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

Supporting Information

Positional Isomerism Effect of Spirobifluorene and Terpyridine Moieties of "$(A)_n$-D-$(A)_n$" Type Electron Transport Materials for Long-lived and Highly efficient TADF-PhOLED

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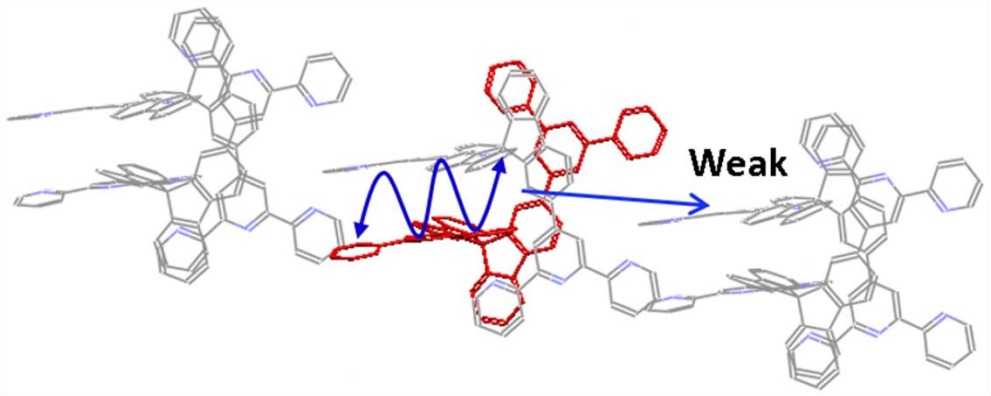

Figure S1. the charge of 22-TPSF oscillate mainly between the two molecules.

