Electronic Supplementary Information

Achieving Enhanced ML or RTP Performance: Alkyl Substituent Effect on the Fine-Tuning of Molecular Packing

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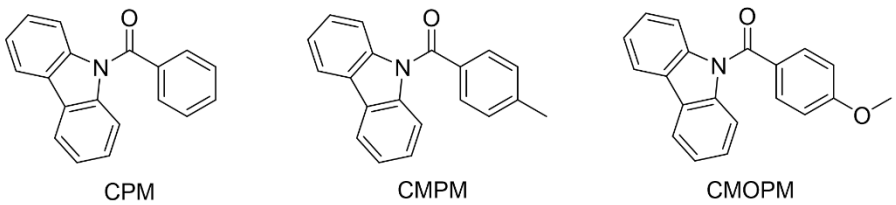
Table of Contents



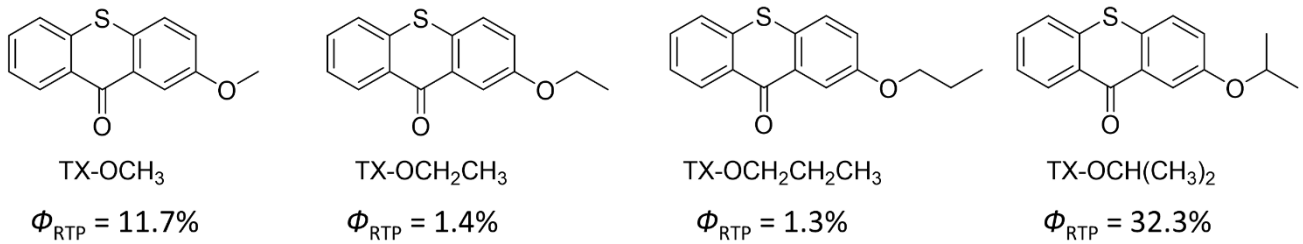
1. The reported RTP compounds with alkyl substituents

Chart S1. The amide derivatives with different substituents.

Chart S2. The thioxanthone (TX) derivatives with different substituents.

2. General experimental procedures

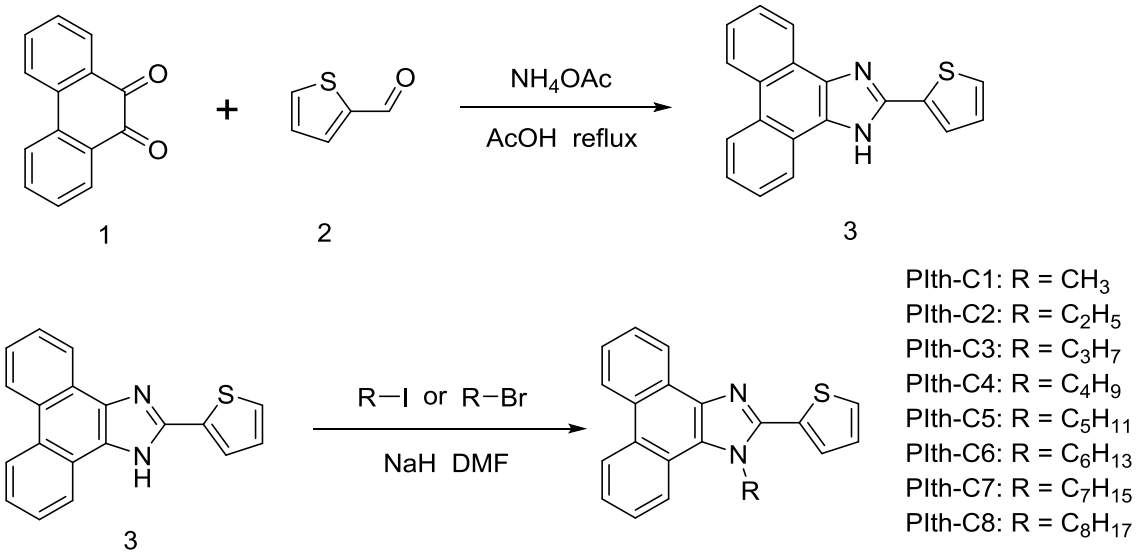
Characterization: ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz Varian Mercury, using $CDCl_3$ as the solvent. Mass spectra were measured on a ZAB 3F-HF mass spectrophotometer.



Elemental analyses of carbon, hydrogen and nitrogen were performed on a Perkin-Elmer microanalyzer. High performance liquid chromatography (HPLC) were performed by an Agilent 1100 Series (85 bar, 1 mL/min, 7% H_2O 93% MeOH). PL spectra were recorded by a Hitachi F-4600 fluorescence spectrophotometer. The ML spectra were measured on a spectrometer of Acton SP2750 with CCD (SPEC-10, Princeton) as a power detector. Absolute photoluminescence quantum yield (PLQY) and luminescence decay were recorded by an Edinburgh FLS980 spectrometer. The powder X-ray diffraction patterns were measured on Rigaku MiniFlex 600 at 25 ^{o}C at 40 kV and 40 mA at a scan rate of 10^{o} (2θ)/min (scan range: 5-60^{o}). The single-crystal X-ray diffraction data were recorded by a Bruker Smart Apex II CCD diffractometer. The CCDC numbers of PIth-C1, PIth-C2, PIth-C3, PIth-C4, PIth-C5, PIth-C6, PIth-C7 and PIth-C8 are 1963678, 19636379, 1963680, 1963681, 1963682, 1963683, 1970707 and 1970708 respectively. Differential scanning calorimetry were performed on

NETZSCHDSC 200 PC instrument from room temperature to 250 ^{o}C at a heating rate of 10 ^{o}C/min under nitrogen. The Gaussian 09 program was utilized to perform the TD-DFT calculations. The ground state (S_0) geometry was obtained from the single crystal structure and no further geometry optimization was conducted in order to maintain the specific molecular configuration and corresponding intermolecular locations.

3. Synthesis



Scheme S1. The synthetic routes of PIth-C derivatives.

Compound 3 (PIth-C): To a round-bottom flask fitted with a reflux condenser, was added 9,10-phenanthrenedione (8.32 g, 40 mmol), 2-thiophenecarboxaldehyde (4.48 g, 40 mmol), ammonium acetate (61.60 g, 800 mmol) and acetic acid (200 mL). The resultant solution was stirred under nitrogen atmosphere at refluxing temperature for 10 h. After the reaction completed, the mixture was cooled to room temperature and quenched with a large amount of water, after stirring for 30 mins, the mixture was filtered and washed with a small amount of methanol to afford a crude product. The crude product was recrystallized by acetone and petroleum ether mixture to give the compound PIth-C as a light yellow solid (11.34g, 93%). And the solid was used in next reactions without further purification. MS (EI), m/z: 300.17, calcd for $C_{19}H_{12}N_2S$: 300.07.

PIth-C1: Under a nitrogen atmosphere, a solution of NaH (0.36 g, 15 mmol) in anhydrous N, N-Dimethylformamide (DMF) (80 mL) was slowly added PIth-C (1.50 g, 5 mmol) at room temperature. The reaction mixture was stirred at 50 ^{o}C for 30 mins, then, a solution of Iodomethane (1.87 mL, 30 mmol) in anhydrous DMF (25 mL) was slowly added. The resultant mixture was stirred at 105 ^{o}C

overnight, allowed to cool to room temperature and quenched with distilled water. The solvent of reaction mixture was removed under reduced pressure, then, the residue was dissolved in 200 mL $CHCl_3$ and rinsed by distilled water for three times. The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuum. The crude product was purified by column chromatography (eluent:petroleum ether/dichloromethane = 1/4) to give the pure compound of PIth-C1 as a white solid (1.01 g, 64%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.81-8.76 (m, 2H, Ar-H), 8.68-8.66 (d, J = 8 Hz, 1H, Ar-H), 8.41-8.39 (d, J = 8 Hz, 1H, Ar-H), 7.72-7.68 (m, 1H, Ar-H), 7.64-7.60 (m, 3H, Ar-H), 7.55-7.54 (d, J = 4 Hz, 1H, Ar-H), 7.50-7.49 (d, J = 4 Hz, 1H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 4.36 (s, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 146.40, 137.69, 132.23, 129.24, 128.46, 128.19, 128.10, 127.85, 127.65, 127.25, 127.15, 126.63, 125.57, 124.95, 124.42, 123.48, 123.02, 122.74, 120.58, 35.92. MS (EI), m/z: 313.94, calcd for $C_{20}H_{14}N_2S$: 314.09. Elemental analyses for $C_{20}H_{14}N_2S$: C, 76.11; H, 4.23; N, 8.87. Found: C, 76.40; H, 4.49; N, 8.91. [CCDC 1963678]

PIth-C2: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of Bromoethane (2.26 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.23 g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.84-8.78 (m, 2H, Ar-H), 8.69-8.67 (d, J = 8 Hz, 1H, Ar-H), 8.32-8.30 (d, J = 8 Hz, 1H, Ar-H), 7.72-7.66 (m, 2H, Ar-H), 7.64-7.60 (m, 2H, Ar-H), 7.56-7.53 (m, 2H, Ar-H), 7.24-7.21 (m, 1H, Ar-H)4.82-4.76 (m, 2H, -CH_2), 1.75-1.70 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.61, 138.05, 132.28, 129.28, 128.16, 128.11, 127.66, 127.25, 127.22, 126.89, 126.29, 125.60, 124.89, 124.52, 123.16, 123.00, 122.74, 120.49, 41.76, 16.21. MS (EI), m/z: 327.93, calcd for $C_{21}H_{16}N_2S$: 328.10. Elemental analyses for $C_{21}H_{16}N_2S$: C, 76.51; H, 4.87; N, 8.42. Found: C, 76.80; H, 4.91; N, 8.53. [CCDC 1963679]

PIth-C3: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromopropane (2.73 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.71 g, 73%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.82-8.79 (m, 2H, Ar-H), 8.68-8.66 (d, J = 8 Hz, 1H, Ar-H), 8.21-8.19 (d, J = 8 Hz, 1H, Ar-H), 7.72-7.60 (m, 4H, Ar-H), 7.55-7.53 (d, J = 8 Hz, 1H, Ar-H), 7.51-7.50 (d, J = 4 Hz, 1H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 4.67-4.63 (m, 2H, -CH_2), 2.12-2.06 (m, 2H, -CH_2), 1.05-1.01 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 146.01, 138.07, 132.37, 129.28, 128.37, 128.14, 127.65, 127.25, 127.23, 126.85, 126.60, 125.61, 124.86, 124.49, 123.26, 123.00, 122.75, 120.45, 48.47, 23.90, 10.85. MS (EI), m/z: 341.84, calcd for $C_{22}H_{18}N_2S$: 342.11. Elemental analyses for $C_{22}H_{18}N_2S$: C, 76.92; H, 5.12; N, 8.14. Found: C, 77.16; H, 5.30; N, 8.18. [CCDC 1963680]

PIth-C4: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromobutane (3.22 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.36 g, 76%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.83-8.78 (m, 2H, Ar-H), 8.68-8.66 (d, J = 8 Hz, 1H, Ar-H), 8.24-8.22 (d, J = 8 Hz, 1H, Ar-H), 7.70-7.60 (m, 4H, Ar-H), 7.55-7.54 (d, J = 4 Hz, 1H, Ar-H), 7.52-7.51 (d, J = 4 Hz, 1H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 4.71-4.67 (m, 2H, -CH_2), 2.06-2.02 (m, 2H, -CH_2), 1.48-1.43 (m, 2H, -CH_2), 0.99-0.95 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.96, 138.08, 132.34, 129.27, 128.40, 128.13, 127.63, 127.25, 127.23, 126.82, 126.59, 125.60, 124.85, 124.49, 123.26, 123.00, 122.74, 120.51, 46.80, 32.52, 19.78, 13.65. MS (EI), m/z: 355.94, calcd for $C_{23}H_{20}N_2S$: 356.13. Elemental analyses for $C_{23}H_{20}N_2S$: C, 77.32; H, 5.71; N, 7.67. Found: C, 77.49; H, 5.66; N, 7.86. [CCDC 1963681]

PIth-C5: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromopentane (3.70 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.32 g, 71%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.85-8.83 (d, J = 8 Hz ,1H, Ar-H), 8.80-8.78 (d, J = 8 Hz, 1H, Ar-H), 8.70-8.68 (d, J = 8 Hz, 1H, Ar-H), 8.27-8.25 (d, J = 8 Hz, 1H, Ar-H), 7.70-7.61 (m, 4H, Ar-H), 7.56-7.54 (d, J = 8 Hz, 1H, Ar-H), 7.53-7.52 (d, J = 4 Hz, 1H, Ar-H), 7.24-7.22 (m, 1H, Ar-H), 4.74-4.70 (m, 2H, -CH_2), 2.08-2.07 (m, 2H, -CH_2), 1.44-1.37 (m, 4H, -CH_2), 0.94-0.90 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.95, 138.10, 132.33, 129.30, 128.42, 128.14, 127.62, 127.26, 127.23, 126.84, 126.59, 125.60, 124.87, 124.52, 123.29, 122.99, 122.75, 120.51, 47.04, 30.26, 28.65, 22.21, 13.98. MS (EI), m/z: 369.84, calcd for $C_{24}H_{22}N_2S$: 370.15. Elemental analyses for $C_{24}H_{22}N_2S$: C, 77.61; H, 6.02; N, 7.41. Found: C, 77.80; H, 5.99; N, 7.56. [CCDC 1963682]

PIth-C6: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromohexane (4.21 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.29 g, 67%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.83-8.78 (m, 2H, Ar-H), 8.69-8.67 (d, J = 8 Hz, 1H, Ar-H), 8.24-8.22 (d, J = 8 Hz, 1H, Ar-H), 7.70-7.60 (m, 4H, Ar-H), 7.55-7.54 (d, J = 4 Hz, 1H, Ar-H), 7.51 (m, 1H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 4.70-4.66 (m, 2H, -CH_2), 2.07-2.03 (m, 2H, -CH_2), 1.45-1.30 (m, 6H, -CH_2), 0.91-0.87 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.93, 138.08, 132.34, 129.27, 128.39, 128.13, 127.62, 127.25, 126.81, 126.58, 125.59, 124.85, 124.49, 123.26, 122.99, 122.75, 120.51, 47.01, 31.21, 30.45, 26.17, 22.54, 13.96. MS (EI), m/z: 383.84, calcd for $C_{25}H_{24}N_2S$: 384.16. Elemental analyses for $C_{25}H_{24}N_2S$: C, 77.96; H, 6.20; N, 7.19. Found: C, 78.09; H, 6.29; N, 7.29. [CCDC 1963683]

PIth-C7: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromoheptane (4.71 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.43 g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.83-8.78 (m, 2H, Ar-H), 8.69-8.67 (d, J = 8 Hz, 1H, Ar-H), 8.24-8.22 (d, J = 8 Hz, 1H, Ar-H), 7.70-7.60 (m, 4H, Ar-H), 7.55-7.54 (d, J = 8 Hz, 1H, Ar-H), 7.52-7.50 (d, J = 8 Hz, 1H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 4.70-4.66 (m, 2H, -CH_2), 2.07-2.03 (m, 2H, -CH_2), 1.42-1.27 (m, 8H, -CH_2), 0.90-0.86 (m, 3H, -CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.93, 138.08, 132.34, 129.28, 128.40, 128.13, 127.62, 127.25, 126.81, 126.58, 125.59, 124.85, 124.49, 123.26, 122.99, 122.75, 120.51, 47.01, 31.66, 30.47, 28.73, 26.44, 22.56, 14.07. MS (EI), m/z: 397.94, calcd for $C_{26}H_{26}N_2S$: 398.18. Elemental analyses for $C_{26}H_{26}N_2S$: C, 78.11; H, 6.65; N, 6.90. Found: C, 78.35; H, 6.58; N, 7.03. [CCDC 1970707]

PIth-C8: Similar procedure to that of **PIth-C1**. A solution of NaH (0.36 g, 15 mmol) in anhydrous DMF (80 mL), PIth-C (1.50 g, 5 mmol), a solution of 1-Bromooctane (5.23 mL, 30 mmol) in anhydrous DMF (25 mL). A white solid (1.57 g, 76%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.84-8.78 (m, 2H, Ar-H), 8.69-8.67 (d, J = 8 Hz, 1H, Ar-H), 8.25-8.23 (d, J = 8 Hz, 1H, Ar-H), 7.70-7.60 (m, 4H, Ar-H), 7.56-7.54 (d, J = 8 Hz, 1H, Ar-H), 7.52-7.51 (d, J = 4 Hz, 1H, Ar-H), 7.24-7.21 (m, 1H, Ar-H), 4.72-4.68 (m, 2H, -CH_2), 2.08-2.04 (m, 2H, -CH_2), 1.45-1.26 (m, 10H, -CH_2), 0.90-0.86 (m, 3H. –CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 145.94, 138.08, 132.33, 129.29, 128.41, 128.13, 127.62, 127.25, 127.23, 126.81, 126.58, 125.60, 124.86, 124.50, 123.27, 122.99, 122.75, 120.52, 47.03, 31.73, 30.47, 29.13, 29.01, 26.47, 22.63, 14.11. MS (EI), m/z: 411.84, calcd for $C_{27}H_{28}N_2S$: 412.19. Elemental analyses for $C_{27}H_{28}N_2S$: C, 78.47; H, 6.91; N, 6.65. Found: C, 78.60; H, 6.84; N, 6.79. [CCDC 1970708]

4. Figures and Tables

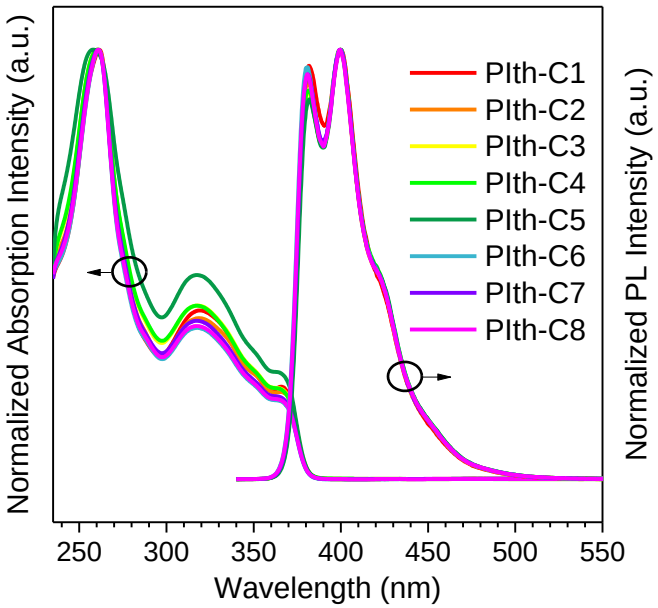


Figure S1. UV and PL spectra of PIth-C derivatives in THF solution. (c = 10^{-5} M)

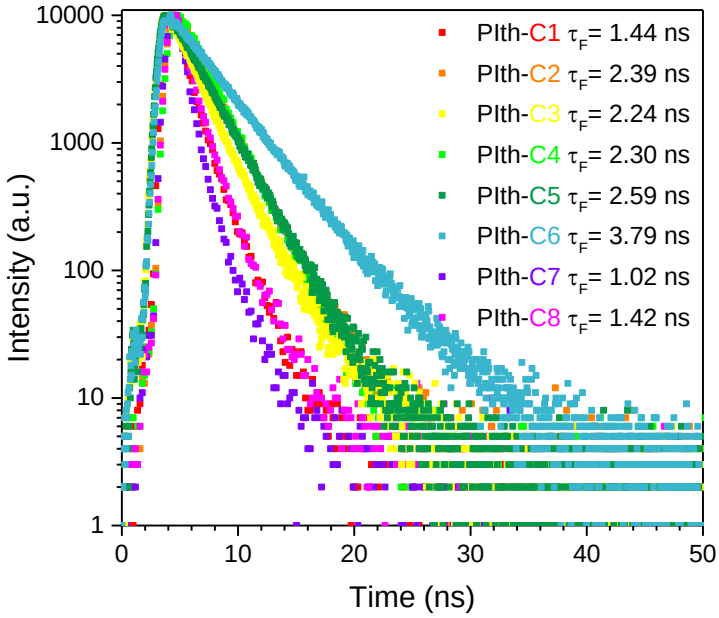


Figure S2. Fluorescence decay of PIth-C derivatives in the solid state.

