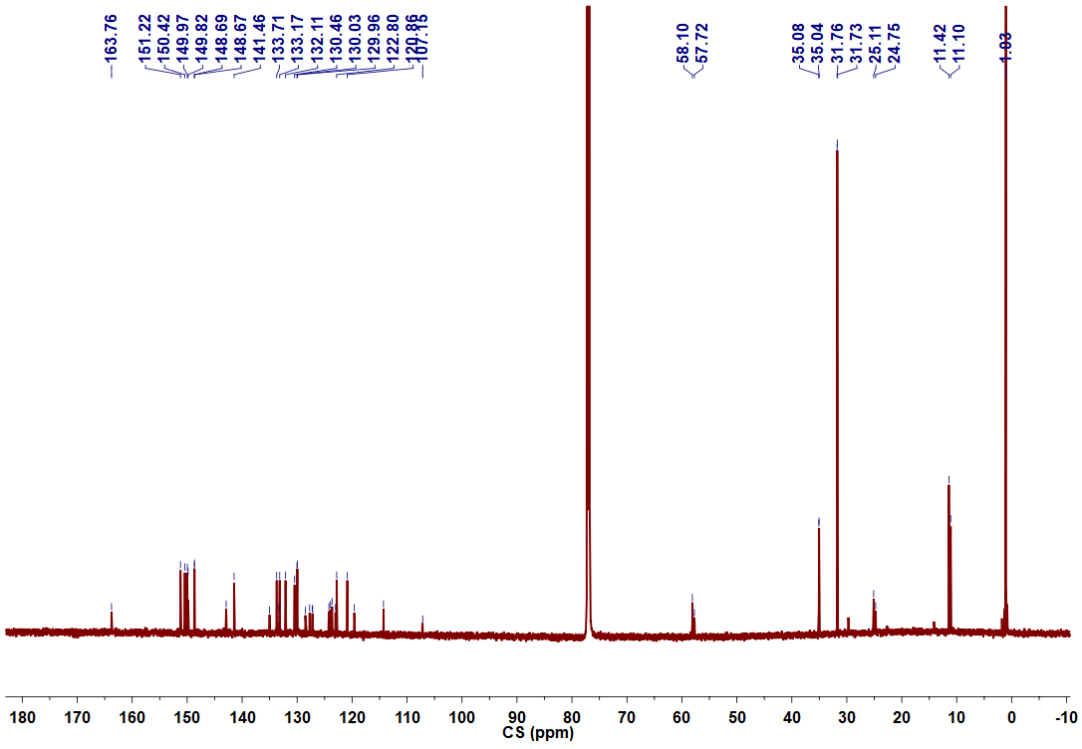


Figure S22. ^{13}C{^{1}H} NMR spectra of **Zn-PDPP** in $CDCl_3$ (175MHz) at 298K

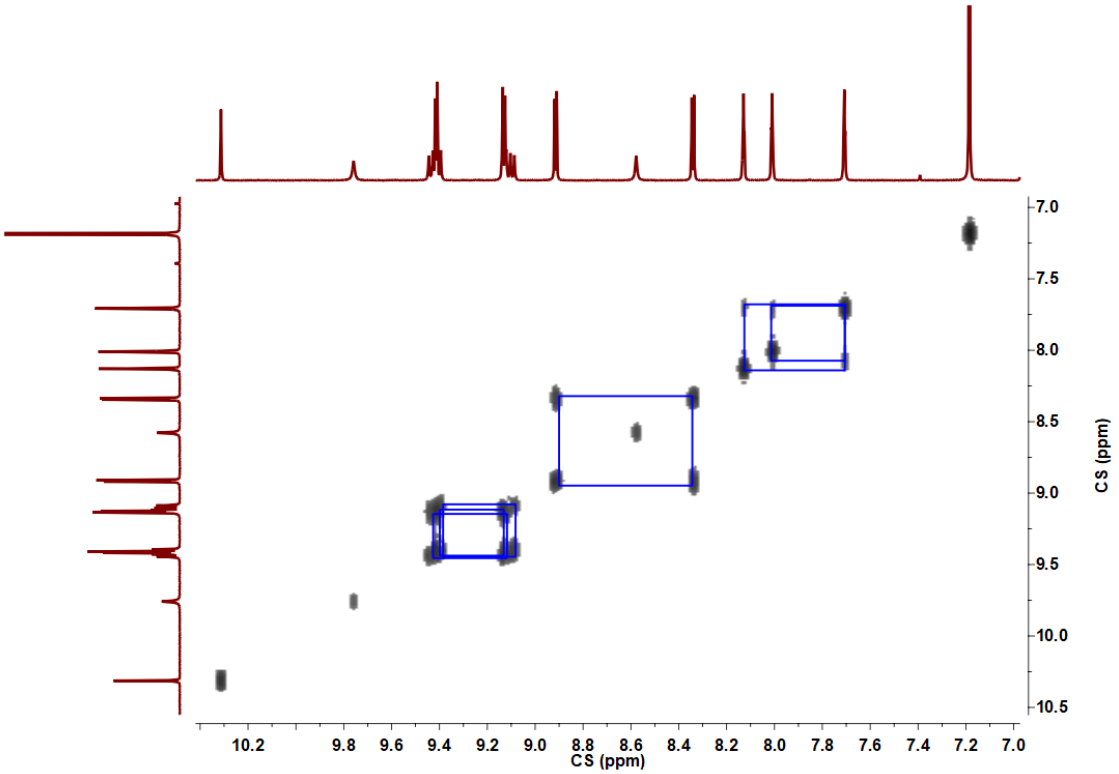


Figure S23. ^{1}H-^{1}H COSY NMR spectra of **Zn-PDPP** in $CDCl_3$ (500 MHz) at 298K

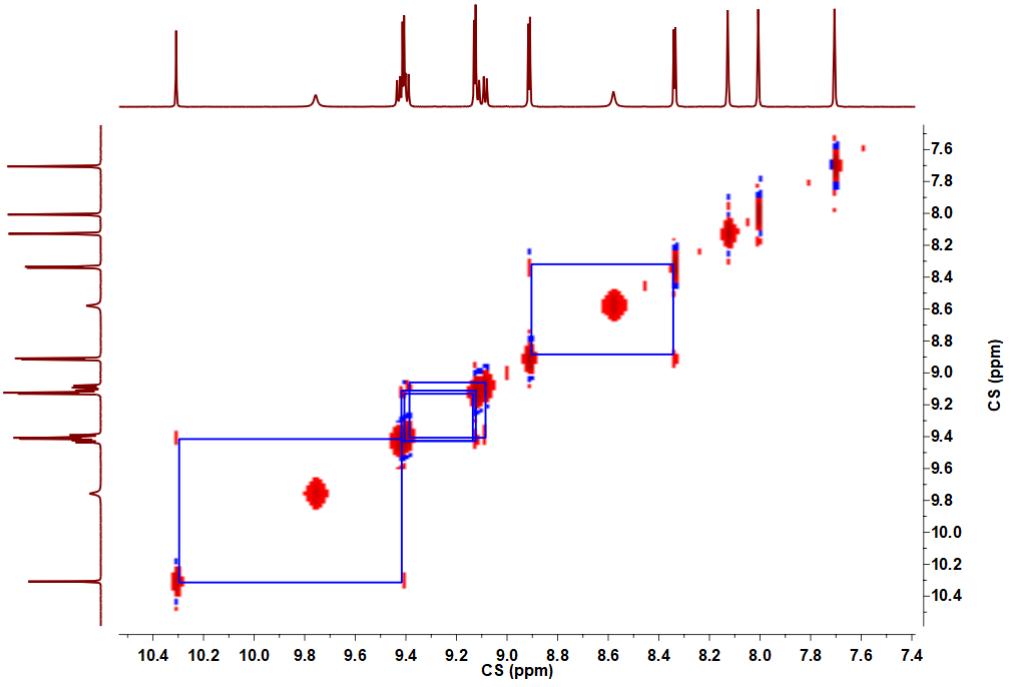


Figure S24. ^{1}H-^{1}H NOESY NMR spectra of **Zn-PDPP** in $CDCl_3$ (500 MHz) at 298K

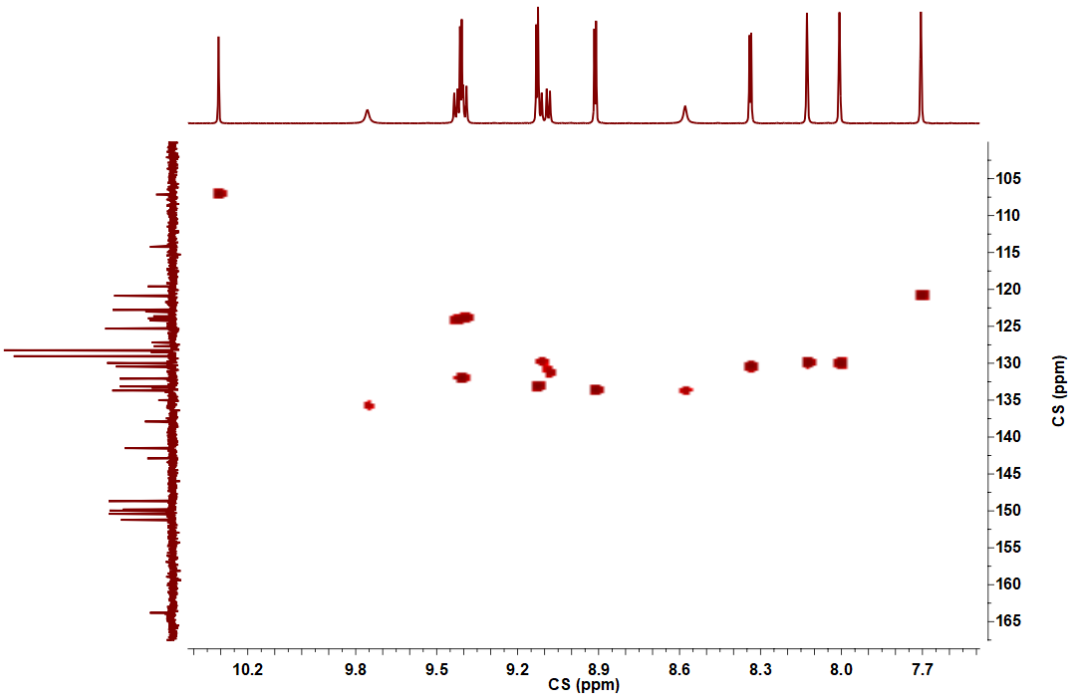


Figure S25. ^{1}H-^{13}C HSQC NMR spectra of **Zn-PDPP** in $CDCl_3$ (500 MHz) at 298K

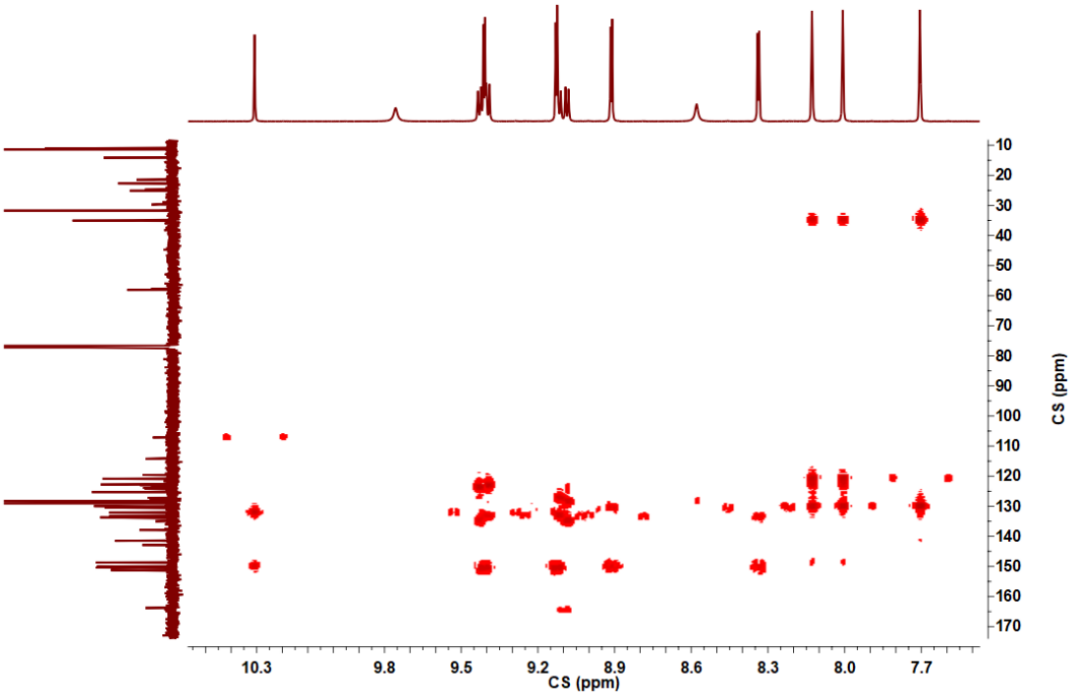


Figure S26. ^{1}H-^{13}C HMBC NMR spectra of **Zn-PDPP** in $CDCl_3$ (500 MHz) at 298K

