

Supporting Information

Synthesis and Structure of 2, 6, 14- and 2, 7, 14-Trisubstituted Triptycene Derivatives

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1. ^1H NMR and ^{13}C NMR spectra of **2~6**.

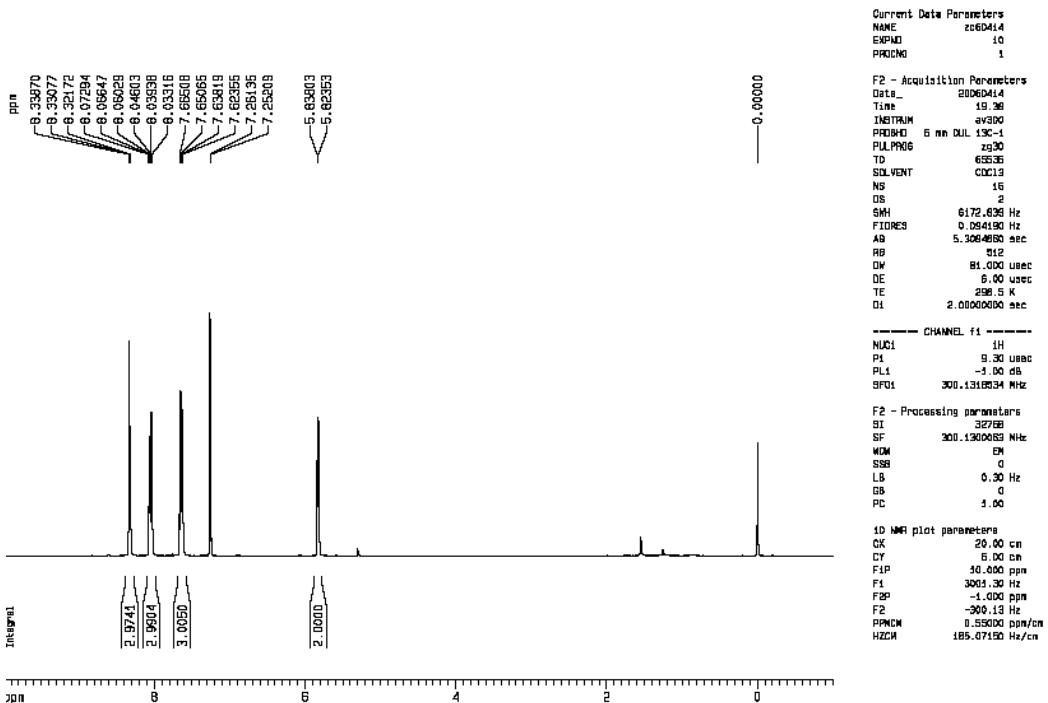


Figure S1. ^1H NMR spectrum of **2a** in CDCl_3 .

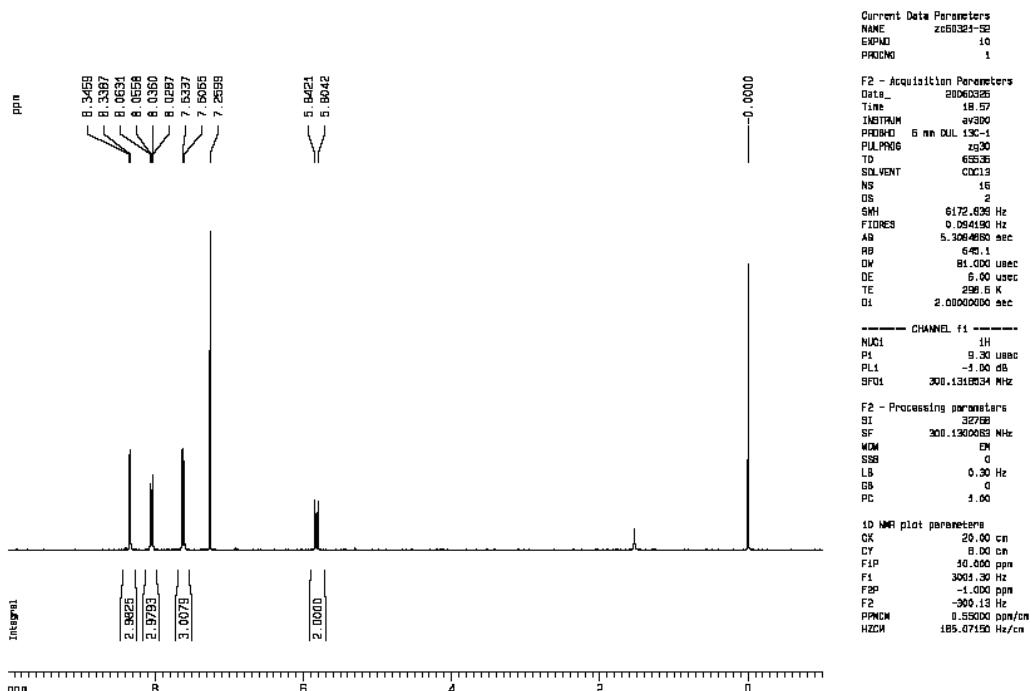


Figure S2. ^1H NMR spectrum of **2b** in CDCl_3 .

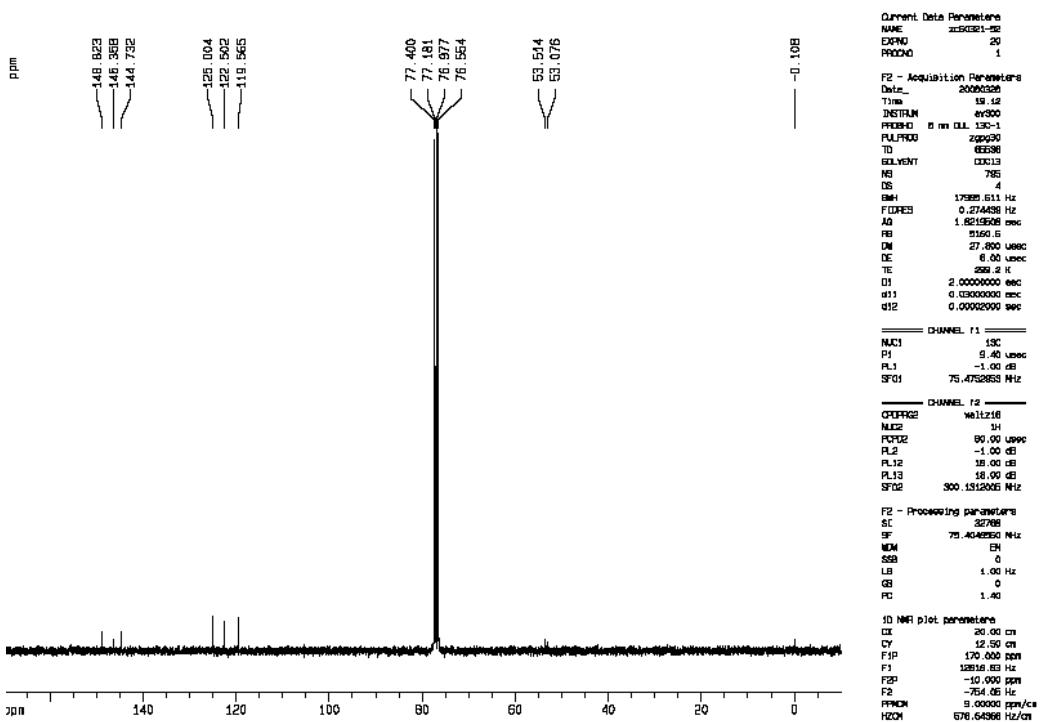


Figure S3. ^{13}C NMR spectrum of **2b** in CDCl_3 .