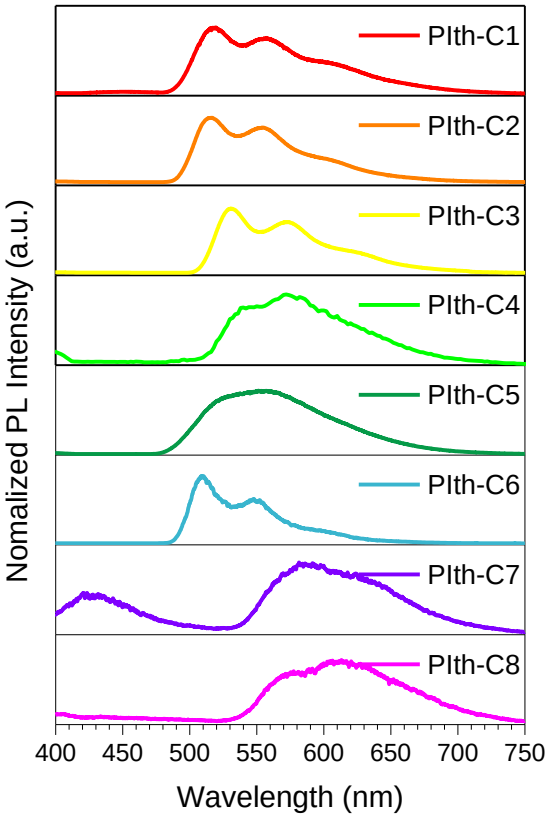


Figure S3. The phosphorescence spectra of PIth-C derivatives in the crystalline state at 77 K.

The phosporescence spectra at 77 K clearly reveal that there are triplet emissions for these PIth-C compounds in solid state under low temperature. The low temperature phosporescence could also help to recognize the emission region of room temperature phosporescence and distingush it from fluorescence.

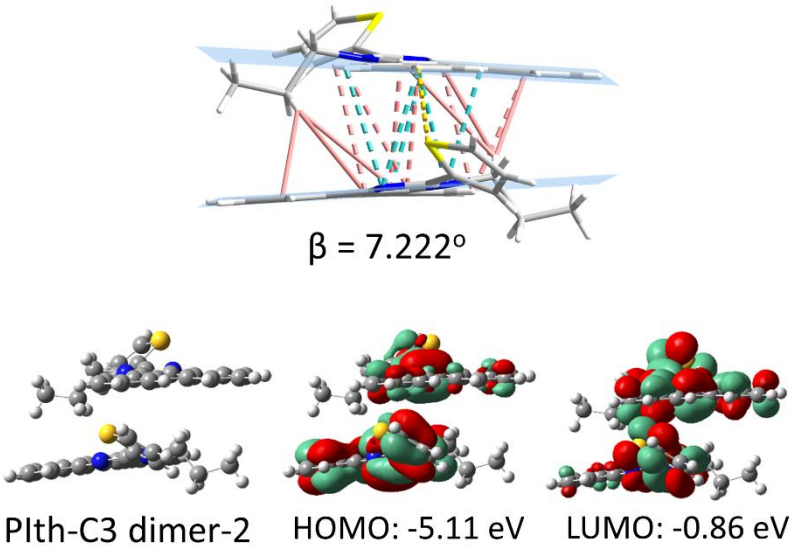


Figure S4. The packing mode and DFT calculations of another molecular dimer in the unit cell of PIth-C3 crystal.

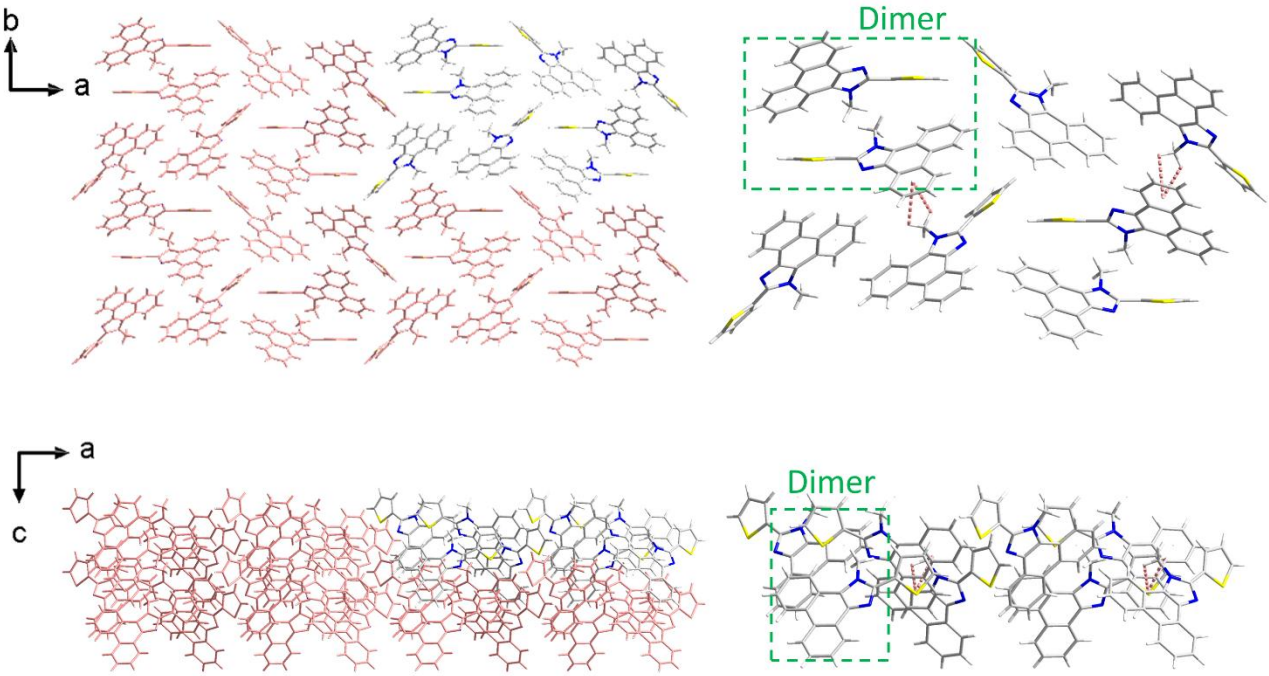


Figure S5. The molecular packing of PIth-C1 from top view and side view.

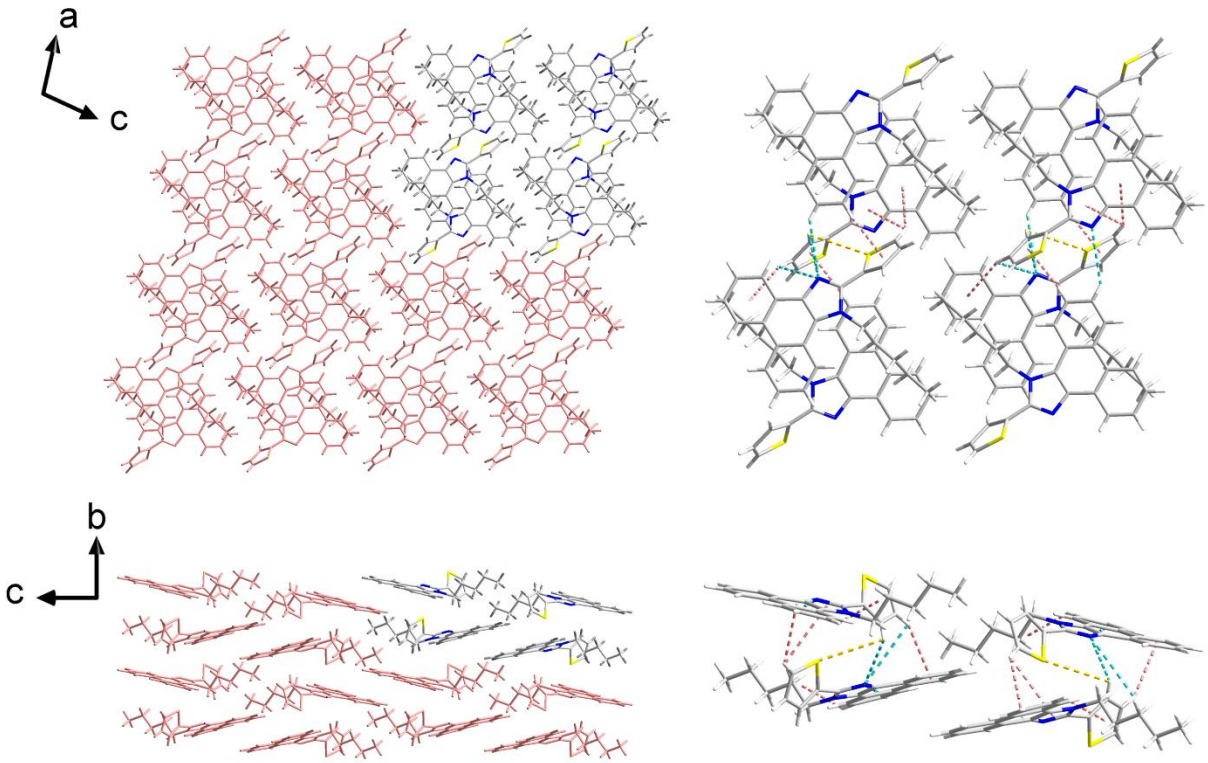


Figure S6. The molecular packing of PIth-C5 from top view and side view.

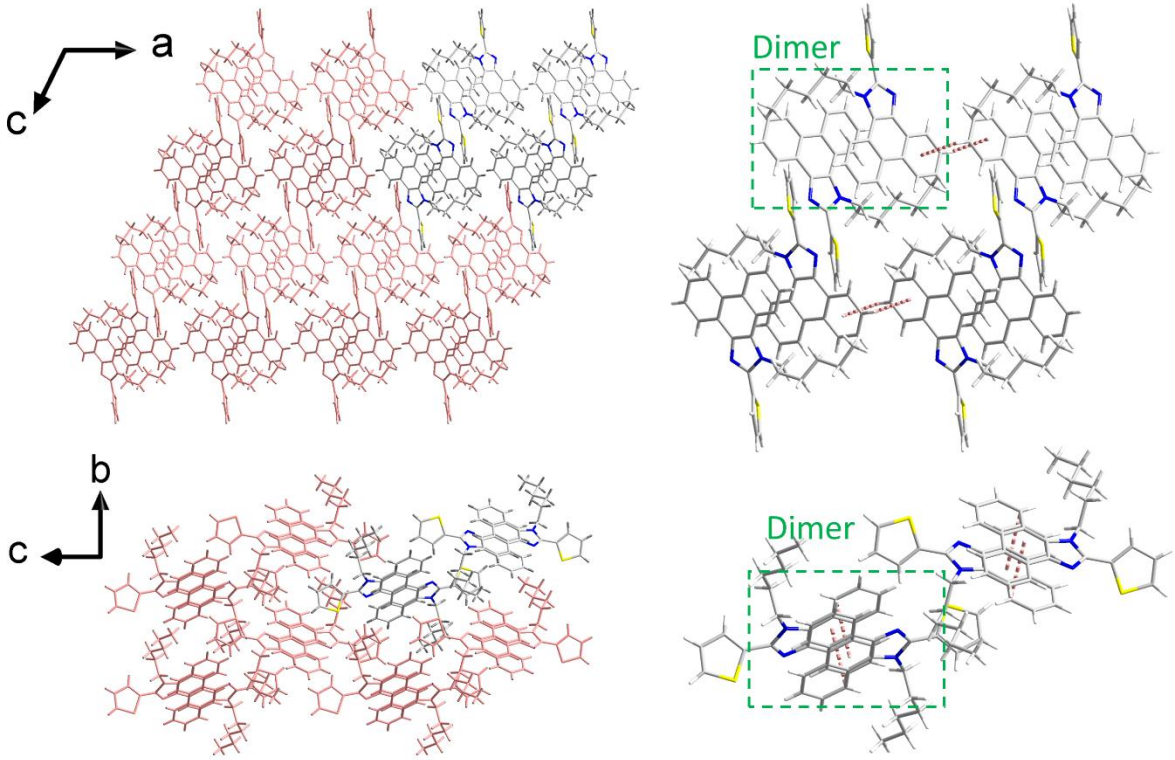


Figure S7. The molecular packing of PIth-C6 from top view and side view.

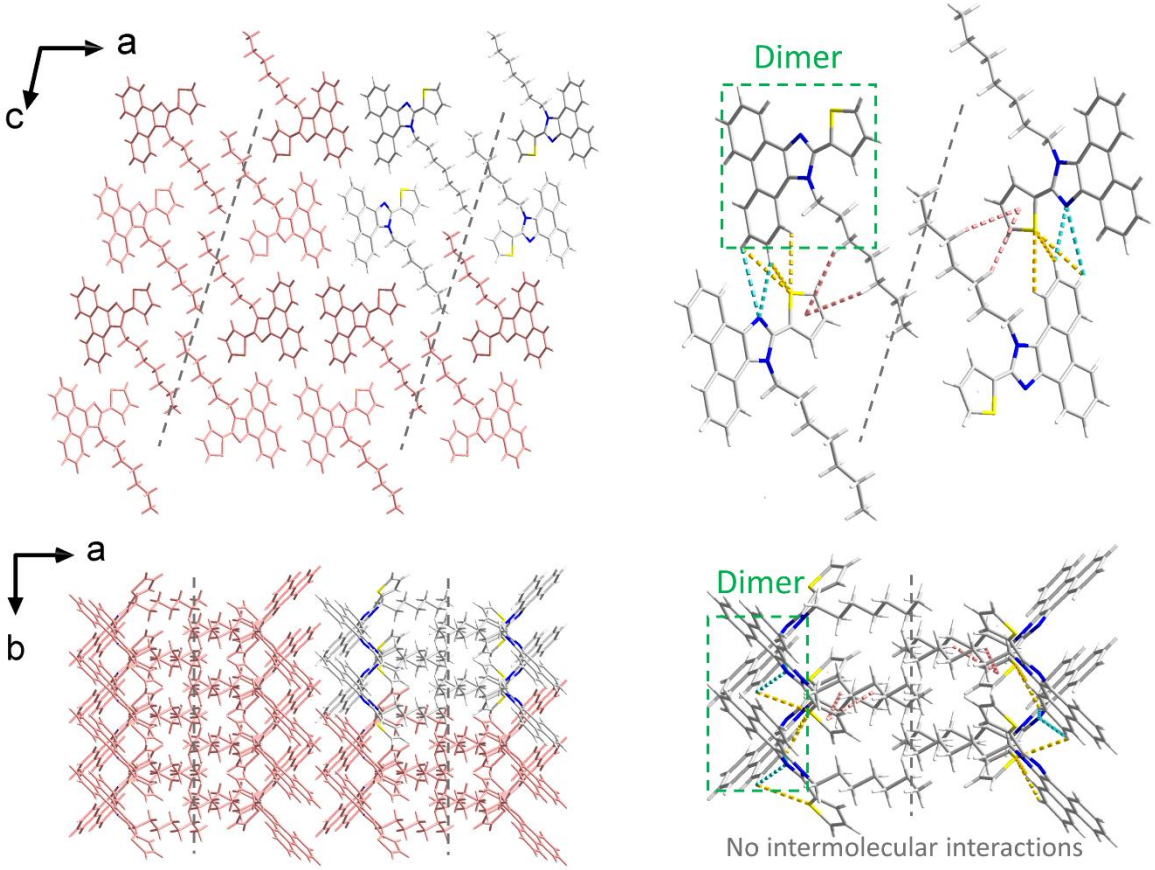


Figure S8. The molecular packing of PIth-C7 from top view and side view.