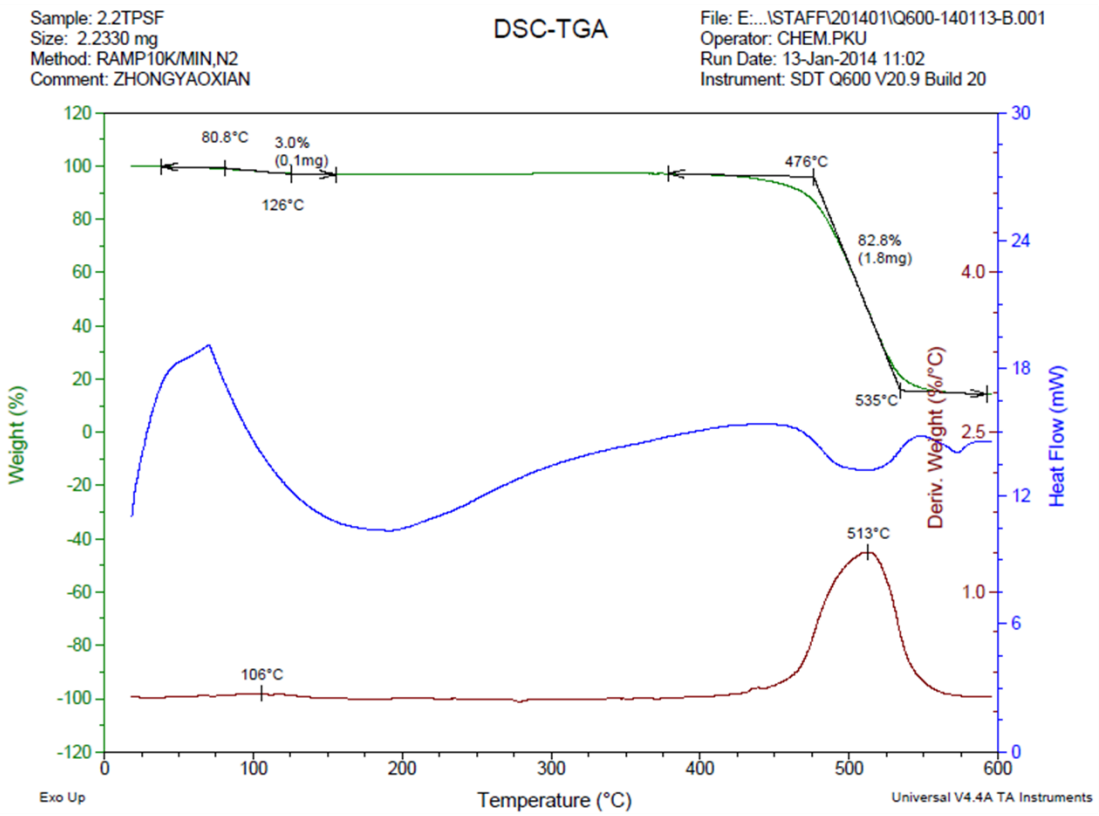

Figure S2. The TGA of 22-TPSF.

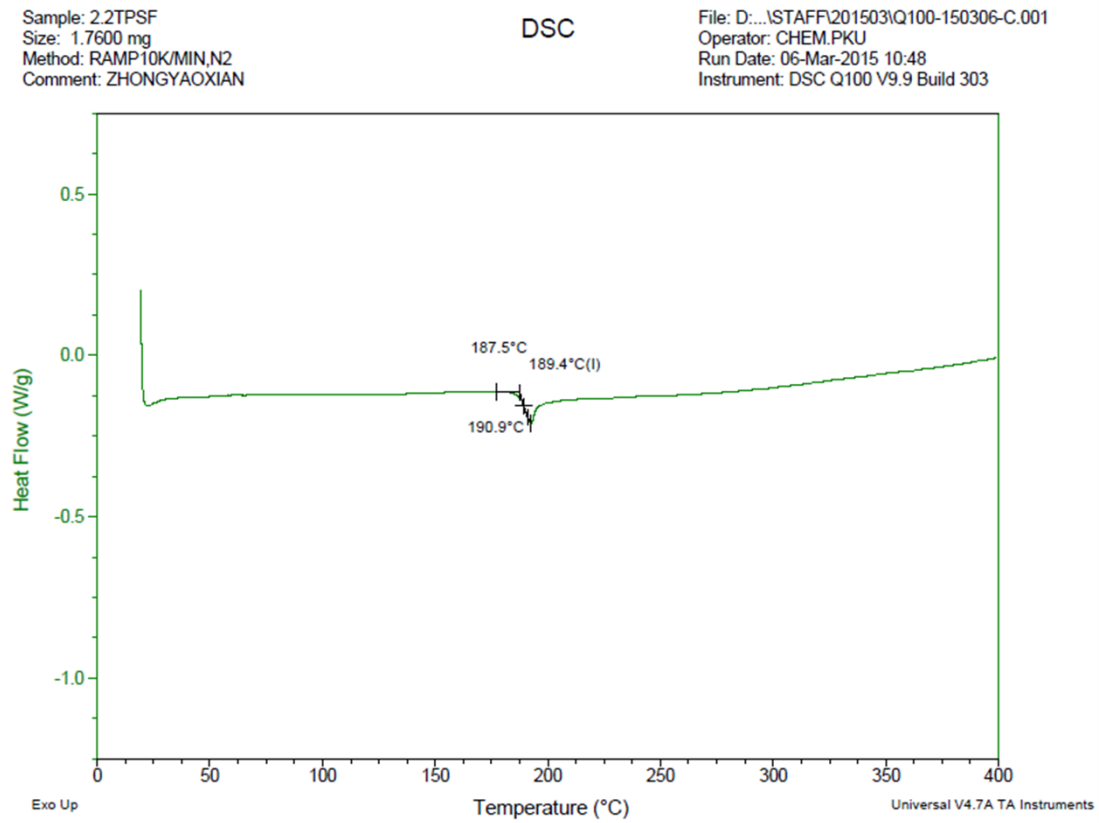

Figure S3. The DSC of 22-TPSF.