Mass spectra

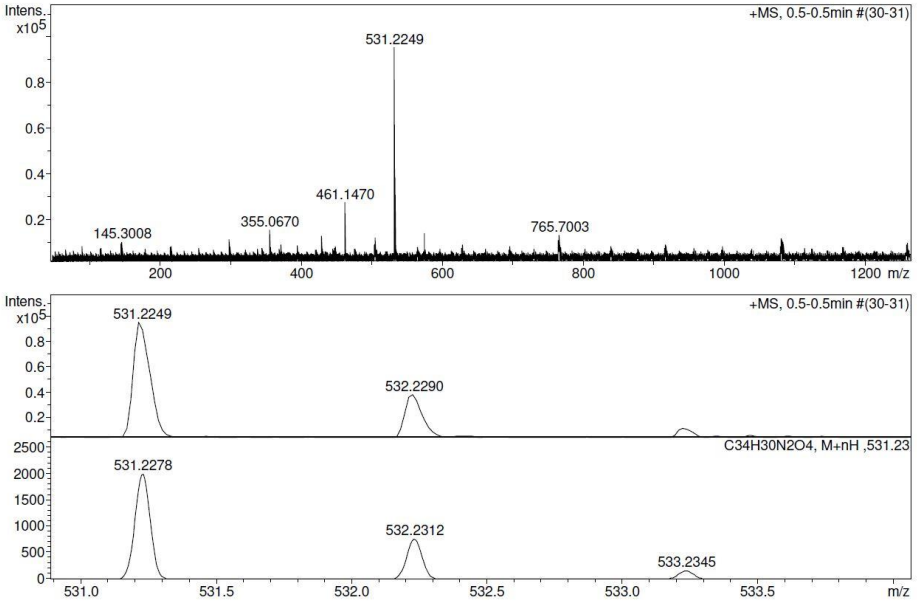


Figure S27. HRMS (ESI/Q-TOF) spectra of **PBI**

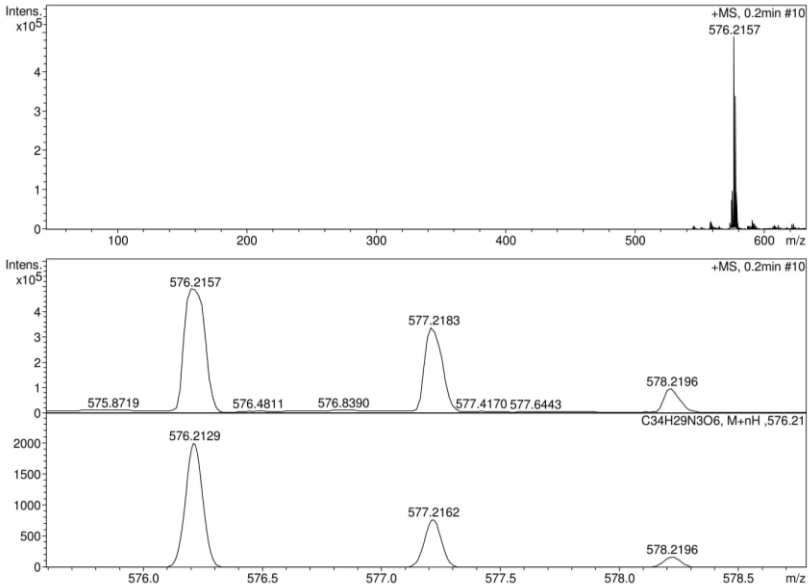


Figure S28. HRMS (ESI/Q-TOF) spectra of **PBNT**

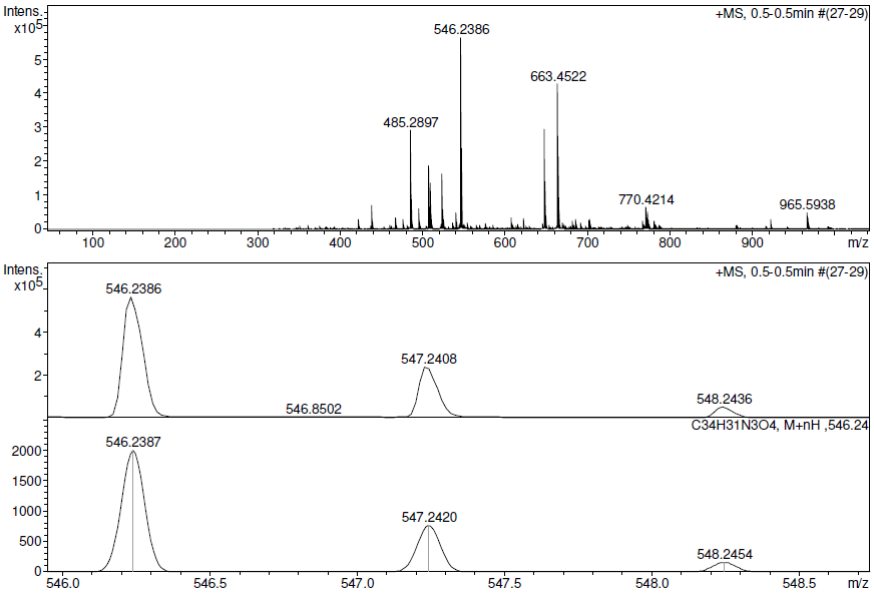


Figure S29. HRMS (ESI/Q-TOF) spectra of **PBN**

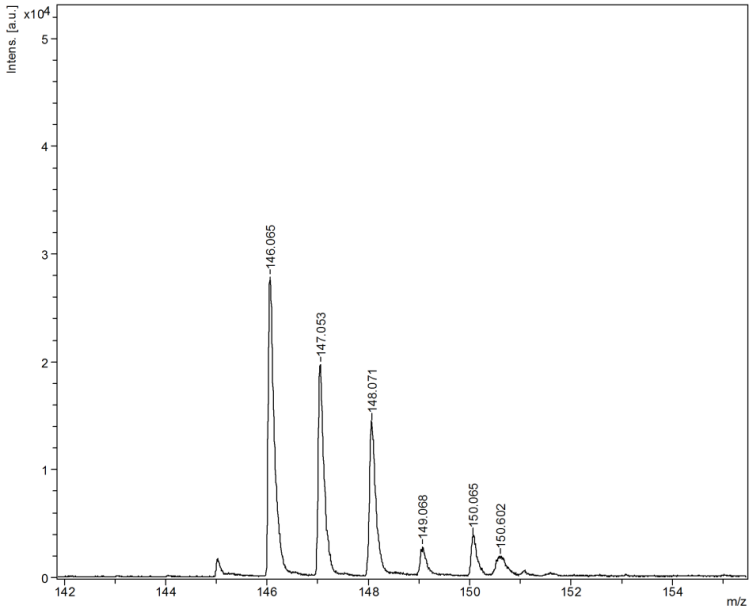


Figure S30. MALDI-TOF spectra of **DPM**

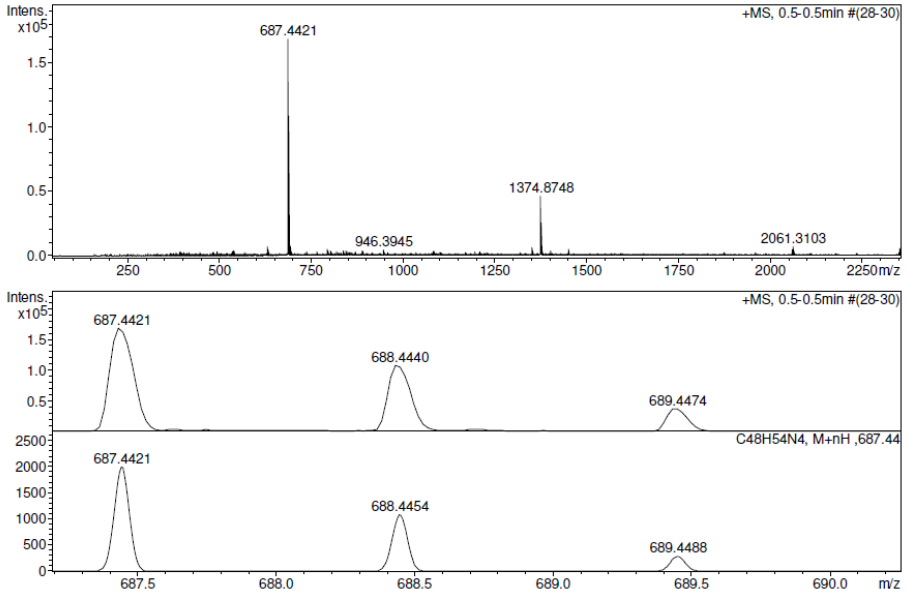


Figure S31. HRMS (ESI/Q-TOF) spectra of **PORP**

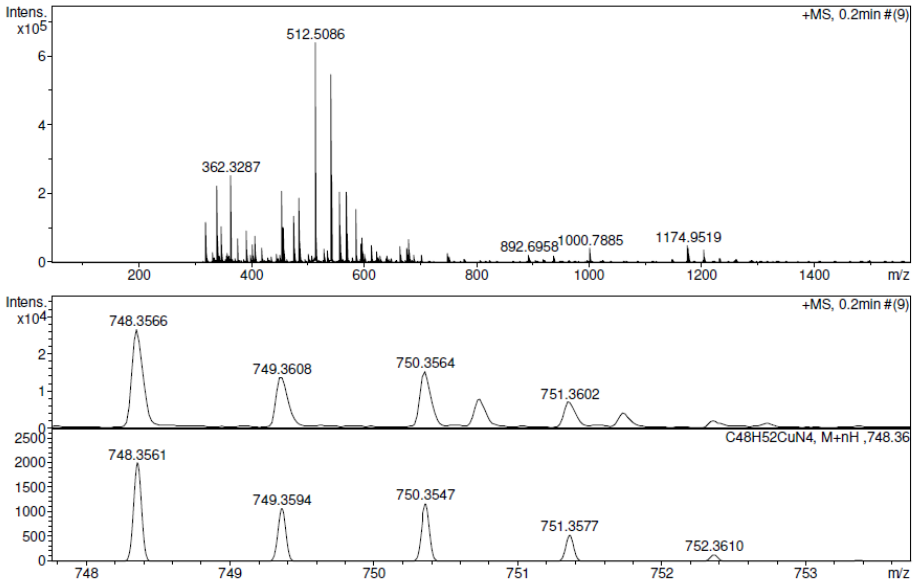


Figure S32. HRMS (ESI/Q-TOF) spectra of **Cu-PORP**

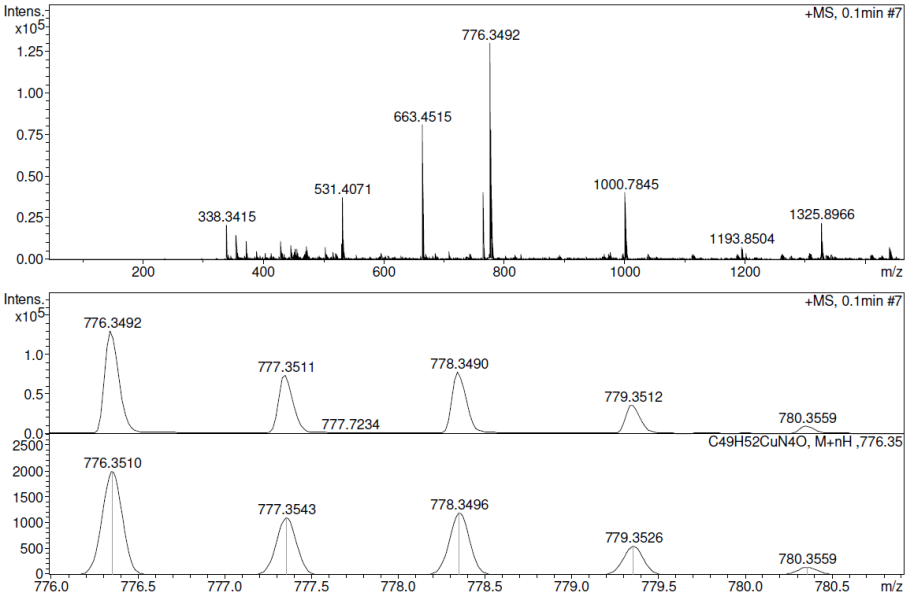


Figure S33. HRMS (ESI/Q-TOF) spectra of **CPHO**

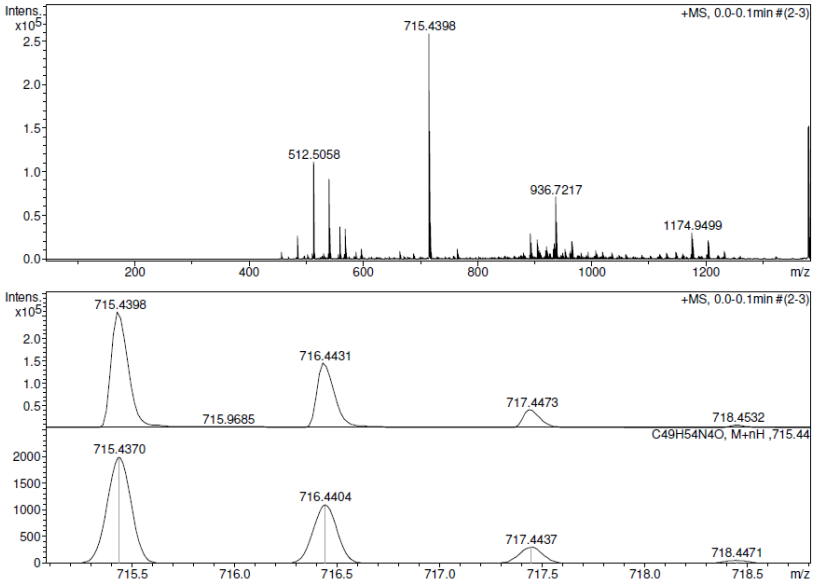


Figure S34. HRMS (ESI/Q-TOF) spectra of **PCHO**

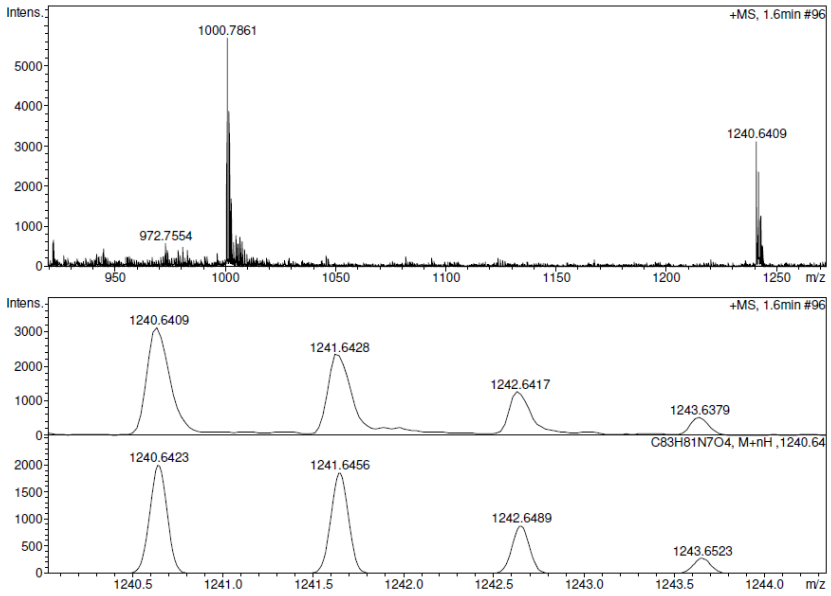


Figure S35. HRMS (APCI/Q-TOF) spectra of **PDPP**

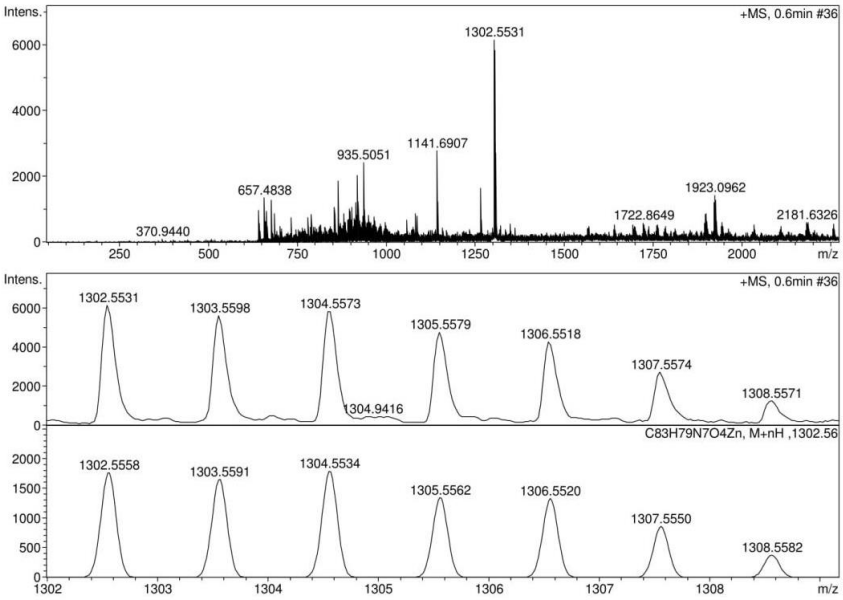


Figure S36. HRMS (APCI/Q-TOF) spectra of **Zn-PDPP**

Fourier Transform-infrared spectra

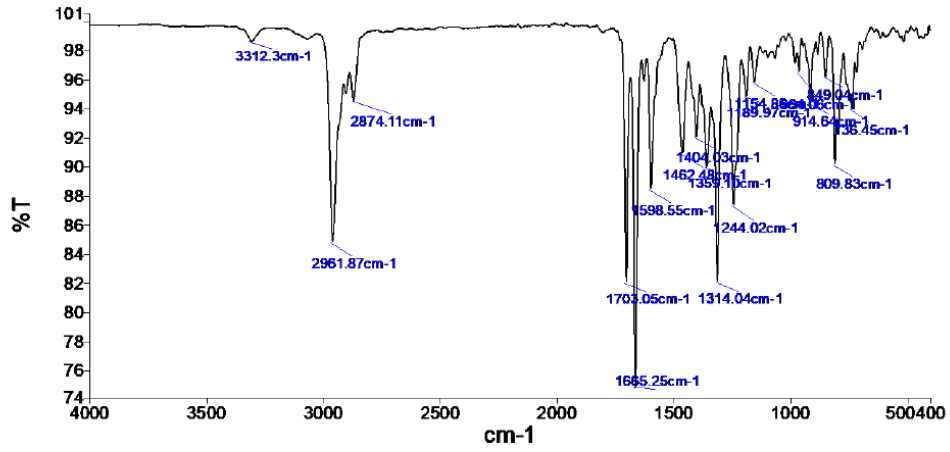


Figure S37. FT-IR spectra of the dyad **PDPP**

Absorption and emission spectra

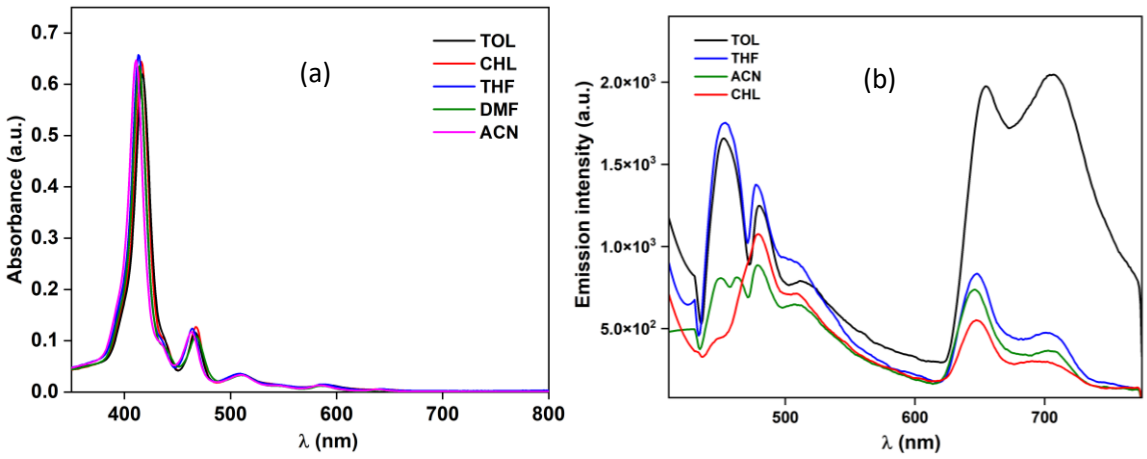


Figure S38. (a) Absorption spectra of **PDPP** in different solvents (b) Emission spectra of **PDPP** in different solvents when excited at 400 nm

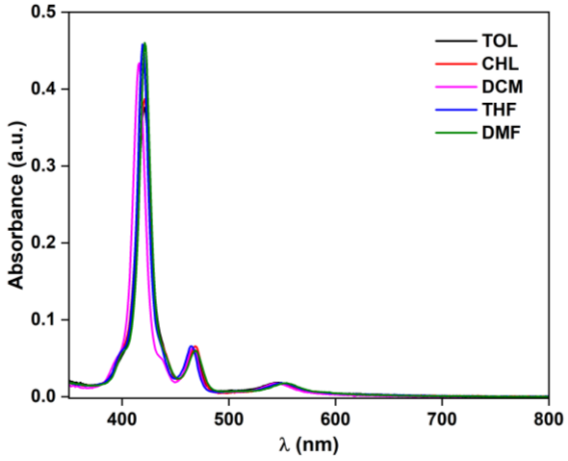


Figure S39. Absorption spectra of **Zn-PDPP** in different solvents

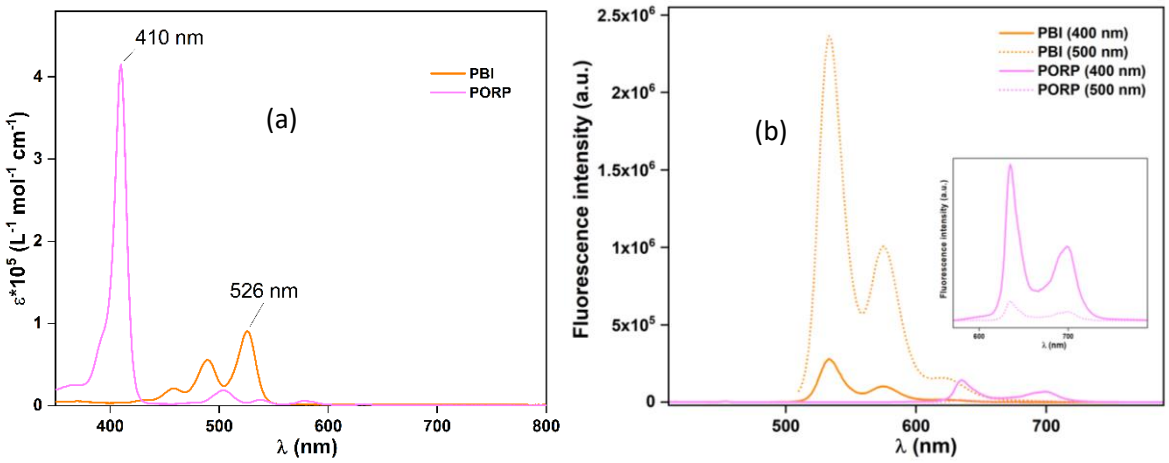


Figure S40. (a) Absorption and (b) emission spectra of **PORP** and **PBI** in toluene solution(10^{-6}M) when excited at 400 nm and 500 nm

