Supplementary Information


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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 CDCl₃ 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, BF₃·Et₂O (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 Na₂SO₄, 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 CH₂Cl₂ and petroleum ether in 20% yield.

Spectral data of 7b: m.p: 263°C; ¹H NMR (500 MHz, CDCl₃, 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); ¹³C NMR (125 MHz, CDCl₃, 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 C₃₄H₂₆N₂: 462.21; Observed 464.29 (M+2); Anal. Calcd. for C₃₄H₂₆N₂: C, 88.28; H, 5.67; N, 6.06 ; Found: C, 88.26; H, 5.65; 6.03.
3. Spectral analyses of 7b:

**Figure SI.** $^1$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 CDCl₃
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, 127°.
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): 2.92 Å, 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(\pi): 2.92 Å, 129°; C20-H20...Ph(\pi): 2.99 Å, 142° and C14-H14...Ph(\pi): 2.98 Å, 143°. The groups which are not involved in hydrogen bonding interactions are omitted for clarity.
Figure S9. Supramolecular assembly of 7b.