# Supplementary Information

## 4,4,9,9-Tetraphenyl Pyrroloindolizine: A Structural Analogue of Calix[2]pyrrole

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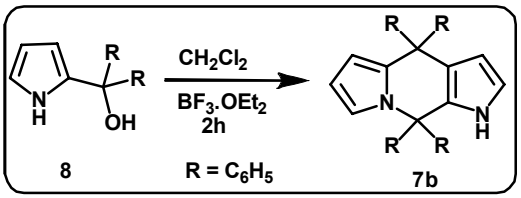
## 1. General Information

All the chemicals were of the best grade commercially available and are used without further purification. NMR spectra were recorded on a Bruker Avance Bruker AMX 500 spectrophotometer with $CDCl_3$ as solvent. Chemical shifts are reported as δ in units of parts per million (ppm) relative to TMS. FAB mass spectra were obtained on a JEOL SX-120/DA6000 spectrometer using argon (6 KV, 10 mA) as the FAB gas. FT-IR spectra were recorded on a Nicolet Impact 400D Infrared spectrophotometer. Melting points were determined on a Buchi melting point apparatus and are uncorrected. The single crystal X-ray diffraction data was collected on a Bruker AXS Kappa Apex 2 CCD diffractometer at 293(2) K for **7b**.

## 2. Synthesis of 7b:




To the stirred solution of 2-(diphenylhydroxymethyl)pyrrole, **8** (450 mg, 3.58 mmol) in dry dichloromethane (250 mL) under argon atmosphere at room temperature, $BF_3.Et_2O$ (0.04mL, 0.36mmol) was added slowly and allowed to stir for 2h. The reaction mixture was then quenched with aq. NaOH solution and extracted with dichloromethane. The organic layer was then washed with water and brine solution. After drying over anhydrous $Na_2SO_4$, the solvent was evaporated under vacuum. The dark residue obtained was purified by silica gel column chromatography (100 – 200 mesh). The colorless fraction eluted with hexane as the eluent was identified as **7b.** The white solid was recrystallized from $CH_2Cl_2$ and petroleum ether in 20% yield.

Spectral data of **7b**: m.p: 263$^0$C; $^1$H NMR (500 MHz, $CDCl_3$, 298 K): δ = 7.60 (brs, NH, 1H), 7.16 (m, CH-phenyl, 6H), 7.06 (s, CH-phenyl, 10H), 6.92 (d, J= 8.5 Hz, CH-phenyl, 4H), 6.68 (t, J= 5.5 Hz, CH-Pyrrole, 1H), 6.42 (m, CH-pyrrole, 1H), 6.13 (t, J= 6.5 Hz, CH-pyrrole, 1H), 5.96 (t, J= 5.5 Hz, CH-pyrrole, 1H), 5.77 (m, CH-pyrrole, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$, 298 K): δ = 147.42, 142.70, 139.02, 130.64, 129.20, 128.61, 127.99, 127.58, 127.19, 125.59, 125.13, 118.69, 117.96, 107.87, 67.97, 51.86 ; FT-IR: (KBr, cm$^{-1}$) = 3408, 3053, 3024, 2961, 2922, 1597, 1486, 1445, 1266, 1181, 1069, 1028, 874, 752, 522, 507; FAB MS (m/z): Calcd. for $C_{34}H_{26}N_2$ 462.21; Observed 464.29 (M+2); Anal. Calcd. for $C_{34}H_{26}N_2$: C, 88.28; H, 5.67; N, 6.06 ; Found: C, 88.26; H, 5.65; 6.03.