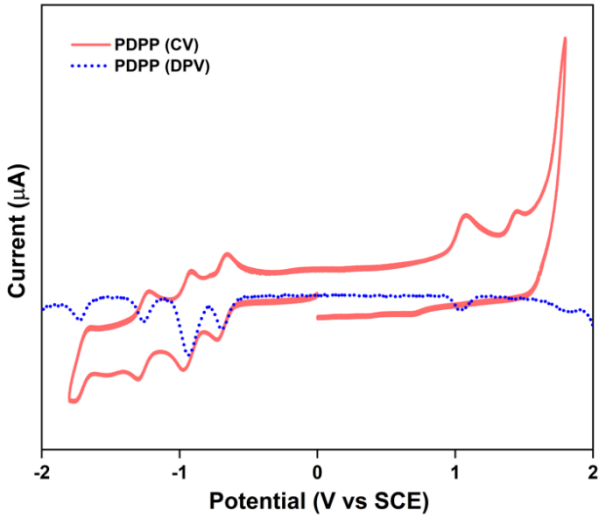


Figure S41. CV and DPV overlayed for **PDPP**

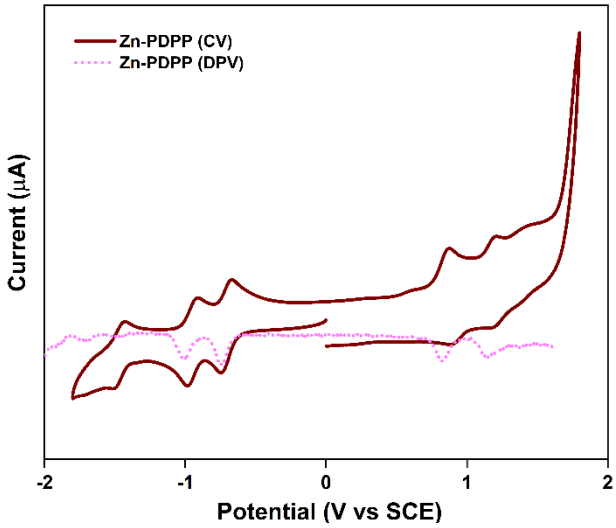


Figure S42. CV and DPV overlayed for **Zn-PDPP**

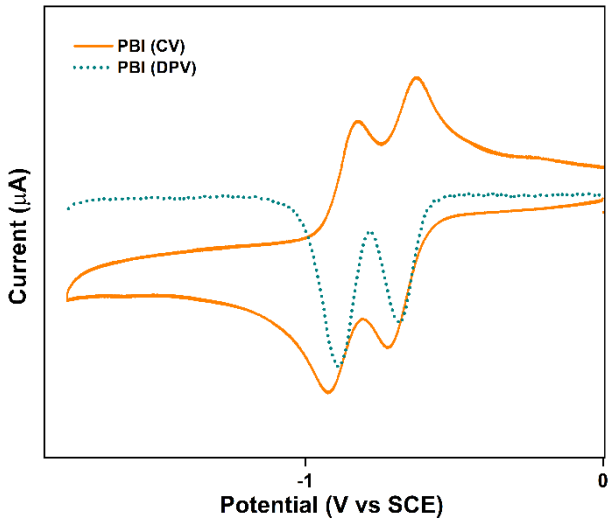


Figure S43. CV and DPV overlayed for **PBI**

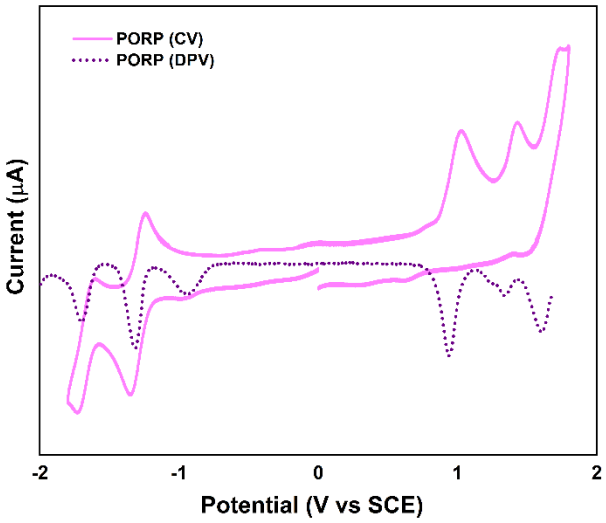


Figure S44. CV and DPV overlayed for **PORP**

Table S1. Table representing complete photophysical and electrochemical data for PBI, PORP, PDPP, and Zn-PDPP.

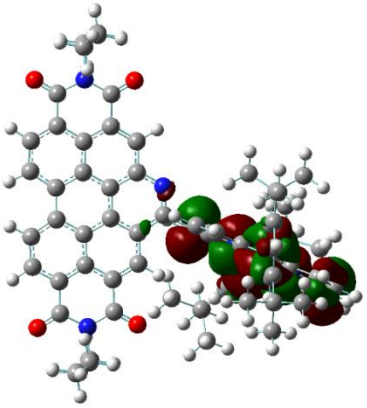
Compound	λ_{em}^{max} (nm) 400nm excitation	E_{opt} (eV)	$E_{1/2}^{red1}$ (V)	$E_{1/2}^{red2}$ (V)	$E_{1/2}^{red3}$ (V)	$E_{1/2}^{oxid1}$ (V)	$E_{1/2}^{oxid2}$ (V)	Band gap E_g (eV)
PDPP	707	1.84	-0.69	-0.94	-1.26	+1.03	+1.32	1.72
Zn-PDPP	-	1.74	-0.75	-1.01	-1.47	+0.82	+1.15	1.57
PBI	533	2.29	-0.69	-0.89	-	-	-	2.3
PORP	635	1.92	-0.94	-1.32	-1.70	+0.94	+1.61	1.88

$E_{1/2}^{red1}$, $E_{1/2}^{red2}$, and $E_{1/2}^{red3}$ represent the first, second, and third reduction potentials, respectively.

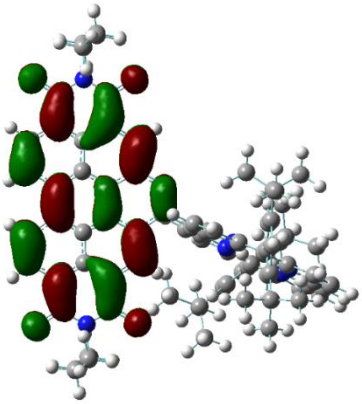
$E_{1/2}^{oxid1}$, and $E_{1/2}^{oxid2}$ represent the first and second oxidation potentials, respectively.

Density functional theory (DFT) calculations

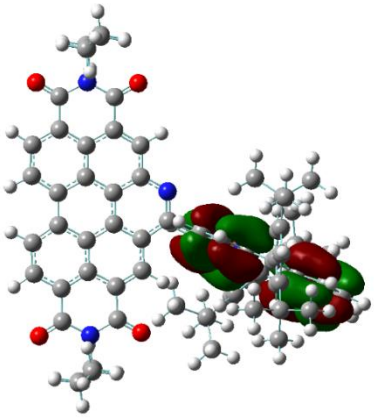
DFT Studies for PDPP



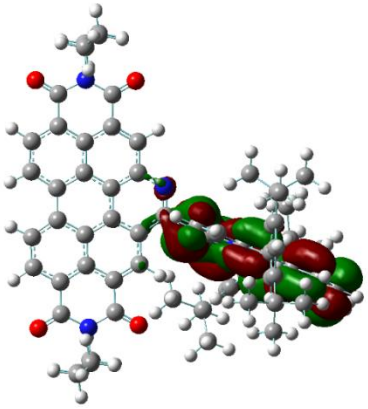
HOMO(PDPP)



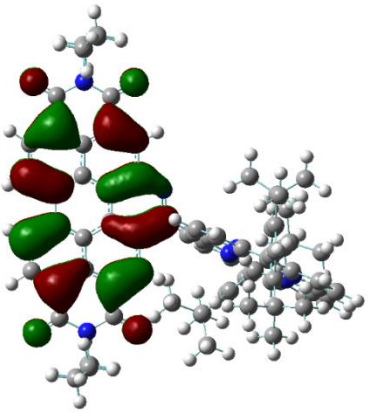
LUMO(PDPP)



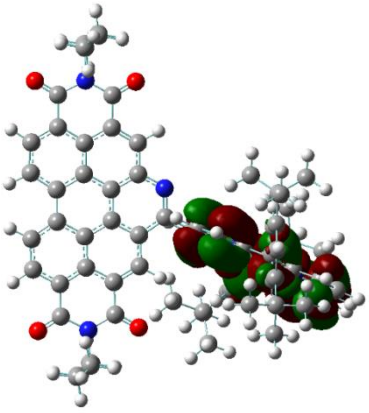
HOMO-1(PDPP)



LUMO+1(PDPP)

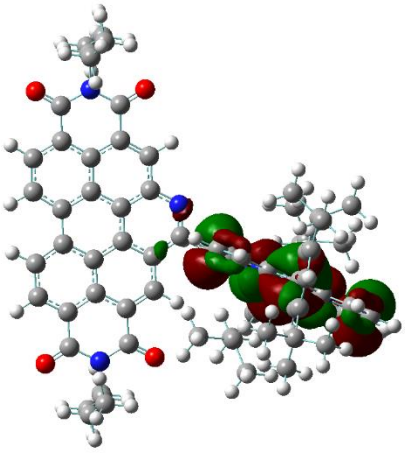


HOMO-2(PDPP)

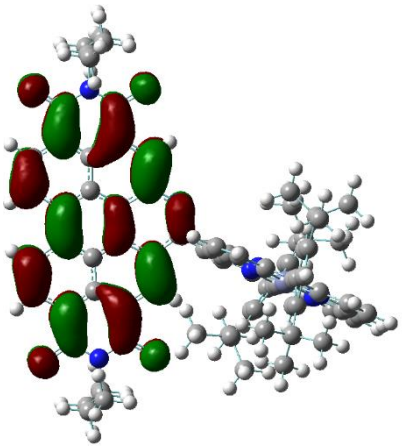


LUMO+2(PDPP)

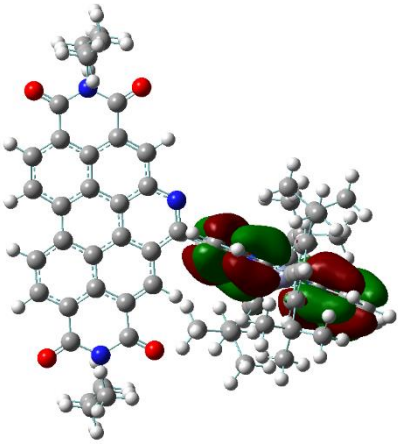
DFT Studies for Zn-PDPP



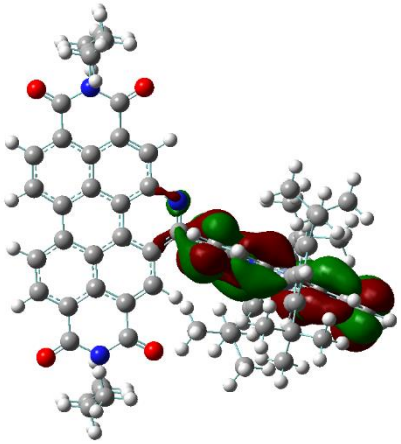
HOMO(Zn-PDPP)



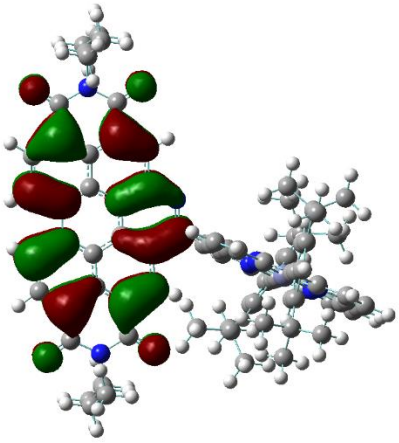
LUMO(Zn-PDPP)



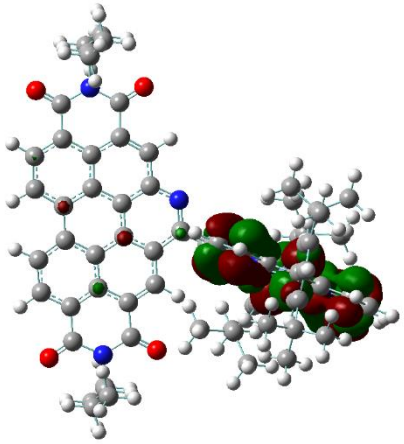
HOMO-1(Zn-PDPP)



LUMO+1(Zn-PDPP)



HOMO-2(Zn-PDPP)



LUMO+2(Zn-PDPP)

Single Crystal X-ray Diffraction Data:

Table S2. Crystal data and structure refinement for PDPP-triflate, and PDPP		
Identification code	**PDPP-triflate**	**PDPP**
CCDC No.	2255971	2255973
Empirical formula	$C_{85}H_{83}F_6N_7O_{10}S_2$	$C_{83}H_{81}N_7O_4$
Formula weight	1540.70	1240.54
Temperature/K	100(2)	100 (2)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	9.458(3)	19.447(11)
b/Å	16.868(5)	20.612(13)
c/Å	24.791(6)	21.648(16)
α/°	77.903(11)	84.15(3)
β/°	80.287(11)	88.97(4)
γ/°	85.773(12)	71.62(3)
Volume/Å^3	3809.0(18)	8191(9)
Z	2	4
ρ_{calc}g/cm^3	1.343	1.006
μ/mm^{-1}	0.150	0.062
F(000)	1616.0	2640.0
Crystal size/mm^3	0.17 × 0.08 × 0.06	0.14 × 0.08 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.784 to 52.044	4.07 to 50.7
Index ranges	$-11 \le h \le 11$, $-20 \le k \le 20$, $-30 \le l \le 30$	$-23 \le h \le 23$, $-24 \le k \le 24$, $-26 \le l \le 26$
Reflections collected	126468	274210
Independent reflections	15014 [R_{int} = 0.4030, R_{sigma} = 0.3283]	29972 [R_{int} = 0.7203, R_{sigma} = 0.4416]
Data/restraints/parameters	15014/187/1037	29972/1981/1886
Goodness-of-fit on F^2	1.021	0.900
Final R indexes [I>=2σ (I)]	R_1 = 0.1146, wR_2 = 0.2621	R_1 = 0.1213, wR_2 = 0.2901
Final R indexes [all data]	R_1 = 0.3382, wR_2 = 0.3737	R_1 = 0.3742, wR_2 = 0.4538
Largest diff. peak/hole / e Å^{-3}	1.08/-0.38	0.54/-0.49

Crystallographic images:

(a) **(b)**

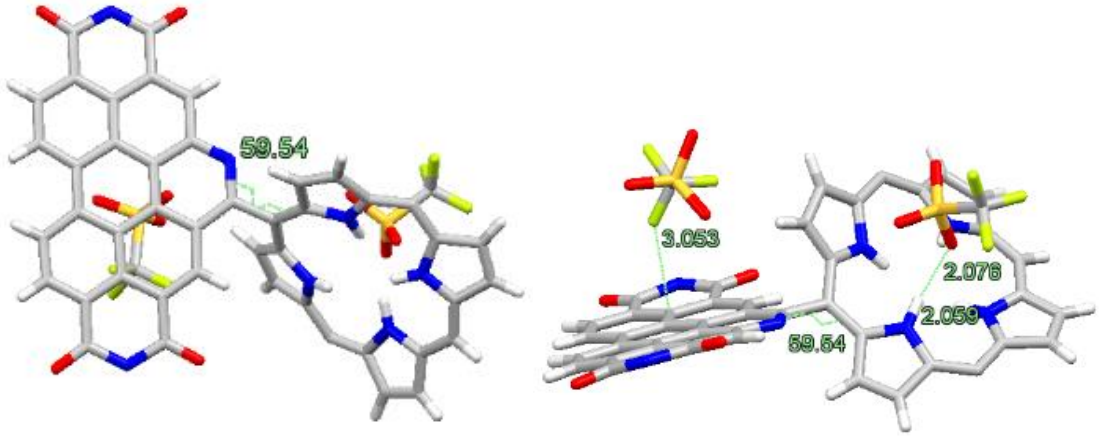
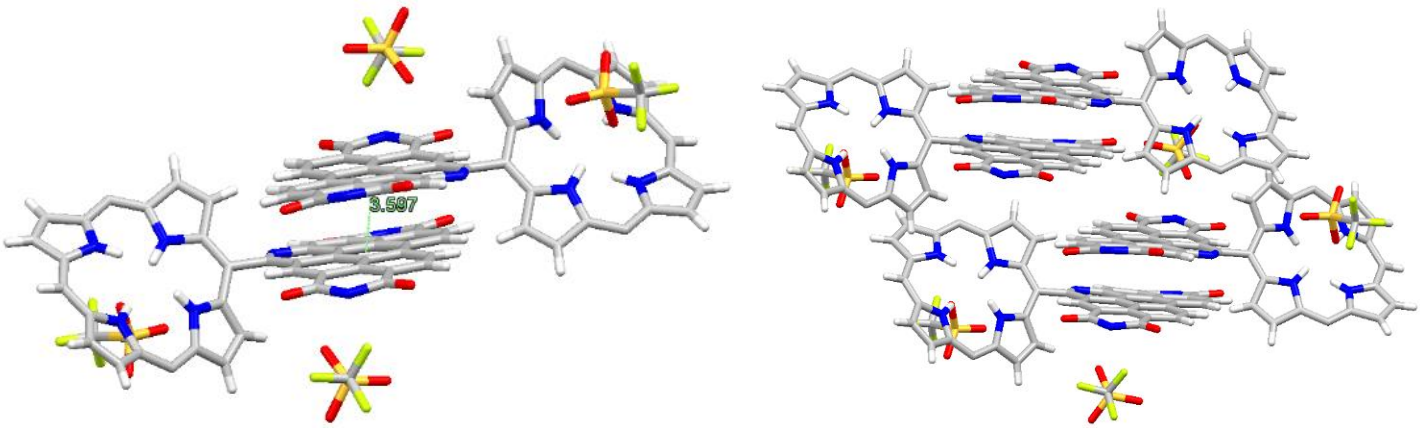


