Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

To Increase Electron Transporting Properties and horizontal molecular orientation via a Meta-Position of Nitrogen for "(A)n–D–(A)n" Structured Terpyridine Electron-Transporting Material

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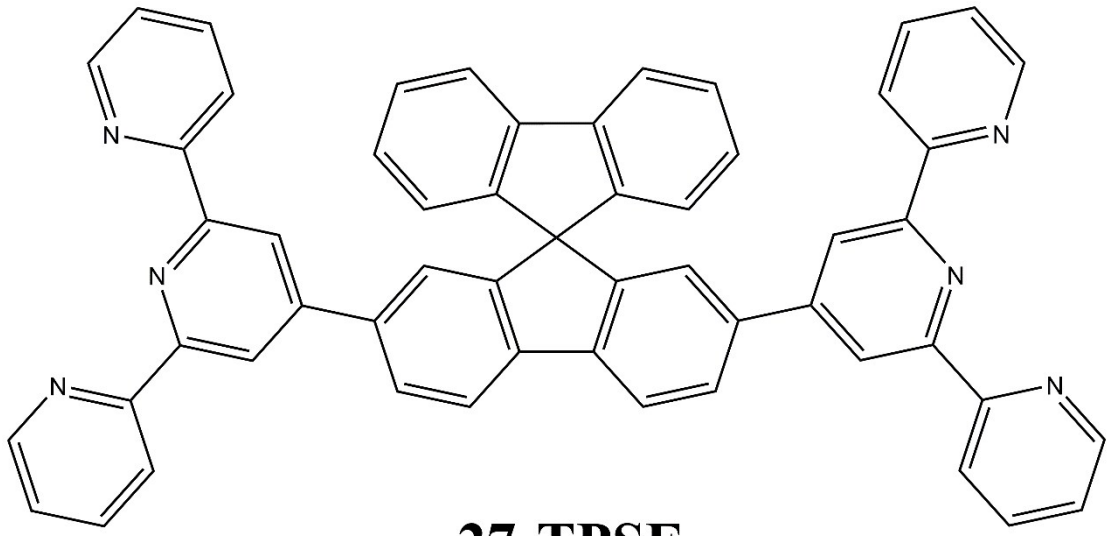