## 3. Spectral analyses of 7b:

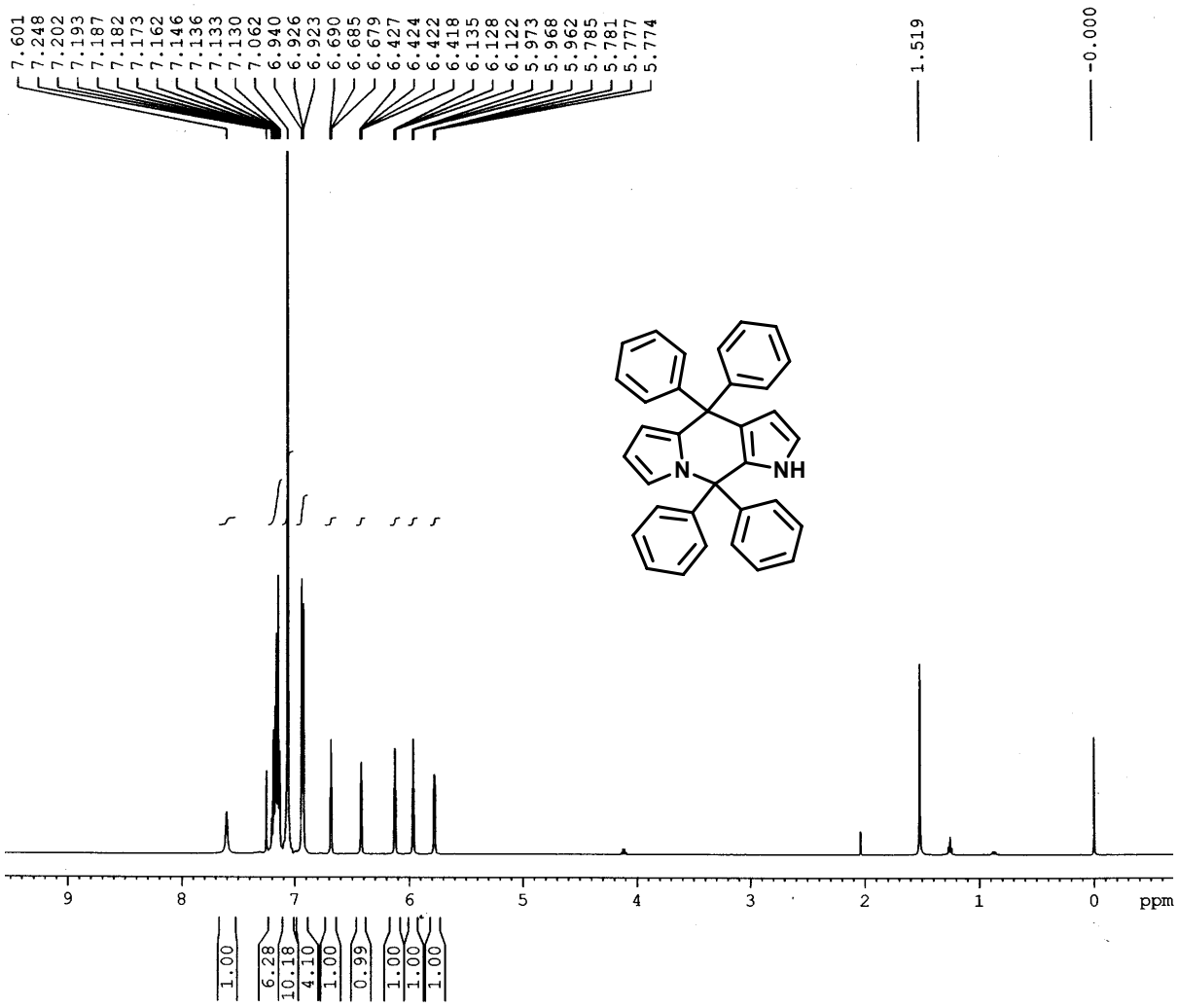



***Figure S1.*** $^{1}$H-NMR Spectrum of **7b** in $CDCl_3$

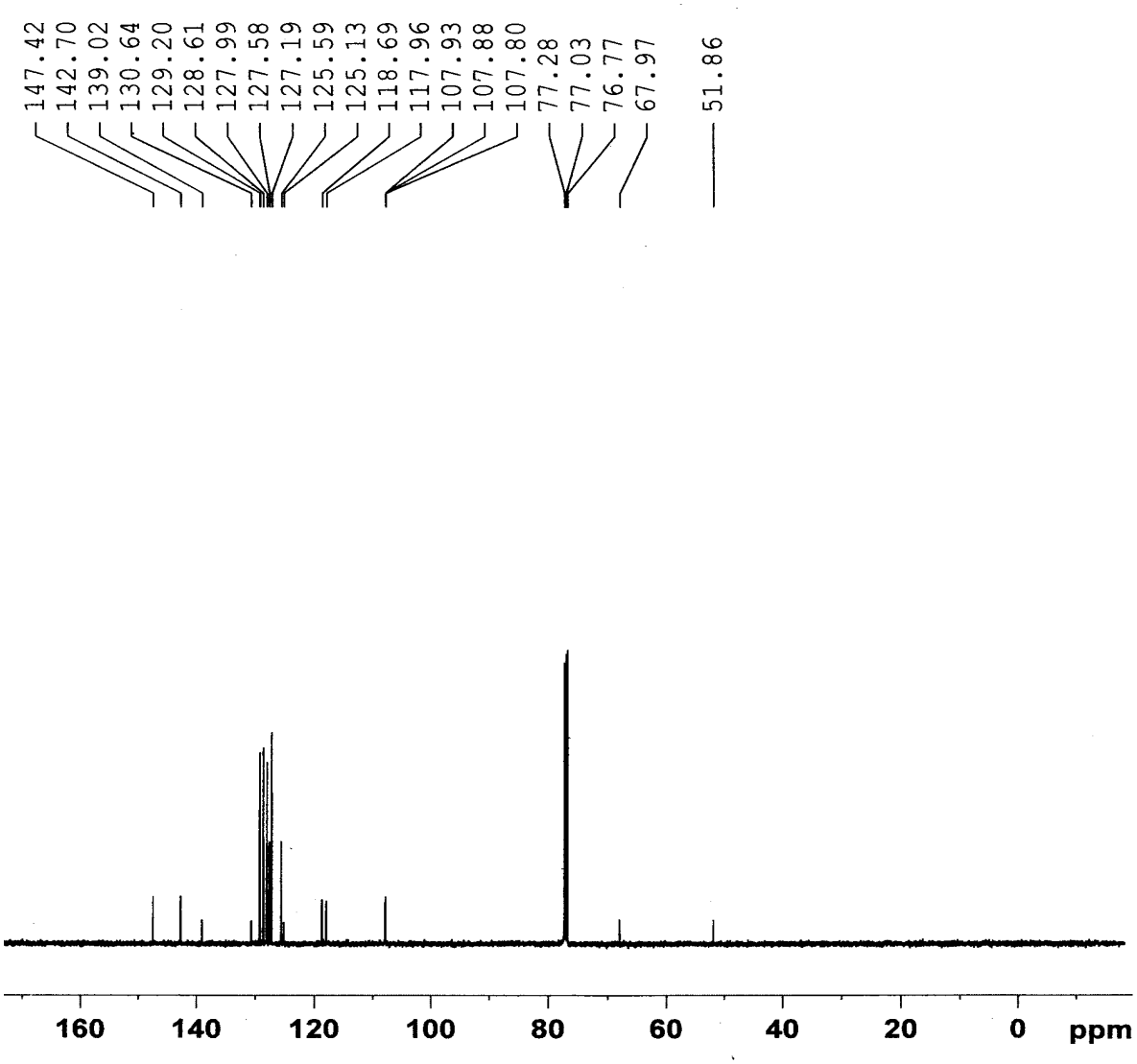