Figure S45. Crystal images for **PDPP-triflate** along different axes **(a)** and **(b).**

(a) **(b)**



(c)

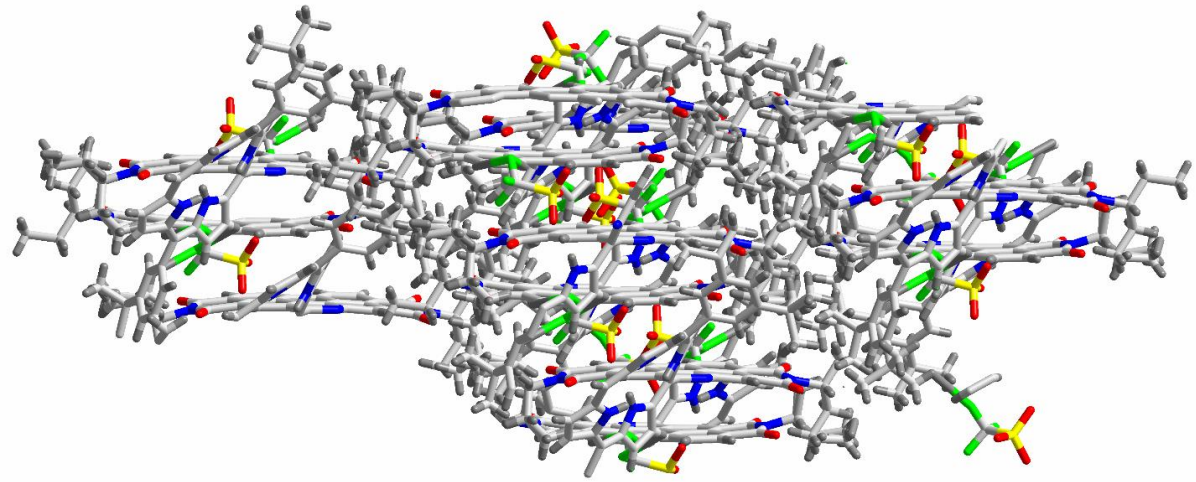
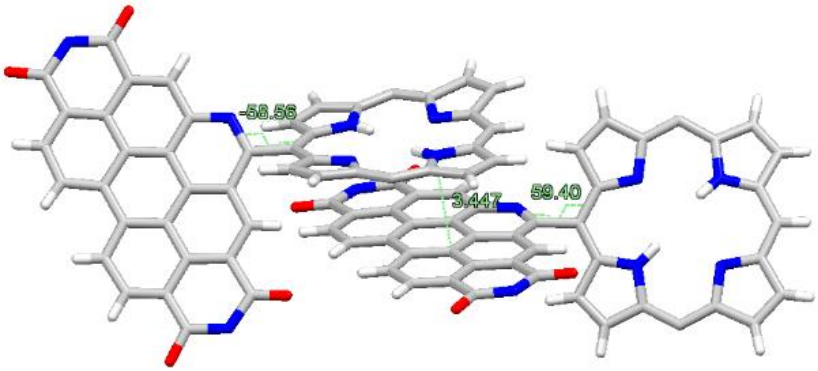


Figure S46. Crystal packing diagram for **PDPP-triflate** through different axes **(a), (b), (c).**

(a)



(b)

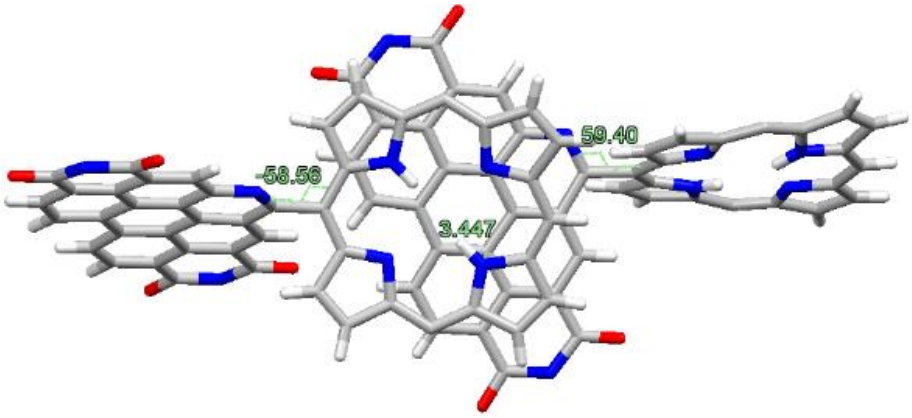
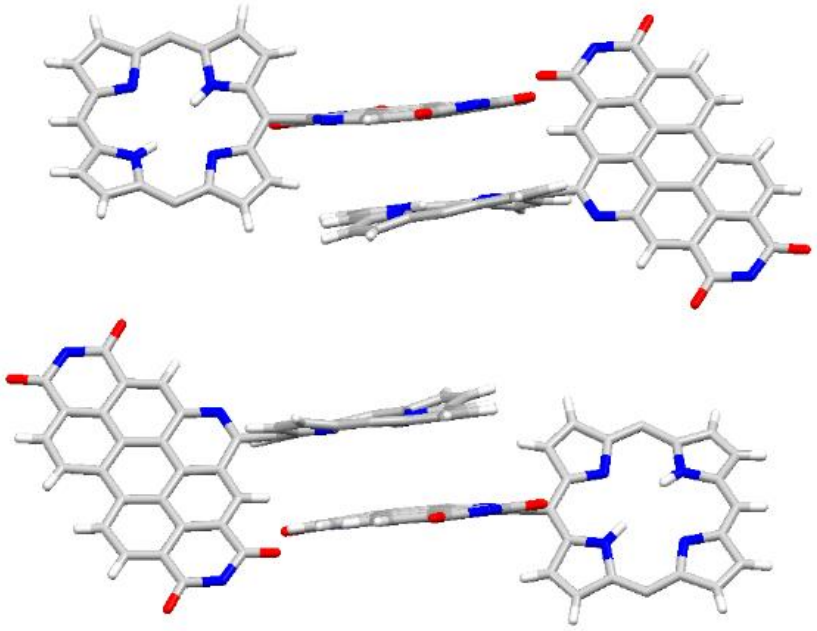
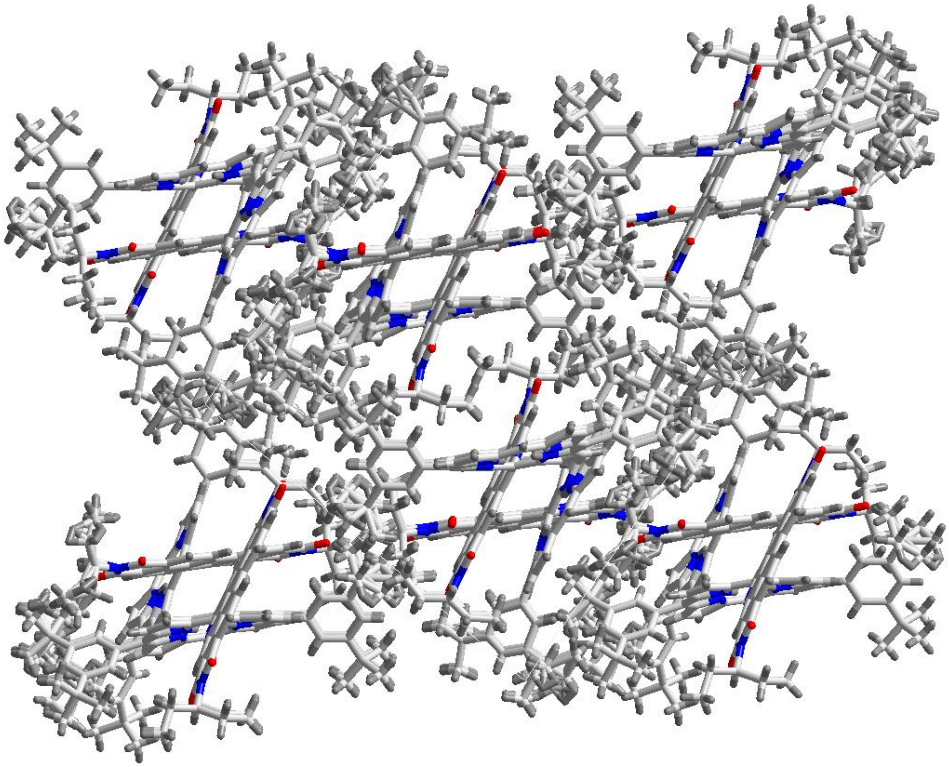


Figure S47. Crystal images for **PDPP** along different axes **(a)** and **(b).**

(a)



(b)



(c)

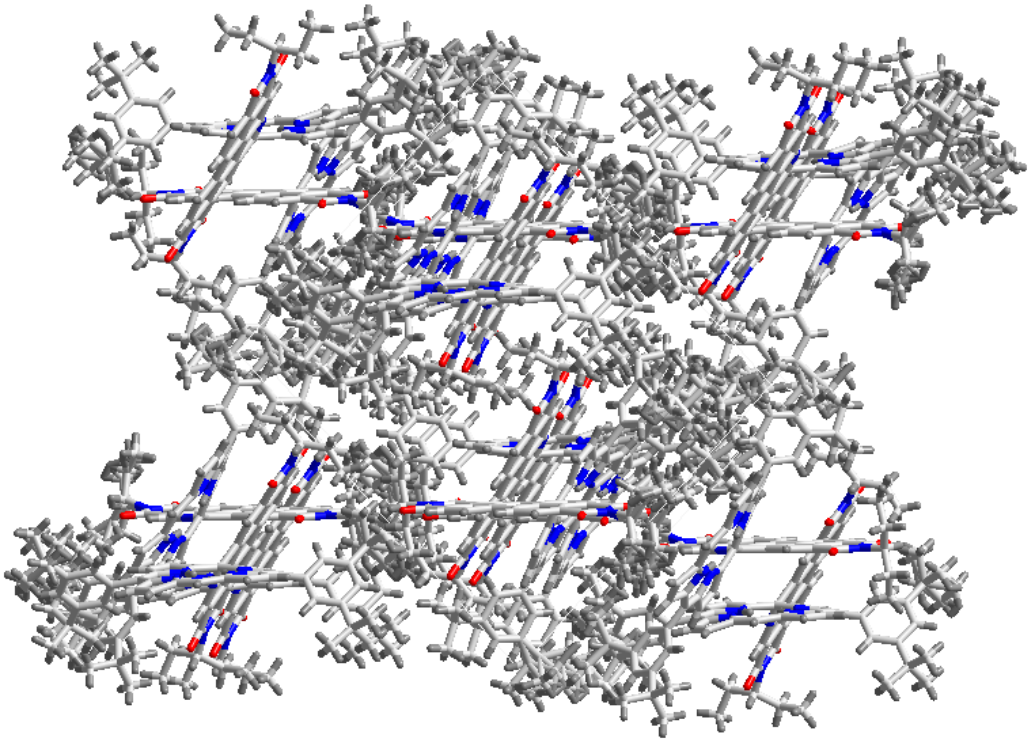


Figure S48. Crystal packing diagram for **PDPP** through different axes **(a), (b), (c).**

Mechanistic details for the formation of PDPP in a single step:

In the TFSA-catalyzed PSR with the 10,20-Bis(3,5-ditertbutylphenyl)-porphyrin-5-carboxaldehyde substrate, no intermediate was observed. The presence of strong oxidizing acid CF_3SO_3H (TFSA) leads to the formation of N-oxide iminium ion which activates the imine for cyclization under heating conditions (~100°C) following a disrotatory mechanism and further aromatization leads to the product **PDPP**.

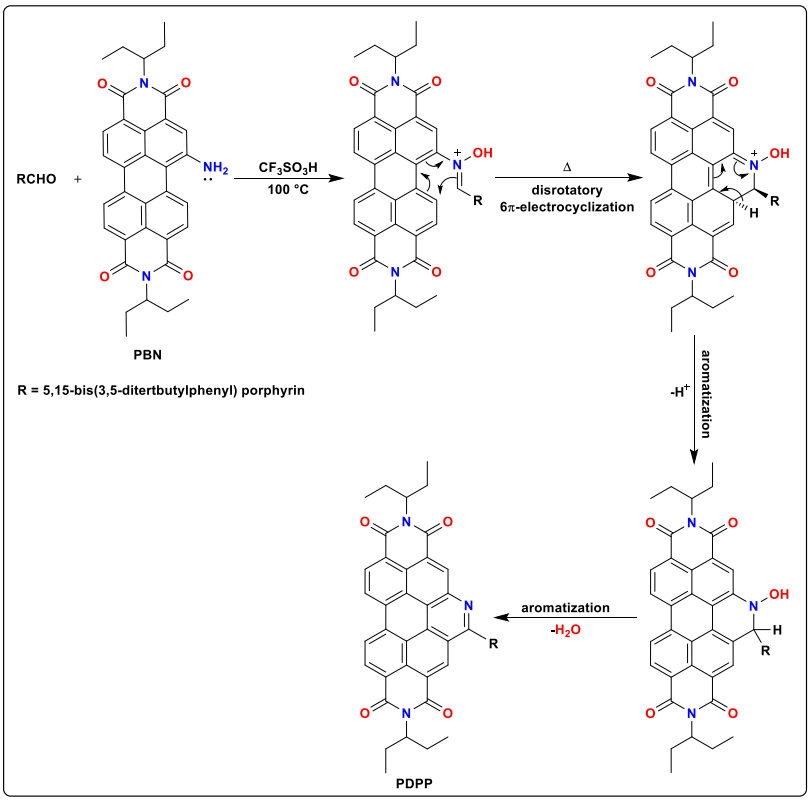


Figure S49. A plausible mechanism for the formation of **PDPP** using triflic acid with porphyrin substrate.

Table S3. Photovoltaic parameters for the **PDPP**:$PC_{71}BM$ based OSCs with different weight ratios of **PDPP** and $PC_{71}BM$ cast from chloroform solvent

Weight ratio	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	PCE (%)
1:0.2	8.31	0.98	0.48	3.91
1:0.6	9.15	0.97	0.50	4.44
1:1.0	9.73	0.98	0.51	4.86
1:1.4	**10.28**	**0.98**	**0.53**	**5.34**
1:1.6	9.63	0.97	0.50	4.67

Table S4. Photovoltaic parameters for the **Zn-PDPP**: $PC_{71}BM$ based OSCs with different weight ratios of **Zn-PDPP** and $PC_{71}BM$ cast from chloroform solvent

Weight ratio	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	PCE (%)
1:0.2	10.18	0.87	0.53	4.69
1:0.6	11.17	0.88	0.56	5.50
1:1.0	13.43	0.86	0.58	6.70
1:1.4	**14.19**	**0.85**	**0.61**	**7.36**
1:1.6	13.54	0.87	0.58	6.83

Table S5. Cartesian coordinates of the single-crystal obtained for compound **PDPP-triflate**.

Number	Label	X	Y	Z
1	S1	0.1008(3)	0.46175(16)	0.31095(9)
2	F1	0.1086(6)	0.3061(3)	0.3564(2)
3	F4	0.3135(6)	0.3544(3)	0.3170(2)
4	F6	0.2146(6)	0.3806(3)	0.39622(19)
5	O1	0.2076(6)	0.5214(4)	0.2992(2)
6	O4	0.0710(6)	0.4382(4)	0.2604(2)
7	O8	-0.0264(6)	0.4744(4)	0.3489(2)
8	C14	0.1880(9)	0.3719(6)	0.3471(4)
9	S2	0.8164(3)	0.55360(19)	0.09048(11)
10	O6	0.9429(7)	0.5437(4)	0.1160(2)
11	O3	0.7011(7)	0.5940(5)	0.1214(3)
12	F3	0.9020(8)	0.6961(5)	0.0366(3)
13	F2	0.9734(8)	0.6018(5)	-0.0079(3)
14	O9	0.7791(8)	0.4820(5)	0.0736(3)
15	F5	0.7521(9)	0.6417(5)	-0.0009(3)
16	C39	0.8664(14)	0.6244(8)	0.0266(4)
17	N1	1.0453(8)	0.3842(5)	0.1554(3)
18	H1	1.018716	0.434144	0.159202
19	N4	0.7972(8)	0.4453(5)	0.2262(3)
20	H4	0.88995	0.450037	0.224573
21	O10	-0.1012(8)	0.8670(4)	0.4548(3)
22	N6	0.9487(7)	0.6046(4)	0.2149(3)
23	H6	0.955762	0.569929	0.192465
24	N7	0.5308(8)	0.6566(5)	0.2992(3)
25	O5	0.7073(8)	0.2850(4)	0.3990(3)
26	N2	1.2137(7)	0.5305(5)	0.1594(3)
27	H2	1.141764	0.509101	0.184287
28	O7	0.1795(8)	0.8962(4)	0.2840(3)
29	N5	0.5477(8)	0.2543(5)	0.4804(3)
30	N3	0.0318(8)	0.8813(5)	0.3676(3)
31	O2	0.4041(9)	0.2320(4)	0.5653(3)
32	C1	0.5559(9)	0.3929(6)	0.4230(3)
33	C4	0.5464(9)	0.5261(6)	0.3618(3)
34	C6	0.4267(9)	0.5503(6)	0.3994(3)
35	C8	1.2420(11)	0.7514(6)	0.1638(3)