27-TPSF

Figure S1. Chemical structure of 27-TPSF

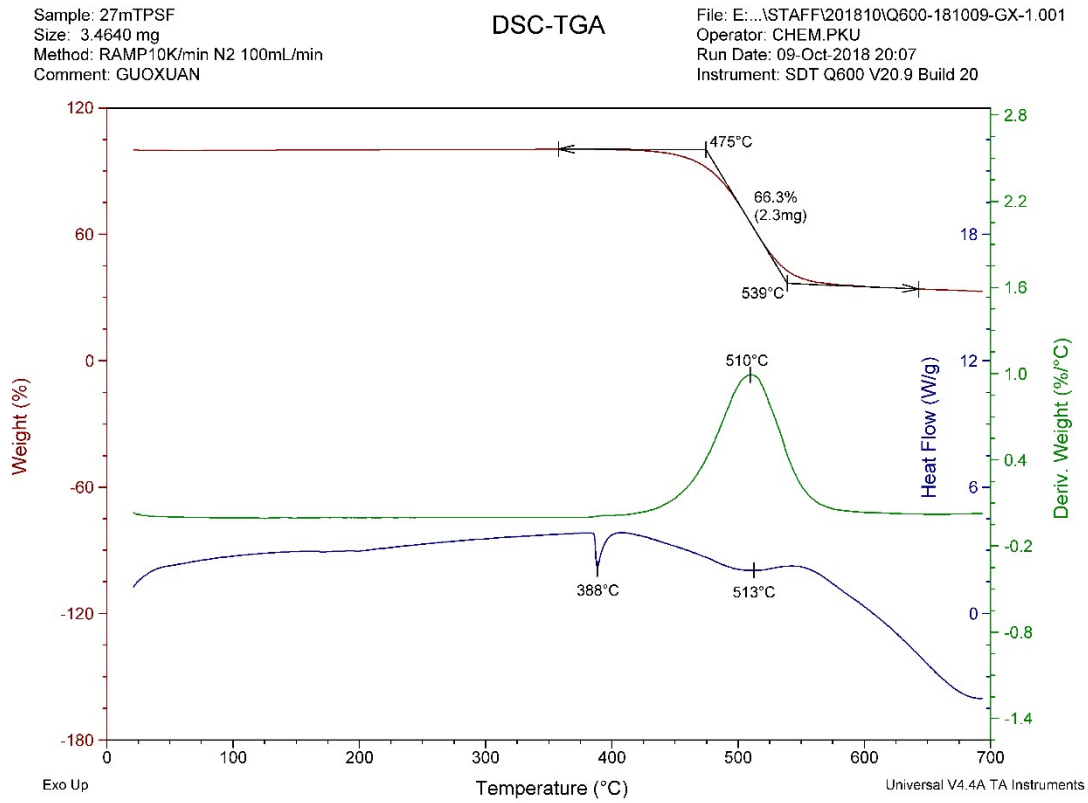

Figure S2. DSC-TGA plots of 27-mTPSF

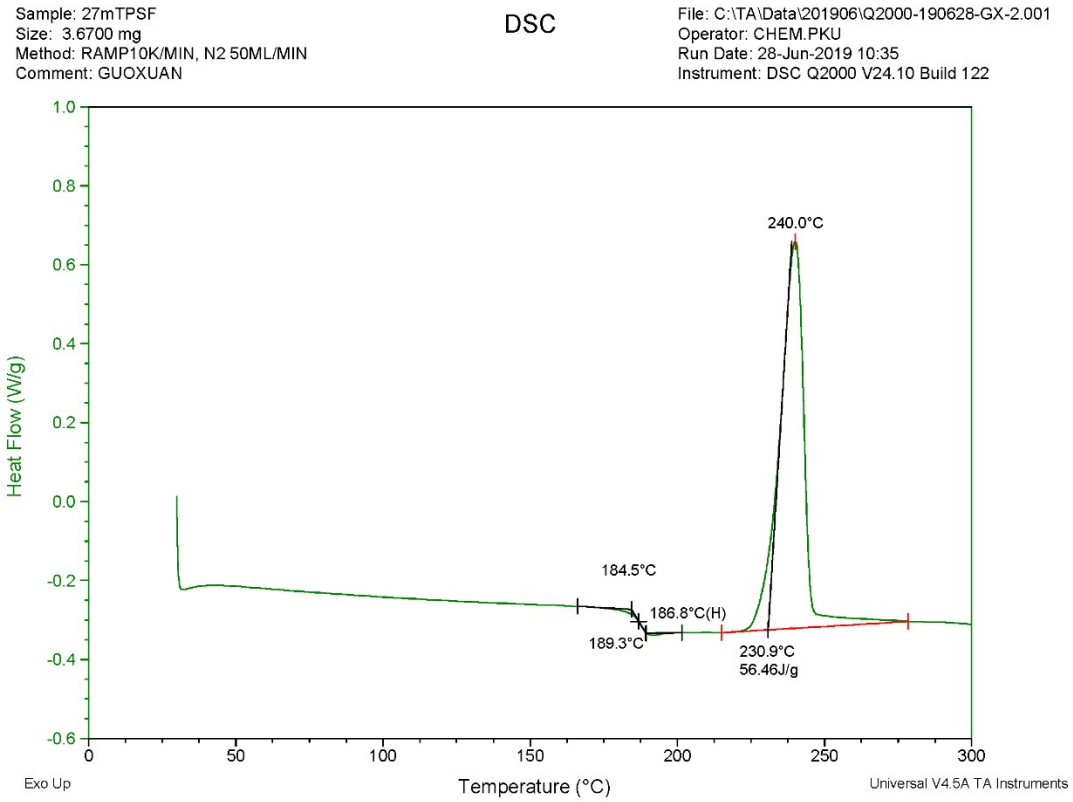

Figure S3. DSC plots of 27-mTPSF

Single carrier devices

In order to compare the electron transport capabilities of 27-TPSF and 27-mTPSF. We used the space-charge-limited current (SCLC) method to estimate the values of electron mobilities of 27-TPSF and 27-mTPSF.[1] The current density-voltage curves were fitted using the equation:

$$J = \frac{9}{8}\varepsilon\varepsilon_0\frac{E^2}{L}\mu_0\, exp(\beta\sqrt{E}) \quad (1)$$

$$\mu(E) = \mu_0\, exp(\beta\sqrt{E}) \quad (2)$$