***Figure S2.*** $^{13}$C-NMR Spectrum of **7b** in $CDCl_3$

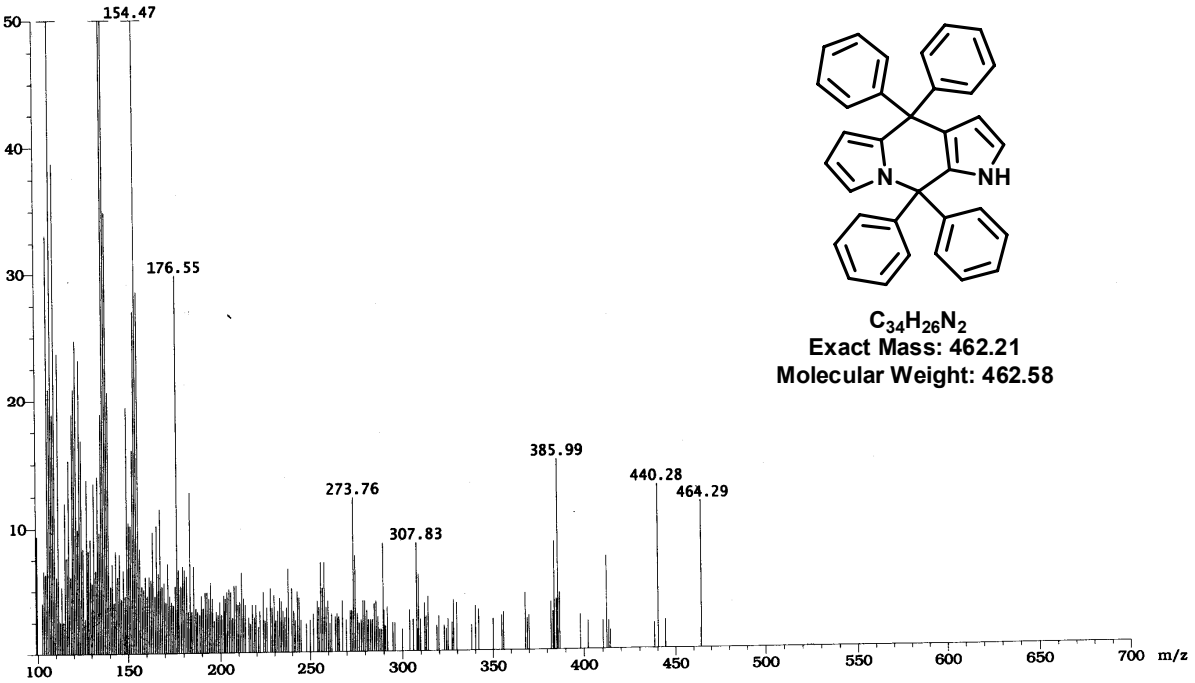



***Figure S3.*** FAB MS spectrum of **7b**

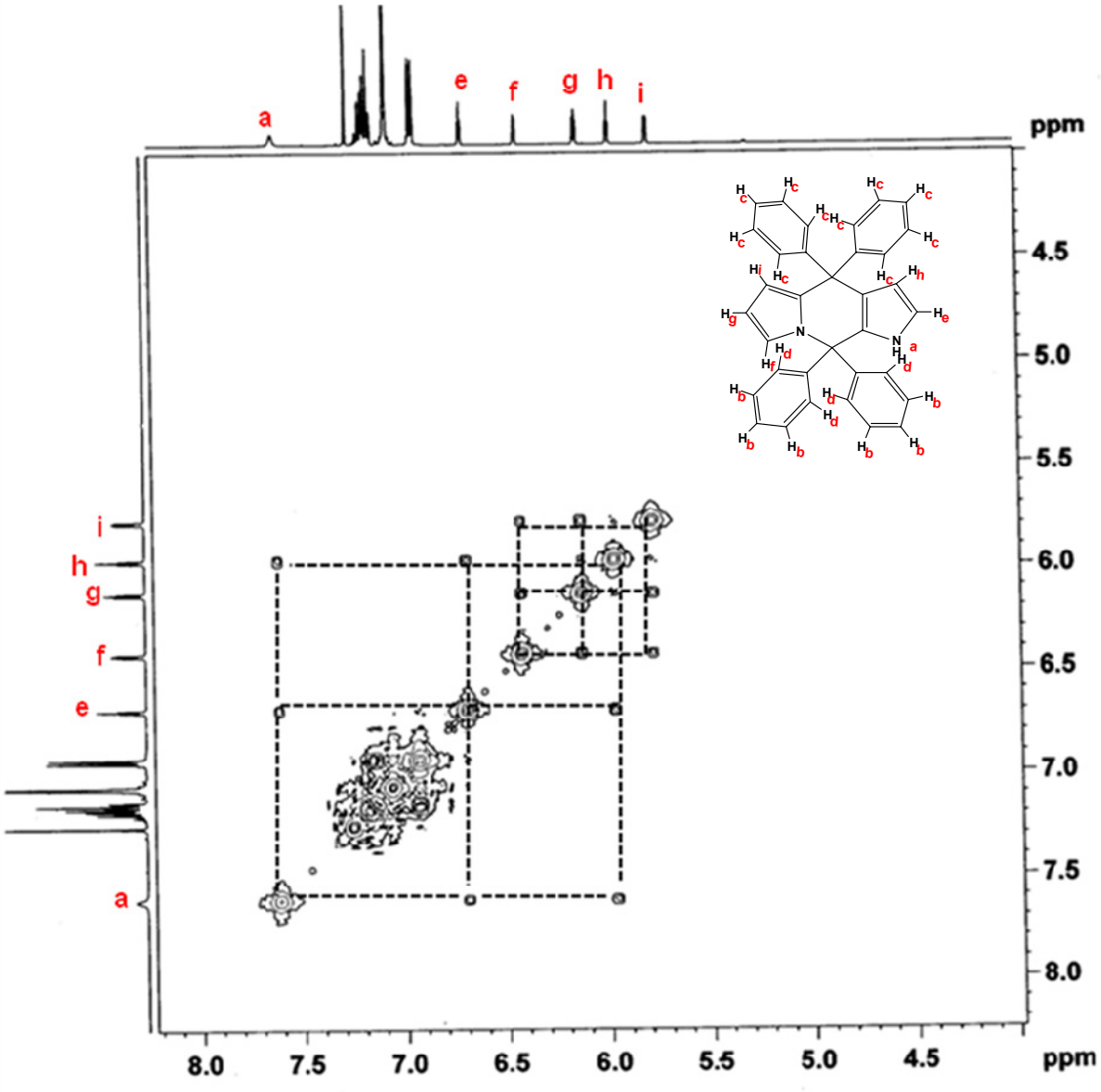