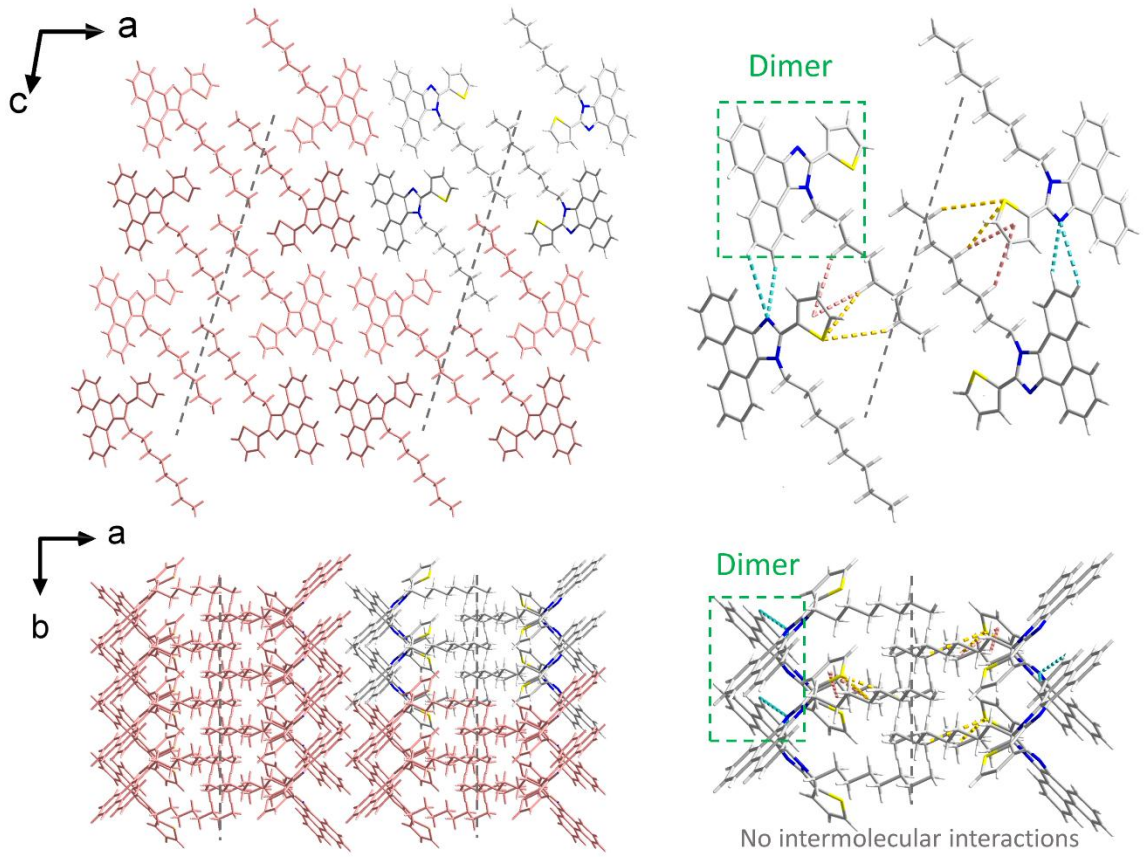


Figure S9. The molecular packing of PIth-C8 from top view and side view.

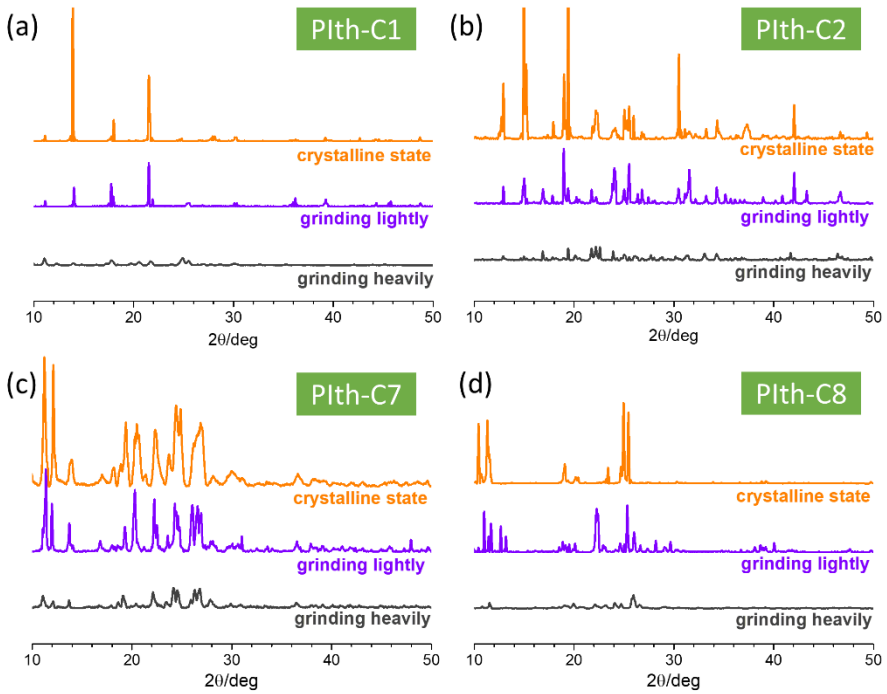


Figure S10. The PXRD patterns of (a) PIth-C1, (b) PIth-C2, (c) PIth-C7 and (d) PIth-C8 in the crystalline state, after light grinding and heavily grinding, respectively.

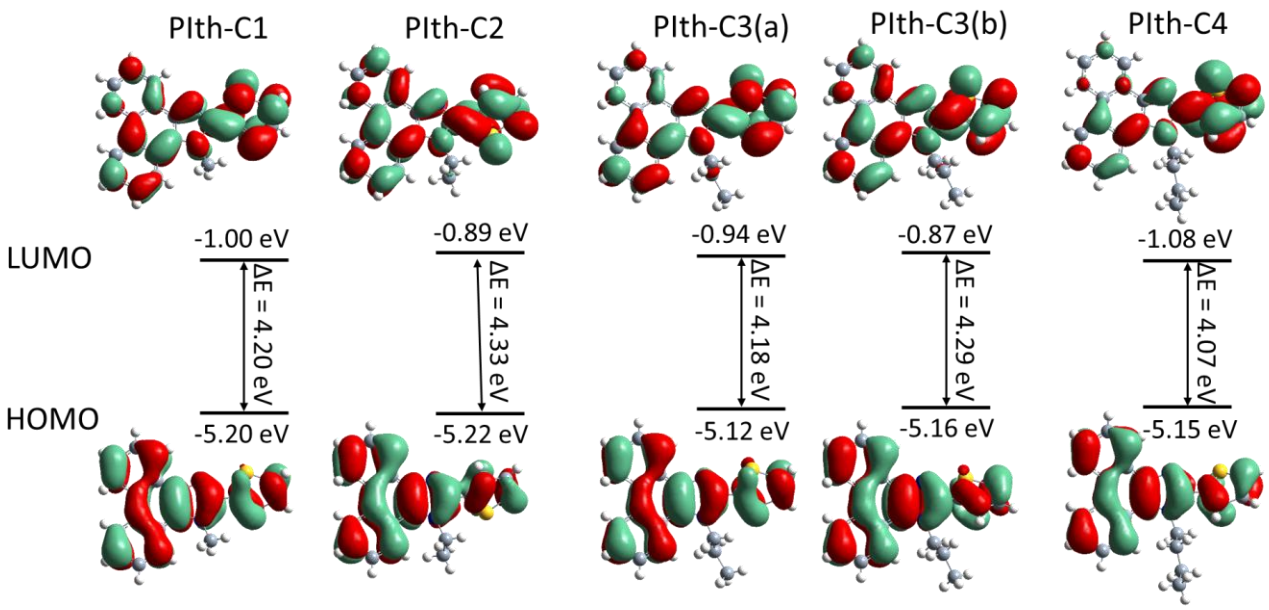


Figure S11. The HOMO and LUMO of the single molecule in the PIth-C derivatives (C1-C4) calculated at B3LYP/6-31G(d, p) level.

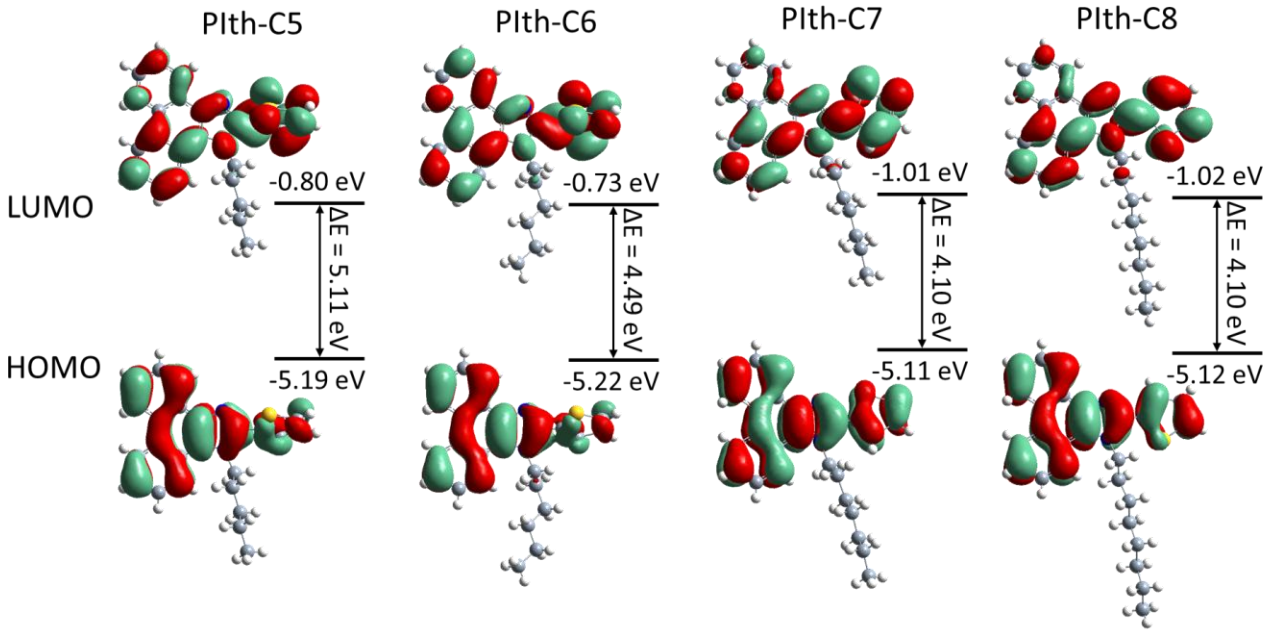


Figure S12. The HOMO and LUMO of the single molecule in the PIth-C derivatives (C5-C8) calculated at B3LYP/6-31G(d, p) level.

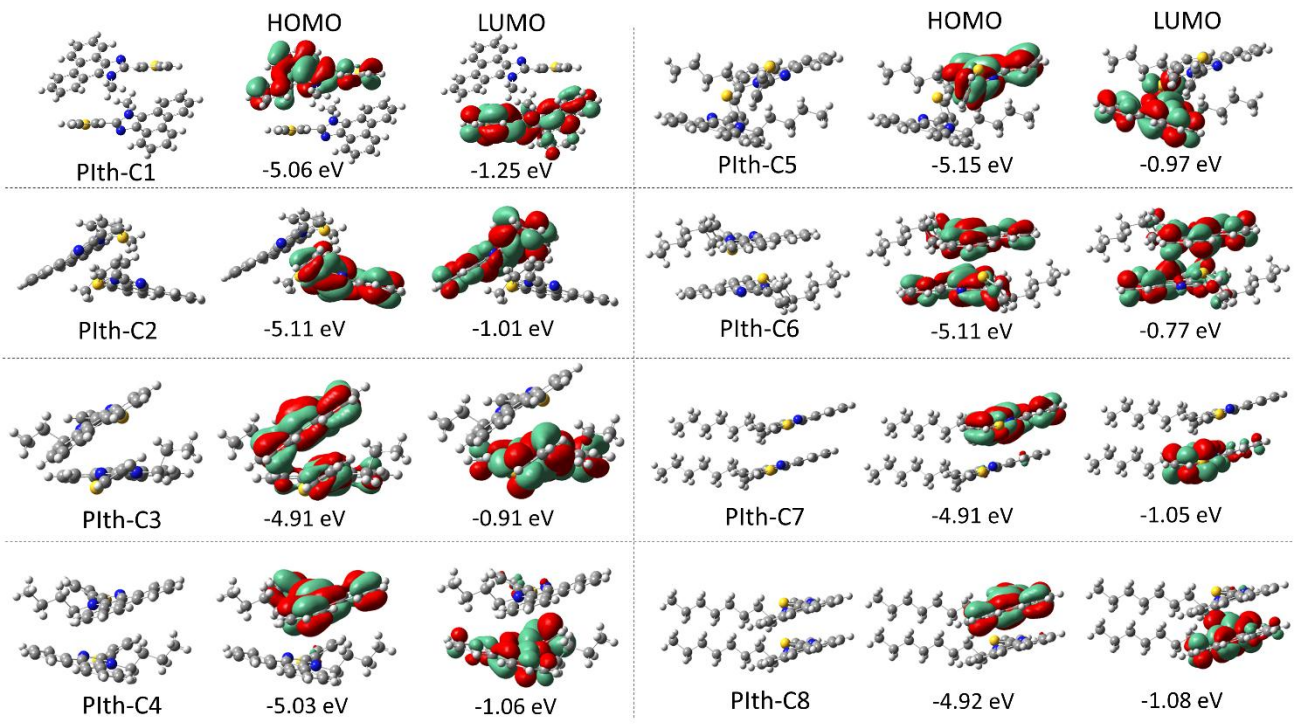


Figure S13. The HOMO and LUMO of the molecular dimers in the PIth-C derivatives calculated at B3LYP/6-31G(d, p) level.

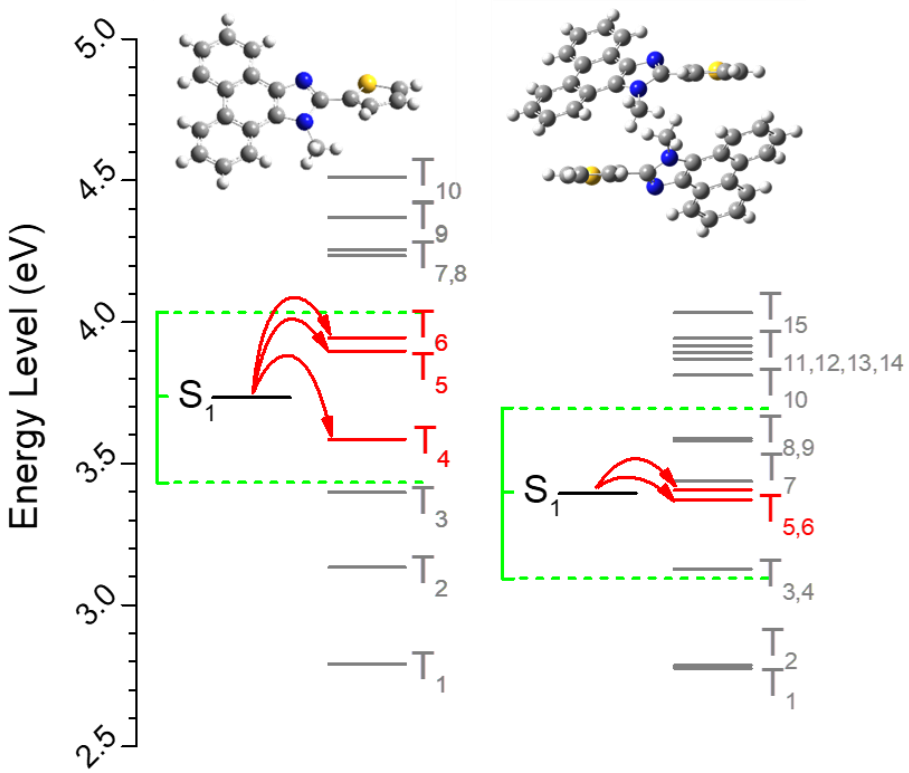


Figure S14. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C1 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C1.

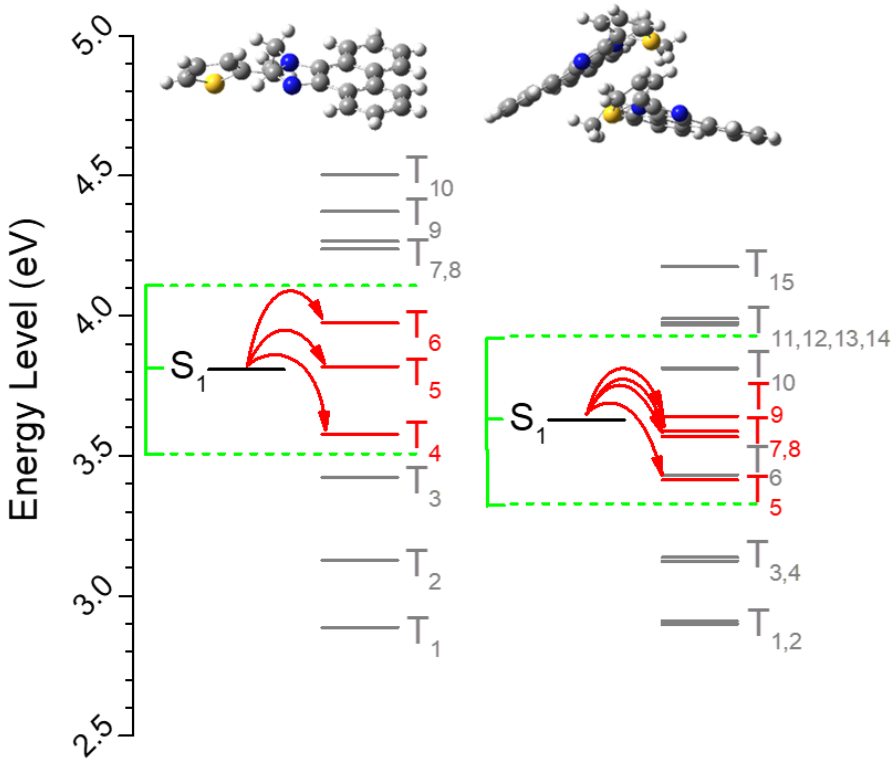


Figure S15. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C2 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C2.