36	C10	0.2581(8)	0.5213(6)	0.4886(3)
37	C12	0.5920(9)	0.5839(6)	0.3117(3)
38	C16	1.4505(10)	0.8326(6)	0.1463(3)
39	C18	1.1834(9)	0.3574(6)	0.1394(3)
40	C20	0.4385(9)	0.4176(6)	0.4620(3)
41	C22	1.2165(10)	0.8968(6)	0.1326(3)
42	C24	1.3648(11)	0.9000(6)	0.1303(3)
43	H24	1.408092	0.950993	0.117208
44	C26	0.5592(10)	0.4684(6)	0.2429(3)
45	H26	0.467615	0.491193	0.255178
46	C28	0.6906(9)	0.4946(6)	0.2481(3)
47	C30	0.3610(9)	0.6271(6)	0.3850(3)
48	C32	0.7346(10)	0.3866(6)	0.2070(3)
49	C34	0.2417(9)	0.6539(6)	0.4205(3)
50	C36	1.1804(10)	0.6707(6)	0.1757(4)
51	C38	0.8353(10)	0.6092(6)	0.2576(4)
52	C40	0.2244(10)	0.7790(6)	0.3508(4)
53	C42	0.6065(10)	0.4483(6)	0.3762(3)
54	H42	0.687807	0.432648	0.351977
55	C44	1.1581(11)	0.8205(6)	0.1494(3)
56	H44	1.057856	0.815968	0.151001
57	C46	0.6457(10)	0.1870(6)	0.0435(4)
58	C48	0.9546(11)	0.3204(6)	0.1648(3)
59	C50	0.7205(10)	0.2614(6)	0.1721(4)
60	C52	1.0487(10)	0.6609(6)	0.2120(3)
61	C54	0.6198(9)	0.2203(6)	0.2138(3)
62	H54	0.611719	0.229572	0.250696
63	C56	1.3075(9)	0.4890(6)	0.1259(4)
64	C58	0.2751(10)	0.3890(7)	0.5475(4)
65	H58	0.240773	0.352587	0.581173
66	C60	1.0443(11)	0.2513(6)	0.1552(3)
67	H60	1.012766	0.197855	0.159483
68	C62	0.1740(10)	0.7283(6)	0.4044(4)
69	C64	0.7146(9)	0.5625(6)	0.2710(3)
70	C66	0.5301(10)	0.1656(6)	0.2028(4)
71	C68	0.8069(10)	0.3249(6)	0.1824(3)
72	C70	0.7286(9)	0.2498(5)	0.1174(3)
73	H70	0.795435	0.278934	0.088386
74	C72	0.2114(11)	0.4647(7)	0.5368(3)
75	H72	0.133367	0.479188	0.562963
76	C74	0.1926(10)	0.6024(7)	0.4735(3)
77	C76	1.3915(10)	0.7586(6)	0.1632(3)
78	H76	1.449869	0.711817	0.174596
79	C78	0.3749(9)	0.4962(6)	0.4504(3)
80	C80	0.4138(9)	0.6788(6)	0.3341(3)
81	C82	1.3018(9)	0.4077(6)	0.1224(3)

82	H82	1.388498	0.383325	0.106674
83	C84	0.9903(10)	0.7042(6)	0.2557(4)
84	H84	1.03258	0.749018	0.263646
85	C85	0.3881(10)	0.3635(7)	0.5110(4)
86	C43	0.3428(10)	0.7547(6)	0.3176(4)
87	H43	0.377862	0.789024	0.283092
88	C11	0.4439(10)	0.2809(7)	0.5223(4)
89	C45	1.1796(10)	0.2742(7)	0.1391(3)
90	H45	1.260012	0.239955	0.129237
91	C23	0.4165(10)	0.1213(6)	0.2494(4)
92	C47	0.5851(11)	0.4040(6)	0.2169(4)
93	H47	0.513824	0.375277	0.207045
94	C3	1.2483(9)	0.6097(6)	0.1487(3)
95	C49	0.0774(10)	0.6326(7)	0.5080(4)
96	H49	0.041691	0.599809	0.543073
97	C25	-0.0099(12)	0.8364(8)	0.4240(4)
98	C51	0.1455(11)	0.8555(6)	0.3309(4)
99	C13	0.8674(10)	0.6714(6)	0.2833(4)
100	H13	0.81102	0.68744	0.315062
101	C53	1.6117(10)	0.8438(6)	0.1410(4)
102	C27	0.6408(10)	0.1967(5)	0.1052(4)
103	C55	0.0585(11)	0.7557(7)	0.4400(4)
104	C7	1.3724(10)	0.6175(7)	0.1053(4)
105	H7	1.419774	0.666145	0.087778
106	C57	0.6132(11)	0.3088(6)	0.4325(4)
107	C29	0.7791(10)	0.2216(6)	0.0049(4)
108	H29A	0.864872	0.192921	0.017801
109	H29B	0.775907	0.21482	-0.03321
110	H29C	0.782417	0.279477	0.005137
111	C59	0.5121(11)	0.2316(6)	0.0234(4)
112	H59A	0.426254	0.209217	0.048269
113	H59B	0.515303	0.289435	0.023666
114	H59C	0.508792	0.224778	-0.01468
115	C15	1.4077(11)	0.5449(7)	0.0943(4)
116	H15	1.488912	0.532165	0.068889
117	C61	0.0143(11)	0.7086(7)	0.4924(4)
118	H61	-0.05963	0.728825	0.517626
119	C31	1.2060(10)	1.0494(6)	0.0895(4)
120	H31A	1.138237	1.094932	0.079825
121	H31B	1.262449	1.061546	0.116269
122	H31C	1.270496	1.040946	0.055654
123	C63	0.3206(11)	0.0714(6)	0.2290(4)
124	H63A	0.266551	0.106698	0.202262
125	H63B	0.378778	0.031079	0.210712
126	H63C	0.253528	0.04356	0.260706
127	C2	1.1225(11)	0.9720(7)	0.1158(4)

128	C65	0.6418(11)	0.0968(6)	0.0415(4)
129	H65A	0.556436	0.073487	0.066149
130	H65B	0.638451	0.091357	0.003138
131	H65C	0.728125	0.068025	0.053895
132	C33	0.5429(10)	0.1567(6)	0.1475(4)
133	H33	0.480698	0.121249	0.138655
134	C67	1.0308(10)	0.9608(6)	0.0726(4)
135	H67A	0.971796	1.010352	0.062701
136	H67B	1.093643	0.949939	0.039006
137	H67C	0.96835	0.915083	0.088405
138	C17	1.6386(11)	0.9127(6)	0.1698(4)
139	H17A	1.585588	0.962183	0.154647
140	H17B	1.605845	0.896945	0.210095
141	H17C	1.741462	0.922673	0.163004
142	C69	0.4993(11)	0.0645(7)	0.2911(4)
143	H69A	0.562892	0.096175	0.304953
144	H69B	0.431321	0.03675	0.322436
145	H69C	0.556571	0.024269	0.272441
146	C35	0.581(3)	0.1670(10)	0.4872(15)
147	H35	0.548659	0.156345	0.528457
148	C71	1.0231(11)	0.9889(6)	0.1691(4)
149	H71A	0.961477	1.037309	0.159147
150	H71B	0.963342	0.94225	0.185641
151	H71C	1.08185	0.997947	0.196082
152	C9	0.3270(11)	0.1840(6)	0.2790(4)
153	H9A	0.391007	0.216315	0.292149
154	H9B	0.272082	0.219755	0.252732
155	H9C	0.260878	0.155947	0.310852
156	C73	1.6727(10)	0.8668(6)	0.0774(4)
157	H73A	1.621972	0.916084	0.060426
158	H73B	1.775314	0.876632	0.072714
159	H73C	1.659093	0.822298	0.059229
160	C37	1.6945(11)	0.7671(7)	0.1649(4)
161	H37A	1.796538	0.778361	0.160161
162	H37B	1.657499	0.749724	0.204673
163	H37C	1.682788	0.724054	0.145079
164	C75	-0.2343(12)	0.8719(7)	0.3233(4)
165	H75A	-0.33739	0.865553	0.325563
166	H75B	-0.18895	0.882787	0.284077
167	H75C	-0.19121	0.822028	0.343181
168	C19	0.398(3)	0.165(2)	0.4237(13)
169	H19A	0.319734	0.133346	0.419366
170	H19B	0.362069	0.219952	0.427111
171	H19C	0.473629	0.167891	0.39098
172	C77	-0.2118(13)	0.9415(7)	0.3496(5)
173	H77A	-0.25987	0.930667	0.38896

174	H77B	-0.25761	0.99139	0.329891
175	C79	-0.0517(12)	0.9562(7)	0.3480(4)
176	H79	-0.01297	0.971872	0.307306
177	C5	-0.0184(13)	1.0264(7)	0.3722(5)
178	H5A	0.086968	1.028184	0.369673
179	H5B	-0.06056	1.017044	0.412305
180	C81	-0.0767(13)	1.1100(8)	0.3423(6)
181	H81A	-0.05177	1.152903	0.359825
182	H81B	-0.03362	1.120363	0.302769
183	H81C	-0.18126	1.109214	0.345433
184	C41	0.758(3)	0.0520(12)	0.5129(9)
185	H41A	0.860261	0.040243	0.515442
186	H41B	0.700952	0.034891	0.549875
187	H41C	0.729951	0.022336	0.486668
188	C83	0.460(2)	0.1243(12)	0.4761(9)
189	H83A	0.382773	0.120324	0.508646
190	H83B	0.494147	0.06835	0.472576
191	C21	0.733(2)	0.1417(11)	0.4927(9)
192	H21A	0.764753	0.170984	0.51897
193	H21B	0.793704	0.158449	0.455867
194	C41A	0.753(3)	0.0602(16)	0.5337(11)
195	H41D	0.7872	0.042308	0.56966
196	H41E	0.707313	0.015314	0.524808
197	H41F	0.834504	0.077483	0.504417
198	C21A	0.646(2)	0.1299(12)	0.5370(8)
199	H21C	0.69386	0.173654	0.547474
200	H21D	0.567162	0.111726	0.567786
201	C35A	0.582(4)	0.1658(10)	0.4856(13)
202	H35A	0.678635	0.175529	0.462412
203	C83A	0.529(2)	0.1330(12)	0.4411(8)
204	H83C	0.538559	0.073082	0.450252
205	H83D	0.591855	0.151684	0.405194
206	C19A	0.374(3)	0.157(3)	0.4332(14)
207	H19D	0.349805	0.132805	0.403479
208	H19E	0.309787	0.137423	0.468124
209	H19F	0.363223	0.216233	0.422947

Table S6. Cartesian coordinates of the single-crystal obtained for compound **PDPP**.

Number	Label	X	Y	Z
1	O1	0.4439(4)	0.4671(3)	0.9729(3)
2	N1	0.5964(4)	0.5902(4)	0.8527(3)
3	N6	0.8226(4)	0.5440(4)	0.8184(3)
4	N8	0.9692(4)	0.5294(5)	0.8293(4)
5	H8	0.92817	0.563165	0.823205
6	N2	0.9309(5)	0.6780(5)	0.8528(4)

7	N9	0.7812(4)	0.6906(4)	0.8440(4)
8	H9	0.821892	0.660362	0.833645
9	O6	0.4202(4)	0.9297(4)	0.5731(4)
10	O8	0.2090(4)	0.5808(4)	0.9088(4)
11	N5	0.3263(5)	0.5237(5)	0.9431(4)
12	C1	0.4987(5)	0.5508(5)	0.8902(4)
13	H1	0.53162	0.516098	0.917176
14	C4	0.4265(5)	0.5561(5)	0.8918(4)
15	O3	0.6493(4)	0.8145(4)	0.6453(4)
16	C6	0.5257(5)	0.5947(4)	0.8502(4)
17	C10	0.7296(5)	0.5090(5)	0.7910(4)
18	H10	0.682014	0.508752	0.781961
19	C16	0.4742(5)	0.6446(4)	0.8099(4)
20	C22	0.3013(5)	0.6169(5)	0.8566(4)
21	C24	0.7918(5)	0.4554(5)	0.7866(4)
22	H24	0.795344	0.411968	0.773351
23	C26	0.3754(5)	0.6077(5)	0.8516(4)
24	C28	0.7146(6)	0.6838(5)	0.8420(5)
25	C32	1.0355(6)	0.5349(6)	0.8434(5)
26	N13	0.5343(5)	0.8721(5)	0.6081(4)
27	C42	0.8498(6)	0.4766(5)	0.8053(5)
28	C48	0.7480(5)	0.5666(5)	0.8117(4)
29	C52	0.9025(6)	0.7471(6)	0.8654(5)
30	C56	0.3753(5)	0.7498(5)	0.7290(4)
31	C60	0.3988(5)	0.6521(5)	0.8106(4)
32	C62	0.4311(6)	0.8386(5)	0.6498(5)
33	C64	0.5735(5)	0.6858(5)	0.7721(4)
34	C68	0.9235(6)	0.4360(5)	0.8090(5)
35	C70	0.4514(5)	0.7423(4)	0.7288(4)
36	C74	0.6189(5)	0.6343(5)	0.8170(5)
37	C76	0.3576(5)	0.8458(5)	0.6507(5)
38	H76	0.325394	0.881122	0.623769
39	C80	0.4011(6)	0.5113(6)	0.9393(5)
40	C82	0.2770(5)	0.7098(5)	0.7780(4)
41	H82	0.242206	0.744607	0.752564
42	C86	0.3302(5)	0.8033(5)	0.6896(4)
43	H86	0.279433	0.810528	0.689521
44	C88	0.6974(5)	0.6284(5)	0.8232(4)
45	C92	0.2542(5)	0.6659(5)	0.8202(4)
46	H92	0.203993	0.671063	0.823152
47	C94	0.3501(5)	0.7037(5)	0.7723(4)
48	C102	0.9796(6)	0.4607(6)	0.8265(5)
49	C104	0.5008(5)	0.6909(4)	0.7699(4)
50	C118	0.7744(6)	0.7538(6)	0.8653(5)
51	C124	0.2740(6)	0.5730(6)	0.9042(5)
52	C126	0.5536(5)	0.7777(5)	0.6904(5)

53	C134	0.4781(5)	0.7868(5)	0.6896(4)
54	C140	0.6626(6)	0.7443(5)	0.8618(5)
55	H140	0.611724	0.752803	0.864348
56	C148	1.0530(6)	0.5930(6)	0.8529(5)
57	H148	1.103028	0.586998	0.858683
58	C156	0.9982(6)	0.3299(6)	0.7660(6)
59	H156	1.024174	0.356887	0.744183
60	C160	0.9637(6)	0.7710(6)	0.8739(5)
61	H160	0.961436	0.816333	0.881179
62	C83	1.0880(6)	0.4659(6)	0.8508(5)
63	H83	1.137846	0.454806	0.861444
64	C43	0.5985(5)	0.7297(5)	0.7312(4)
65	H43	0.648514	0.725895	0.732028
66	C87	1.0544(6)	0.4220(6)	0.8400(5)
67	H87	1.075483	0.373629	0.840987
68	C89	0.9410(6)	0.3611(6)	0.8026(6)
69	C91	0.8304(6)	0.7816(6)	0.8726(5)
70	C93	0.5842(6)	0.8221(6)	0.6468(5)
71	C47	0.4603(7)	0.8825(6)	0.6091(6)
72	C97	1.0058(6)	0.6592(7)	0.8548(5)
73	C99	0.8081(7)	0.8532(7)	0.8909(6)
74	C101	0.6988(6)	0.7866(6)	0.8760(5)
75	H101	0.678106	0.83045	0.8906
76	C103	1.0262(7)	0.7161(6)	0.8694(5)
77	H103	1.07438	0.716575	0.87505
78	C53	0.9023(6)	0.3232(6)	0.8339(6)
79	H53	0.864849	0.345194	0.860744
80	C109	0.8351(7)	0.8679(7)	0.9460(6)
81	H109	0.867961	0.832362	0.972262
82	C111	0.7604(7)	0.9072(7)	0.8541(6)
83	H111	0.74281	0.897355	0.816657
84	C113	1.0824(7)	0.2212(6)	0.7200(6)
85	C57	0.8120(8)	0.9377(8)	0.9619(7)
86	C29	0.5593(8)	0.9207(8)	0.5634(7)
87	H29	0.514241	0.95466	0.544023
88	C117	1.0189(7)	0.2588(6)	0.7600(6)
89	C15	0.2482(16)	0.5250(15)	1.0393(12)
90	H15A	0.196645	0.540724	1.026027
91	H15B	0.25292	0.491717	1.076554
92	C123	0.2905(17)	0.4876(12)	0.9899(10)
93	H123	0.334267	0.459125	1.01495
94	C63	0.9160(7)	0.2528(6)	0.8276(7)
95	C2	0.7684(8)	0.9843(8)	0.9226(7)
96	H2	0.75767	1.030179	0.932678
97	C129	0.7359(8)	0.9773(8)	0.8694(7)
98	C65	0.9771(7)	0.2207(6)	0.7880(6)

99	H65	0.988052	0.173649	0.781477
100	C131	0.8860(17)	0.2178(13)	0.8851(13)
101	C135	0.895(2)	0.2414(19)	0.9494(13)
102	H13A	0.875763	0.291581	0.947267
103	H13B	0.868993	0.220975	0.980667
104	H13C	0.946803	0.226476	0.960879
105	C137	0.6799(9)	1.0294(8)	0.8256(7)
106	C69	0.2637(18)	0.5784(15)	1.0562(15)
107	H69A	0.231166	0.597884	1.089379
108	H69B	0.314005	0.563872	1.071297
109	H69C	0.257441	0.613131	1.020509
110	C35	0.6448(8)	1.0945(7)	0.8558(7)
111	H35A	0.62603	1.083128	0.896342
112	H35B	0.604885	1.124911	0.829289
113	H35C	0.680795	1.117815	0.861318
114	C141	1.0511(7)	0.2023(6)	0.6632(7)
115	H14A	1.017697	0.176665	0.676397
116	H14B	1.090437	0.173786	0.639432
117	H14C	1.024811	0.24429	0.637112
118	C9	0.8045(16)	0.239(2)	0.865(2)
119	H9A	0.783831	0.289601	0.862472
120	H9B	0.800293	0.223488	0.824936
121	H9C	0.778158	0.218815	0.896418
122	C145	0.3209(14)	0.3717(12)	0.9654(12)
123	H14D	0.3021	0.339669	0.945961
124	H14E	0.364087	0.375692	0.943385
125	H14F	0.333586	0.354576	1.008925
126	C147	1.1259(7)	0.2683(6)	0.6969(7)
127	H14G	1.094948	0.30773	0.670534
128	H14H	1.167078	0.242938	0.672906
129	H14I	1.143831	0.284423	0.732516
130	C149	1.1317(7)	0.1576(7)	0.7584(7)
131	H14J	1.15808	0.171962	0.789743
132	H14K	1.166341	0.128961	0.731002
133	H14L	1.102258	0.131231	0.778987
134	C75	0.917(2)	0.1383(13)	0.889(2)
135	H75A	0.911582	0.12276	0.848977
136	H75B	0.968618	0.123652	0.901009
137	H75C	0.890808	0.118151	0.920796
138	C151	0.5952(9)	0.9602(8)	0.5937(8)
139	H15C	0.601423	0.996635	0.562694
140	H15D	0.644201	0.929672	0.606715
141	C153	0.6013(9)	0.8850(8)	0.5109(8)
142	H15E	0.61092	0.91988	0.479996
143	H15F	0.648668	0.853745	0.52724
144	C39	0.5603(9)	0.9925(7)	0.6473(8)