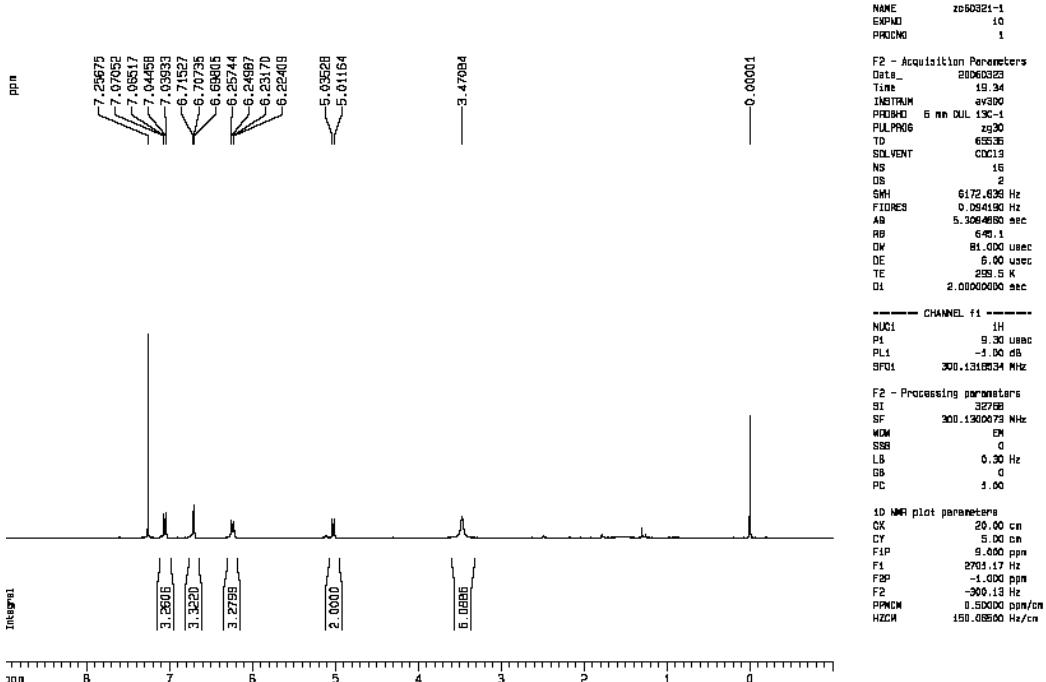


Figure S4. ^1H NMR spectrum of **3a** in CDCl_3 .

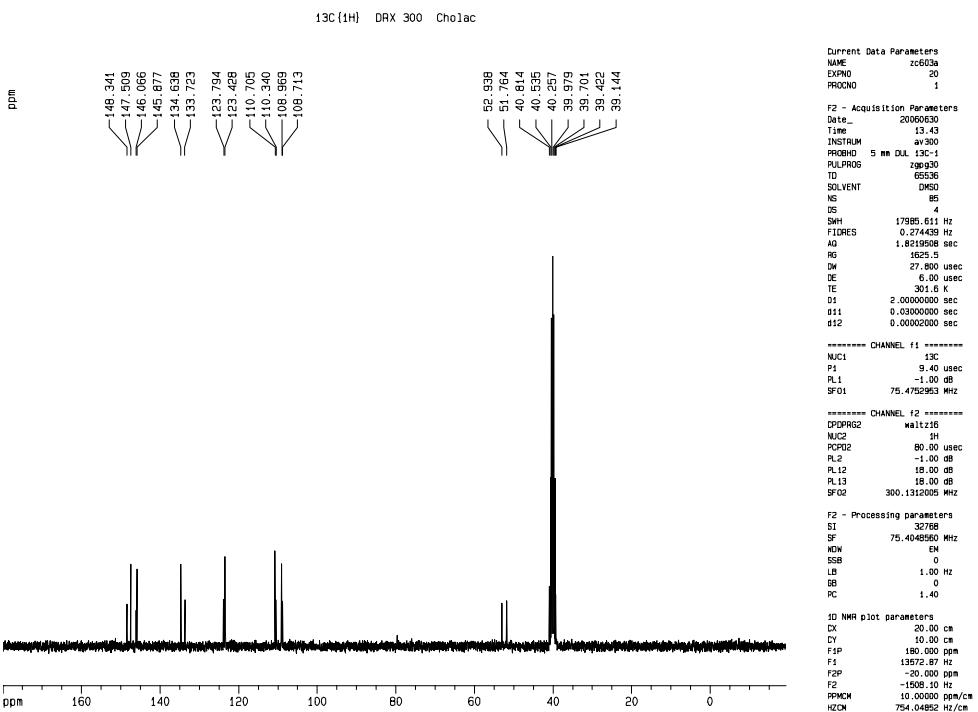


Figure S5. ^{13}C NMR spectrum of **3a** in DMSO.

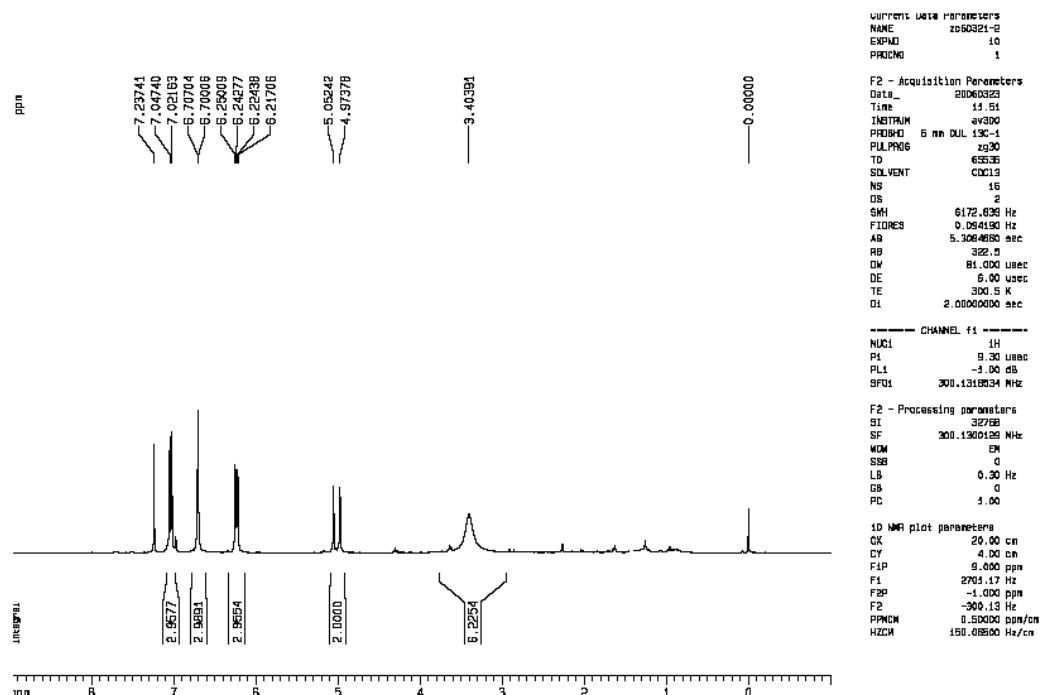


Figure S6. ^1H NMR spectrum of **3b** in CDCl_3 .