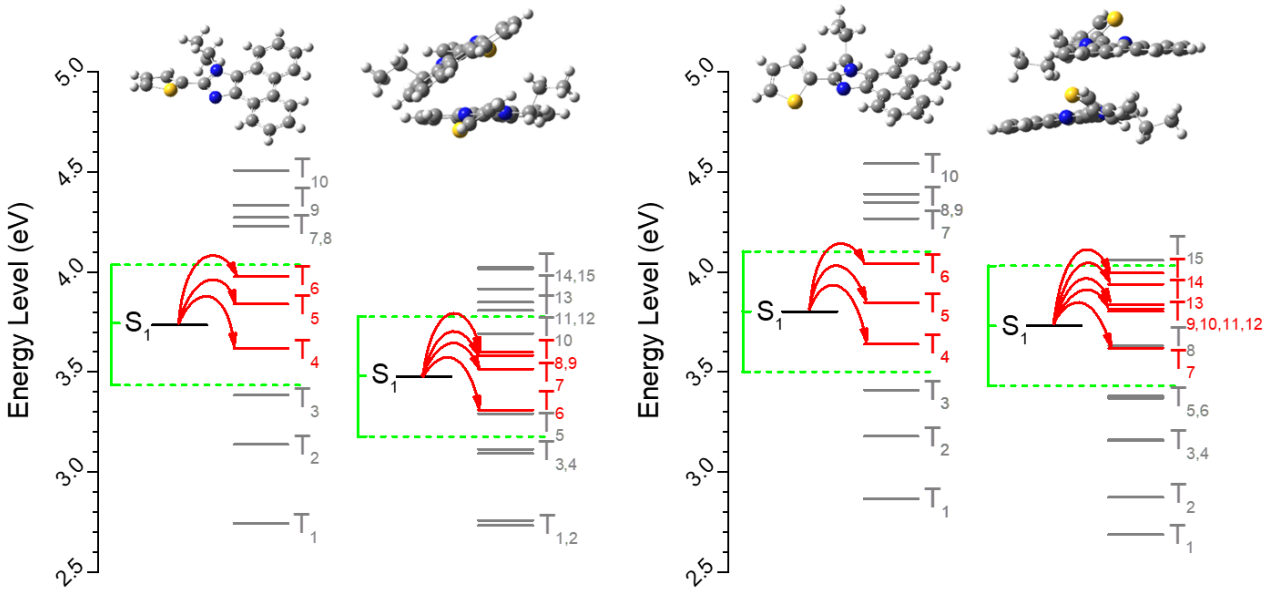


Figure S16. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C3 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C3.(a, b represent two monomers with different configurations and two dimers with different packing modes in the single crystal of PIth-C3)

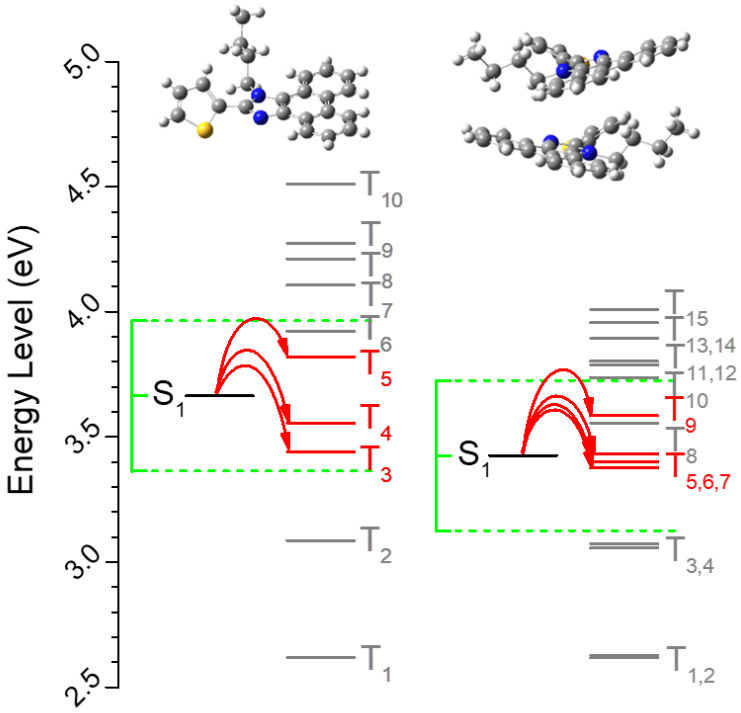


Figure S17. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C4 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C4.

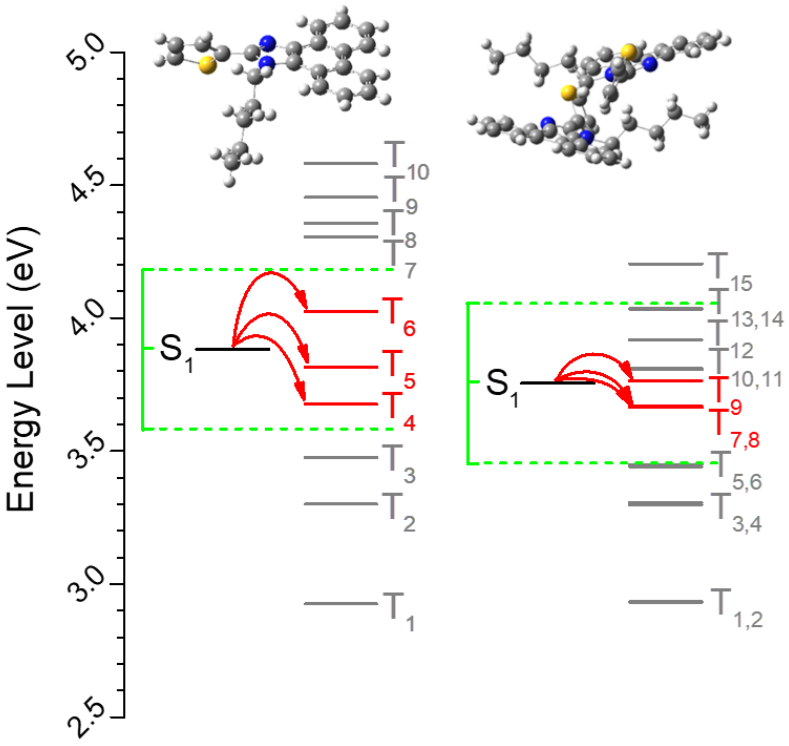


Figure S18. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C5 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C5.

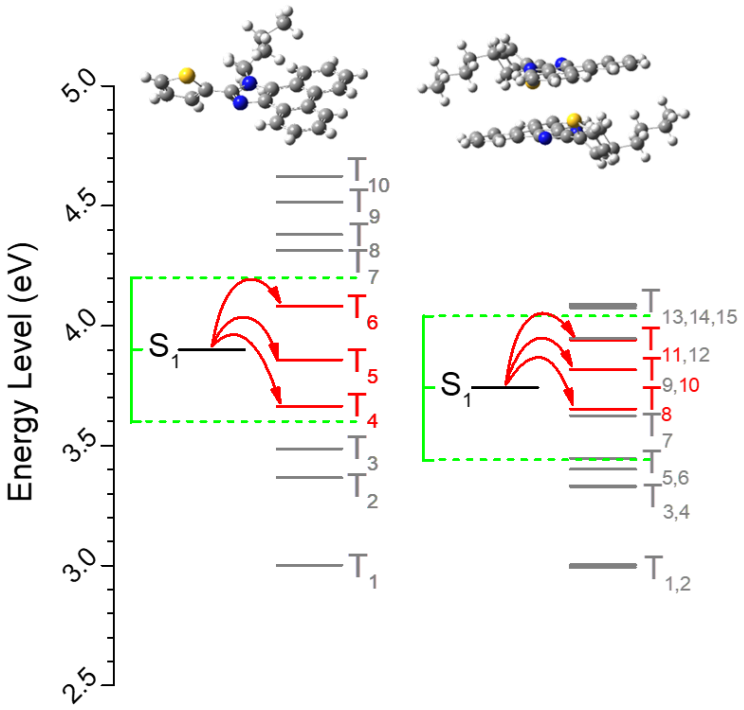


Figure S19. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C6 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C6.

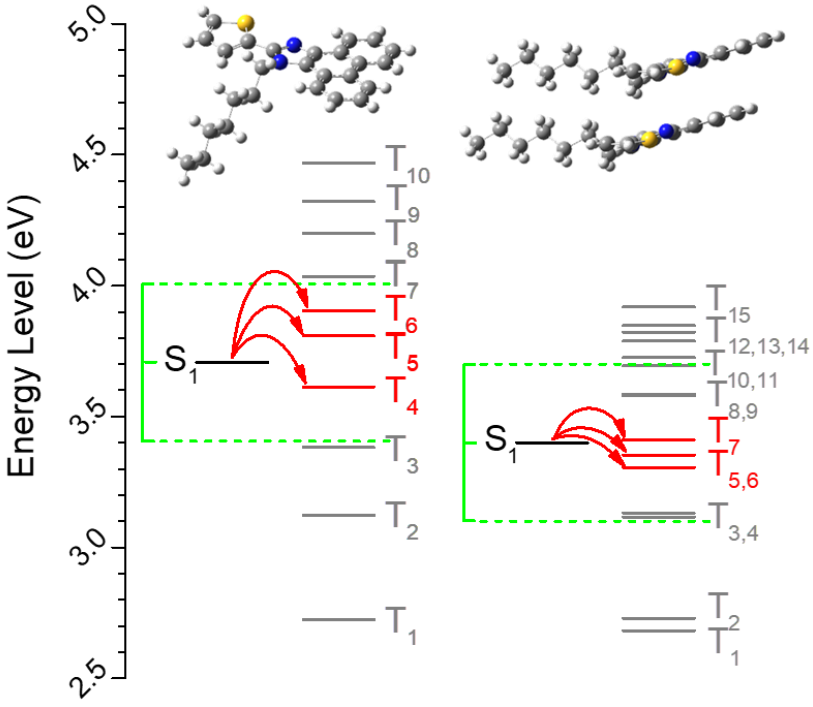


Figure S20. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C7 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C7.

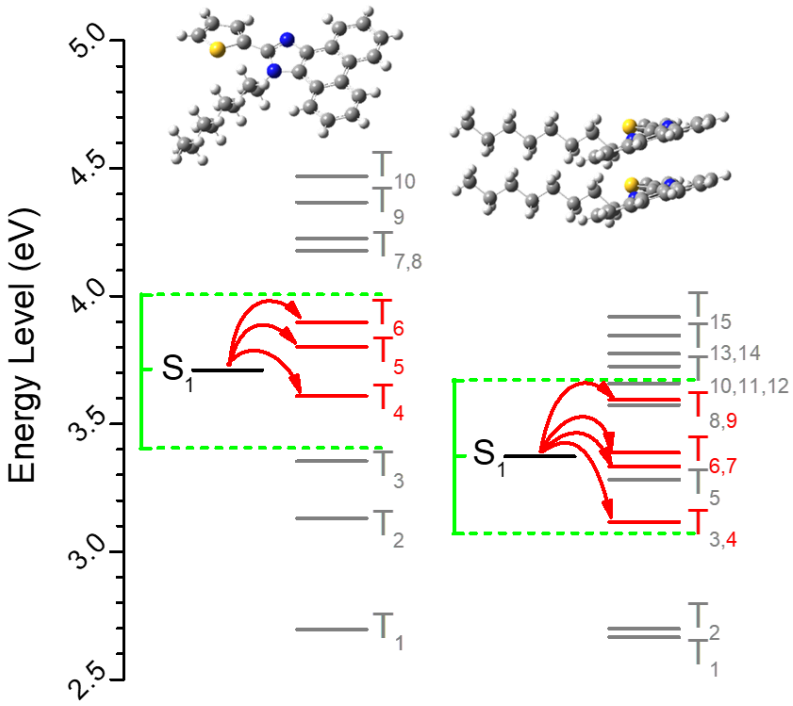


Figure S21. The lowest singlet (S_1) and triplet (T_n) states of a PIth-C8 monomer and its dimer obtained by TD-DFT calculations based on the single crystal structure data of PIth-C8.

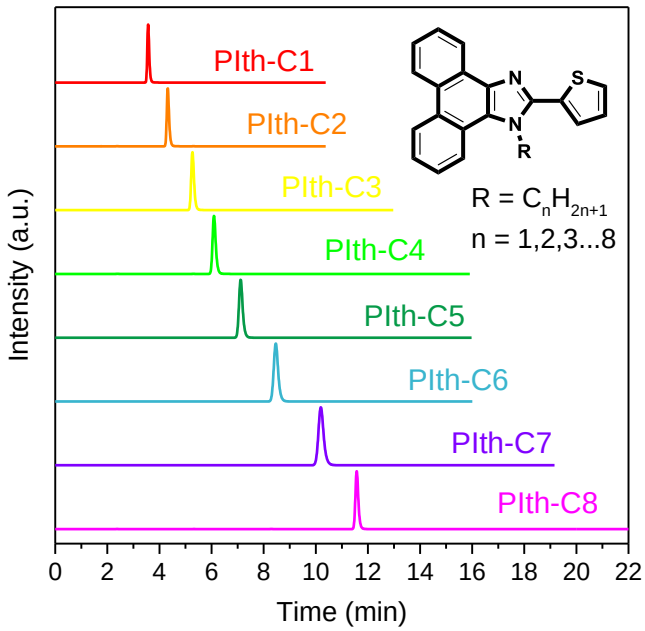


Figure S22. The High Performance Liquid Chromatography (HPLC) of the PIth-C derivatives.

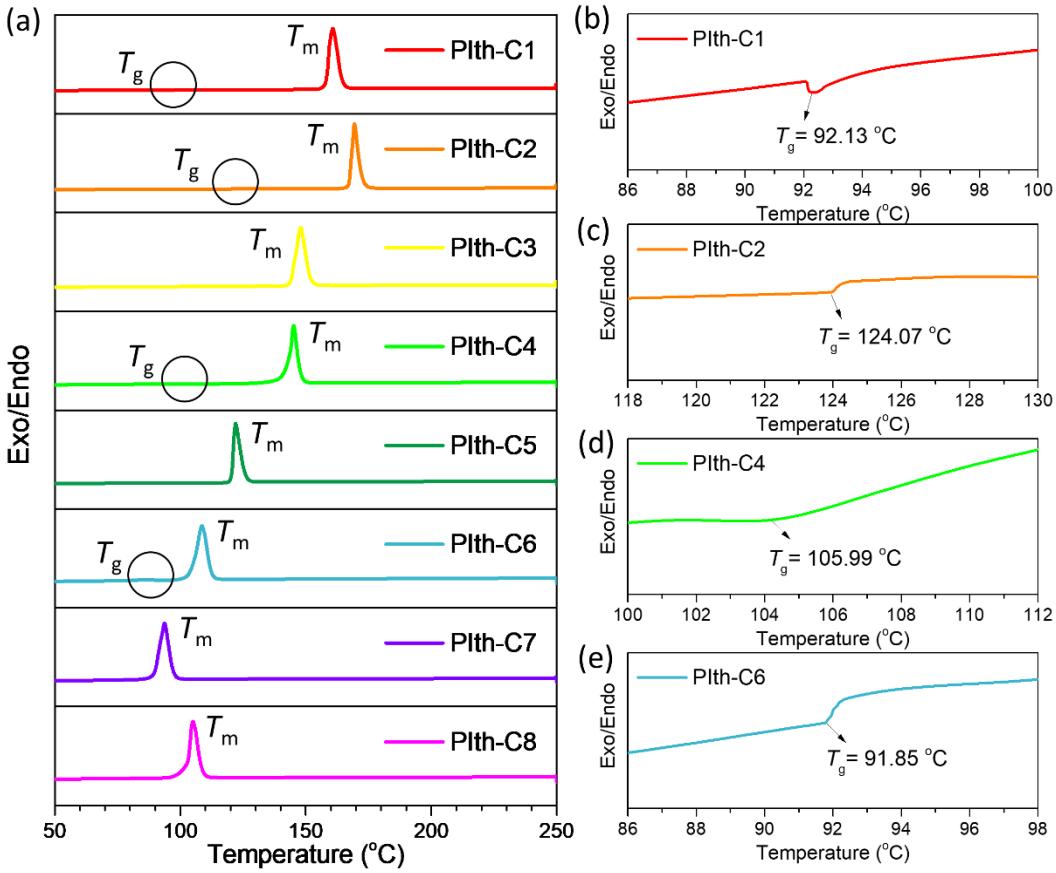


Figure S23. The Differential Scanning Calorimetry (DSC) curves of the PIth-C derivatives. (T_g: glass transition temperature; T_m: melting temperature).

According to the DSC curves, almost all of them have high melting points (T_m) over 100 °C. The glass transition temperatures (T_g) were only found for PIth-C1, PIth-C2, PIth-C4 and PIth-C6, which were around 100 °C.

Table S1. Excited wavelength for luminescence measurement of all the Pith-C derivatives.