where E is the electric field, ε and ε_0 are the relative dielectric constant and the permittivity of the free space, respectively, and L is the thickness of the organic layer.

Then the electron mobilities were derived from Figure 4a. As shown in **Figure S4**, for the electric field at 0.8 MV/cm, the estimated electron mobility of 27-TPSF is 1.0×10^{-6} cm²/V s and the electron mobility of 27-mTPSF is 3.3×10^{-6} cm²/V s.

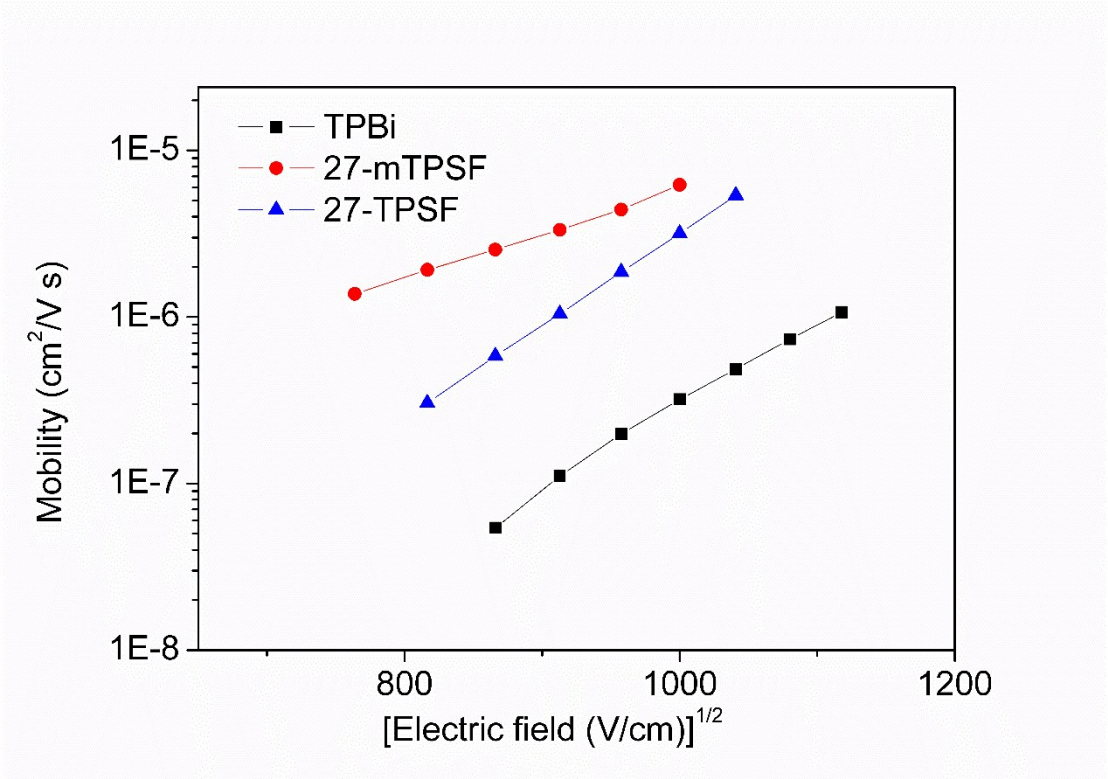

Figure S4. Mobility-[Electric field (V/cm)]$^{1/2}$ curves of electron-dominant devices: ITO/BCP (10 nm)/27-mTPSF or 27-TPSF or TPBi (30 nm)/LiF/Al.