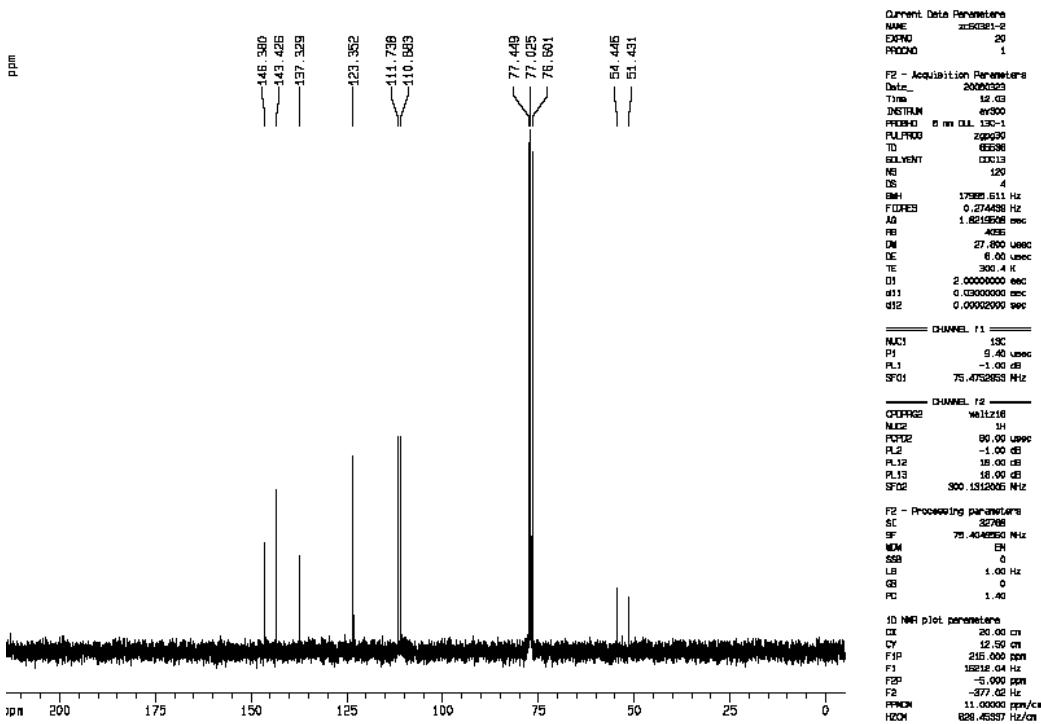


Figure S7. ^{13}C NMR spectrum of **3b** in CDCl_3 .

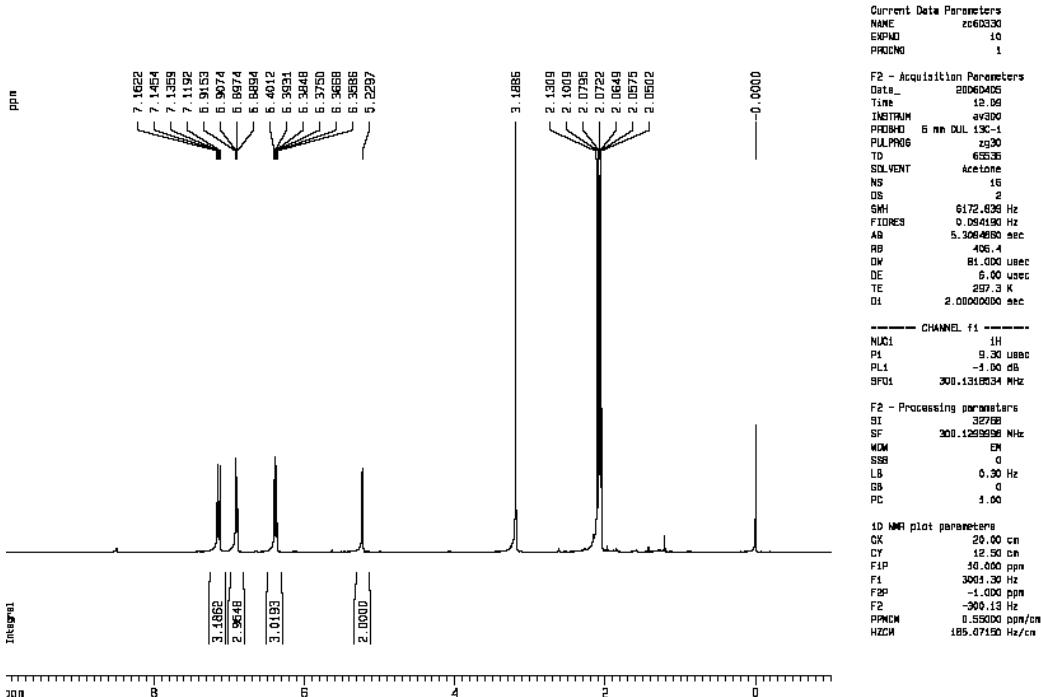


Figure S8. ^1H NMR spectrum of **4a** in d^6 -acetone.