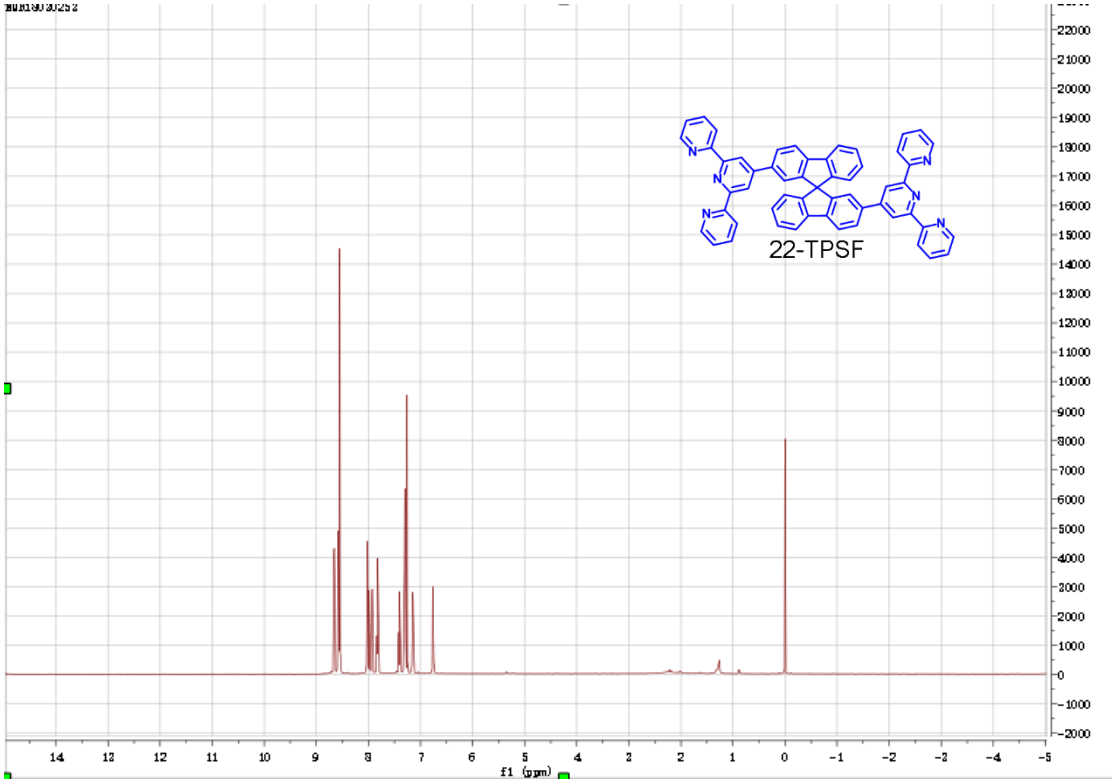

Figure S4. The ^{1}H NMR spectrum of 22-TPSF.