***Figure S4.*** $^{1}$H- $^{1}$H COSY Spectrum of **7b** in $CDCl_3$

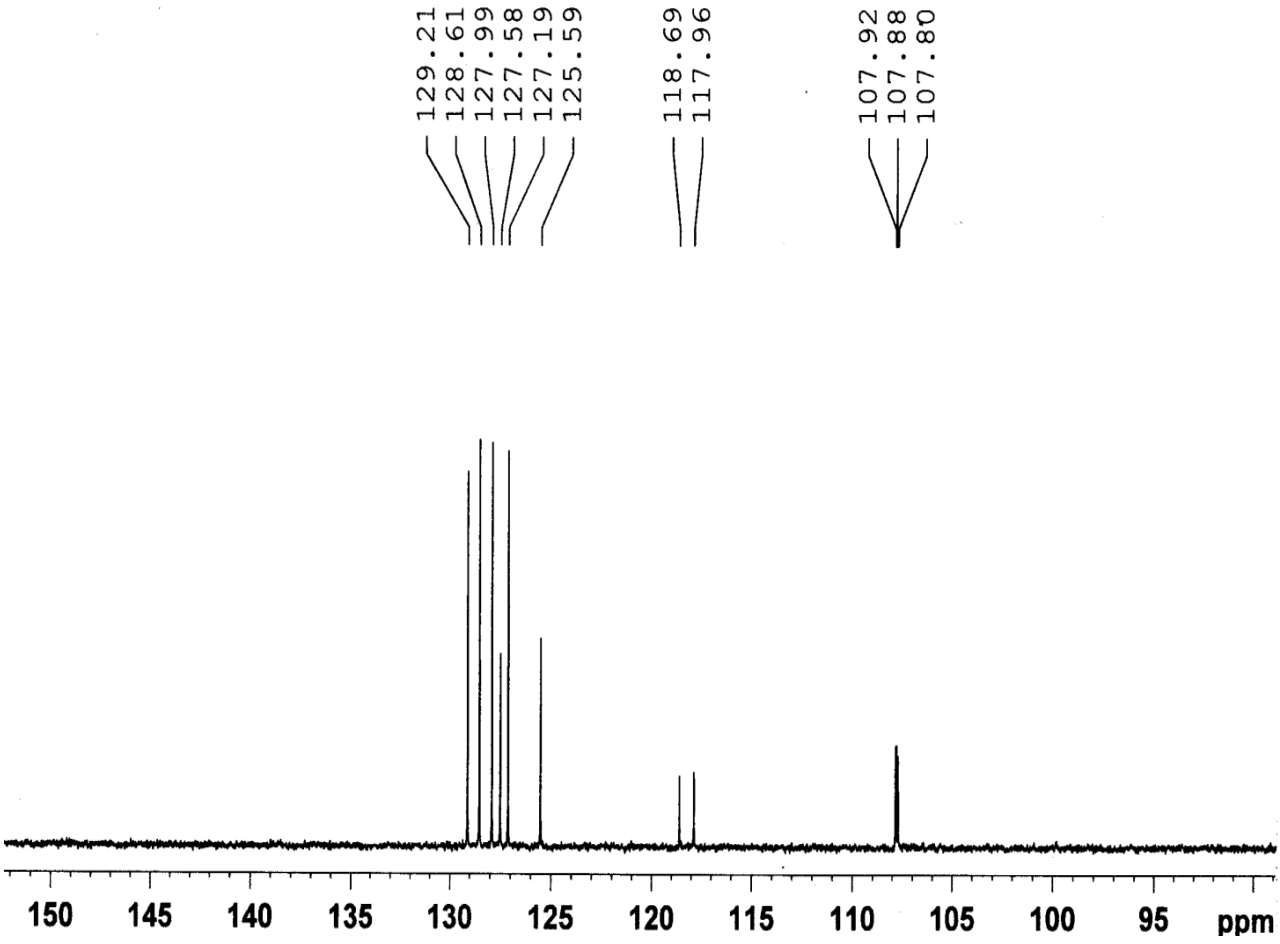



***Figure S5.*** DEPT 45 Spectrum of **7b** in $CDCl_3$

## 4. Single crystal