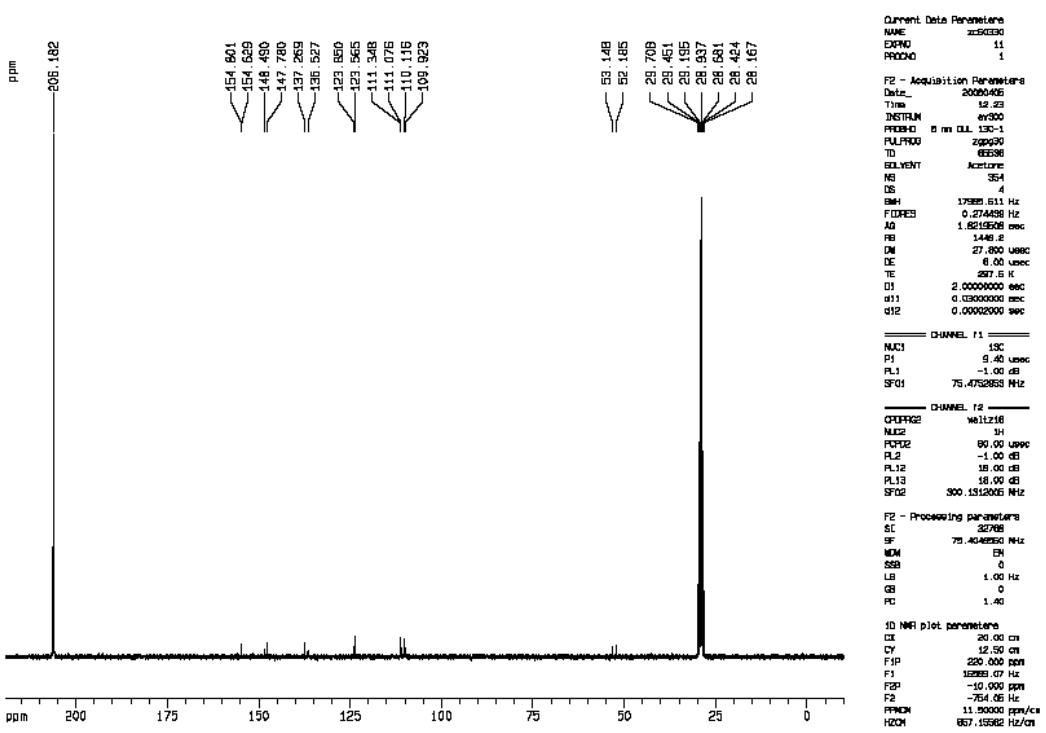


Figure S9. ^{13}C NMR spectrum of **4a** in d^6 -acetone.

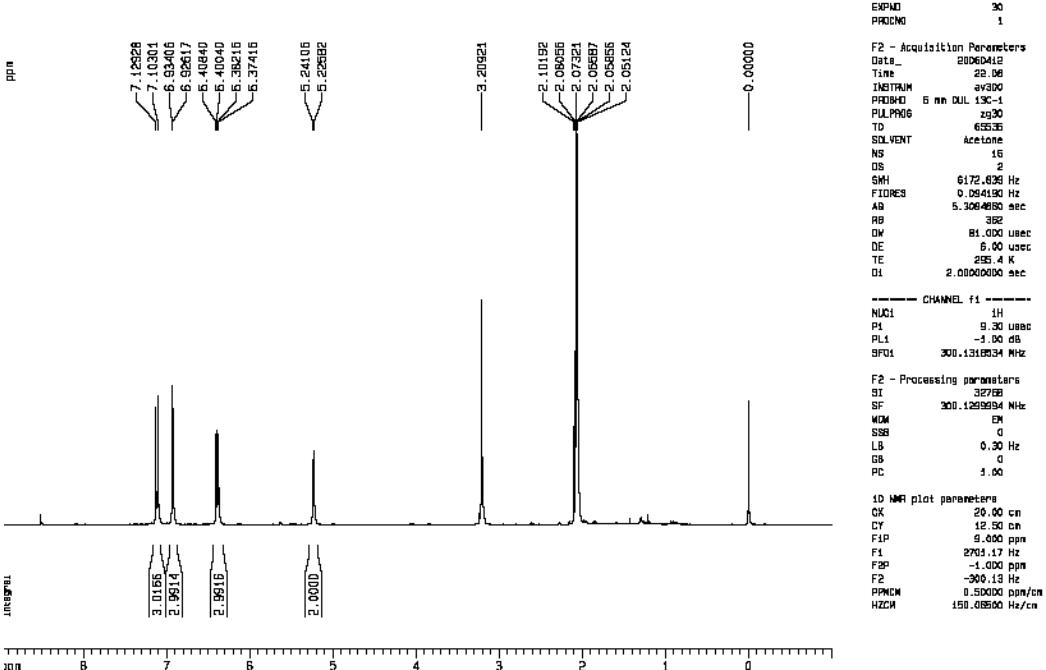


Figure S10. ^1H NMR spectrum of **4b** in d^6 -acetone.

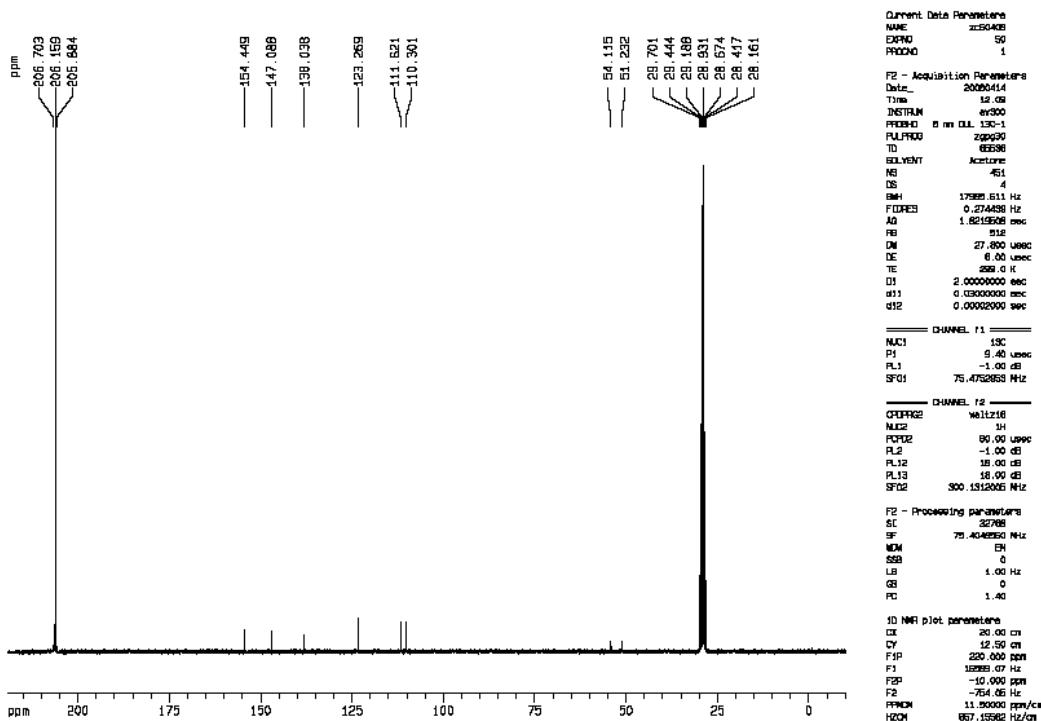


Figure S11. ¹³C NMR spectrum of **4b** in *d*⁶-acetone.