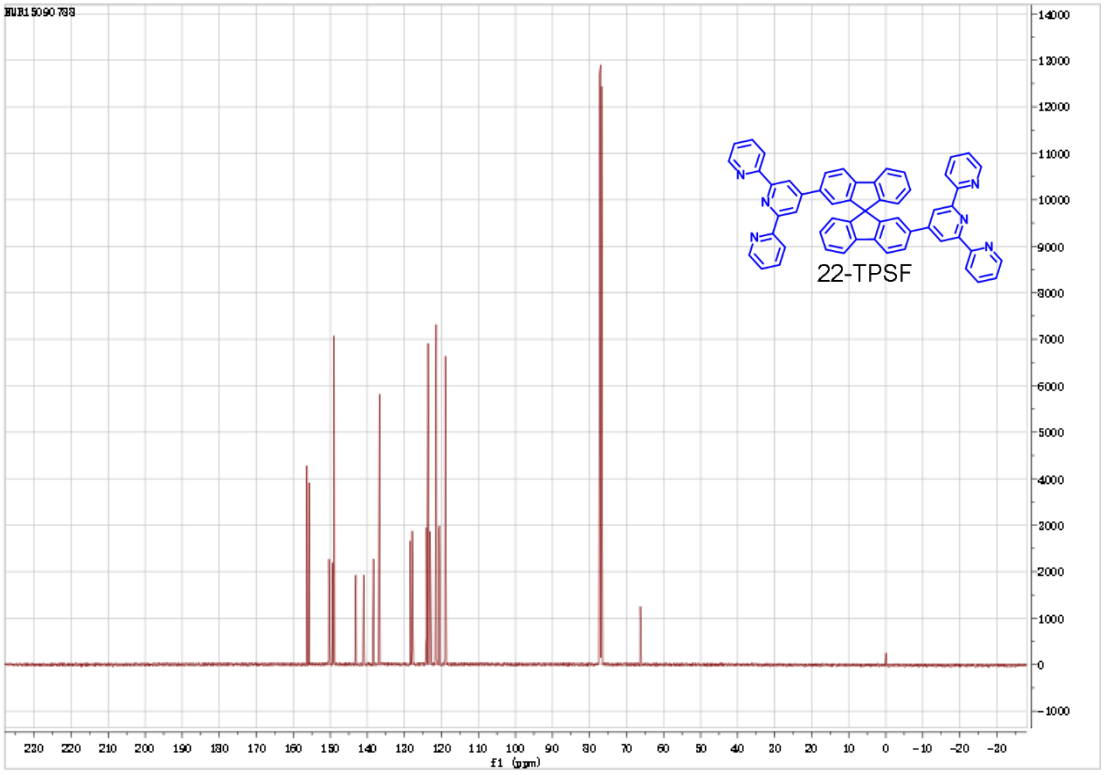

Figure S5. The ^{13}C NMR spectrum of 22-TPSF.

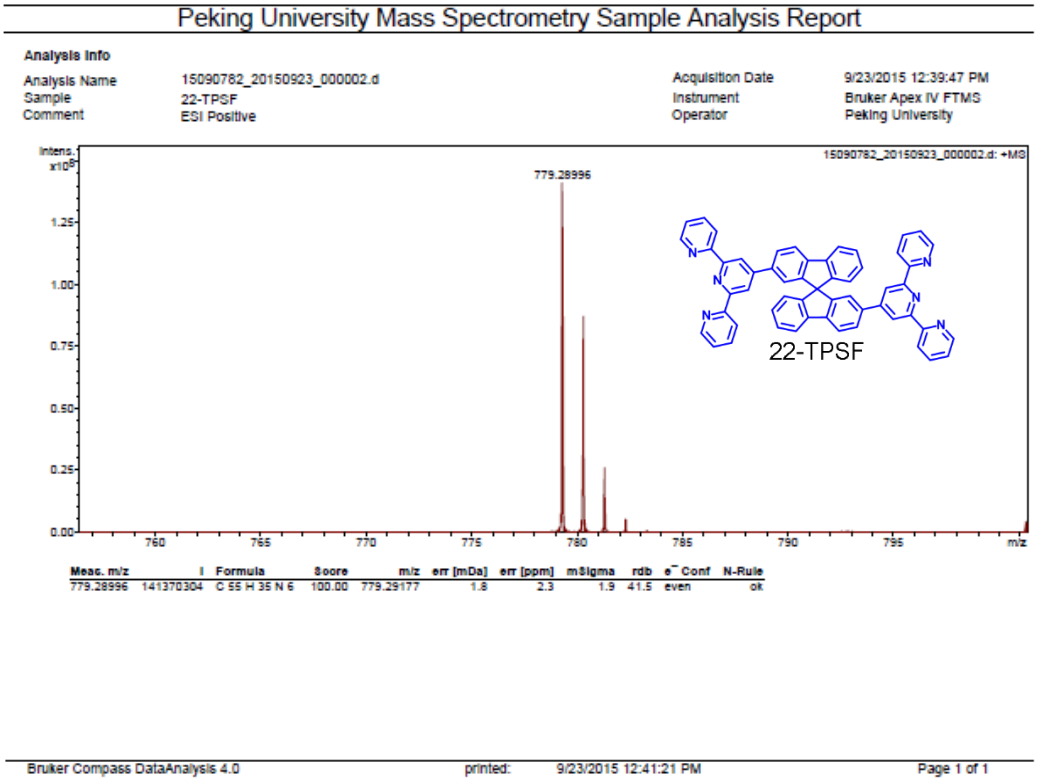

Figure S6. The HRMS spectrum of 22-TPSF.