Measurement	PL in solution	PL in crystalline state	RTP in crystalline state	Phoporscence in crystalline state at 77 K	Lifetime in crystalline state (τ_F/τ_P)	PLQY in crystalline state
Excited wavelength	320 nm	370 nm	395 nm	370 nm	375/395 nm	370 nm

PL: photoluminescence; RTP: room temperature phosphorescence; PLQY: photoluminescence quantum yield.

Table S2. Structure data of crystals PIth-C1, PIth-C2, PTth-C3 and PIth-C4.

Name	PIth-C1	PIth-C2	PIth-C3	PIth-C4
Empirical formula	$C_{20}H_{14}N_2S$	$C_{21}H_{16}N_2S$	$C_{22}H_{18}N_2S$	$C_{23}H_{20}N_2S$
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	orthorhombic	orthorhombic	monoclinic	orthorhombic
Space group	*Pna*2_1 (33)	*Pbca* (61)	*P*2_1 (4)	*Aba2* (41)
Unit cell angles (^{o})	α = 90 β = 90 γ = 90	α = 90 β = 90 γ = 90	α = 90 β = 102.982(4) γ = 90	α = 90 β = 90 γ = 90
Unit cell length (Å)	a = 29.597(9) b = 16.762(5) c = 6.172(2)	a = 10.801(3) b = 11.135(3) c = 27.335(8)	a = 12.895(3) b = 7.3292(18) c = 18.213(4)	a = 14.577(8) b = 25.798(15) c = 9.910(5)
Unit cell volume (Å^3)	3062.0(17)	3287.6(16)	1677.3(7)	3727(4)
Z	4	8	4	8
Density (g/cm^3)	1.364	1.327	1.356	1.303
F(000)	1312.0	1376.0	720.0	1544.0
CCDC number	1963678	19636379	1963680	1963681

Table S3. Structure data of crystals PIth-C5, PIth-C6, PIth-C7 and PIth-C8.

Name	PIth-C5	PIth-C6	PIth-C7	PIth-C8
Empirical formula	$C_{24}H_{22}N_2S$	$C_{25}H_{24}N_2S$	$C_{26}H_{26}N_2S$	$C_{27}H_{28}N_2S$
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_{1/}c$ (14)	$P2_1/c$ (14)
Unit cell angles (^{o})	α = 90 β = 102.378(6) γ = 90	α = 90 β = 116.04(3) γ = 90	α = 90 β = 102.670(12) γ = 90	α = 90 β = 99.930(2) γ = 90
Unit cell length (Å)	a = 10.069(3) b = 8.451(3) c = 22.933(8)	a = 11.753(4) b = 9.213(3) c = 20.432(7)	a = 22.385(5) b = 5.0506(12) c = 18.722(4)	a = 23.057(3) b = 5.0554(6) c = 18.693(2)
Unit cell volume ($Å^3$)	1906.1(11)	1987.8(12)	2065.2(8)	2146.3(5)
Z	4	4	4	4
Density (g/cm^3)	1.291	1.285	1.282	1.277
F(000)	784.0	816.0	848.0	880.0
CCDC number	1963682	1963683	1970707	1970708

Table S4. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C1.

Dimer-PIth-C1 67.149°				
Position of interaction	Type of Interaction		d /Å	Number(8)
	1	C-H…π	3.992	1
Alkyl chain	2	C-H…π	3.958	1
	3	C-H…π	3.943	1
Alkyl chain	4	C-H…π	3.861	1
Alkyl chain	5	C-H…π	3.775	1
	6	C-H…π	3.586	1
	7	C-H…π	3.148	1
	8	C-H…π	2.994	1
	Type of Interaction		d /Å	Number(5)
	1	C-H…N	3.528	1
	2	C-H…N	3.527	1
	3	C-H…N	3.322	1
Alkyl chain	4	C-H…N	3.147	1
Alkyl chain	5	C-H…N	2.852	1
	Type of Interaction		d /Å [a]	Number(4)
	1	C-H…S	3.931	1
	2	C-H…S	3.637	1
Alkyl chain	3	C-H…S	3.249	1
	4	C-H…S	3.182	1

Table S5. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C2.

Dimer-PIth-C2 42.616°				
Position of interaction	Type of Interaction		d /Å	Number(8)
	1	C-H…π	3.628	1
Alkyl chain	2	C-H…π	3.583	1
Alkyl chain	3	C-H…π	3.426	1
	4	C-H…π	3.227	1
	5	C-H…π	3.171	1
Alkyl chain	6	C-H…π	3.169	1
	7	C-H…π	3.146	1
Alkyl chain	8	C-H…π	3.052	1
	Type of Interaction		d /Å	Number(5)
	1	C-H…N	3.649	1
	2	C-H…N	3.629	1
	3	C-H…N	3.506	1
	4	C-H…N	2.917	1
	5	C-H…N	2.877	1
	Type of Interaction		d /Å	Number(3)
	1	C-H…S	3.892	1
Alkyl chain	2	C-H…S	3.870	1
Alkyl chain	3	C-H…S	3.172	1

Table S6. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C3.

Dimer-PIth-C3 31.563°				
Position of interaction	Type of Interaction		d /Å	Number(4)
	1	π…π	3.656	1
	2	π…π	3.813	1
	3	π…π	3.895	1
	4	π…π	3.961	1
	Type of Interaction		d /Å	Number(9)
	1	C-H…π	3.256	1
	2	C-H…π	3.447	1
	3	C-H…π	3.748	1
Alkyl chain	4	C-H…π	3.780	1
	5	C-H…π	3.797	1
	6	C-H…π	3.800	1
	7	C-H…π	3.820	1
	8	C-H…π	3.869	1
Alkyl chain	9	C-H…π	3.903	1
	Type of Interaction		d /Å	Number(4)
Alkyl chain	1	C-H…N	2.810	1
Alkyl chain	2	C-H…N	3.381	1
Alkyl chain	3	C-H…N	3.595	1
	4	C-H…N	3.657	1
	Type of Interaction		d /Å	Number(4)
Alkyl chain	1	C-H…S	3.198	1
Alkyl chain	2	C-H…S	3.419	1
Alkyl chain	3	C-H…S	3.504	1
	4	C-H…S	3.800	1

Table S7. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C3.

Dimer-PIth-C3 7.222°				
Position of interaction	Type of Interaction		d /Å	Number(3)
	1	π…π	3.772	1
	2	π…π	3.878	1
	3	π…π	3.896	1
	Type of Interaction		d /Å	Number(12)
Alkyl chain	1	C-H…π	3.553	1
	2	C-H…π	3.603	1
Alkyl chain	3	C-H…π	3.651	1
Alkyl chain	4	C-H…π	3.689	1
Alkyl chain	5	C-H…π	3.747	1
	6	C-H…π	3.780	1
Alkyl chain	7	C-H…π	3.797	1
Alkyl chain	8	C-H…π	3.836	1
	9	C-H…π	3.836	1
	10	C-H…π	3.905	1
	11	C-H…π	3.907	1
	12	C-H…π	3.954	1
	Type of Interaction		d /Å	Number(10)
	1	C-H…N	3.506	2
	2	C-H…N	3.636	2
	3	C-H…N	3.698	2
	4	C-H…N	3.756	2
	5	C-H…N	3.989	2
	Type of Interaction		d /Å	Number(1)
	1	C-H…S	3.332	1

Table S8. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C4.

Dimer-PTth-C4 27.942°				
Position of interaction	Type of Interaction		d /Å	Number(2)
	1	π…π	3.852	1
	2	π…π	3.887	1
	Type of Interaction		d /Å	Number(15)
	1	C-H…π	3.080	1
	2	C-H…π	3.109	1
	3	C-H…π	3.323	1
Alkyl chain	4	C-H…π	3.411	1
	5	C-H…π	3.444	1
	6	C-H…π	3.496	1
Alkyl chain	7	C-H…π	3.644	1
Alkyl chain	8	C-H…π	3.650	1
Alkyl chain	9	C-H…π	3.664	1
	10	C-H…π	3.783	1
Alkyl chain	11	C-H…π	3.790	1
Alkyl chain	12	C-H…π	3.920	1
	13	C-H…π	3.923	1
	14	C-H…π	3.945	1
	15	C-H…π	3.985	1
	Type of Interaction		d /Å	Number(4)
Alkyl chain	1	C-H…N	2.754	1
	2	C-H…N	3.072	1
	3	C-H…N	3.573	1
	4	C-H…N	3.635	1
	Type of Interaction		d /Å	Number(4)
	1	C-H…S	3.544	1
Alkyl chain	2	C-H…S	3.846	1
	3	C-H…S	3.891	1
Alkyl chain	4	C-H…S	3.969	1

Table S9. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C5.

Dimer-PIth-C5 29.194°				
Position of interaction	Type of Interaction		d /Å	Number(18)
Alkyl chain	1	C-H…π	3.039	1
Alkyl chain	2	C-H…π	3.153	1
Alkyl chain	3	C-H…π	3.258	1
Alkyl chain	4	C-H…π	3.297	1
Alkyl chain	5	C-H…π	3.300	1
Alkyl chain	6	C-H…π	3.310	1
Alkyl chain	7	C-H…π	3.402	1
	8	C-H…π	3.513	1
Alkyl chain	9	C-H…π	3.563	1
Alkyl chain	10	C-H…π	3.667	1
Alkyl chain	11	C-H…π	3.684	1
	12	C-H…π	3.693	1
Alkyl chain	13	C-H…π	3.734	1
Alkyl chain	14	C-H…π	3.756	1
	15	C-H…π	3.778	1
Alkyl chain	16	C-H…π	3.865	1
Alkyl chain	17	C-H…π	3.886	1
Alkyl chain	18	C-H…π	3.889	1
	Type of Interaction		d /Å	Number(2)
	1	C-H…N	3.350	1
	2	C-H…N	3.870	1
	Type of Interaction		d /Å	Number(2)
	1	C-H…S	3.089	1
	2	C-H…S	3.152	1

Table S10. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C6.

Dimer-PTth-C6 0°				
Position of interaction	Type of Interaction		d /Å	Number(4)
	1	π…π	3.583	2
	2	π…π	3.703	2
	Type of Interaction		d /Å	Number(20)
Alkyl chain	1	C-H…π	3.355	2
	2	C-H…π	3.603	2
Alkyl chain	3	C-H…π	3.611	2
	4	C-H…π	3.659	2
Alkyl chain	5	C-H…π	3.756	2
	6	C-H…π	3.867	2
Alkyl chain	7	C-H…π	3.875	2
	8	C-H…π	3.908	2
Alkyl chain	9	C-H…π	3.981	2
	10	C-H…π	3.985	2
	Type of Interaction		d /Å	Number(8)
	1	C-H…N	3.470	2
	2	C-H…N	3.500	2
	3	C-H…N	3.713	2
	4	C-H…N	3.835	2
	Type of Interaction		d /Å	Number(2)
	1	C-H…S	3.083	2

Table S11. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C7.

Dimer-PIth-C7 0°				
Position of interaction	Type of Interaction		d /Å	Number(3)
	1	π…π	3.842	1
	2	π…π	3.744	1
	3	π…π	3.660	1
	Type of Interaction		d /Å	Number(11)
	1	C-H…π	3.836	1
	2	C-H…π	3.826	1
	3	C-H…π	3.764	1
	4	C-H…π	3.754	1
	5	C-H…π	3.741	1
Alkyl chain	6	C-H…π	3.712	1
Alkyl chain	7	C-H…π	3.590	1
	8	C-H…π	3.454	1
Alkyl chain	9	C-H…π	3.274	1
Alkyl chain	10	C-H…π	3.268	1
Alkyl chain	11	C-H…π	2.621	1
	Type of Interaction		d /Å	Number(3)
	1	C-H…N	3.999	1
	2	C-H…N	3.761	1
Alkyl chain	3	C-H…N	3.625	1
	Type of Interaction		d /Å	Number(2)
	1	C-H…S	3.699	1
	2	C-H…S	3.492	1

Table S12. Summarization of intermolecular interactions in the molecular dimer derived from the unit cell of PIth-C8.

Dimer-PIth-C8 0°				
Position of interaction	Type of Interaction		d /Å	Number(3)
	1	π…π	3.853	1
	2	π…π	3.740	1
	3	π…π	3.703	1
	Type of Interaction		d /Å	Number(12)
	1	C-H…π	3.885	1
	2	C-H…π	3.863	1
	3	C-H…π	3.830	1
	4	C-H…π	3.765	1
	5	C-H…π	3.761	1
	6	C-H…π	3.760	1
Alkyl chain	7	C-H…π	3.664	1
Alkyl chain	8	C-H…π	3.548	1
	9	C-H…π	3.447	1
Alkyl chain	10	C-H…π	3.243	1
Alkyl chain	11	C-H…π	3.215	1
Alkyl chain	12	C-H…π	2.590	1
	Type of Interaction		d /Å	Number(3)
	1	C-H…N	3.700	1
	2	C-H…N	3.640	1
Alkyl chain	3	C-H…N	3.590	1
	Type of Interaction		d /Å	Number(3)
Alkyl chain	1	C-H…S	3.975	1
Alkyl chain	2	C-H…S	3.859	1
	3	C-H…S	3.693	1

Table S13. Summarization of intermolecular interactions between the molecular dimer in the unit cell of PIth-C derivatives.

Unit cells	C-H…π (d /Å) (number)	C-H…N(d /Å) (number)	C-H…S(d /Å) (number)
PIth-C1	3.083(2), 3.122(2)	\	\
PIth-C2	3.095(4), 3.563(4), 3.641(4)	2.796 (4), 3.808 (4)	\
PIth-C3	3.041 (2), 3.272(1), 3.513(1), 3.669(1), 3.958(1), 3.977(1)	3.044(2), 3.101(2)	3.340(2), 3.412(2), 3.429(2), 3.557(2), 3.579(2), 3.802(2)
PIth-C4	3.237(4), 3.451(4), 3.653(2), 3.837(4)	\	3.741(4), 3.803(4), 3.909(4)
PIth-C5	2.817(4), 3.546(2), 3.611(2), 3.700(2)	3.175(4), 3.268(2), 3.716(2)	3.498(2)
PIth-C6	3.568(4)	\	\
PIth-C7	3.309(2), 3.713(2)	2.877(2), 3.770(2)	3.201(2), 3.482(4)
PIth-C8	3.171(2), 3.721(2)	2.858(2), 3.738(2)	3.495(2), 3.657(4)

Table S14. Singlet and triplet excited state transition configurations of PIth-C1 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C1		Dimer-PIth-C1	
	T1: 2.7911 eV		T1: 2.7768 eV
	T2: 3.1329 eV		T2: 2.7869 eV
	T3: 3.3984 eV		T3: 3.1259 eV
	T4: 3.5861 eV H-1 -> L (20.6%) H -> L (3.4%)		T4: 3.1278 eV
S1: 3.7331 eV H-1 -> L (2.0%) H-1 -> L+2 (4.0%) H -> L (71.6%) H -> L+1 (20.0%)			T5: 3.3718 eV H ->L (39.5%)
	T5: 3.8974 eV H-1 -> L (5.8%) H -> L (3.8%)	S1: 3.3941 eV H ->L (99.7%)	
	T6: 3.9450 eV H-1 -> L (42.2%) H-1 -> L+2 (10.8%)		T6: 3.4065 eV H ->L (58.9%)
	T7: 4.2338 eV		T7: 3.4374 eV
	T8: 4.2553 eV		T8: 3.5802 eV
	T9: 4.3696 eV		T9: 3.5895 eV
	T10: 4.5124 eV		T10: 3.8117 eV
			T11: 3.8692 eV
			T12: 3.8920 eV
			T13: 3.9158 eV
			T14: 3.9431 eV
			T15: 4.0321 eV

Table S15. Singlet and triplet excited state transition configurations of PIth-C2 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C2	Dimer-PIth-C2
T1: 2.7912 eV	T1: 2.8989 eV
T2: 3.1498 eV	T2: 2.9103 eV
T3: 3.4179 eV	T3: 3.1238 eV
T4: 3.6228 eV H -> L (3.2%)	T4: 3.1373 eV
S1: 3.7535 eV H-1 -> L+2 (4.0%) H -> L (70.7%) H -> L+1 (21.5%)	T5: 3.4140 eV H ->L+1 (5.8%)
T5: 3.8532 eV H -> L (3.2%)	T6: 3.4323 eV
T6: 3.9714 eV H-1 -> L+2 (14.1%)	T7: 3.5685 eV H ->L (13.2%) H ->L+1 (4.9%)
T7: 4.2239 eV	T8: 3.5869 eV
T8: 4.2800 eV	S1: 3.6288 eV H ->L (95.2%) H ->L+1 (2.3%)
T9: 4.3238 eV	T9: 3.6400 eV H ->L (78.3%)
T10: 4.4931 eV	T10: 3.8115 eV
	T11: 3.8130 eV
	T12: 3.9672 eV
	T13: 3.9759 eV
	T14: 3.9900 eV
	T15: 4.1759 eV

Table S16. Singlet and triplet excited state transition configurations of PIth-C3 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C3	Dimer-PIth-C3
T1: 2.8663 eV	T1: 2.7331 eV
T2: 3.1795 eV	T2: 2.7586 eV
T3: 3.4098 eV	T3: 3.0936 eV
T4: 3.6390 eV H-1 -> L (15.5%) H -> L (4.8%)	T4: 3.1134 eV
S1: 3.8016 eV H-1 -> L (2.5%) H-1 -> L+2 (4.1%) H -> L (52.8%) H -> L+1 (38.6%)	T5: 3.2921 eV
T5: 3.8471 eV H -> L (4.1%) H -> L+1 (3.1%)	T6: 3.3106 eV H-1 ->L (4.7%) H ->L (2.9%)
T6: 4.0405 eV H-1 -> L (53.8%) H-1 -> L+2 (17.5%)	S1: 3.4767 eV H-1 ->L (2.1%) H ->L (94.3%)
T7: 4.2669 eV	T7: 3.5157 eV H-1 ->L (30.2%) H ->L (47.0%)
T8: 4.3487 eV	T8: 3.5833 eV H-1 ->L (2.5%)
T9: 4.3893 eV	T9: 3.6001 eV H-1 ->L (6.8%) H ->L (6.0%)
T10: 4.5406 eV	T10: 3.6933 eV
	T11: 3.8082 eV
	T12: 3.8479 eV
	T13: 3.9162 eV
	T14: 4.0144 eV
	T15: 4.0215 eV