145	H39A	0.510113	1.019924	0.63638
146	H39B	0.586457	1.022368	0.660563
147	H39C	0.560648	0.957018	0.68116
148	C157	0.7116(9)	1.0364(8)	0.7646(7)
149	H15G	0.753478	1.052523	0.768534
150	H15H	0.675409	1.069535	0.736501
151	H15I	0.727239	0.99166	0.747848
152	C159	0.2720(14)	0.4312(11)	0.9625(13)
153	H15J	0.228312	0.425548	0.983528
154	H15K	0.258686	0.446577	0.918259
155	C161	0.6130(9)	1.0065(8)	0.8110(8)
156	H16A	0.629161	0.964716	0.789582
157	H16B	0.578399	1.043145	0.784413
158	H16C	0.589642	0.99719	0.849892
159	C163	0.5658(10)	0.8468(9)	0.4807(8)
160	H16D	0.582348	0.84348	0.437788
161	H16E	0.513321	0.869881	0.480754
162	H16F	0.576932	0.800639	0.502615
163	C155	0.8213(15)	0.9244(13)	1.0731(10)
164	H15L	0.842973	0.875128	1.069709
165	H15M	0.83955	0.936244	1.110914
166	H15N	0.768436	0.935864	1.075071
167	C81	0.8074(13)	1.0424(10)	1.0215(11)
168	H81A	0.820458	1.068139	0.985109
169	H81B	0.754604	1.05396	1.023396
170	H81C	0.825718	1.05434	1.059239
171	C79	0.8412(12)	0.9650(10)	1.0166(9)
172	C165	0.9245(12)	0.9381(13)	1.0210(14)
173	H16G	0.94474	0.960548	0.98656
174	H16H	0.940552	0.948209	1.060534
175	H16I	0.941174	0.888287	1.018765
176	O4	0.1370(4)	0.8415(3)	0.7243(4)
177	N4	0.3108(4)	0.6339(4)	0.6351(4)
178	N10	0.3341(4)	0.5162(4)	0.7335(4)
179	H10A	0.35617	0.510538	0.697709
180	N12	0.4605(4)	0.6177(4)	0.6312(4)
181	H12	0.430837	0.600012	0.652814
182	N14	0.4832(4)	0.4974(4)	0.7293(4)
183	N7	0.1196(4)	0.5443(4)	0.6740(3)
184	O2	-0.0142(5)	0.3857(4)	0.6181(4)
185	N11	0.0179(6)	0.9050(5)	0.7300(4)
186	O5	-0.2544(4)	0.5013(4)	0.6342(3)
187	C8	-0.0072(5)	0.6112(5)	0.6802(4)
188	O7	-0.1019(4)	0.9687(4)	0.7354(4)
189	N3	-0.1353(5)	0.4433(5)	0.6279(4)
190	C12	0.4398(6)	0.6698(5)	0.5857(5)

191	C14	0.3101(6)	0.6796(5)	0.5867(5)
192	C18	0.2169(5)	0.5902(5)	0.6853(4)
193	C20	0.2373(5)	0.7051(5)	0.5575(5)
194	H20	0.222905	0.735859	0.520877
195	C30	0.4277(6)	0.4216(5)	0.7935(5)
196	C34	0.1023(5)	0.7243(5)	0.7063(4)
197	H34	0.151913	0.72142	0.709128
198	C36	0.6041(6)	0.4299(5)	0.7461(5)
199	H36	0.655445	0.414923	0.743241
200	C38	0.3573(6)	0.4594(5)	0.7776(5)
201	C40	0.0848(5)	0.6652(5)	0.6946(4)
202	C44	0.3056(6)	0.8130(5)	0.5060(5)
203	H44	0.27861	0.825147	0.542379
204	C46	0.2593(5)	0.5381(5)	0.7274(5)
205	C50	0.2414(5)	0.6322(5)	0.6409(5)
206	C54	0.5052(5)	0.6843(5)	0.5646(5)
207	H54	0.507883	0.719233	0.533407
208	C58	0.5355(6)	0.5958(5)	0.6393(5)
209	C66	0.1363(5)	0.5992(5)	0.6856(4)
210	C72	0.1956(6)	0.6762(5)	0.5932(4)
211	H72	0.145219	0.68367	0.58759
212	C78	-0.0433(5)	0.7312(5)	0.7013(4)
213	C84	-0.0771(6)	0.8534(6)	0.7172(5)
214	C90	0.5614(6)	0.6392(5)	0.5973(5)
215	H90	0.610684	0.637058	0.592744
216	C96	0.3592(6)	0.7488(5)	0.5064(5)
217	C98	-0.1721(6)	0.5592(6)	0.6562(4)
218	C100	-0.1016(5)	0.5581(5)	0.6618(4)
219	C106	0.5644(5)	0.3983(5)	0.7774(5)
220	H106	0.58211	0.3555	0.802163
221	C108	0.3974(6)	0.7315(5)	0.4530(5)
222	H108	0.431794	0.687112	0.452401
223	C110	-0.1387(5)	0.6777(5)	0.6842(4)
224	C112	0.4070(6)	0.3090(5)	0.8229(5)
225	H112	0.377112	0.317223	0.786826
226	C114	-0.0237(5)	0.7906(5)	0.7105(4)
227	C116	0.0469(5)	0.5483(5)	0.6719(4)
228	C120	0.0114(5)	0.6693(5)	0.6932(4)
229	C122	0.4411(6)	0.3566(6)	0.8351(5)
230	C128	-0.1193(5)	0.7366(5)	0.6962(4)
231	C130	0.2900(5)	0.4497(5)	0.8012(5)
232	H130	0.286732	0.415042	0.832495
233	C132	0.4882(6)	0.4391(5)	0.7682(5)
234	C136	-0.0433(6)	0.4954(5)	0.6520(4)
235	C138	0.3324(6)	0.8407(5)	0.4008(5)
236	H138	0.323281	0.87199	0.364294

237	C142	-0.0828(5)	0.6157(5)	0.6761(4)
238	C144	0.0523(6)	0.7834(5)	0.7133(4)
239	C146	0.5531(6)	0.4935(5)	0.7162(5)
240	C150	0.0747(7)	0.8445(6)	0.7217(5)
241	C152	0.2344(6)	0.4969(5)	0.7721(5)
242	H152	0.184912	0.502059	0.780256
243	C154	-0.0608(7)	0.4358(6)	0.6318(5)
244	C158	0.5774(6)	0.5399(5)	0.6764(5)
245	H158	0.628304	0.531555	0.675096
246	C162	0.3691(6)	0.6994(5)	0.5623(5)
247	C164	-0.1703(6)	0.8014(5)	0.7021(4)
248	H164	-0.22054	0.807152	0.698549
249	C166	-0.2255(6)	0.6196(6)	0.6639(5)
250	H166	-0.27455	0.620694	0.660618
251	C21	-0.1914(7)	0.5010(7)	0.6399(5)
252	C85	0.3866(6)	0.7774(6)	0.4005(5)
253	C11	0.2918(6)	0.8588(5)	0.4528(5)
254	C45	-0.1478(6)	0.8573(6)	0.7132(5)
255	H45	-0.18374	0.900032	0.718047
256	C23	0.4164(7)	0.2494(6)	0.8631(6)
257	C95	0.0280(5)	0.4920(5)	0.6570(4)
258	H95	0.064991	0.450555	0.650273
259	C3	0.4862(6)	0.3445(6)	0.8869(5)
260	H3	0.508457	0.377567	0.89553
261	C49	-0.2120(6)	0.6786(6)	0.6762(5)
262	H49	-0.25095	0.719759	0.679383
263	C25	0.4297(7)	0.7584(6)	0.3409(5)
264	C51	0.5490(7)	0.2699(6)	0.9840(6)
265	C13	0.4989(7)	0.2837(6)	0.9263(6)
266	C105	0.2301(6)	0.9280(6)	0.4536(4)
267	C107	-0.0564(7)	0.9113(7)	0.7272(6)
268	C27	0.4841(7)	0.6864(6)	0.3478(5)
269	H27A	0.515707	0.681318	0.383901
270	H27B	0.513424	0.679117	0.310302
271	H27C	0.458174	0.652526	0.353522
272	C55	-0.1515(7)	0.3838(7)	0.6021(6)
273	H55	-0.103	0.353345	0.590115
274	C7	0.4620(6)	0.2387(6)	0.9143(6)
275	H7	0.468119	0.198714	0.942383
276	C115	0.3753(7)	0.7626(6)	0.2888(5)
277	H11A	0.349578	0.729243	0.299888
278	H11B	0.401339	0.752243	0.250021
279	H11C	0.340409	0.809016	0.28335
280	C59	0.3756(8)	0.2004(7)	0.8512(7)
281	C119	0.0388(9)	0.9669(7)	0.7400(7)
282	H119	0.09163	0.942377	0.735581

283	C121	0.2347(9)	0.9686(7)	0.5100(6)
284	H12A	0.194165	1.011597	0.507556
285	H12B	0.232112	0.940623	0.548881
286	H12C	0.280552	0.978903	0.508848
287	C61	0.4670(7)	0.8096(6)	0.3214(5)
288	H61A	0.431642	0.85583	0.317563
289	H61B	0.489986	0.79994	0.281244
290	H61C	0.504088	0.806895	0.352513
291	C31	0.6078(9)	0.2016(7)	0.9826(8)
292	H31A	0.636156	0.202443	0.944808
293	H31B	0.639681	0.193263	1.019104
294	H31C	0.585741	0.164932	0.982994
295	C125	0.5872(9)	0.3256(8)	0.9851(7)
296	H12D	0.550666	0.370828	0.986055
297	H12E	0.61854	0.315456	1.022168
298	H12F	0.616597	0.32563	0.947866
299	C127	-0.1761(8)	0.3404(7)	0.6533(6)
300	H12G	-0.22351	0.368046	0.668506
301	H12H	-0.14091	0.328719	0.688394
302	C33	0.4316(7)	0.1301(6)	0.8444(7)
303	H33A	0.407238	0.099153	0.830356
304	H33B	0.455527	0.110797	0.884671
305	H33C	0.46785	0.135438	0.814001
306	C133	0.2211(9)	0.9770(7)	0.3925(6)
307	H13D	0.181119	1.019322	0.396769
308	H13E	0.26601	0.988133	0.384345
309	H13F	0.210437	0.954329	0.357844
310	C67	-0.1832(7)	0.2742(7)	0.6330(6)
311	H67A	-0.23041	0.283891	0.612409
312	H67B	-0.17944	0.240826	0.669456
313	H67C	-0.14451	0.255191	0.604046
314	C17	0.4990(9)	0.2782(8)	1.0400(6)
315	H17D	0.463346	0.324303	1.035756
316	H17E	0.473874	0.243702	1.041996
317	H17F	0.527814	0.272032	1.078106
318	C139	0.1558(7)	0.9129(8)	0.4648(8)
319	H13G	0.116429	0.956468	0.465344
320	H13H	0.146875	0.887842	0.43136
321	H13I	0.158133	0.885195	0.504733
322	C71	0.3302(7)	0.2200(6)	0.7917(7)
323	H71A	0.361401	0.222982	0.756207
324	H71B	0.292971	0.26461	0.794013
325	H71C	0.306915	0.185031	0.78663
326	C143	-0.1591(9)	0.4494(9)	0.4919(7)
327	H14M	-0.17214	0.444308	0.449594
328	H14N	-0.10637	0.430783	0.497686

329	H14O	-0.17542	0.498139	0.498748
330	C73	-0.1948(9)	0.4109(8)	0.5376(7)
331	H73A	-0.20029	0.37111	0.518509
332	H73B	-0.24395	0.441358	0.546004
333	C37	0.0397(9)	1.0005(8)	0.6244(7)
334	H37A	0.035961	1.042974	0.597939
335	H37B	0.086136	0.965758	0.61737
336	H37C	-7.9E-05	0.983555	0.614341
337	C19	0.0461(9)	0.9296(8)	0.8556(7)
338	H19A	0.061602	0.881768	0.845965
339	H19B	-0.00282	0.941373	0.872655
340	H19C	0.079671	0.935431	0.88627
341	C77	0.3304(8)	0.1922(7)	0.9076(7)
342	H77A	0.294875	0.170332	0.89683
343	H77B	0.305146	0.237497	0.921173
344	H77C	0.36216	0.163504	0.941326
345	C5	0.0460(10)	0.9720(8)	0.8026(8)
346	H5A	0.092226	0.982203	0.805434
347	H5B	0.007666	1.015273	0.809798
348	C41	0.0358(10)	1.0131(8)	0.6849(8)
349	H41A	-0.01027	1.050915	0.687737
350	H41B	0.074816	1.033351	0.690726
351	C167	0.1808(19)	0.928(2)	0.3968(14)
352	H16M	0.139546	0.970616	0.393192
353	H16N	0.209106	0.925706	0.358653
354	H16O	0.163157	0.888499	0.403038
355	C1A	0.2748(19)	0.9791(16)	0.439(2)
356	H1AA	0.242251	1.026452	0.437436
357	H1AB	0.312072	0.971034	0.470879
358	H1AC	0.297865	0.971593	0.39821
359	C1B	0.188(2)	0.951(2)	0.5141(12)
360	H1BA	0.151539	0.996374	0.504593
361	H1BB	0.164533	0.917734	0.530136
362	H1BC	0.22242	0.954668	0.545404
363	C79A	0.8556(12)	0.9324(13)	1.0249(9)
364	C168	0.7936(15)	0.9670(17)	1.0673(12)
365	H16J	0.764949	1.011867	1.046872
366	H16K	0.762402	0.938006	1.075629
367	H16L	0.813753	0.973388	1.106587
368	C81A	0.9088(17)	0.9725(17)	1.0068(16)
369	H81D	0.882985	1.016003	0.982526
370	H81E	0.929533	0.982031	1.044486
371	H81F	0.94773	0.945176	0.9819
372	C1C	0.8944(16)	0.8641(12)	1.0629(12)
373	H1CA	0.93554	0.837716	1.039479
374	H1CB	0.911959	0.873177	1.102269

375	H1CC	0.860608	0.837795	1.071312
376	C169	0.8639(9)	0.2127(7)	0.8520(9)
377	C9A	0.7879(8)	0.2474(8)	0.8224(10)
378	H9AA	0.770177	0.295582	0.831188
379	H9AB	0.790667	0.245276	0.777359
380	H9AC	0.754559	0.223492	0.839766
381	C1D	0.8626(10)	0.2153(8)	0.9243(9)
382	H1DA	0.91155	0.192861	0.941623
383	H1DB	0.845647	0.263238	0.933666
384	H1DC	0.829789	0.191271	0.942736
385	C75A	0.8885(10)	0.1374(7)	0.8365(11)
386	H75D	0.936766	0.113359	0.85457
387	H75E	0.85409	0.114593	0.853725
388	H75F	0.890199	0.136377	0.791318
389	C170	0.2707(13)	0.3722(10)	1.0080(11)
390	H17A	0.251404	0.357824	0.97209
391	H17B	0.317267	0.338138	1.021038
392	H17C	0.236475	0.375912	1.042244
393	C1E	0.2802(14)	0.4329(10)	0.9925(11)
394	H1EA	0.23082	0.457602	0.975638
395	H1EB	0.309388	0.420868	0.955016
396	C15A	0.2642(16)	0.5468(14)	1.0446(13)
397	H15O	0.215185	0.571127	1.026891
398	H15P	0.257551	0.522682	1.08511
399	C69A	0.2935(14)	0.5949(12)	1.0565(12)
400	H69D	0.262101	0.625533	1.084471
401	H69E	0.341321	0.572795	1.076179
402	H69F	0.298662	0.621573	1.017559
403	C1F	0.3007(16)	0.4931(11)	1.0032(9)
404	H1F	0.347993	0.470802	1.025783
405	C31A	0.564(3)	0.1918(11)	1.000(3)
406	H31D	0.574478	0.168838	0.961907
407	H31E	0.605841	0.173563	1.028561
408	H31F	0.521448	0.183602	1.019813
409	C17A	0.535(3)	0.295(3)	1.0478(15)
410	H17G	0.485845	0.295714	1.060772
411	H17H	0.570461	0.264438	1.077635
412	H17I	0.537955	0.341764	1.046242
413	C171	0.6256(17)	0.272(3)	0.972(3)
414	H17J	0.640896	0.256926	0.930793
415	H17K	0.626257	0.319723	0.972336
416	H17L	0.658763	0.242397	1.00373

Table S7. Bond distance data of **PDPP-triflate**.