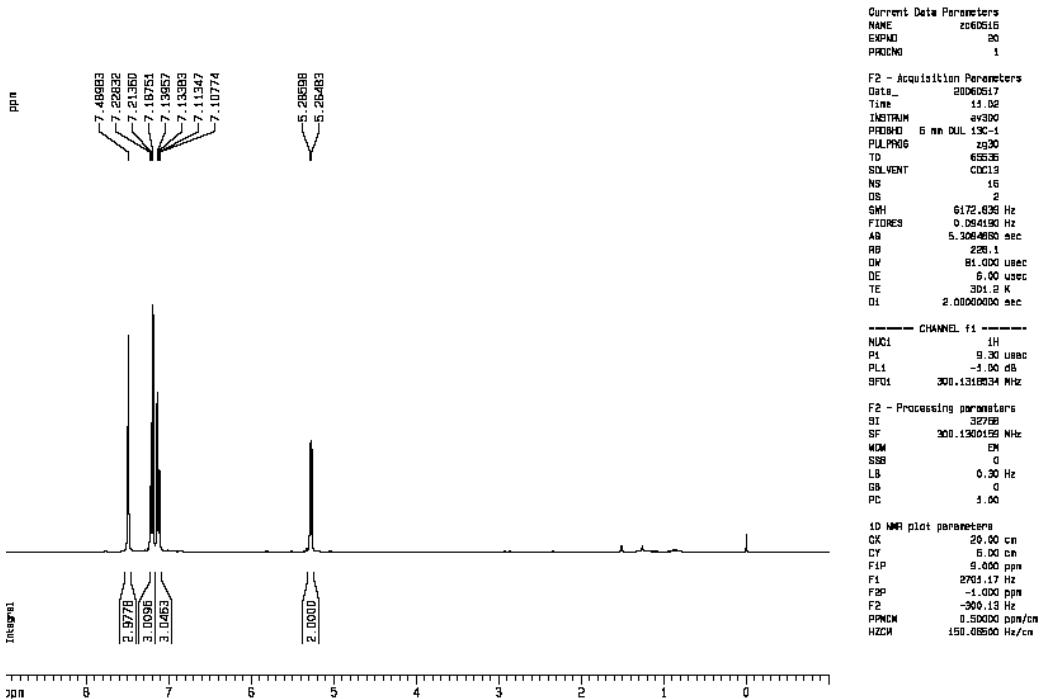


Figure S12. ¹H NMR spectrum of **5a** in CDCl₃.

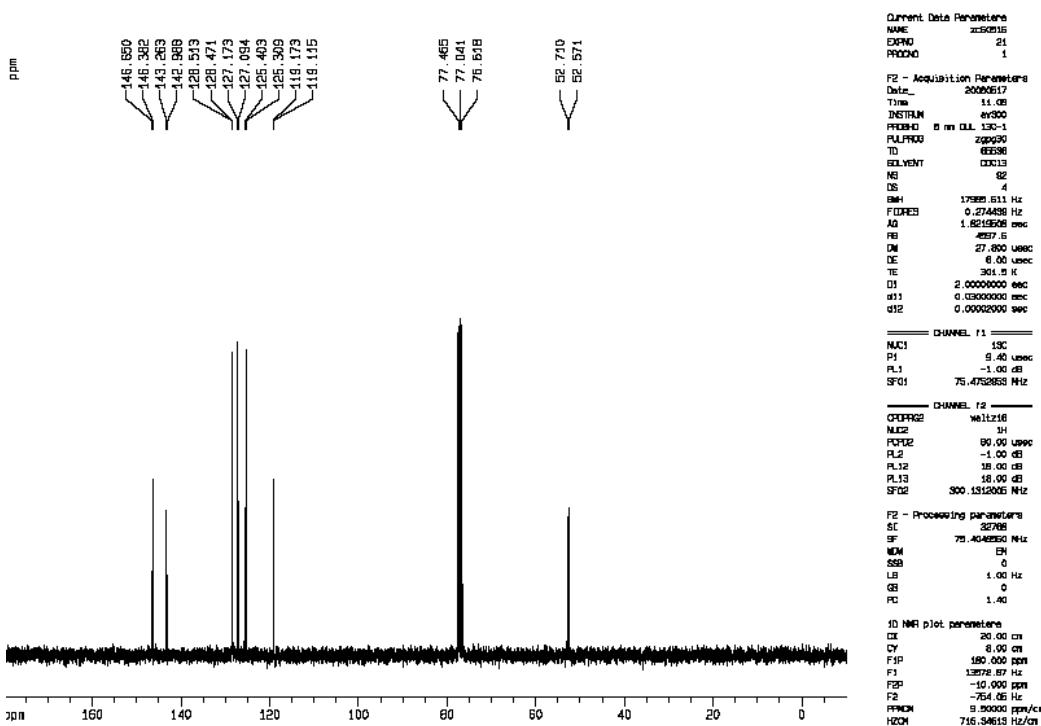


Figure S13. ^{13}C NMR spectrum of **5a** in CDCl_3 .

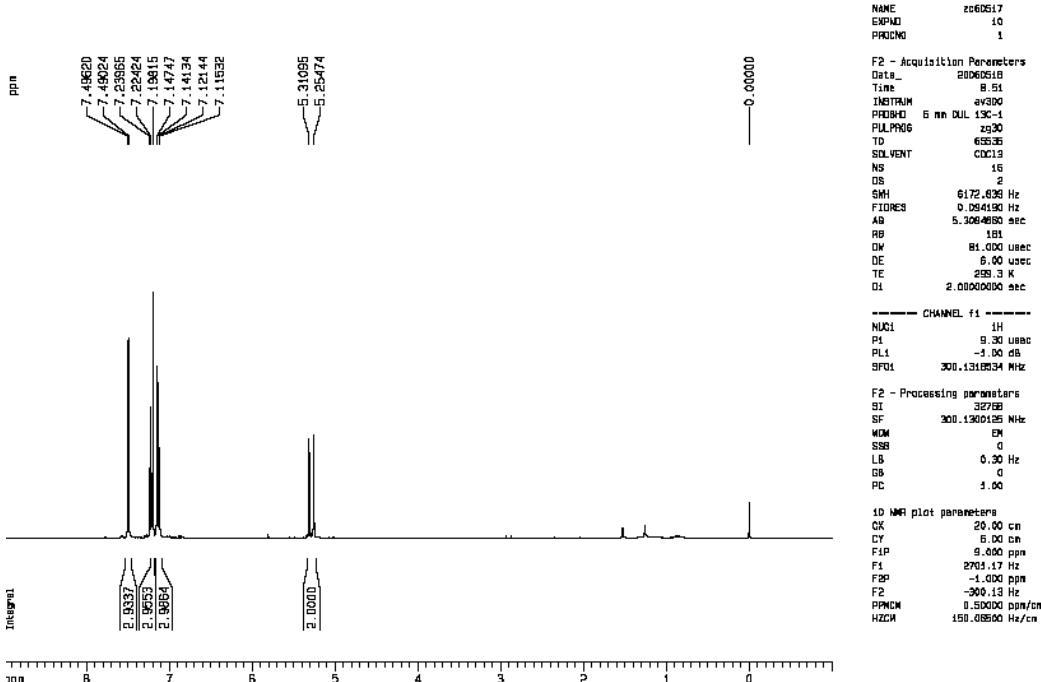


Figure S14. ^1H NMR spectrum of **5b** in CDCl_3 .