Table S17. Singlet and triplet excited state transition configurations of PIth-C3 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C3	Dimer-PIth-C3
	T1: 2.6877 eV T2: 2.8739 eV T3: 3.1564 eV T4: 3.1629 eV T5: 3.3692 eV
T1: 2.7445 eV	
	T6: 3.3804 eV
T2: 3.1379 eV	
	T7: 3.6186 eV H-1 ->L+2 (2.9%) H ->L (5.1%)
T3: 3.3853 eV	
	T8: 3.6320 eV
T4: 3.6186 eV H -> L (3.8%)	
	S1: 3.7313 eV H-1 ->L (12.4%) H-1 ->L+1 (19.7%) H-1 ->L+2 (28.4%) H ->L (24.5%) H ->L+3 (4.4%)
S1: 3.7352 eV H-1 -> L+2 (2.9%) H -> L (70.7%) H -> L+1 (22.9%)	
	T9: 3.8038 eV H-1 ->L (21.1%) H ->L (34.0%)
T5: 3.8389 eV H -> L (3.3%) H -> L+1 (2.8%)	
	T10: 3.8154 eV H-1 ->L (10.4%) H-1 ->L+1 (47.3%) H ->L (5.4%)
T6: 3.9763 eV H-1 -> L+2 (13.2%)	
	T11: 3.8364 eV H-1 ->L (11.7%) H-1 ->L+1 (5.3%) H ->L (3.0%)
T7: 4.2284 eV	
	T12: 3.8378 eV H-1 ->L+1 (2.7%) H ->L (9.4%)
T8: 4.2719 eV	
	T13: 3.9380 eV H-1 ->L+2 (9.5%) H ->L+3 (34.2%)
T9: 4.3327 eV	
	T14: 3.9955 eV H-1 ->L+2 (20.5%) H ->L+3 (11.2%)
T10: 4.5071 eV	
	T15: 4.0581 eV

Table S18. Singlet and triplet excited state transition configurations of PIth-C4 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C4		Dimer-PIth-C4	
	T1: 2.6189 eV		T1: 2.6173 eV
	T2: 3.0860 eV		T2: 2.6260 eV
	T3: 3.4401 eV H -> L: (2.8%) H -> L+1 (82.0%)		T3: 3.0562 eV
	T4: 3.5549 H -> L (13.1%) eV		T4: 3.0727 eV
S1: 3.6639 eV H -> L (94.1%) H -> L+1 (2.7%)			T5: 3.3761 eV H ->L (8.2%)
	T5: 3.8204 eV H -> L (4.3%)		T6: 3.4005 eV H ->L (2.7%)
	T6: 3.9235 eV	S1: 3.4261 eV H ->L (98.7%)	
	T7: 4.1064 eV		T7: 3.4327 eV H ->L (66.8%)
	T8: 4.2113 eV		T8: 3.5556 eV
	T9: 4.2733 eV		T9: 3.5850 eV H ->L (9.6%)
	T10: 4.5103 eV		T10: 3.7375 eV
			T11: 3.7882 eV
			T12: 3.8014 eV
			T13: 3.8949 eV
			T14: 3.9561 eV
			T15: 4.0099 eV

Table S19. Singlet and triplet excited state transition configurations of PIth-C5 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C5		Dimer-PIth-C5	
	T1: 2.9249 eV		T1: 2.9312 eV
	T2: 3.3003 eV		T2: 2.9338 eV
	T3: 3.4758 eV		T3: 3.2980 eV
	T4: 3.6766 eV H-1 -> L (14.9%) H -> L (7.4%)		T4: 3.3057 eV
	T5: 3.8164 eV H-1 -> L (3.0%) H -> L+1 (4.2%)		T5: 3.4407 eV
S1: 3.8830 eV H-1 -> L (4.1%) H-1 -> L+2 (4.4%) H -> L (51.9%) H -> L+1 (36.6%)			T6: 3.4489 eV
	T6: 4.0247 eV H-1 -> L (51.7%) H-1 -> L+2 (17.8%)		T7: 3.6637 eV H ->L (2.9%)
	T7: 4.3052 eV		T8: 3.6680 eV H ->L (2.7%)
	T8: 4.3572 eV	S1: 3.7546 eV H ->L (98.9%)	
	T9: 4.4539 eV		T9: 3.7637 eV H ->L (88.7%)
	T10: 4.5805 eV		T10: 3.8062 eV
			T11: 3.8112 eV
			T12: 3.9182 eV
			T13: 4.0331 eV
			T14: 4.0363 eV
			T15: 4.2033 eV

Table S20. Singlet and triplet excited state transition configurations of PIth-C6 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C6	Dimer-PIth-C6
	T1: 2.9927 eV T2: 3.0033 eV T3: 3.3289 eV T4: 3.3324 eV T5: 3.4016 eV T6: 3.4467 eV
T1: 3.0023 eV	
	T7: 3.6244 eV
T2: 3.3662 eV	
	T8: 3.6535 eV H ->L+2 (2.1%)
T3: 3.4871 eV	
T4: 3.6655 eV H-1 -> L (20.8%) H-1 -> L+1 (19.2%) H -> L (5.1%) H -> L+1 (2.7%)	S1: 3.7416 eV H ->L (85.9%) H ->L+2 (6.8%)
T5: 3.8585 eV H-1 -> L+1 (6.3%) H -> L (3.1%)	
	T9: 3.8155 eV
S1: 3.9007 eV H-1 -> L (3.6%) H-1 -> L+1 (2.5%) H-1 -> L+2 (4.9%) H -> L (53.6%) H -> L+1 (34.3%)	
	T10: 3.8175 eV H ->L (2.8%)
T6: 4.0818 eV H-1 -> L (39.7%) H-1 -> L+1 (29.7%) H-1 -> L+2 (22.0%)	
	T11: 3.9407 eV H ->L (27.3%) H ->L+2 (7.7%)
T7: 4.3135 eV	T12: 3.9484 eV
T8: 4.3798 eV	T13: 4.0742 eV
T9: 4.5160 eV	T14: 4.0836 eV
T10: 4.6241 eV	T15: 4.0899 eV

Table S21. Singlet and triplet excited state transition configurations of PIth-C7 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C7		Dimer-PIth-C7	
	T1: 2.7252 eV		T1: 2.6829 eV
	T2: 3.1230 eV		T2: 2.7294 eV
	T3: 3.3821 eV		T3: 3.1163 eV
	T4: 3.6133 eV H -> L （2.5%）		T4: 3.1309 eV
S1: 3.7065 eV H-1 -> L+2 (2.5%) H -> L (79.4%) H -> L+1 (14.4%)			T5: 3.3058 eV H ->L (3.9%)
	T5: 3.8086 eV H -> L+1 (3.9%)		T6: 3.3535 eV H ->L (3.4%)
	T6: 3.9044 eV H-1 -> L+2 (11.1%)	S1: 3.4006 eV H ->L (98.1%)	
	T7: 4.0357 eV		T7: 3.4109 eV H ->L (85.0%)
	T8: 4.1983 eV		T8: 3.5786 eV
	T9: 4.3206 eV		T9: 3.5866 eV
	T10: 4.4686 eV		T10: 3.6933 eV
			T11: 3.7252 eV
			T12: 3.7883 eV
			T13: 3.8228 eV
			T14: 3.8474 eV
			T15: 3.9179 eV

Table S22. Singlet and triplet excited state transition configurations of PIth-C8 monomer and dimer revealed by TD-DFT calculations.

Monomer-PIth-C8		Dimer-PIth-C8	
	T1: 2.6962 eV		T1: 2.6654 eV
	T2: 3.1304 eV		T2: 2.6981 eV
	T3: 3.3540 eV		T3: 3.1159 eV
	T4: 3.6086 eV H-1 -> L (17.6%) H -> L (2.4%)		T4: 3.1174 eV H -> L (10.0%)
S1: 3.7110 eV H-1 -> L (2.4%） H-1 -> L+2 (2.8%) H -> L (69.6%) H -> L+1 (22.5%)			T5: 3.2820 eV
	T5: 3.8009 eV H-1 -> L (13.9%) H -> L+1 (5.2%)		T6: 3.3330 eV H -> L (5.6%)
	T6: 3.8983 eV H-1 -> L (46.1%) H-1 -> L+2 (10.9%)	S1: 3.3724 eV H -> L (98.0%)	
	T7: 4.1776 eV		T7: 3.3880 eV H -> L (76.6%)
	T8: 4.2256 eV		T8: 3.5741 eV
	T9: 4.3671 eV		T9: 3.5935 eV H -> L (3.3%)
	T10: 4.4691 eV		T10: 3.6586 eV
			T11: 3.7253 eV
			T12: 3.7749 eV
			T13: 3.8457 eV
			T14: 3.8475 eV
			T15: 3.9190 eV

5. Structure Information

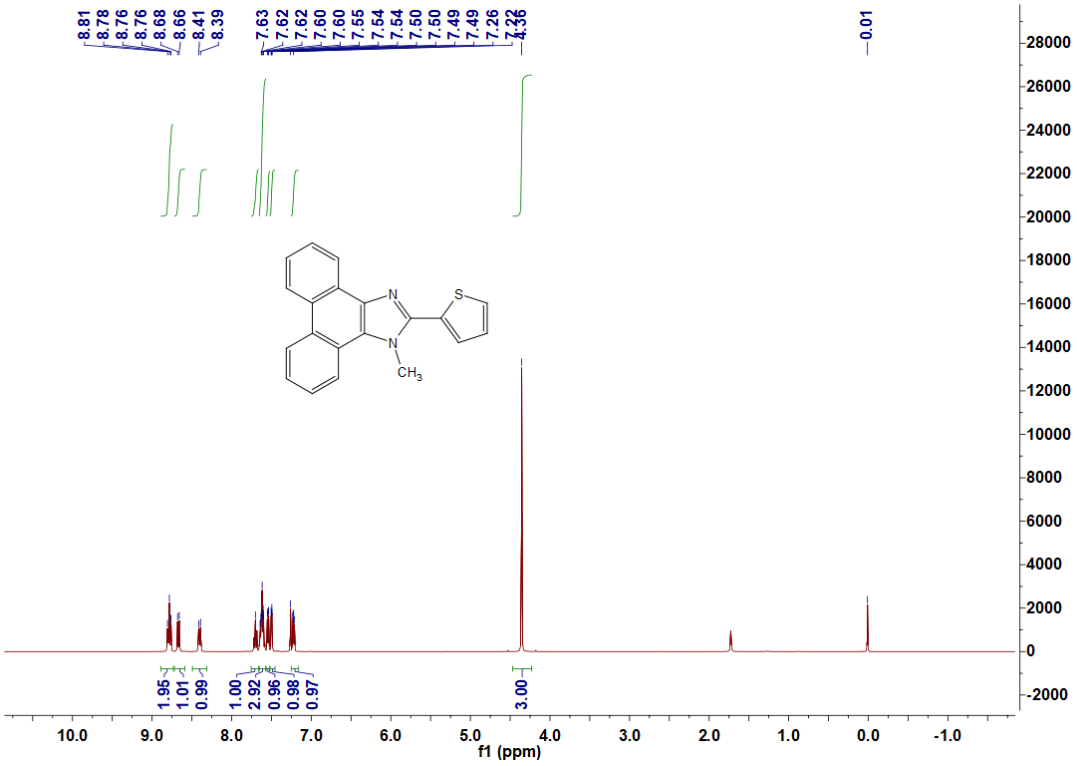


Figure S24. ^{1}H NMR spectrum of PIth-C1 conducted in $CDCl_3$.

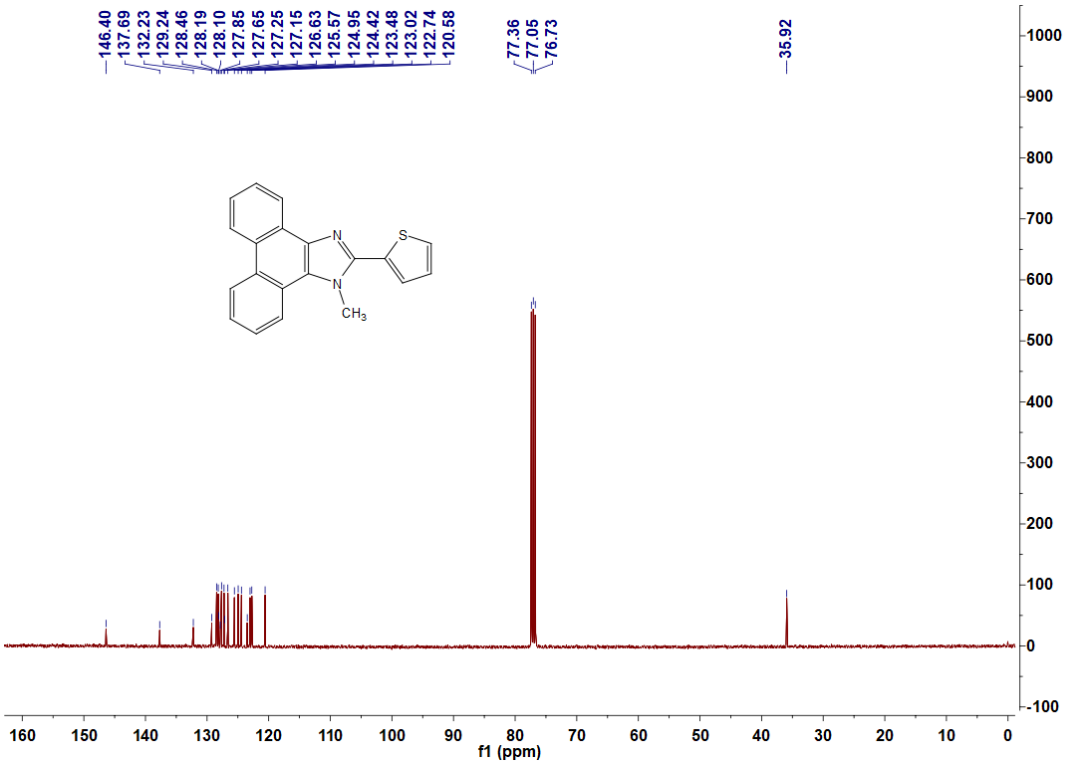


Figure S25. ^{13}C NMR spectrum of PIth-C1 conducted in $CDCl_3$.

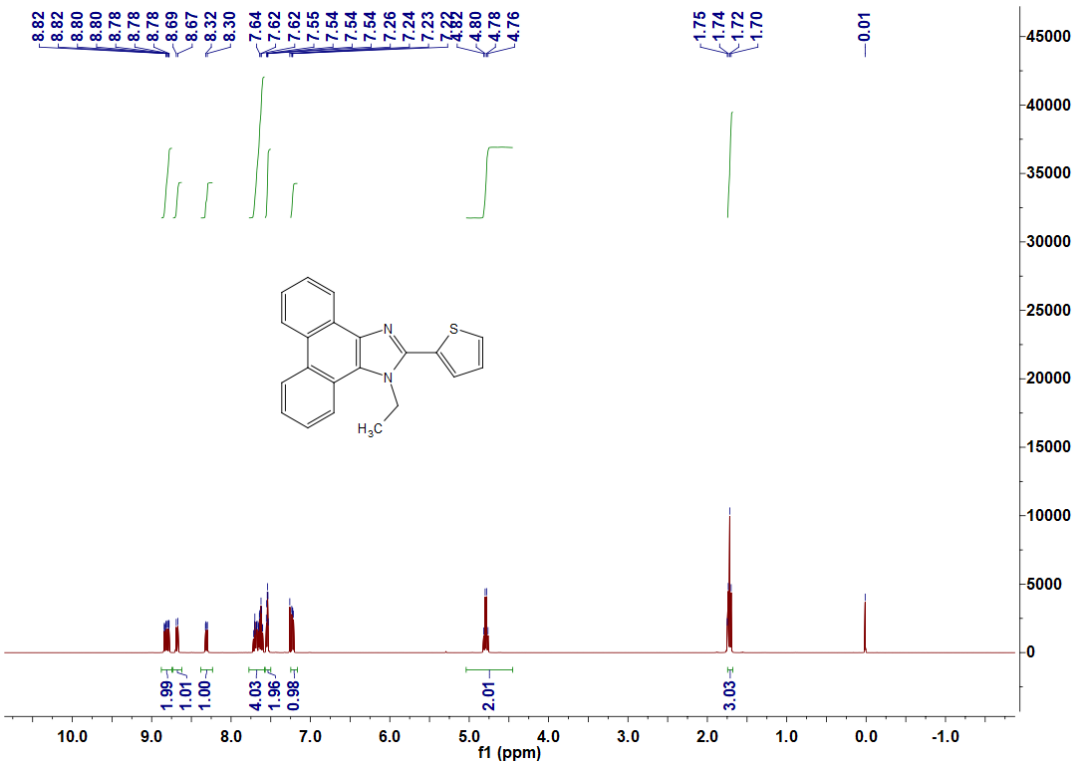


Figure S26. ^{1}H NMR spectrum of PIth-C2 conducted in $CDCl_3$.