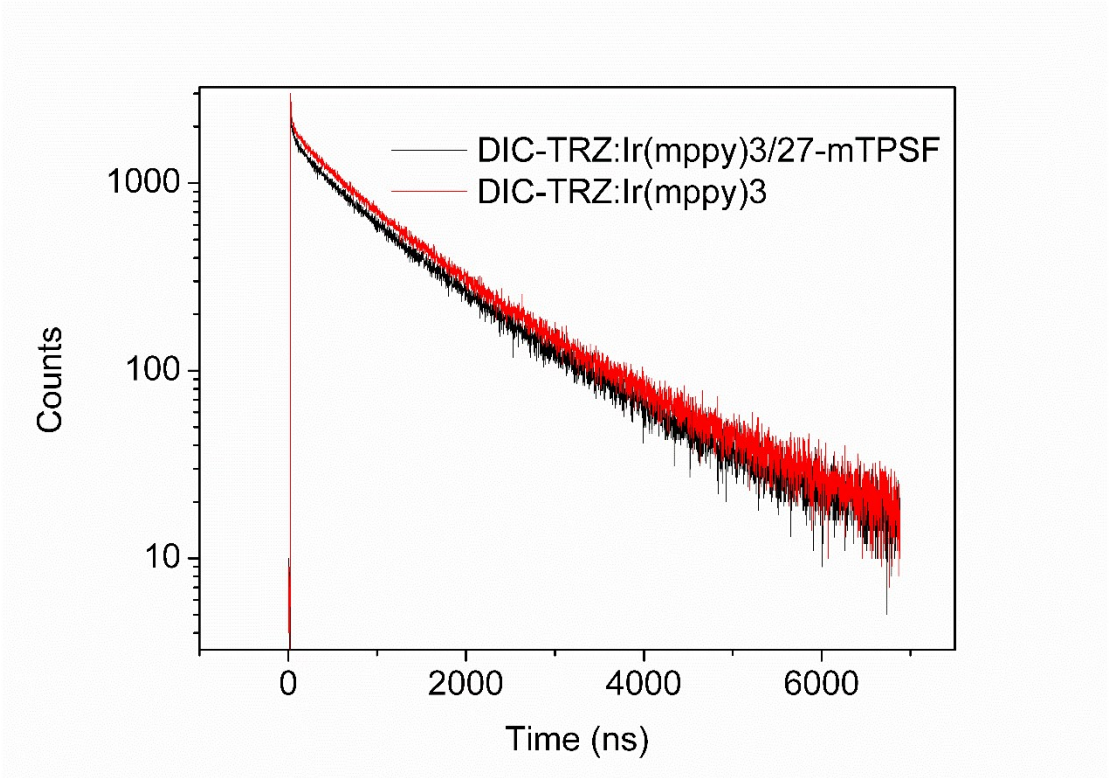

Figure S5. The transient decay curves of DIC-TRZ: Ir(mppy)3 (8 wt%, 30nm) and DIC-TRZ: Ir(mppy)3 (8 wt%, 30nm)/27-mTPSF(50nm) films.