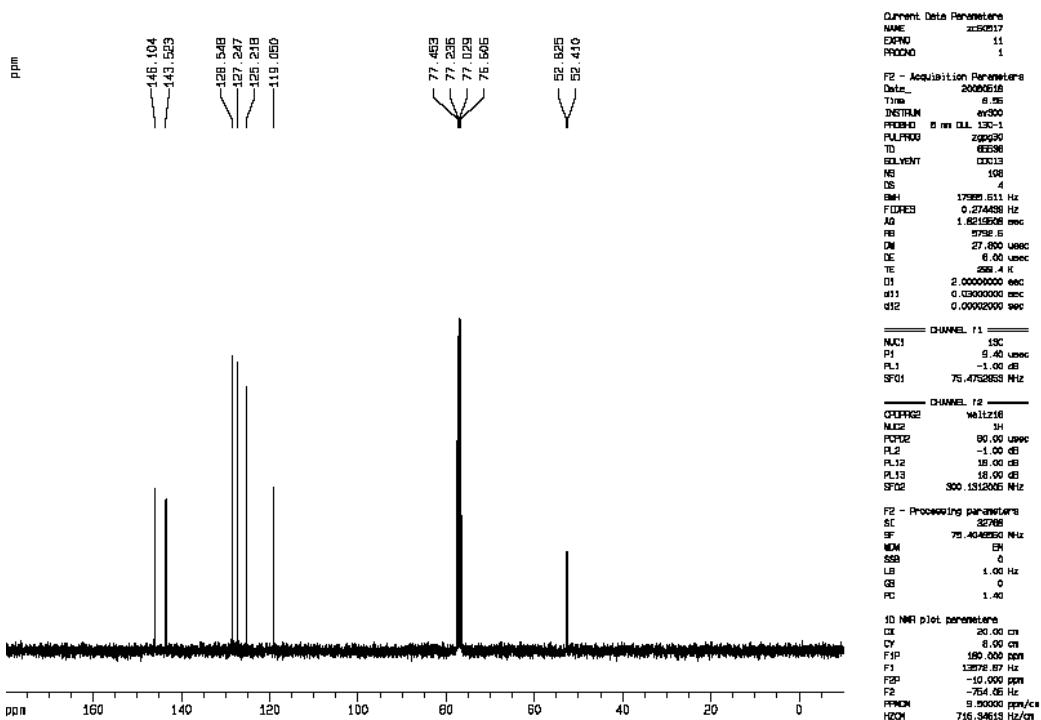


Figure S15. ^{13}C NMR spectrum of **5b** in CDCl_3 .

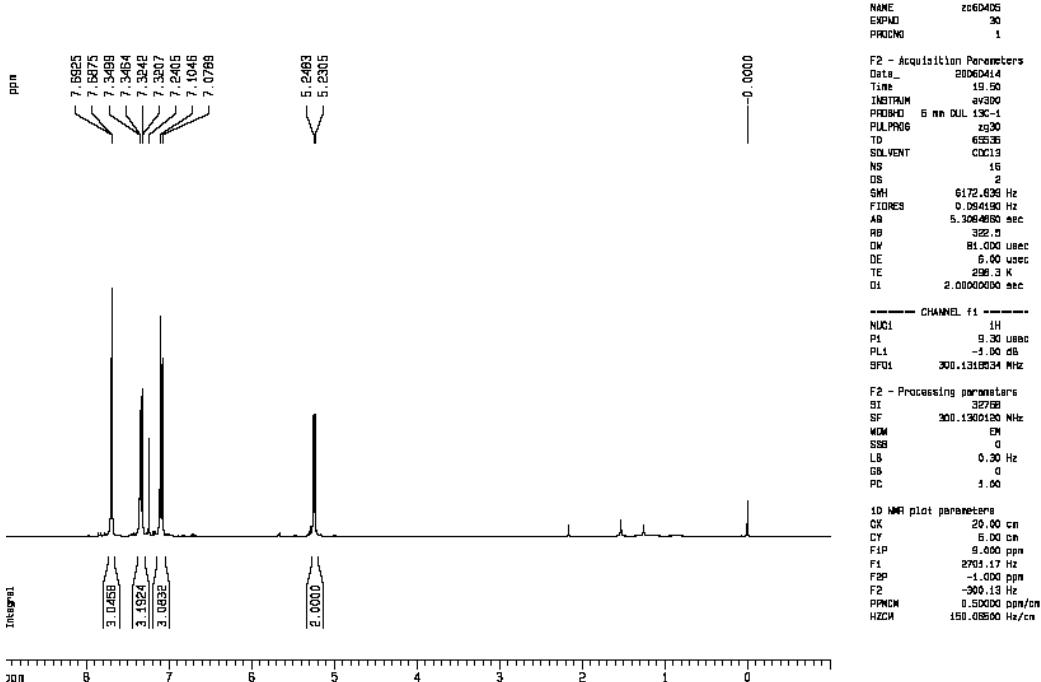


Figure S16. ^1H NMR spectrum of **6a** in CDCl_3 .

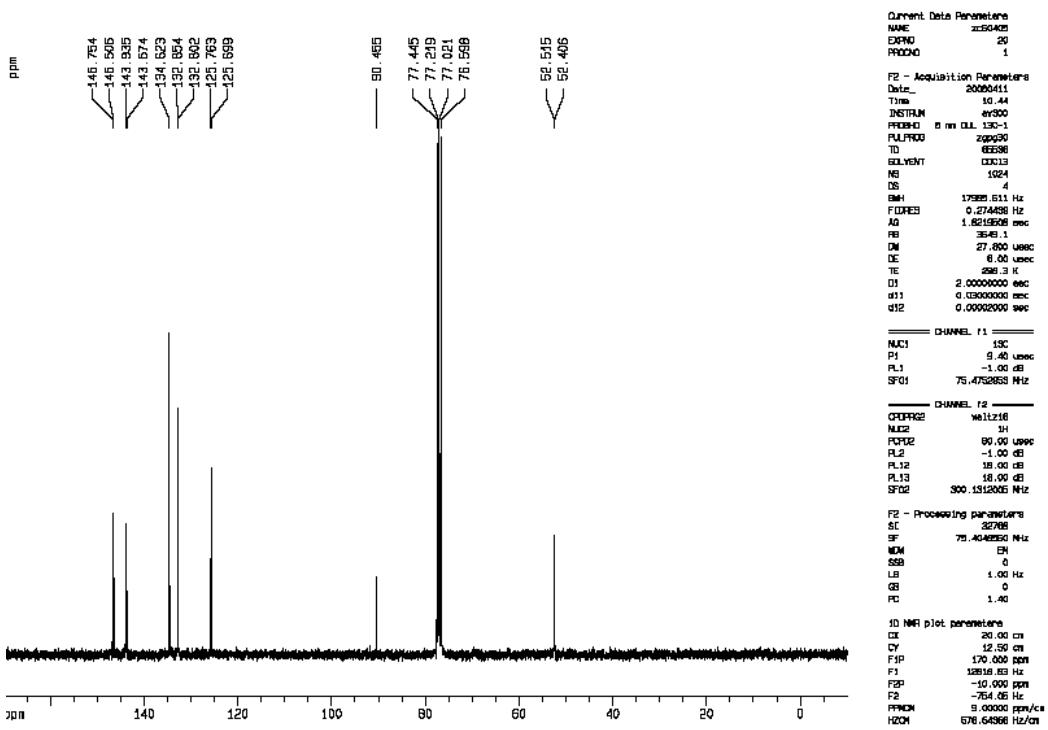


Figure S17. ^{13}C NMR spectrum of **6a** in CDCl_3 .