Table S1. Summary of the crystal data for 22-TPSF.

Parameter	22-TPSF
Empirical formula	$C_{55}H_{34}N_6$
Formula weight [g mol^{-1}]	778.92
Temperature [K]	180
Wavelength [Å]	0.71073
Crystal system	Monoclinic
Space group	P 21/*n*
6Crystal color and size [mm^{-3}]	Colorless, 0.35×0.2×0.15
a [Å]	16.5689 (5)
b [Å]	35.4714 (9)
c [Å]	16.5839 (5)
α [°]	90

β [°]	107.626 (3)
γ [°]	90
Volume [Å^3]	9289.1 (5)
Z	4
Density, calcd [g cm^{-3}]	1.175
Absorption coefficient [mm^{-1}]	0.125
F(000)	3416.0
θ range for data collection [°]	1.727 to 25.027
Reflections collected	54830
Independent reflections	16408
R_{int}	0.0342
Restraints / parameters	0/1126
Goodness-of-fit on F^2	1.019
Final R indices [I> 2σ(I)]	R_1 = 0.0965, wR_2 = 0.2167
R indices (all data)	R_1 = 0.1088, wR_2 = 0.2225

Table S2. Summary of the crystal data for 27-TPSF.

Parameter	27-TPSF
Empirical formula	$C_{55}H_{34}N_6$
Formula weight [g mol^{-1}]	778.92
Temperature [K]	180
Wavelength [Å]	0.71073
Crystal system	Monoclinic
Space group	C 2/c
Crystal color and size [mm^{-3}]	Colorless, 0.6×0.5×0.02
a [Å]	19.5621 (10)
b [Å]	24.2721 (18)
c [Å]	12.7702 (7)
α [°]	90

β [°]	129.729 (5)
γ [°]	90
Volume [Å^3]	4663.3 (6)
Z	4
Density, calcd [g cm^{-3}]	1.351
Absorption coefficient [mm^{-1}]	0.301
F(000)	1960.0
θ range for data collection [°]	2.668 to 23.253
Reflections collected	12016
Independent reflections	3351
R_{int}	0.0416
Restraints / parameters	2/303
Goodness-of-fit on F^2	1.042
Final R indices [I> 2σ(I)]	R_1 = 0.1018, wR_2 = 0.2208
R indices (all data)	R_1 = 0.1371, wR_2 = 0.2426

Table S3. The calculated transfer integral of hole and electron at B3LYP/6-31G(d) level, the centroids and the nearest distance of different molecule for 22-TPSF.

	Hole/meV	**Electron/meV**	**Centroids/Å**	**Nearest distance/Å**
P1	-80.259	-42.204	1.194	3.159
P2	0.004	0.467	16.459	2.529
P3	0.023	0.690	16.793	3.596
P4	0.000	0.804	16.584	3.273
P5	0.000	0.805	16.584	3.273
P6	0.025	-1.846	16.595	3.754
P7	0.000	0.001	19.5741	4.551
P8	0.000	0.001	19.5741	4.551
P9	0.000	-0.003	16.6283	6.957
P10	0.000	0.000	16.5689	6.151

P11	0.000	0.000	16.5689	6.058

Table S4. The calculated transfer integral of hole and electron at B3LYP/6-31G(d) level, the centroids and the nearest distance of different molecule for 27-TPSF.

	P1	**P2**	**P3**	**P4**	**P5**	**P6**
Hole/meV	-0.048	0.048	0.127	0.127	0.000	0.000
Electron/meV	-8.846	8.846	0.149	0.149	0.000	-0.000
Centroids/Å	19.562	19.562	15.056	15.056	12.770	12.770
Nearest distance/Å	4.146	4.146	2.264	2.264	3.334	3.334