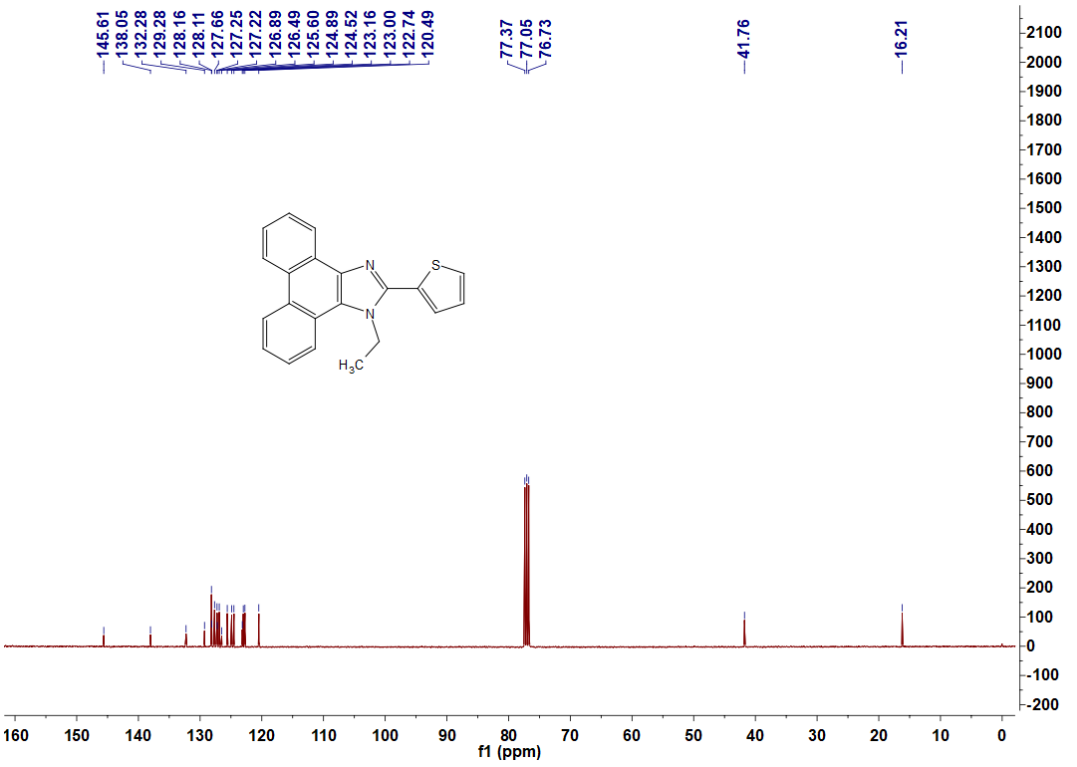


Figure S27. ^{13}C NMR spectrum of PIth-C2 conducted in $CDCl_3$.

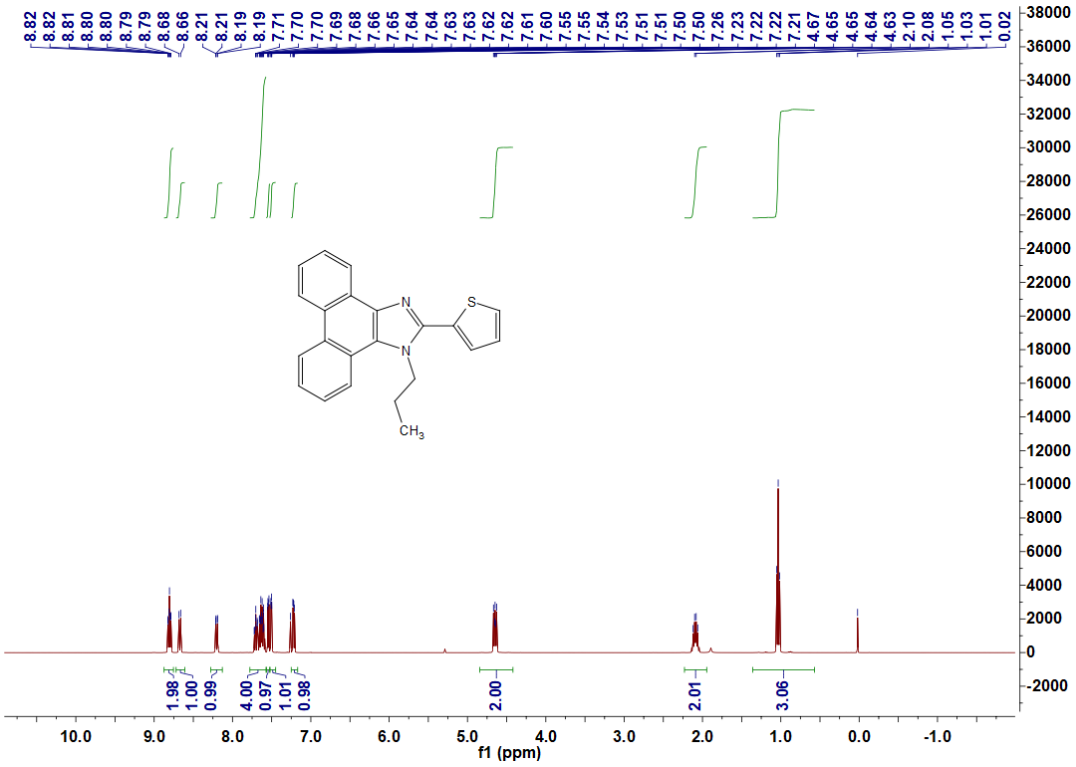


Figure S28. ^{1}H NMR spectrum of PIth-C3 conducted in $CDCl_3$.

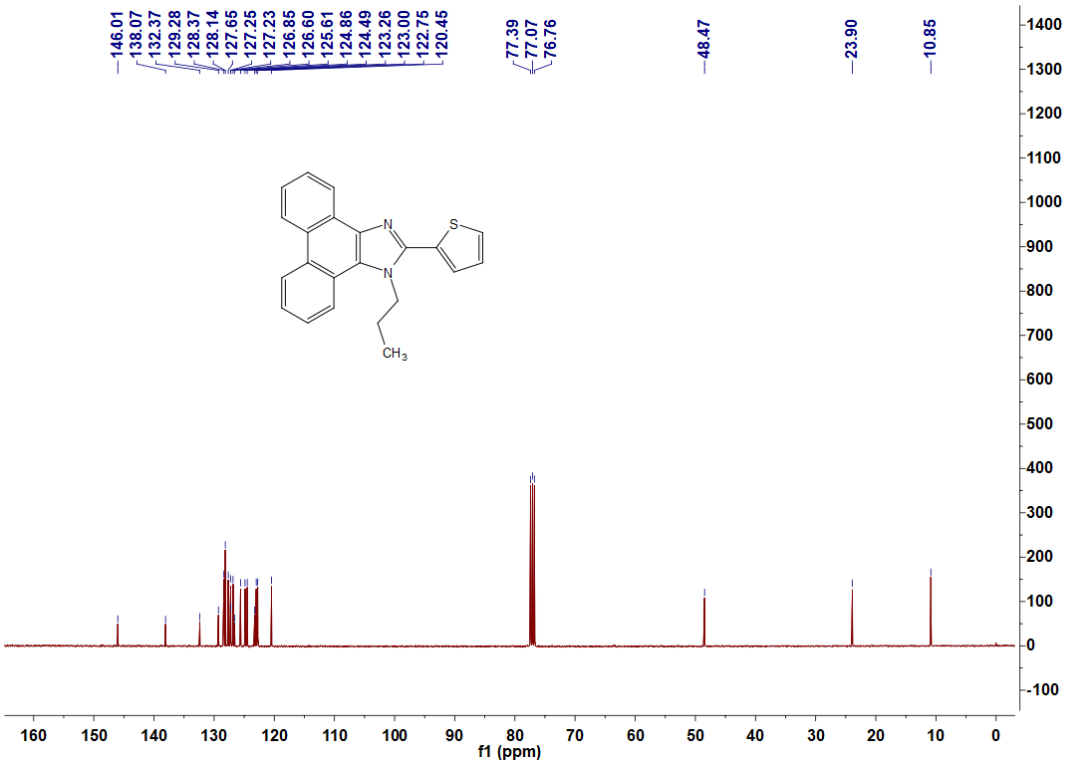


Figure S29. ^{13}C NMR spectrum of PIth-C3 conducted in $CDCl_3$.

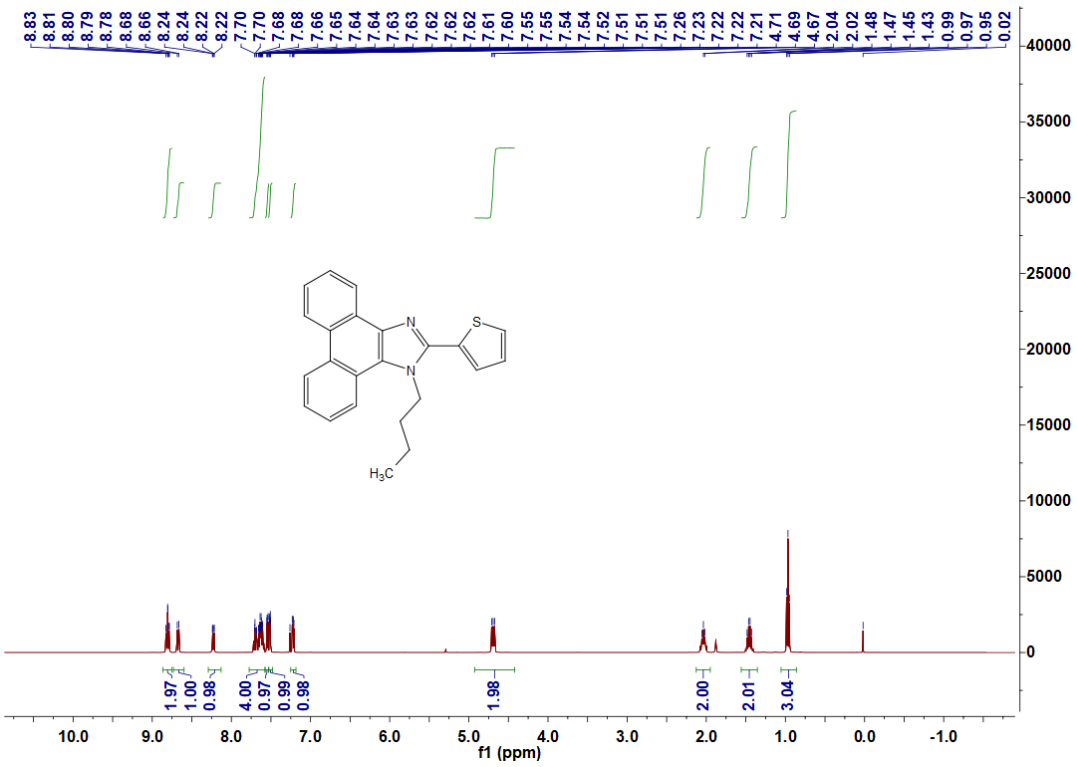


Figure S30. ^{1}H NMR spectrum of PIth-C4 conducted in $CDCl_3$.

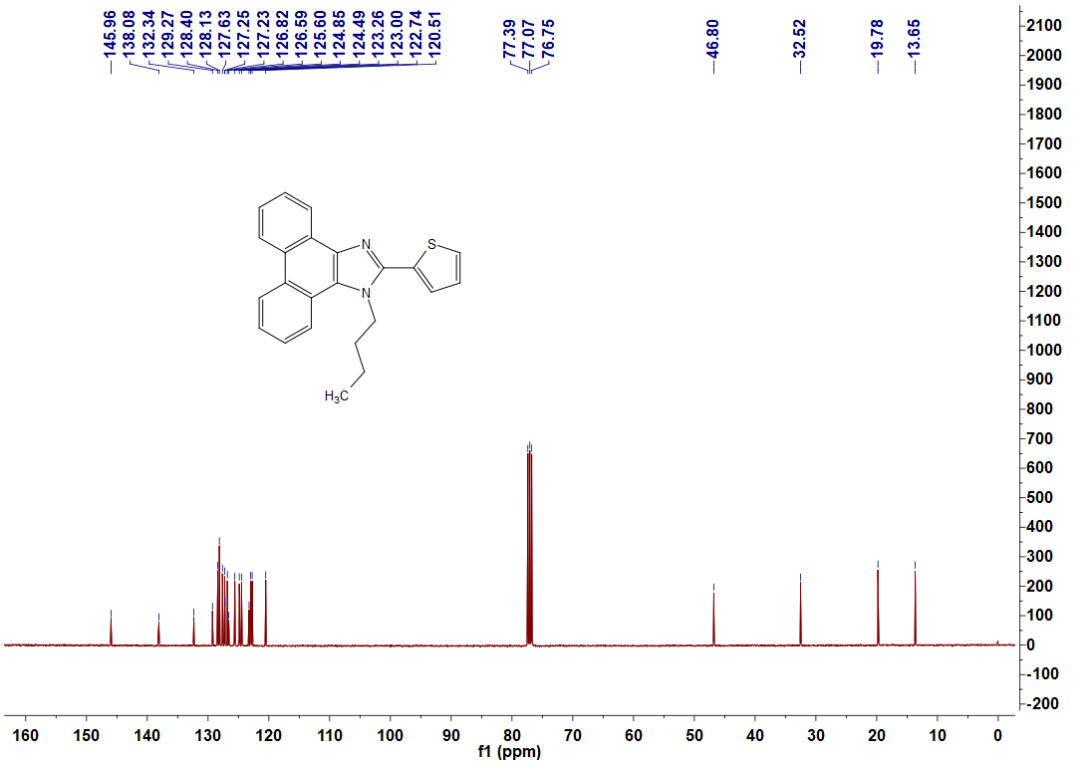


Figure S31. ^{13}C NMR spectrum of PIth-C4 conducted in $CDCl_3$.

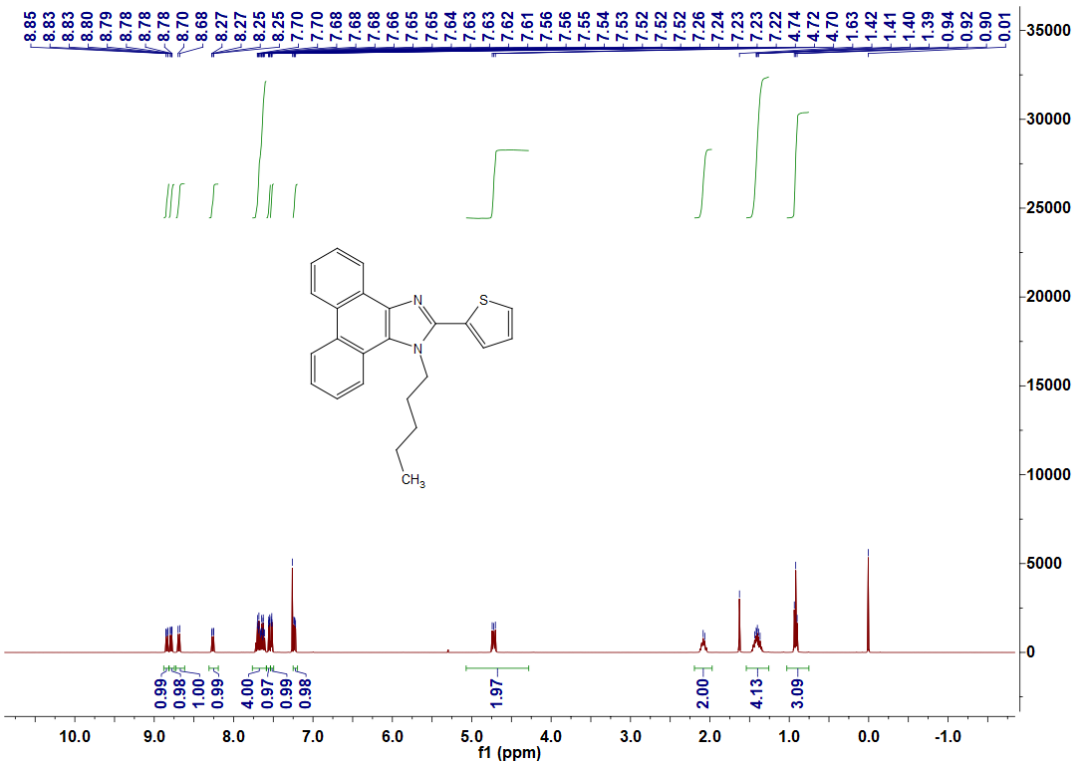


Figure S32. ^{1}H NMR spectrum of PIth-C5 conducted in $CDCl_3$.

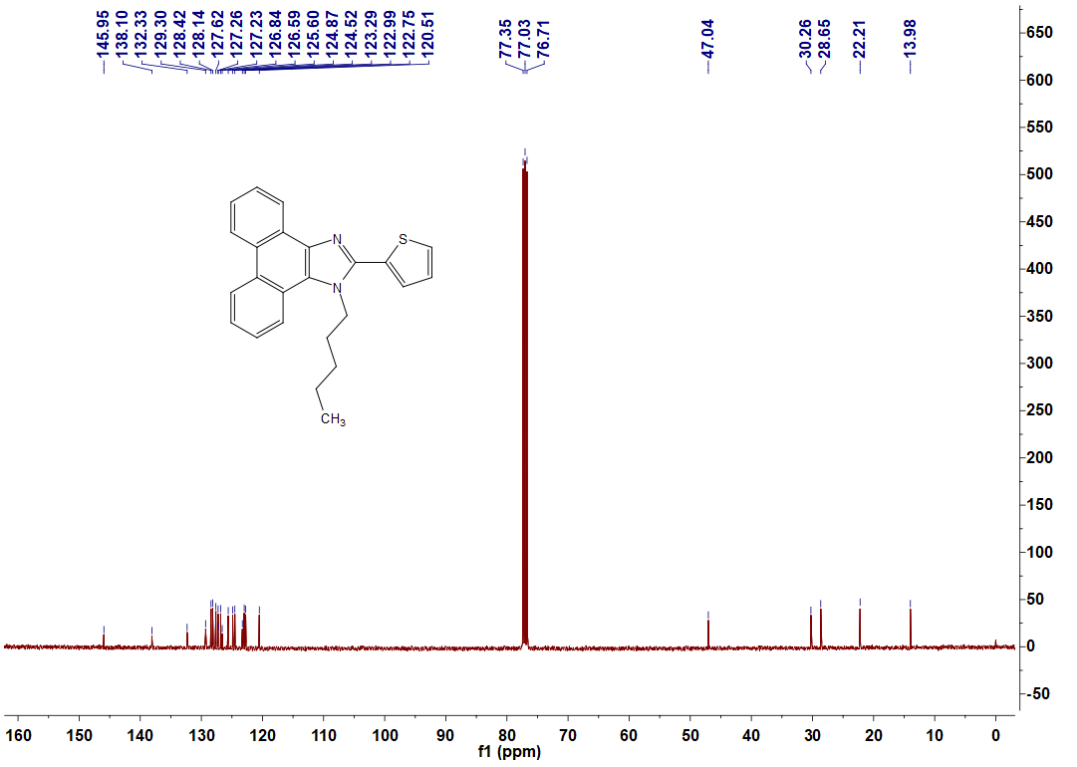


Figure S33. ^{13}C NMR spectrum of PIth-C5 conducted in $CDCl_3$.