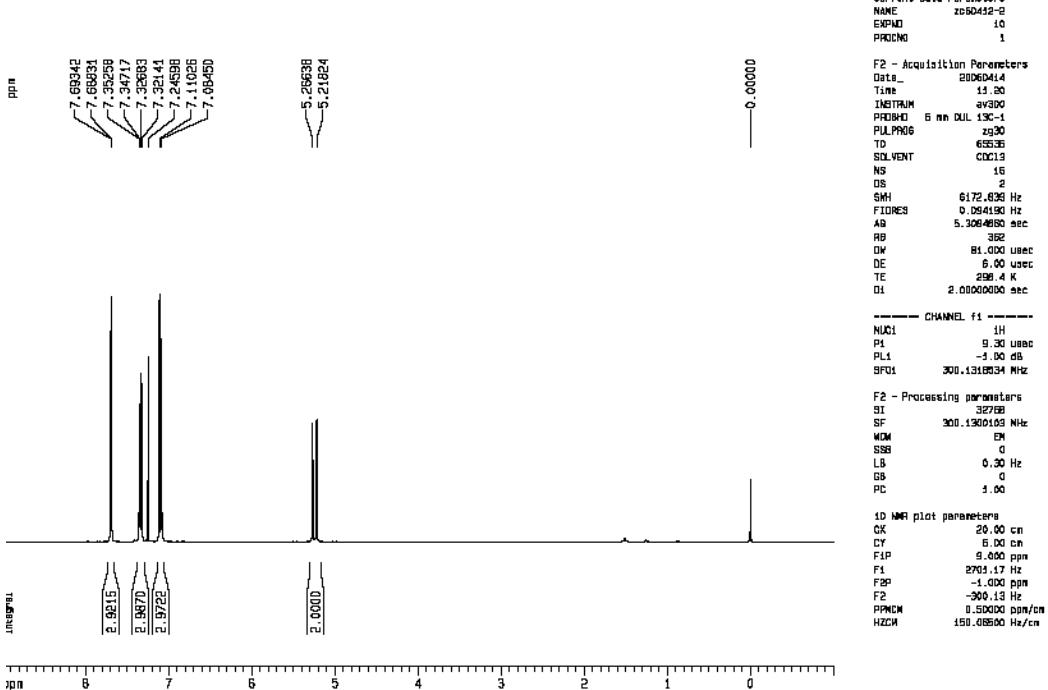


Figure S18. ^1H NMR spectrum of **6b** in CDCl_3 .

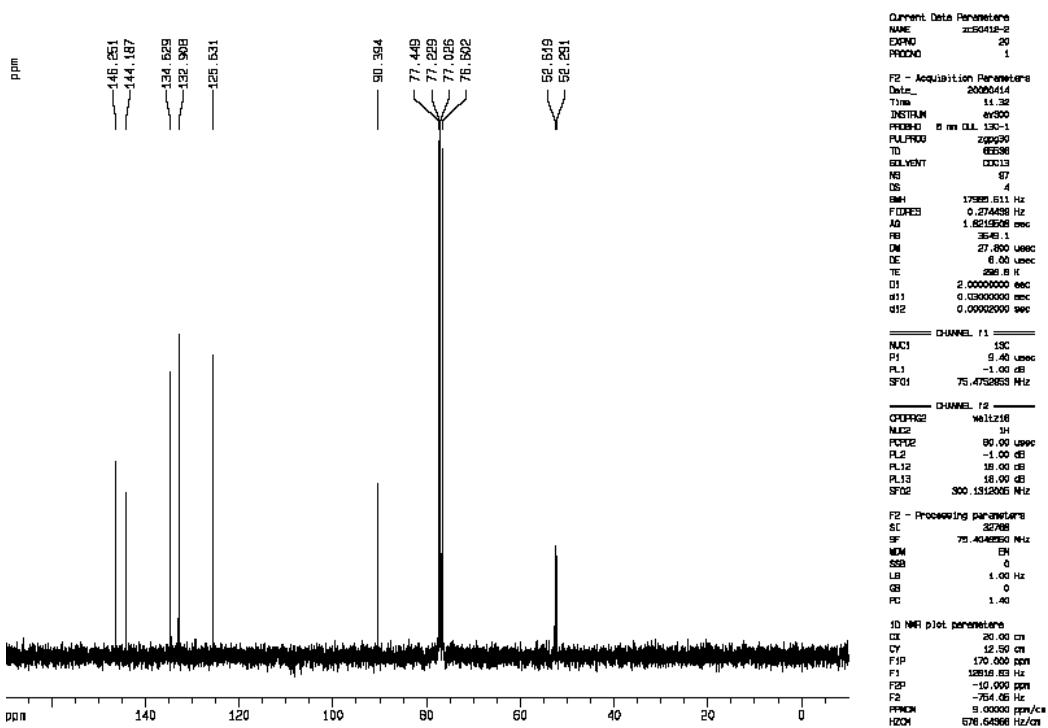


Figure S19. ^{13}C NMR spectrum of **6b** in CDCl_3 .