Number	Atom1	Atom2	Length
1	S1	O1	1.430(7)
2	S1	O4	1.467(7)
3	S1	O8	1.429(6)
4	S1	C14	1.810(9)
5	F1	C14	1.34(1)
6	F4	C14	1.34(1)
7	F6	C14	1.32(1)
8	S2	O6	1.429(7)
9	S2	O3	1.438(8)
10	S2	O9	1.44(1)
11	S2	C39	1.79(1)
12	F3	C39	1.36(2)
13	F2	C39	1.30(1)
14	F5	C39	1.36(2)
15	N1	H1	0.881
16	N1	C18	1.37(1)
17	N1	C48	1.38(1)
18	N4	H4	0.88
19	N4	C28	1.37(1)
20	N4	C32	1.39(1)
21	O10	C25	1.21(1)
22	N6	H6	0.88
23	N6	C38	1.38(1)
24	N6	C52	1.37(1)
25	N7	C12	1.32(1)
26	N7	C80	1.37(1)
27	O5	C57	1.22(1)
28	N2	H2	0.88
29	N2	C56	1.37(1)
30	N2	C3	1.36(1)
31	O7	C51	1.22(1)
32	N5	C11	1.42(1)
33	N5	C57	1.42(1)
34	N5	C35	1.46(2)
35	N3	C25	1.45(1)
36	N3	C51	1.39(1)
37	N3	C79	1.48(1)
38	O2	C11	1.22(1)
39	C1	C20	1.44(1)
40	C1	C42	1.37(1)
41	C1	C57	1.47(1)
42	C4	C6	1.43(1)
43	C4	C12	1.43(1)

44	C4	C42	1.39(1)
45	C6	C30	1.40(1)
46	C6	C78	1.43(1)
47	C8	C36	1.47(1)
48	C8	C44	1.38(1)
49	C8	C76	1.43(1)
50	C10	C72	1.39(1)
51	C10	C74	1.46(1)
52	C10	C78	1.43(1)
53	C12	C64	1.48(1)
54	C16	C24	1.37(1)
55	C16	C76	1.36(1)
56	C16	C53	1.53(1)
57	C18	C82	1.41(1)
58	C18	C45	1.41(2)
59	C20	C78	1.41(1)
60	C20	C85	1.39(1)
61	C22	C24	1.40(1)
62	C22	C44	1.39(1)
63	C22	C2	1.52(1)
64	C24	H24	0.95
65	C26	H26	0.95
66	C26	C28	1.38(1)
67	C26	C47	1.36(1)
68	C28	C64	1.43(1)
69	C30	C34	1.42(1)
70	C30	C80	1.41(1)
71	C32	C68	1.39(1)
72	C32	C47	1.41(1)
73	C34	C62	1.38(1)
74	C34	C74	1.44(1)
75	C36	C52	1.41(1)
76	C36	C3	1.40(1)
77	C38	C64	1.39(1)
78	C38	C13	1.41(2)
79	C40	C62	1.45(1)
80	C40	C43	1.36(1)
81	C40	C51	1.48(1)
82	C42	H42	0.95
83	C44	H44	0.95
84	C46	C27	1.56(1)
85	C46	C29	1.52(1)
86	C46	C59	1.53(1)
87	C46	C65	1.54(1)
88	C48	C60	1.43(1)
89	C48	C68	1.39(1)

90	C50	C54	1.39(1)
91	C50	C68	1.48(2)
92	C50	C70	1.40(1)
93	C52	C84	1.44(1)
94	C54	H54	0.95
95	C54	C66	1.39(1)
96	C56	C82	1.40(1)
97	C56	C15	1.40(1)
98	C58	H58	0.95
99	C58	C72	1.36(2)
100	C58	C85	1.38(1)
101	C60	H60	0.95
102	C60	C45	1.33(1)
103	C62	C55	1.40(1)
104	C66	C23	1.54(1)
105	C66	C33	1.39(1)
106	C70	H70	0.95
107	C70	C27	1.38(1)
108	C72	H72	0.95
109	C74	C49	1.40(1)
110	C76	H76	0.95
111	C80	C43	1.42(1)
112	C82	H82	0.95
113	C84	H84	0.95
114	C84	C13	1.34(1)
115	C85	C11	1.44(2)
116	C43	H43	0.95
117	C45	H45	0.95
118	C23	C63	1.49(2)
119	C23	C69	1.53(1)
120	C23	C9	1.54(1)
121	C47	H47	0.95
122	C3	C7	1.45(1)
123	C49	H49	0.95
124	C49	C61	1.38(2)
125	C25	C55	1.47(2)
126	C13	H13	0.95
127	C53	C17	1.54(2)
128	C53	C73	1.56(1)
129	C53	C37	1.52(1)
130	C27	C33	1.37(1)
131	C55	C61	1.39(1)
132	C7	H7	0.95
133	C7	C15	1.32(2)
134	C29	H29A	0.98
135	C29	H29B	0.98

136	C29	H29C	0.98
137	C59	H59A	0.98
138	C59	H59B	0.98
139	C59	H59C	0.98
140	C15	H15	0.95
141	C61	H61	0.95
142	C31	H31A	0.98
143	C31	H31B	0.98
144	C31	H31C	0.98
145	C31	C2	1.54(1)
146	C63	H63A	0.98
147	C63	H63B	0.98
148	C63	H63C	0.981
149	C2	C67	1.54(2)
150	C2	C71	1.55(1)
151	C65	H65A	0.98
152	C65	H65B	0.98
153	C65	H65C	0.98
154	C33	H33	0.95
155	C67	H67A	0.981
156	C67	H67B	0.98
157	C67	H67C	0.98
158	C17	H17A	0.98
159	C17	H17B	0.98
160	C17	H17C	0.98
161	C69	H69A	0.98
162	C69	H69B	0.979
163	C69	H69C	0.98
164	C35	H35	1
165	C35	C83	1.49(4)
166	C35	C21	1.49(3)
167	C71	H71A	0.98
168	C71	H71B	0.98
169	C71	H71C	0.98
170	C9	H9A	0.98
171	C9	H9B	0.98
172	C9	H9C	0.979
173	C73	H73A	0.98
174	C73	H73B	0.98
175	C73	H73C	0.98
176	C37	H37A	0.98
177	C37	H37B	0.979
178	C37	H37C	0.98
179	C75	H75A	0.98
180	C75	H75B	0.979
181	C75	H75C	0.98

182	C75	C77	1.50(2)
183	C19	H19A	0.98
184	C19	H19B	0.98
185	C19	H19C	0.98
186	C19	C83	1.53(4)
187	C77	H77A	0.99
188	C77	H77B	0.99
189	C77	C79	1.54(2)
190	C79	H79	1
191	C79	C5	1.51(2)
192	C5	H5A	0.99
193	C5	H5B	0.99
194	C5	C81	1.56(2)
195	C81	H81A	0.98
196	C81	H81B	0.98
197	C81	H81C	0.98
198	C41	H41A	0.98
199	C41	H41B	0.98
200	C41	H41C	0.98
201	C41	C21	1.51(3)
202	C83	H83A	0.99
203	C83	H83B	0.99
204	C21	H21A	0.99
205	C21	H21B	0.99

Table S8. Bond distance data of **PDPP**.

Number	Atom1	Atom2	Length
1	O1	C80	1.21(1)
2	N1	C6	1.35(1)
3	N1	C74	1.31(1)
4	N6	C42	1.38(1)
5	N6	C48	1.38(1)
6	N8	H8	0.879
7	N8	C32	1.37(2)
8	N8	C102	1.37(2)
9	N2	C52	1.41(2)
10	N2	C97	1.38(1)
11	N9	H9	0.881
12	N9	C28	1.35(1)
13	N9	C118	1.39(2)
14	O6	C47	1.25(1)
15	O8	C124	1.23(1)
16	N5	C80	1.40(2)
17	N5	C124	1.41(1)
18	N5	C123	1.49(3)

19	C1	H1	0.95
20	C1	C4	1.37(1)
21	C1	C6	1.40(1)
22	C4	C26	1.43(1)
23	C4	C80	1.49(2)
24	O3	C93	1.23(1)
25	C6	C16	1.42(1)
26	C10	H10	0.95
27	C10	C24	1.37(1)
28	C10	C48	1.46(2)
29	C16	C60	1.43(1)
30	C16	C104	1.43(1)
31	C22	C26	1.40(1)
32	C22	C92	1.33(1)
33	C22	C124	1.50(2)
34	C24	H24	0.95
35	C24	C42	1.41(2)
36	C26	C60	1.38(1)
37	C28	C88	1.39(2)
38	C28	C140	1.44(1)
39	C32	C148	1.38(2)
40	C32	C83	1.46(1)
41	N13	C93	1.39(1)
42	N13	C47	1.39(2)
43	N13	C29	1.51(2)
44	C42	C68	1.41(1)
45	C48	C88	1.39(1)
46	C52	C160	1.45(2)
47	C52	C91	1.37(1)
48	C56	C70	1.44(1)
49	C56	C86	1.39(1)
50	C56	C94	1.46(1)
51	C60	C94	1.39(1)
52	C62	C76	1.39(2)
53	C62	C134	1.39(1)
54	C62	C47	1.44(2)
55	C64	C74	1.44(1)
56	C64	C104	1.39(1)
57	C64	C43	1.39(1)
58	C68	C102	1.41(2)
59	C68	C89	1.49(2)
60	C70	C104	1.43(1)
61	C70	C134	1.40(1)
62	C74	C88	1.50(1)
63	C76	H76	0.949
64	C76	C86	1.37(1)

65	C82	H82	0.95
66	C82	C92	1.39(1)
67	C82	C94	1.39(1)
68	C86	H86	0.95
69	C92	H92	0.95
70	C102	C87	1.44(1)
71	C118	C91	1.40(2)
72	C118	C101	1.44(1)
73	C126	C134	1.42(1)
74	C126	C43	1.35(1)
75	C126	C93	1.49(2)
76	C140	H140	0.95
77	C140	C101	1.34(2)
78	C148	H148	0.95
79	C148	C97	1.39(2)
80	C156	H156	0.95
81	C156	C89	1.38(2)
82	C156	C117	1.41(2)
83	C160	H160	0.95
84	C160	C103	1.38(1)
85	C83	H83	0.95
86	C83	C87	1.31(2)
87	C43	H43	0.95
88	C87	H87	0.95
89	C89	C53	1.37(2)
90	C91	C99	1.49(2)
91	C97	C103	1.42(2)
92	C99	C109	1.41(2)
93	C99	C111	1.39(2)
94	C101	H101	0.95
95	C103	H103	0.95
96	C53	H53	0.95
97	C53	C63	1.41(2)
98	C109	H109	0.95
99	C109	C57	1.44(2)
100	C111	H111	0.95
101	C111	C129	1.44(2)
102	C113	C117	1.54(2)
103	C113	C141	1.52(2)
104	C113	C147	1.52(2)
105	C113	C149	1.53(2)
106	C57	C2	1.31(2)
107	C57	C79	1.55(3)
108	C29	H29	1
109	C29	C151	1.44(3)
110	C29	C153	1.50(2)

111	C117	C65	1.39(2)
112	C15	H15A	0.99
113	C15	H15B	0.99
114	C15	C123	1.47(4)
115	C15	C69	1.32(5)
116	C123	H123	1
117	C123	C159	1.50(4)
118	C63	C65	1.47(2)
119	C63	C131	1.57(3)
120	C2	H2	0.95
121	C2	C129	1.37(2)
122	C129	C137	1.53(2)
123	C65	H65	0.95
124	C131	C135	1.55(4)
125	C131	C9	1.56(4)
126	C131	C75	1.55(4)
127	C135	H13A	0.98
128	C135	H13B	0.98
129	C135	H13C	0.98
130	C137	C35	1.51(2)
131	C137	C157	1.46(2)
132	C137	C161	1.56(3)
133	C69	H69A	0.98
134	C69	H69B	0.98
135	C69	H69C	0.98
136	C35	H35A	0.98
137	C35	H35B	0.98
138	C35	H35C	0.98
139	C141	H14A	0.98
140	C141	H14B	0.98
141	C141	H14C	0.98
142	C9	H9A	0.99
143	C9	H9B	0.97
144	C9	H9C	0.98
145	C145	H14D	0.98
146	C145	H14E	0.98
147	C145	H14F	0.98
148	C145	C159	1.29(3)
149	C147	H14G	0.98
150	C147	H14H	0.98
151	C147	H14I	0.98
152	C149	H14J	0.98
153	C149	H14K	0.98
154	C149	H14L	0.98
155	C75	H75A	0.97
156	C75	H75B	0.98

157	C75	H75C	0.98
158	C151	H15C	0.99
159	C151	H15D	0.99
160	C151	C39	1.45(2)
161	C153	H15E	0.99
162	C153	H15F	0.99
163	C153	C163	1.41(3)
164	C39	H39A	0.98
165	C39	H39B	0.98
166	C39	H39C	0.98
167	C157	H15G	0.98
168	C157	H15H	0.98
169	C157	H15I	0.98
170	C159	H15J	0.99
171	C159	H15K	0.99
172	C161	H16A	0.98
173	C161	H16B	0.98
174	C161	H16C	0.98
175	C163	H16D	0.98
176	C163	H16E	0.98
177	C163	H16F	0.98
178	C155	H15L	0.98
179	C155	H15M	0.98
180	C155	H15N	0.98
181	C155	C79	1.52(3)
182	C81	H81A	0.98
183	C81	H81B	0.98
184	C81	H81C	0.98
185	C81	C79	1.54(3)
186	C79	C165	1.54(3)
187	C165	H16G	0.98
188	C165	H16H	0.98
189	C165	H16I	0.98
190	O4	C150	1.20(2)
191	N4	C14	1.33(1)
192	N4	C50	1.36(1)
193	N10	H10A	0.879
194	N10	C38	1.39(1)
195	N10	C46	1.38(1)
196	N12	H12	0.879
197	N12	C12	1.35(1)
198	N12	C58	1.39(1)
199	N14	C132	1.37(1)
200	N14	C146	1.36(1)
201	N7	C66	1.32(1)
202	N7	C116	1.39(1)

203	O2	C154	1.20(1)
204	N11	C150	1.41(1)
205	N11	C107	1.41(2)
206	N11	C119	1.49(2)
207	O5	C21	1.23(2)
208	C8	C116	1.41(1)
209	C8	C120	1.41(2)
210	C8	C142	1.45(1)
211	O7	C107	1.26(1)
212	N3	C154	1.41(2)
213	N3	C21	1.38(1)
214	N3	C55	1.52(2)
215	C12	C54	1.45(2)
216	C12	C162	1.40(2)
217	C14	C20	1.47(1)
218	C14	C162	1.41(2)
219	C18	C46	1.39(1)
220	C18	C50	1.41(1)
221	C18	C66	1.52(1)
222	C20	H20	0.95
223	C20	C72	1.34(2)
224	C30	C38	1.37(1)
225	C30	C122	1.49(1)
226	C30	C132	1.42(2)
227	C34	H34	0.95
228	C34	C40	1.41(2)
229	C34	C144	1.32(1)
230	C36	H36	0.95
231	C36	C106	1.30(2)
232	C36	C146	1.47(1)
233	C38	C130	1.46(2)
234	C40	C66	1.44(1)
235	C40	C120	1.40(1)
236	C44	H44	0.95
237	C44	C96	1.40(1)
238	C44	C11	1.39(1)
239	C46	C152	1.40(2)
240	C50	C72	1.42(1)
241	C54	H54	0.95
242	C54	C90	1.35(1)
243	C58	C90	1.41(2)
244	C58	C158	1.37(1)
245	C72	H72	0.95
246	C78	C114	1.43(2)
247	C78	C120	1.40(1)
248	C78	C128	1.45(1)

249	C84	C114	1.40(1)
250	C84	C45	1.36(2)
251	C84	C107	1.41(2)
252	C90	H90	0.95
253	C96	C108	1.38(2)
254	C96	C162	1.47(1)
255	C98	C100	1.37(2)
256	C98	C166	1.37(1)
257	C98	C21	1.44(2)
258	C100	C136	1.46(1)
259	C100	C142	1.41(2)
260	C106	H106	0.95
261	C106	C132	1.46(1)
262	C108	H108	0.949
263	C108	C85	1.38(1)
264	C110	C128	1.43(2)
265	C110	C142	1.42(1)
266	C110	C49	1.43(2)
267	C112	H112	0.95
268	C112	C122	1.39(2)
269	C112	C23	1.40(2)
270	C114	C144	1.44(2)
271	C116	C95	1.39(2)
272	C122	C3	1.39(2)
273	C128	C164	1.41(1)
274	C130	H130	0.95
275	C130	C152	1.32(1)
276	C136	C154	1.48(2)
277	C136	C95	1.37(2)
278	C138	H138	0.95
279	C138	C85	1.40(1)
280	C138	C11	1.38(2)
281	C144	C150	1.48(2)
282	C146	C158	1.41(2)
283	C152	H152	0.95
284	C158	H158	0.95
285	C164	H164	0.95
286	C164	C45	1.40(2)
287	C166	H166	0.95
288	C166	C49	1.37(2)
289	C85	C25	1.54(2)
290	C11	C105	1.55(1)
291	C45	H45	0.95
292	C23	C7	1.39(2)
293	C23	C59	1.51(2)
294	C95	H95	0.95

295	C3	H3	0.95
296	C3	C13	1.40(2)
297	C49	H49	0.95
298	C25	C27	1.52(2)
299	C25	C115	1.54(2)
300	C25	C61	1.48(2)
301	C51	C13	1.54(2)
302	C51	C31	1.51(2)
303	C51	C125	1.55(2)
304	C51	C17	1.53(2)
305	C13	C7	1.39(2)
306	C105	C121	1.57(2)
307	C105	C133	1.56(2)
308	C105	C139	1.58(2)
309	C27	H27A	0.98
310	C27	H27B	0.98
311	C27	H27C	0.98
312	C55	H55	1
313	C55	C127	1.52(2)
314	C55	C73	1.60(2)
315	C7	H7	0.95
316	C115	H11A	0.98
317	C115	H11B	0.98
318	C115	H11C	0.98
319	C59	C33	1.53(2)
320	C59	C71	1.52(2)
321	C59	C77	1.52(2)
322	C119	H119	1
323	C119	C5	1.38(2)
324	C119	C41	1.44(2)
325	C121	H12A	0.98
326	C121	H12B	0.98
327	C121	H12C	0.98
328	C61	H61A	0.98
329	C61	H61B	0.98
330	C61	H61C	0.98
331	C31	H31A	0.98
332	C31	H31B	0.98
333	C31	H31C	0.98
334	C125	H12D	0.98
335	C125	H12E	0.98
336	C125	H12F	0.98
337	C127	H12G	0.99
338	C127	H12H	0.99
339	C127	C67	1.52(2)
340	C33	H33A	0.98

341	C33	H33B	0.98
342	C33	H33C	0.98
343	C133	H13D	0.98
344	C133	H13E	0.98
345	C133	H13F	0.98
346	C67	H67A	0.98
347	C67	H67B	0.98
348	C67	H67C	0.98
349	C17	H17D	0.98
350	C17	H17E	0.98
351	C17	H17F	0.98
352	C139	H13G	0.98
353	C139	H13H	0.98
354	C139	H13I	0.98
355	C71	H71A	0.98
356	C71	H71B	0.98
357	C71	H71C	0.98
358	C143	H14M	0.98
359	C143	H14N	0.98
360	C143	H14O	0.98
361	C143	C73	1.50(2)
362	C73	H73A	0.99
363	C73	H73B	0.99
364	C37	H37A	0.98
365	C37	H37B	0.98
366	C37	H37C	0.98
367	C37	C41	1.36(2)
368	C19	H19A	0.98
369	C19	H19B	0.98
370	C19	H19C	0.98
371	C19	C5	1.37(2)
372	C77	H77A	0.98
373	C77	H77B	0.98
374	C77	H77C	0.98
375	C5	H5A	0.99
376	C5	H5B	0.99
377	C41	H41A	0.99
378	C41	H41B	0.99