X-ray structure and analysis of 7b:

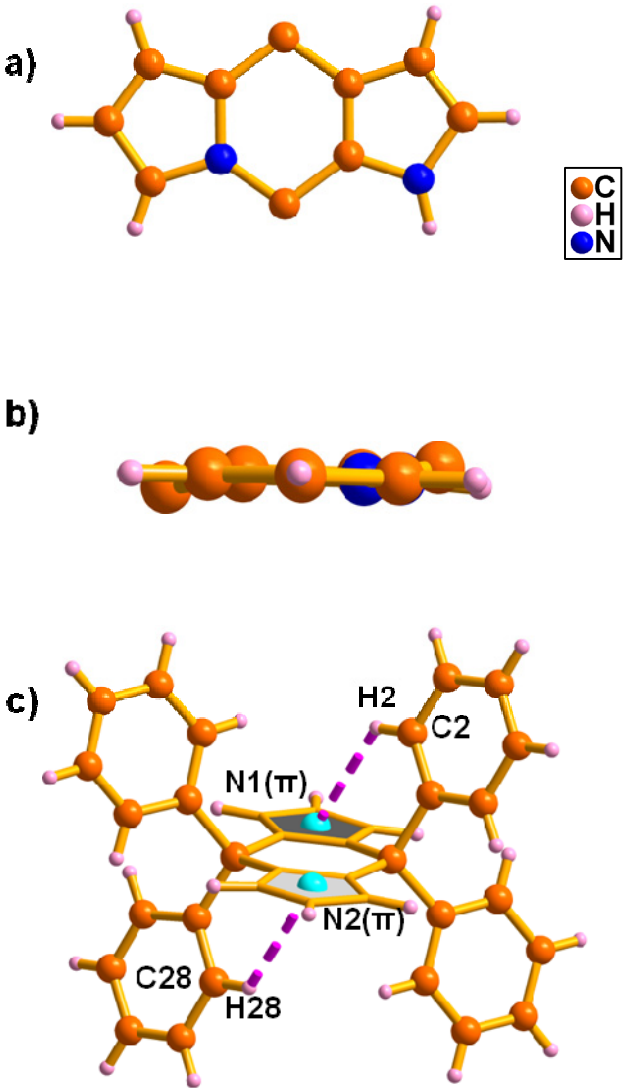



***Figure S6***. Single crystal X-ray structure of **7b**. a) top view, b) side view and c) top view with intramolecular hydrogen bonding interactions. The *meso*-diaryl groups in (a and b) are omitted for clarity. The distances and angles are C28-H28…N1: 2.83 Å, 127˚ and C2-H2…N2: 2.81 Å, 127º.