2. Crystal packing of **2b**.

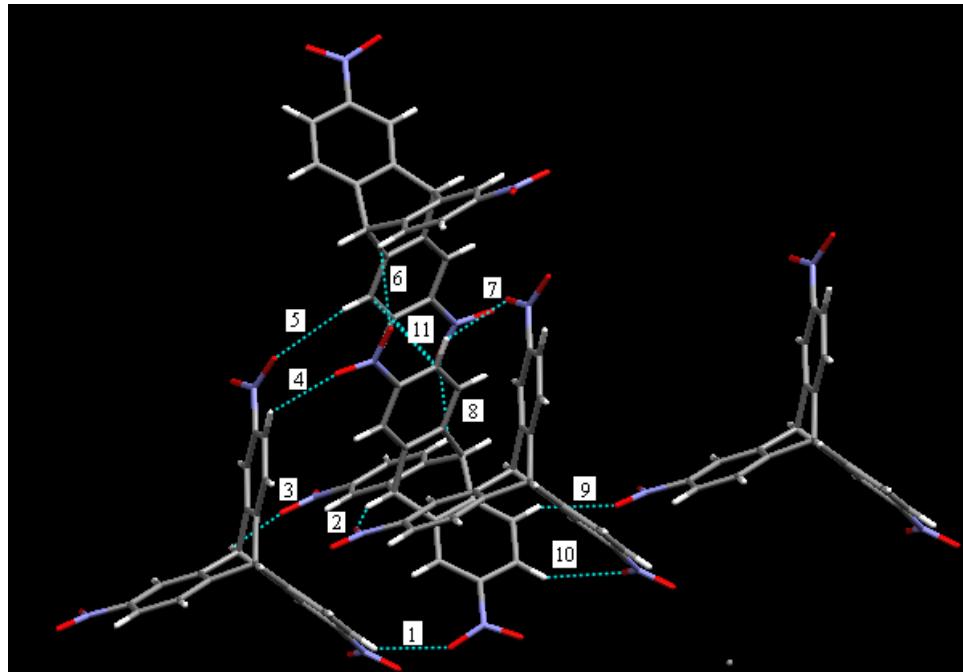


Figure S20. The C-H---O-N hydrogen bonds and π - π stacking interactions existed in the crystal packing of **2b**: (1) $d_{\text{C-H---O}}$: 2.55 Å, $\theta_{\text{C-H---O}}$: 146.0°; (2) $d_{\text{C-H---O}}$: 2.64 Å, $\theta_{\text{C-H---O}}$: 129.1°; (3) $d_{\text{C-H---O}}$: 2.64 Å, $\theta_{\text{C-H---O}}$: 129.1°; (4) $d_{\text{C-H---O}}$: 2.69 Å, $\theta_{\text{C-H---O}}$: 140.9°; (5) $d_{\text{C-H---O}}$: 2.63 Å, $\theta_{\text{C-H---O}}$: 150.9°; (6) $d_{\text{C-H---O}}$: 2.66 Å, $\theta_{\text{C-H---O}}$: 103.3°; (7) $d_{\text{C-H---O}}$: 2.55 Å, $\theta_{\text{C-H---O}}$: 146.0°; (8) $d_{\text{C-H---O}}$: 2.66 Å, $\theta_{\text{C-H---O}}$: 103.3°; (9) $d_{\text{C-H---O}}$: 2.42 Å, $\theta_{\text{C-H---O}}$: 144.5°; (10) $d_{\text{C-H---O}}$: 2.69 Å, $\theta_{\text{C-H---O}}$: 149.0°; (11) $d_{\pi---\pi}$: 3.16 Å.

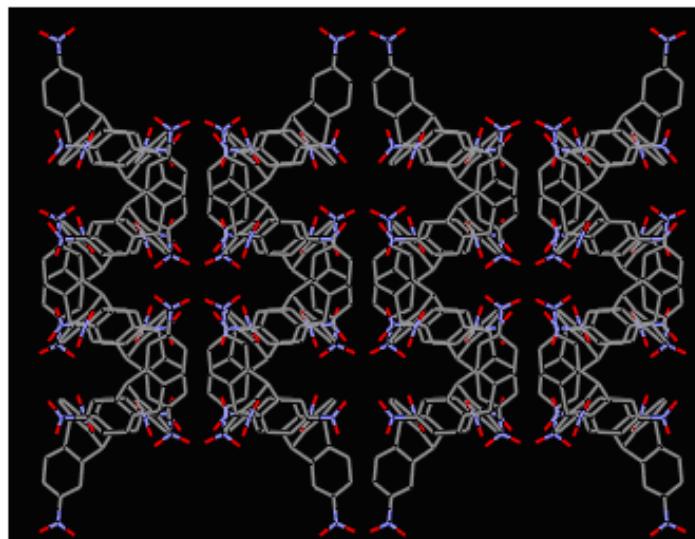


Figure S21. The crystal packing of **2b** viewed along *c*-axis. Hydrogen atoms are omitted for clarity.

3. Crystal packing of **6b**.

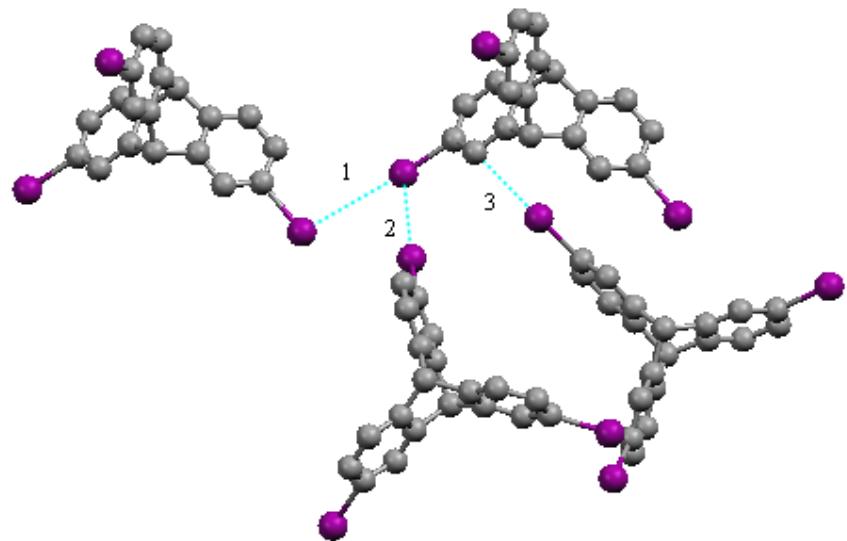


Figure S22. The iodine bonds involved in the crystal packing of **6b**: (1) $d_{\text{I}-\text{I}^{'}}$: 3.94 Å; (2) $d_{\text{I}-\text{C}}$: 3.83 Å; (3) $d_{\text{C}-\text{I}-\pi}$: 3.50 Å.

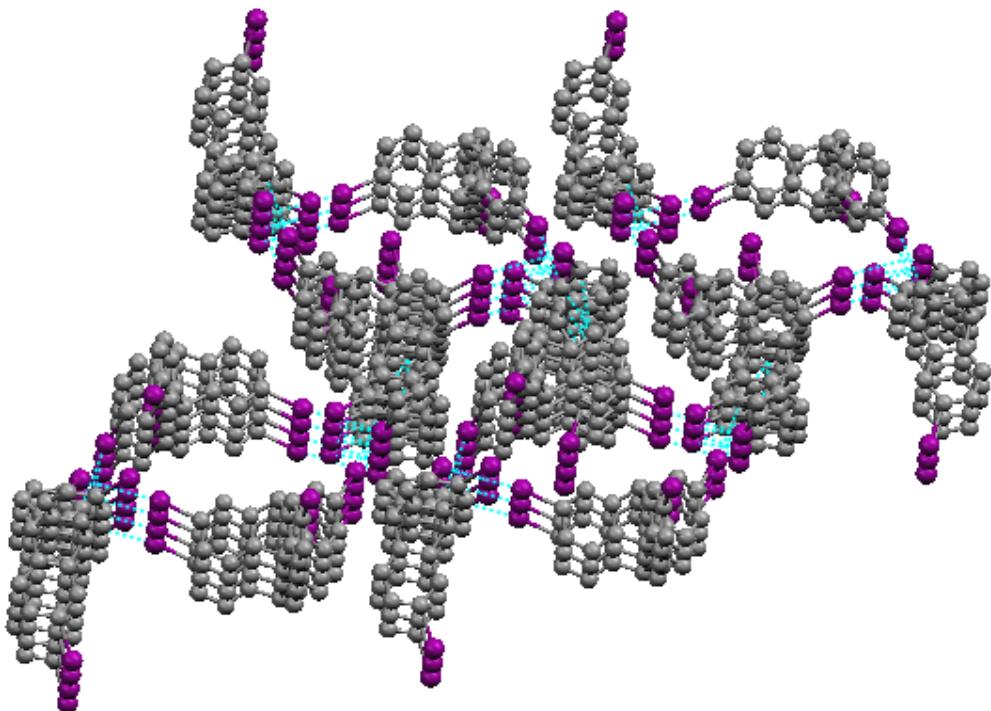


Figure S23. The packing diagram of **6b** viewed along *a*-axis. Solvent molecules and hydrogen atoms are omitted for clarity.