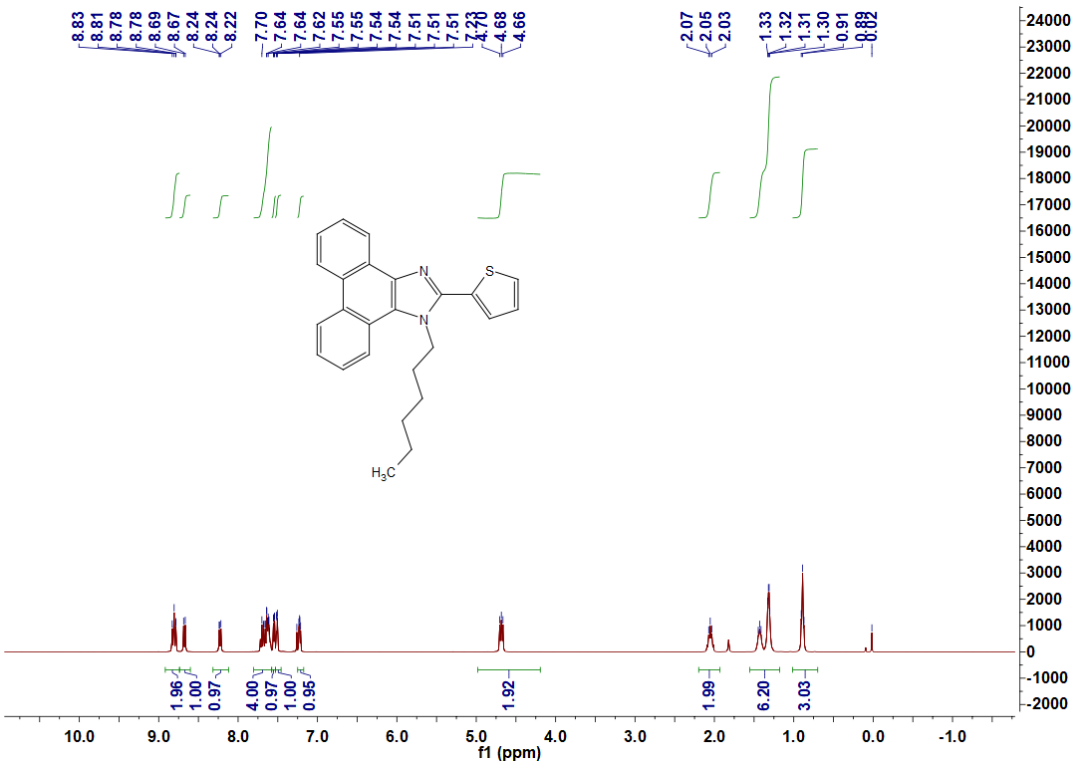


Figure S34. ^{1}H NMR spectrum of PIth-C6 conducted in $CDCl_3$.

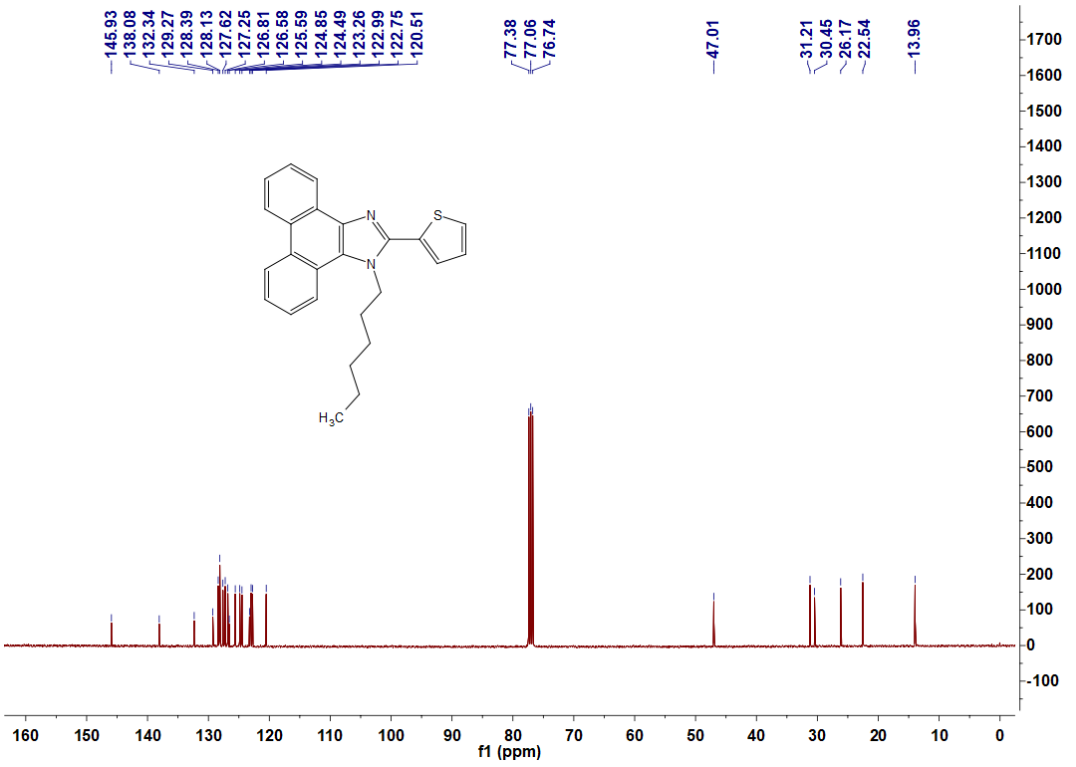


Figure S35. ^{13}C NMR spectrum of PIth-C6 conducted in $CDCl_3$.

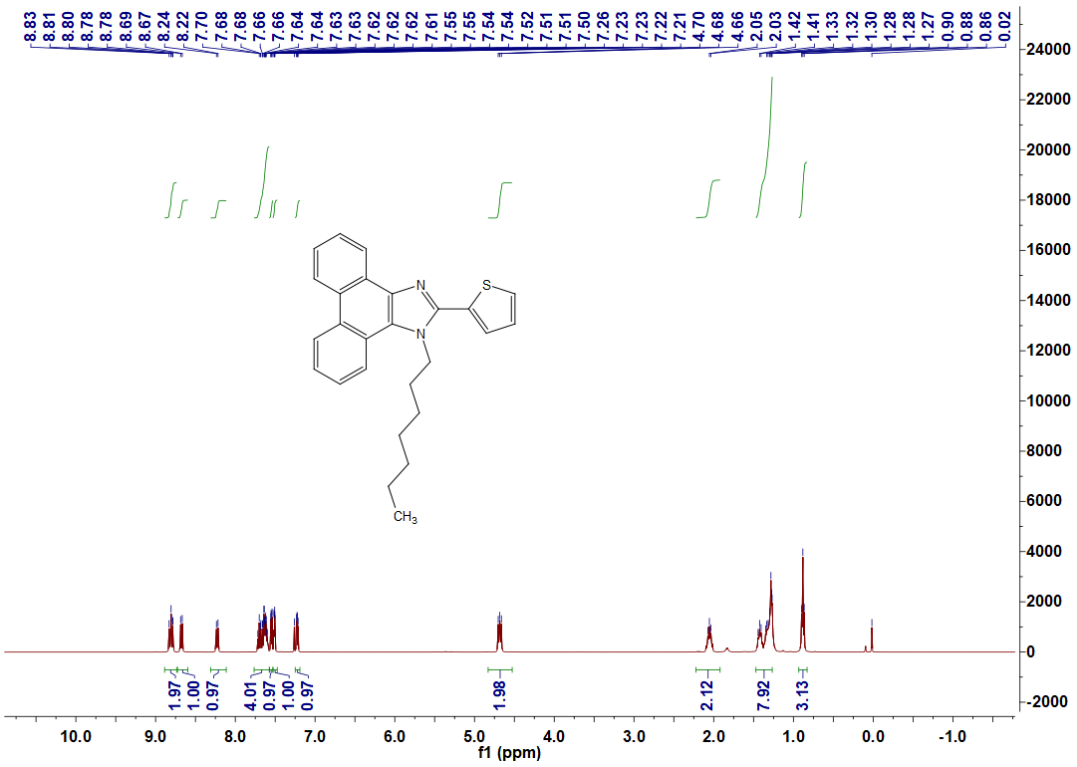


Figure S36. ^{1}H NMR spectrum of PIth-C7 conducted in $CDCl_3$.

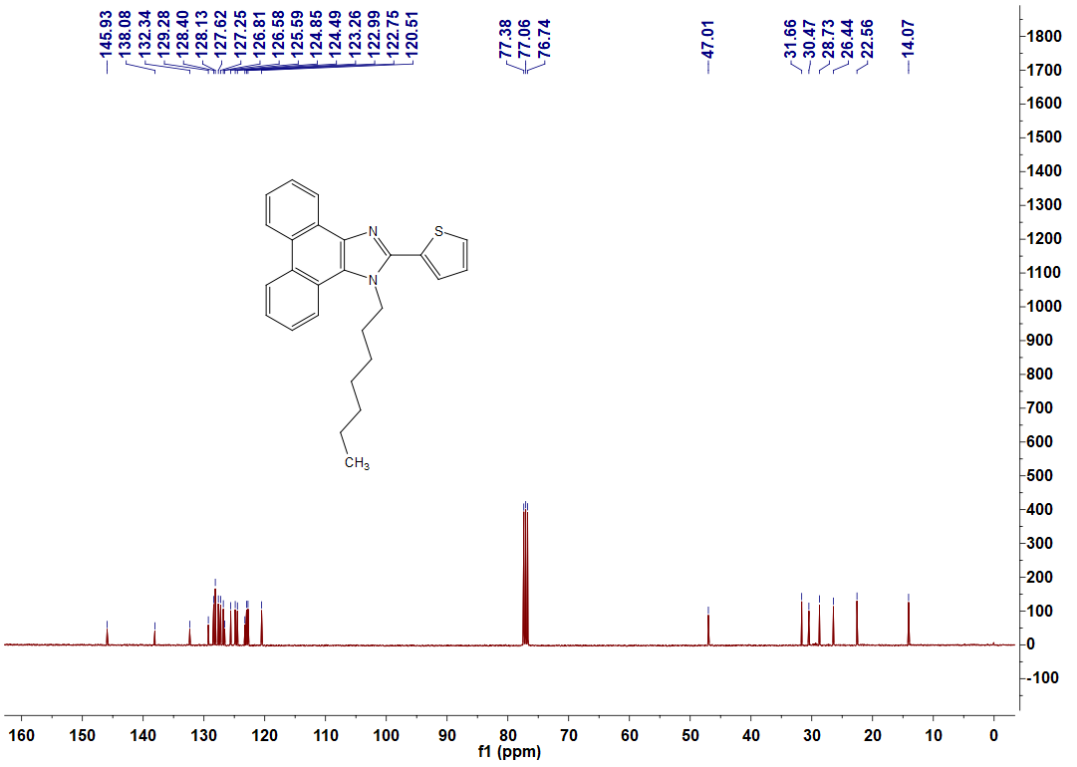


Figure S37. ^{13}C NMR spectrum of PIth-C7 conducted in $CDCl_3$.

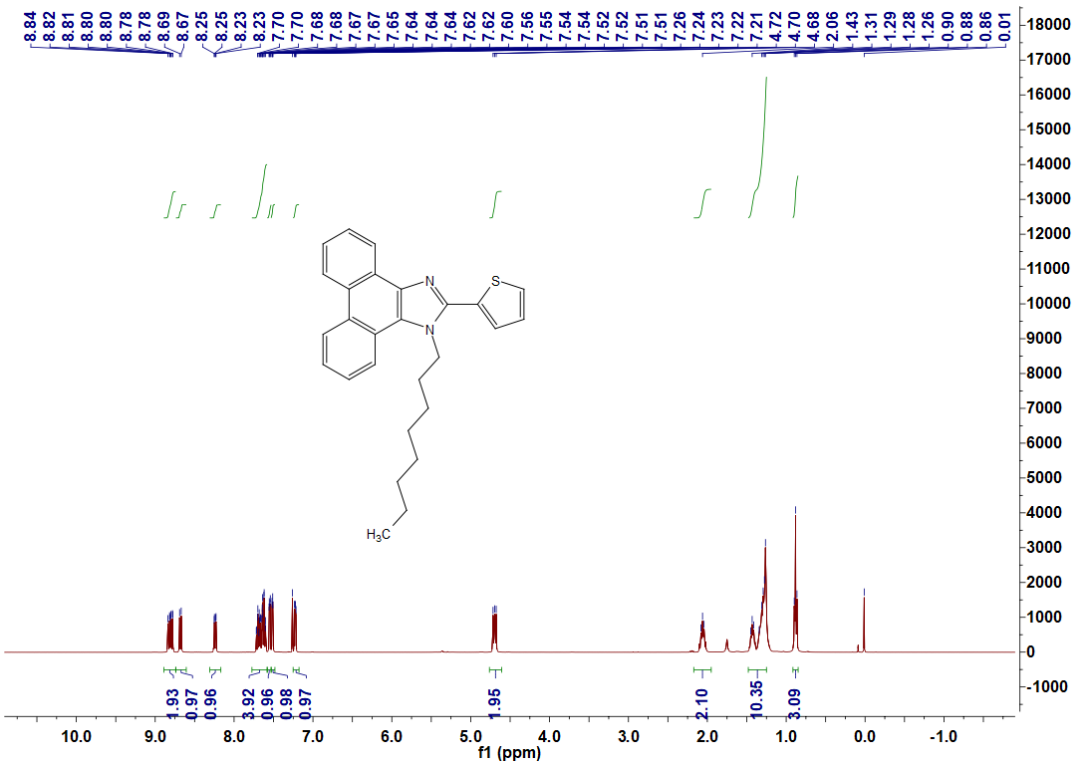


Figure S38. ^{1}H NMR spectrum of PIth-C8 conducted in $CDCl_3$.

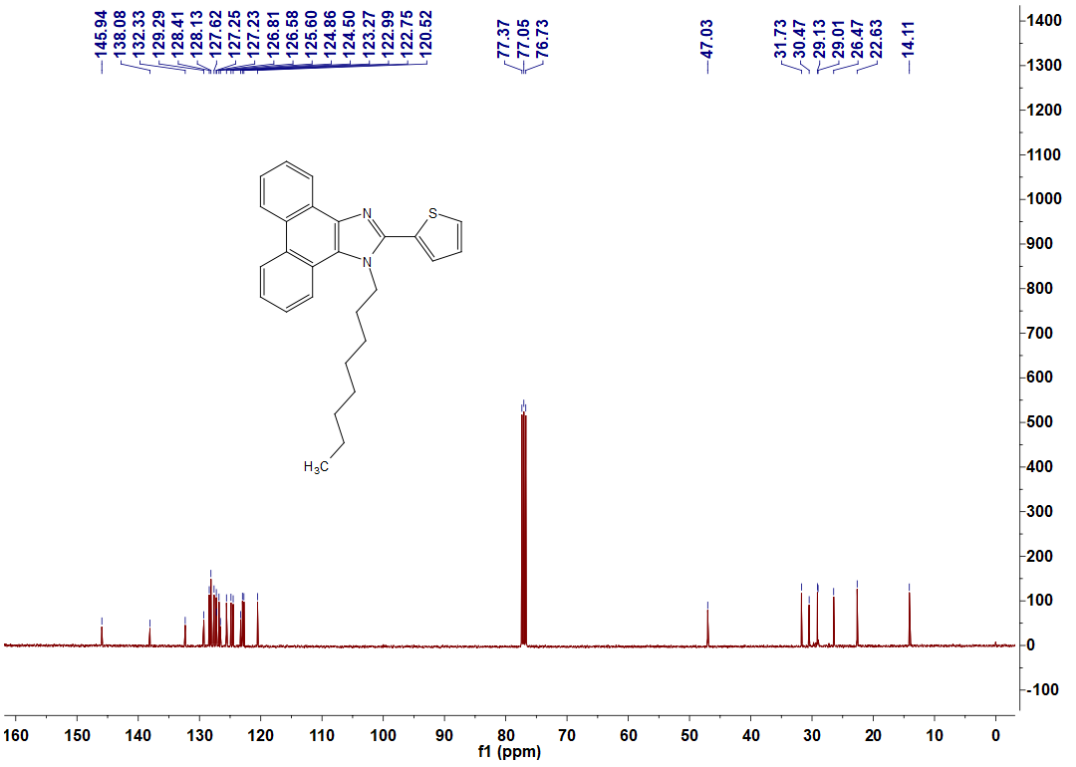


Figure S39. ^{13}C NMR spectrum of PIth-C8 conducted in $CDCl_3$.