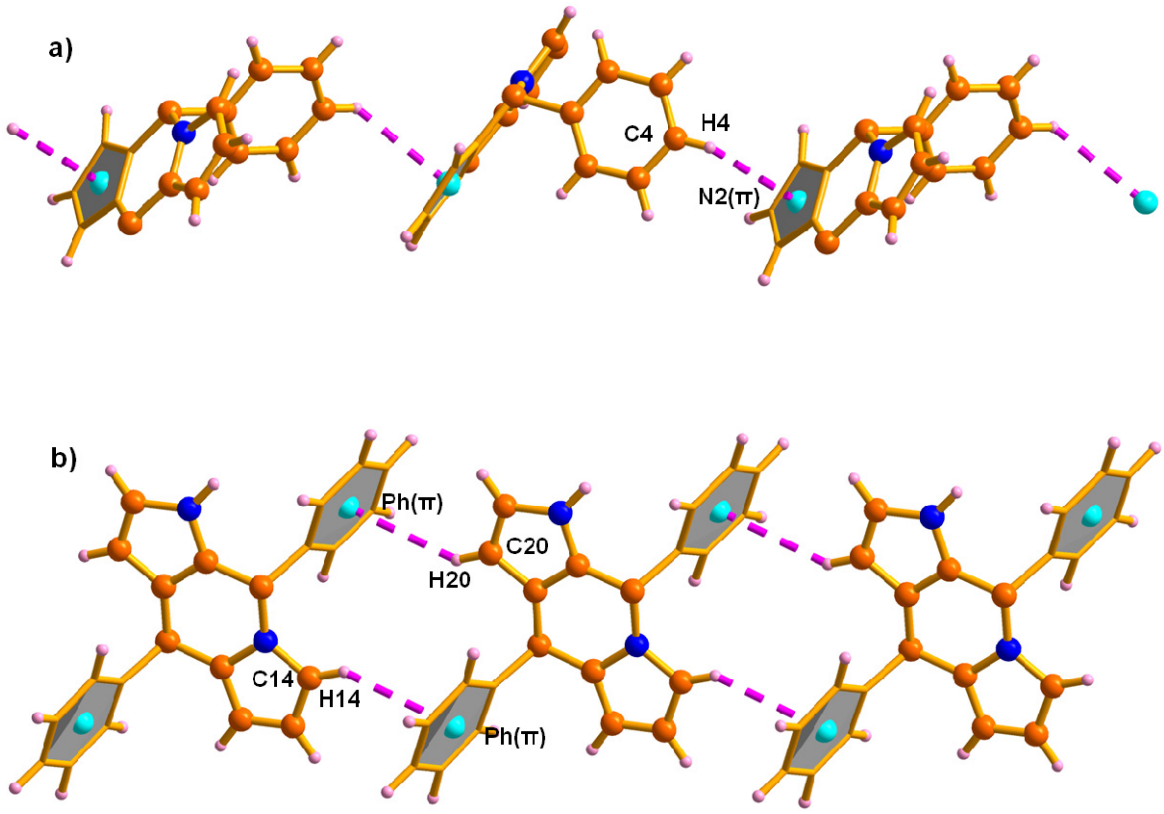



***Figure S7***. Single crystal X-ray analysis of **7b**. a) and b) are 1-D arrays. The intermolecular hydrogen bonding interactions are formed in a) between one of the *meso*-phenyl rings and *α,β*- linked pyrrolic π-cloud; b) between the pyrrolic *β*-CH and one of the *meso*-phenyl rings π-cloud and N,*α* pyrrolic *α*-CH and one of the meso-phenyl rings π-cloud. The distances and angles in (a and b) are: C4-H4...N2(π): 2.92Å, 129˚; C20-H20...Ph(π): 2.99 Å, 142˚ and C14-H14...Ph(π): 2.98 Å, 143˚. The groups which are not involved in hydrogen bonding interactions are omitted for clarity.