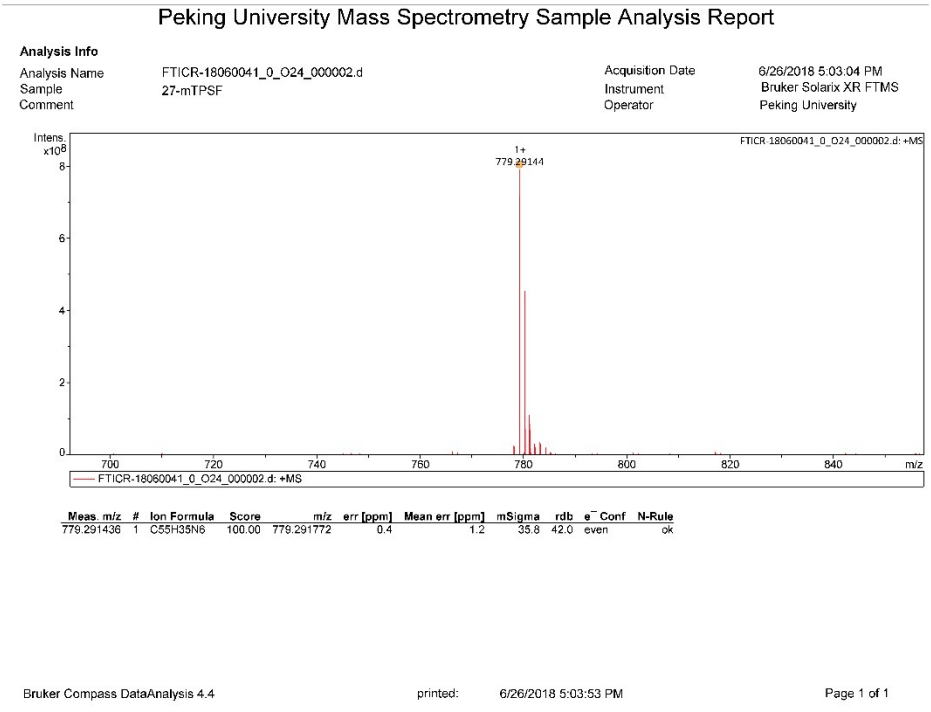

Figure S6. The mass spectrometry analysis of 27-mTPSF

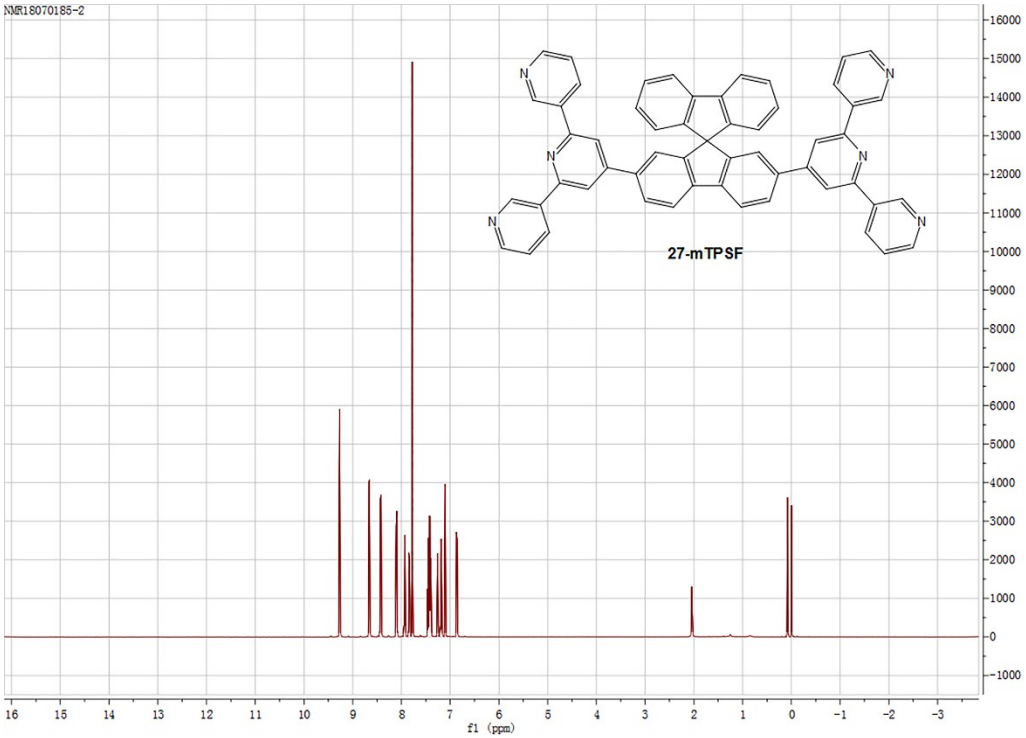

Figure S7. The ^{1}H NMR spectrum of 27-mTPSF

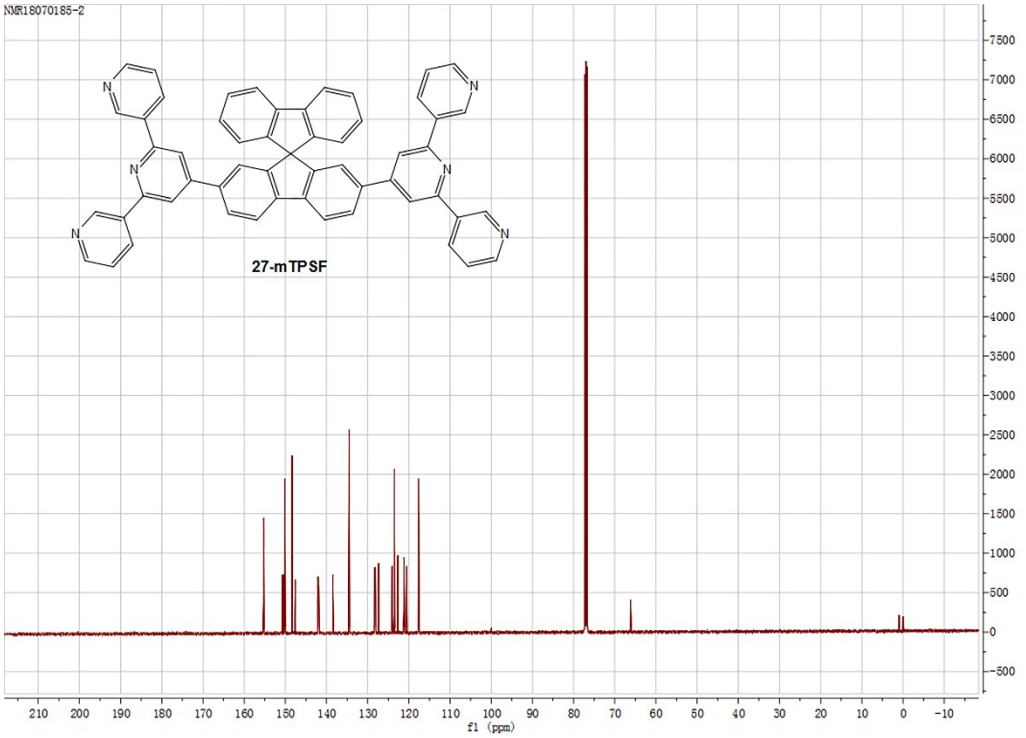

Figure S8. The ^{13}C NMR spectrum of 27-mTPSF

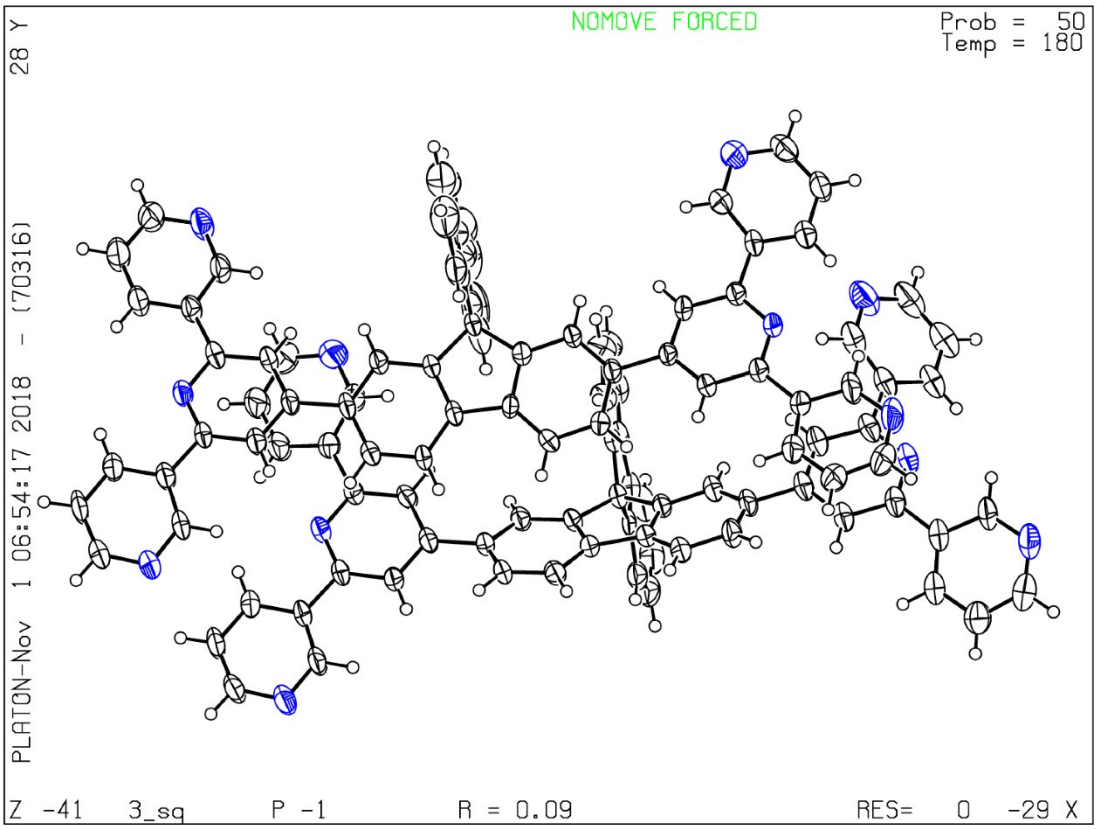

Figure S9. The single crystal structure of 27-mTPSF

Table S1. Summary of the crystal data for 27-mTPSF

Parameter	27-mTPSF
Bond precision: C-C = 0.0063 A	Wavelength=0.71073
Cell	a=12.1535(8) b=17.2039(13) c=21.2434(14)
	alpha=85.915(6) beta=82.611(5) gamma=70.949(6)
Temperature	180 K
Volume	4161.6(5)
Space group	P -1
Hall group	-P 1
Sum formula	C55 H34 N6
Mr	778.88
Dx,g cm^{-3}	1.243
Z	4
Mu (mm^{-1})	0.074
F000	1624.0
h, k, l_{max}	14, 20, 25
Nref	14715
T_{min}, T_{max}	0.775, 1.000
Correction method= # Reported T Limits: T_{min}=0.775 T_{max}=1.000	

AbsCorr = MULTI-SCAN	
Data completeness = 0.999	Theta(max)= 25.027
R(reflections)= 0.0869(7748)	wR2(reflections)= 0.1973(14715)
S = 1.035	Npar= 1099

References

1. M. A. Khan, W. Xu, H. Khizar ul, Y. Bai, X. Y. Jiang, Z. L. Zhang, W. Q. Zhu, Z. L. Zhang and W. Q. Zhu, *Journal of Applied Physics*, 2008, **103**, 014509.