Table S9. Cartesian coordinates of the optimized geometry for compound **PDPP**.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-4.619835	4.859119	0.753330

2	6	0	-3.963319	6.012109	0.622202
3	6	0	-2.672935	5.670486	0.516857
4	7	0	-2.568947	4.409035	0.580576
5	6	0	-3.703780	3.871581	0.768428
6	6	0	-2.020056	-0.311307	0.998627
7	6	0	-3.172326	0.326479	1.209049
8	6	0	-3.013490	1.597096	0.800624
9	7	0	-1.802363	1.654066	0.400182
10	6	0	-1.162702	0.549924	0.421507
11	6	0	-3.961035	2.553738	0.920554
12	6	0	2.837938	2.135627	-0.930218
13	6	0	2.205086	0.974207	-0.803004
14	6	0	1.025549	1.217575	-0.202383
15	7	0	0.958037	2.481652	-0.058312
16	6	0	2.027586	3.075561	-0.416656
17	6	0	0.108407	0.252179	0.067535
18	6	0	0.527683	7.314407	0.124443
19	6	0	1.692440	6.691683	-0.081602
20	6	0	1.453627	5.370299	-0.194557
21	7	0	0.202527	5.249767	0.003862
22	6	0	-0.402935	6.352800	0.178327
23	6	0	-1.705372	6.585713	0.373993
24	6	0	2.350402	4.390991	-0.433503
25	6	0	3.629664	4.741618	-0.724433
26	6	0	-5.228481	2.171871	1.217640
27	6	0	4.669086	4.118487	-0.136172
28	6	0	5.954991	4.415899	-0.395481
29	6	0	6.178030	5.404211	-1.279637
30	6	0	5.190989	6.077623	-1.899372
31	6	0	3.929047	5.716364	-1.604243
32	6	0	-5.955224	2.774191	2.176923
33	6	0	-7.225040	2.433787	2.463383
34	6	0	-7.767261	1.443275	1.731771
35	6	0	-7.099302	0.796374	0.759041
36	6	0	-5.827044	1.175117	0.538137
37	6	0	5.526435	7.184924	-2.909550
38	6	0	6.337661	6.583177	-4.078373
39	6	0	4.288505	7.881290	-3.521967
40	6	0	6.357343	8.283227	-2.208051
41	6	0	7.082024	3.653744	0.315938
42	6	0	6.935139	2.139638	0.038667
43	6	0	8.502706	4.060616	-0.139190
44	6	0	6.994267	3.914696	1.835784
45	6	0	-7.729233	-0.316724	-0.089900
46	6	0	-7.655755	0.054381	-1.589041
47	6	0	-7.983392	3.161412	3.583197
48	6	0	-7.260382	2.920866	4.927141
49	6	0	-8.023802	4.676045	3.277792

50	6	0	-9.447512	2.697309	3.763488
51	6	0	3.473043	-7.030764	0.417436
52	6	0	2.243023	-6.947380	-0.102824
53	6	0	1.592546	-5.774711	-0.225607
54	6	0	2.249021	-4.679688	0.213434
55	6	0	3.499620	-4.743962	0.735996
56	6	0	4.121071	-5.933867	0.841657
57	6	0	1.617734	-3.495354	0.113403
58	6	0	2.235808	-2.379792	0.519139
59	6	0	3.474309	-2.444714	1.028178
60	6	0	4.118108	-3.618781	1.145499
61	6	0	0.352709	-5.662034	-0.762593
62	6	0	0.381051	-3.366076	-0.396594
63	6	0	-0.325264	-6.725506	-1.234973
64	6	0	-1.541280	-6.613342	-1.779747
65	6	0	-2.141144	-5.416770	-1.871485
66	6	0	-1.494807	-4.333365	-1.401163
67	6	0	-0.260775	-4.459131	-0.856717
68	6	0	-2.053345	-3.113140	-1.499299
69	6	0	-1.354209	-2.044196	-1.078427
70	6	0	-0.166084	-2.132327	-0.454411
71	6	0	5.375412	-6.056776	1.360635
72	6	0	5.374884	-3.636876	1.673270
73	6	0	-3.377944	-5.336797	-2.434645
74	6	0	-3.299355	-2.933923	-2.026271
75	7	0	5.984643	-4.878478	1.774238
76	7	0	-3.975746	-4.088739	-2.399178
77	6	0	7.350688	-4.946684	2.350034
78	6	0	8.422571	-4.240544	1.489776
79	6	0	7.416624	-4.537775	3.838826
80	6	0	6.398927	-5.302781	4.697051
81	6	0	-5.397870	-3.978165	-2.800830
82	6	0	-5.601796	-4.027767	-4.329233
83	6	0	-4.821173	-2.937207	-5.075127
84	8	0	5.939291	-2.628673	2.039439
85	8	0	5.930167	-7.131801	1.455585
86	8	0	-3.942952	-6.294097	-2.917483
87	7	0	1.687394	-1.245718	0.447397
88	6	0	0.509129	-1.053330	0.020294
89	6	0	-6.356341	-4.948083	-2.063582
90	8	0	-3.810938	-1.839290	-2.140953
91	6	0	-6.023375	-5.139722	-0.576037
92	6	0	-6.954445	-1.628844	0.147860
93	6	0	-9.215673	-0.597155	0.232400
94	6	0	8.397372	-4.711376	0.028610
95	1	0	-5.712152	4.804780	0.834055
96	1	0	-4.405366	7.016365	0.594460
97	1	0	-1.855311	-1.355095	1.295535

98	1	0	-4.039852	-0.145048	1.688600
99	1	0	-1.370360	2.535454	0.041631
100	1	0	3.817122	2.230546	-1.416315
101	1	0	2.635268	0.039772	-1.185364
102	1	0	0.382329	8.395929	0.243759
103	1	0	2.646657	7.230366	-0.135349
104	1	0	-0.297315	4.333035	-0.006517
105	1	0	-2.012057	7.647055	0.418030
106	1	0	4.464039	3.352152	0.628555
107	1	0	7.211831	5.683581	-1.518275
108	1	0	3.101412	6.197712	-2.144140
109	1	0	-5.476429	3.552888	2.791362
110	1	0	-8.802014	1.150292	1.937932
111	1	0	-5.275671	0.684605	-0.279950
112	1	0	6.573550	7.353322	-4.847262
113	1	0	7.311603	6.156190	-3.752815
114	1	0	5.766138	5.769741	-4.580927
115	1	0	4.586681	8.686988	-4.230525
116	1	0	3.657809	8.367702	-2.743500
117	1	0	3.658520	7.174835	-4.108500
118	1	0	7.335456	7.912973	-1.830252
119	1	0	6.590098	9.122202	-2.902105
120	1	0	5.801371	8.708016	-1.341166
121	1	0	7.762036	1.558888	0.506472
122	1	0	5.991399	1.711596	0.442024
123	1	0	6.955974	1.932650	-1.055770
124	1	0	9.282650	3.468142	0.390628
125	1	0	8.723616	5.128899	0.084242
126	1	0	8.656929	3.879804	-1.227250
127	1	0	6.041700	3.551336	2.280391
128	1	0	7.814857	3.398541	2.383626
129	1	0	7.073912	5.003441	2.057239
130	1	0	-8.145542	-0.718816	-2.223414
131	1	0	-8.168661	1.023871	-1.783212
132	1	0	-6.613727	0.141614	-1.967181
133	1	0	-7.797396	3.411447	5.770398
134	1	0	-7.198035	1.832333	5.155455
135	1	0	-6.224261	3.324862	4.937920
136	1	0	-8.602875	5.230833	4.050375
137	1	0	-8.505801	4.869603	2.292343
138	1	0	-7.014323	5.141745	3.254451
139	1	0	-10.053382	2.867312	2.844596
140	1	0	-9.513573	1.622398	4.046438
141	1	0	-9.953575	3.261781	4.579241
142	1	0	3.918482	-8.038676	0.472804
143	1	0	1.824132	-7.914266	-0.415712
144	1	0	3.935835	-1.494678	1.347902
145	1	0	0.060895	-7.754415	-1.219211

146	1	0	-2.014813	-7.541825	-2.141549
147	1	0	-1.769676	-1.045047	-1.263840
148	1	0	7.716093	-6.002805	2.373643
149	1	0	8.311827	-3.133531	1.518663
150	1	0	9.434395	-4.450181	1.914307
151	1	0	8.441199	-4.743236	4.233732
152	1	0	7.259708	-3.444285	3.973899
153	1	0	5.353362	-5.067684	4.393858
154	1	0	6.543226	-6.403719	4.607686
155	1	0	6.501706	-5.033904	5.773515
156	1	0	-5.801939	-2.985521	-2.479743
157	1	0	-5.305098	-5.023814	-4.731240
158	1	0	-6.688019	-3.905805	-4.559050
159	1	0	-5.018617	-2.984719	-6.170851
160	1	0	-5.114093	-1.921026	-4.725310
161	1	0	-3.723058	-3.052157	-4.930717
162	1	0	-7.400420	-4.557121	-2.146092
163	1	0	-6.392229	-5.945235	-2.558090
164	1	0	-6.848009	-5.671512	-0.047986
165	1	0	-5.102490	-5.746891	-0.430464
166	1	0	-5.859299	-4.168573	-0.060916
167	1	0	-7.411052	-2.459815	-0.434943
168	1	0	-6.973155	-1.918082	1.223230
169	1	0	-5.888363	-1.562106	-0.162748
170	1	0	-9.853762	0.298904	0.058200
171	1	0	-9.626443	-1.403585	-0.416606
172	1	0	-9.358175	-0.945213	1.280488
173	1	0	9.213603	-4.232169	-0.559695
174	1	0	8.532586	-5.814853	-0.041338
175	1	0	7.434035	-4.451194	-0.465717

Table S10. Cartesian coordinates of the optimized geometry for compound **Zn-PDPP**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.328993	-2.374143	-1.682558
2	6	0	7.121322	-1.263465	-1.702027
3	6	0	6.259742	-0.128713	-1.466111
4	7	0	4.963423	-0.553481	-1.308843
5	6	0	4.973265	-1.922671	-1.440030
6	6	0	0.297820	-2.380540	-0.763859
7	6	0	1.372743	-3.176441	-1.027500
8	6	0	2.534413	-2.315996	-1.088785
9	7	0	2.149063	-1.011612	-0.869982
10	6	0	0.789612	-1.023564	-0.665214
11	6	0	3.845804	-2.760744	-1.345360
12	6	0	0.390600	3.680845	-0.085532
13	6	0	-0.410538	2.578315	-0.066475
14	6	0	0.433051	1.437047	-0.347147

15	7	0	1.728732	1.857746	-0.532327
16	6	0	1.732524	3.227220	-0.382413
17	6	0	-0.009102	0.104521	-0.408036
18	6	0	6.397146	3.685646	-1.133441
19	6	0	5.325953	4.491655	-0.878866
20	6	0	4.168275	3.629225	-0.749752
21	7	0	4.550260	2.320774	-0.933817
22	6	0	5.903248	2.328958	-1.167831
23	6	0	6.688331	1.199114	-1.406286
24	6	0	2.856655	4.069163	-0.486537
25	6	0	2.642413	5.544495	-0.301922
26	6	0	4.056967	-4.236140	-1.531624
27	6	0	2.098189	6.313967	-1.331369
28	6	0	1.893449	7.697548	-1.181895
29	6	0	2.249838	8.276545	0.040826
30	6	0	2.798330	7.533673	1.104562
31	6	0	2.990205	6.162208	0.910828
32	6	0	4.234478	-4.770547	-2.812929
33	6	0	4.430225	-6.145413	-3.010123
34	6	0	4.448572	-6.972652	-1.875682
35	6	0	4.277158	-6.473498	-0.574491
36	6	0	4.078572	-5.093069	-0.425194
37	6	0	3.159562	8.245118	2.424114
38	6	0	1.889480	8.895322	3.025760
39	6	0	3.742238	7.277421	3.472921
40	6	0	4.214362	9.344652	2.148130
41	6	0	1.297490	8.509273	-2.349625
42	6	0	-0.102749	7.951344	-2.704235
43	6	0	1.143761	10.005306	-2.012305
44	6	0	2.222758	8.389044	-3.585484
45	6	0	4.302653	-7.378878	0.674031
46	6	0	5.447665	-6.927789	1.613988
47	6	0	4.610787	-6.691816	-4.441192
48	6	0	3.352097	-6.362074	-5.280835
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50	6	0	4.817065	-8.219058	-4.470519
51	6	0	-8.368858	-1.194941	0.393277
52	6	0	-7.576065	-1.389623	1.524476
53	6	0	-6.185269	-1.194438	1.489079
54	6	0	-5.601964	-0.788640	0.252380
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57	6	0	-4.198186	-0.572547	0.138963
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59	6	0	-4.458691	0.024731	-2.222875
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61	6	0	-5.311101	-1.384619	2.653746
62	6	0	-3.351644	-0.757491	1.258877
63	6	0	-5.783517	-1.779581	3.916641
64	6	0	-4.920044	-1.946738	4.999144

65	6	0	-3.548983	-1.724998	4.861163
66	6	0	-3.033578	-1.329860	3.616033
67	6	0	-3.908777	-1.158991	2.509523
68	6	0	-1.631293	-1.096303	3.458782
69	6	0	-1.112486	-0.710480	2.245317
70	6	0	-1.960790	-0.536003	1.111365
71	6	0	-8.667386	-0.595891	-2.006178
72	6	0	-6.666804	0.028543	-3.336517
73	6	0	-2.651999	-1.907974	6.030598
74	6	0	-0.713300	-1.269107	4.617913
75	7	0	-8.046594	-0.192717	-3.206119
76	7	0	-1.282335	-1.668687	5.845583
77	6	0	-8.933064	0.005547	-4.400524
78	6	0	-8.953968	1.469909	-4.878172
79	6	0	-8.618295	-0.987777	-5.535042
80	6	0	-8.656887	-2.461291	-5.114327
81	6	0	-0.347595	-1.840698	7.006602
82	6	0	-0.633190	-0.839768	8.142120
83	6	0	-0.632330	0.629474	7.704882
84	8	0	-6.181974	0.380820	-4.405051
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91	6	0	0.070213	-4.318459	6.409427
92	6	0	2.952394	-7.263402	1.423134
93	6	0	4.528809	-8.863108	0.324969
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95	1	0	6.626146	-3.404204	-1.814598
96	1	0	8.191427	-1.210605	-1.855837
97	1	0	-0.734365	-2.685332	-0.664269
98	1	0	1.382522	-4.246075	-1.176812
99	1	0	0.105250	4.708356	0.085584
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101	1	0	7.427890	3.976445	-1.290235
102	1	0	5.311094	5.568080	-0.789737
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104	1	0	1.838099	5.819564	-2.262313
105	1	0	2.099587	9.339990	0.180620
106	1	0	3.407426	5.544171	1.697053
107	1	0	4.210729	-4.092655	-3.660667
108	1	0	4.600318	-8.034369	-2.009067
109	1	0	3.942777	-4.661696	0.561842
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112	1	0	1.125877	8.138845	3.236895
113	1	0	3.981122	7.830053	4.387817
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115	1	0	3.031575	6.488318	3.740746
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117	1	0	4.478230	9.859665	3.079218
118	1	0	5.129087	8.912504	1.727971
119	1	0	-0.536534	8.515969	-3.537755
120	1	0	-0.059962	6.899364	-3.001728
121	1	0	-0.783393	8.031002	-1.849496
122	1	0	0.718181	10.531962	-2.873078
123	1	0	2.106712	10.474536	-1.783223
124	1	0	0.471019	10.166623	-1.162987
125	1	0	2.336648	7.350590	-3.910469
126	1	0	1.809086	8.958298	-4.426075
127	1	0	3.221208	8.782957	-3.366368
128	1	0	5.476265	-7.560847	2.508577
129	1	0	6.418440	-7.003915	1.112134
130	1	0	5.321292	-5.891919	1.942556
131	1	0	3.467236	-6.741347	-6.302961
132	1	0	2.459362	-6.823904	-4.845217
133	1	0	3.174316	-5.284349	-5.343175
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135	1	0	6.757563	-6.252027	-4.526506
136	1	0	5.746271	-4.941063	-5.151354
137	1	0	5.713930	-8.522102	-3.919420
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139	1	0	4.940268	-8.550994	-5.506922
140	1	0	-9.441422	-1.349552	0.435306
141	1	0	-8.061155	-1.698400	2.443130
142	1	0	-4.014070	0.334542	-3.162091
143	1	0	-6.840534	-1.962026	4.070977
144	1	0	-5.299511	-2.251547	5.968443
145	1	0	-0.045330	-0.540606	2.162285
146	1	0	-9.924303	-0.233612	-4.012453
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148	1	0	-9.695917	1.513957	-5.685890
149	1	0	-9.378584	-0.815060	-6.307676
150	1	0	-7.651089	-0.746303	-5.983787
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152	1	0	-9.620288	-2.726803	-4.664597
153	1	0	-8.498796	-3.112075	-5.980544
154	1	0	0.624035	-1.591020	6.577796
155	1	0	-1.578805	-1.090248	8.630396
156	1	0	0.158691	-0.993055	8.886593
157	1	0	-0.766868	1.287447	8.569680
158	1	0	0.309130	0.903695	7.215837
159	1	0	-1.446497	0.843915	7.003900
160	1	0	0.485167	-3.323657	8.278345
161	1	0	-1.230205	-3.570704	7.977774
162	1	0	0.167579	-5.320867	6.839141
163	1	0	-0.702786	-4.370761	5.634848
164	1	0	1.017379	-4.068588	5.918354

165	1	0	2.958427	-7.898236	2.316892
166	1	0	2.122236	-7.584289	0.784260
167	1	0	2.750716	-6.237391	1.744992
168	1	0	5.488113	-9.024083	-0.178693
169	1	0	4.536985	-9.457306	1.244949
170	1	0	3.733181	-9.259399	-0.315220
171	1	0	-9.400851	3.491580	-4.215954
172	1	0	-10.301267	2.243928	-3.338160
173	1	0	-8.587505	2.517438	-2.991508
174	30	0	3.346837	0.655318	-0.907504

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