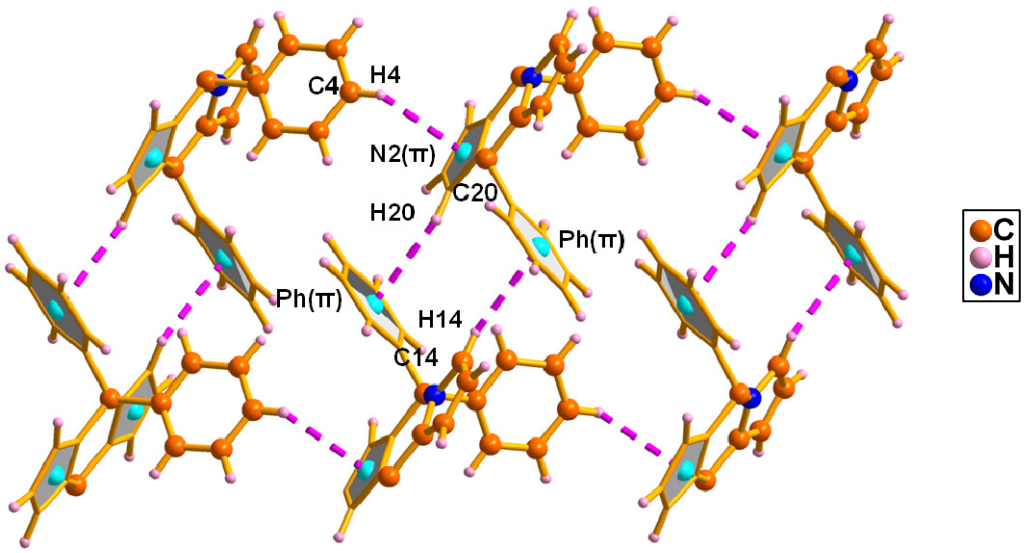



***Figure S8***. 2D array of **7b**. The intermolecular hydrogen bonding interactions are generated by combining the two one-dimensional interactions (*Figure S7*) .The distances and angles are: C4-H4...N2(π): 2.92Å, 129˚; C20-H20...Ph(π): 2.99 Å, 142˚ and C14-H14...Ph(π): 2.98 Å, 143˚. The groups which are not involved in hydrogen bonding interactions are omitted for clarity.

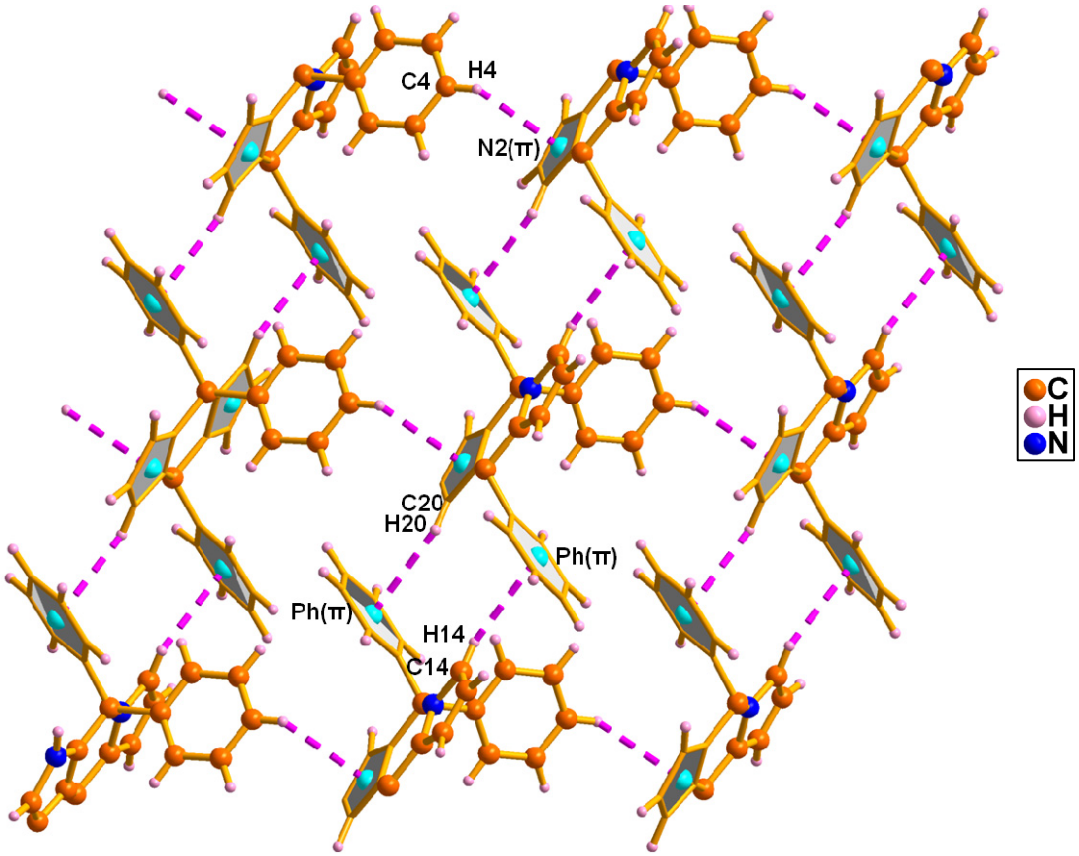



***Figure S9***. Supramolecular assembly of **7b**.