

## Supplementary Information for

### Symmetric and unsymmetric thienyl-substituted fluorenone dyes: static excimer-induced emission enhancement

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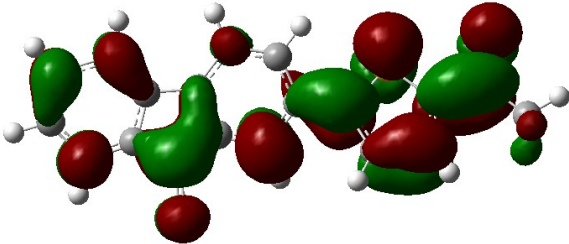
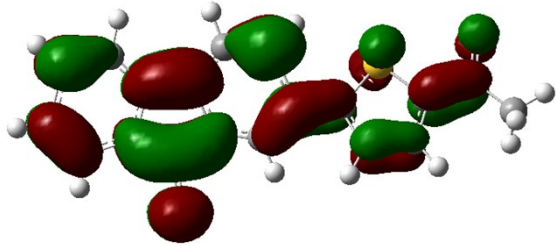
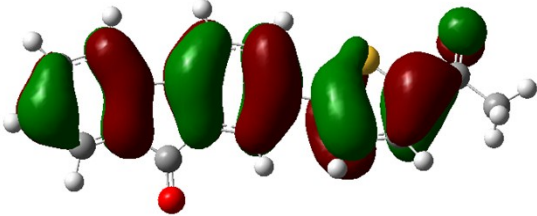
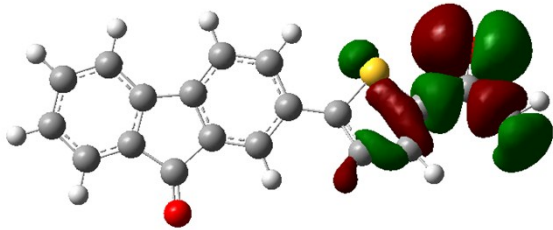
## 1. Single-Crystal Structure

**Table S1.** Selected Crystallographic Data for **ATPF**.

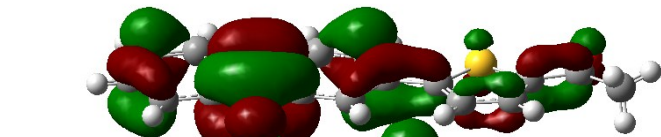
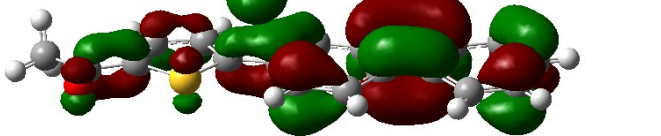
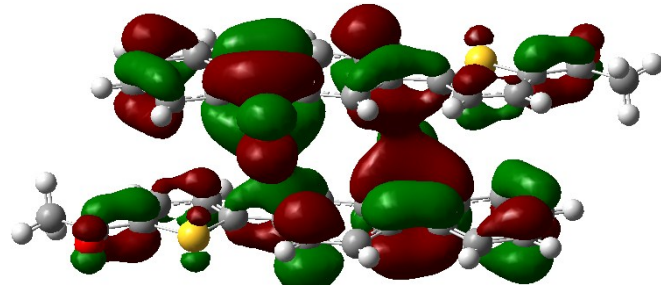
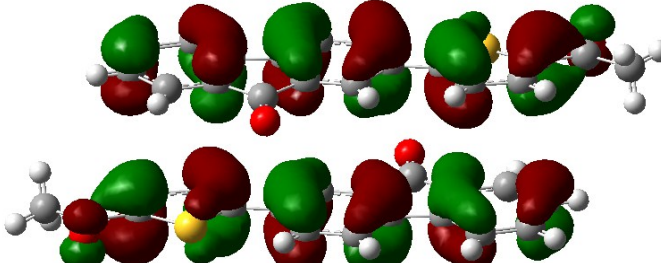
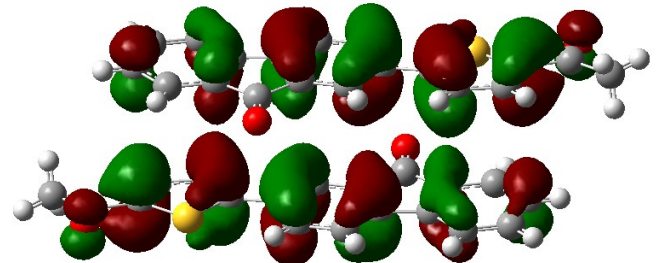
Compound	<b>ATPF</b>
Empirical formula	C <sub>19</sub> H <sub>12</sub> O <sub>2</sub> S
Formula mass	304.35
Crystal color	yellow
crystal size (mm <sup>3</sup> )	0.48×0.31×0.10
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	6.1090(6)
<i>c</i> [Å]	15.5179(14)
<i>V</i> [Å <sup>3</sup> ]	699.34(11)
<i>Z</i>	2
$\rho$ (calcd, g/cm <sup>3</sup> )	1.445
$\mu$ [mm <sup>-1</sup> ]	0.235
<i>F</i> (000)	316
$\theta_{\min}$ - $\theta_{\max}$ [°]	2.702-23.81
<i>T</i> / K	298(2)
Collected reflections	2387
Unique reflections	1549
<i>R</i> / <i>wR</i>	0.1030/0.2690

## 2. Theoretical Calculation

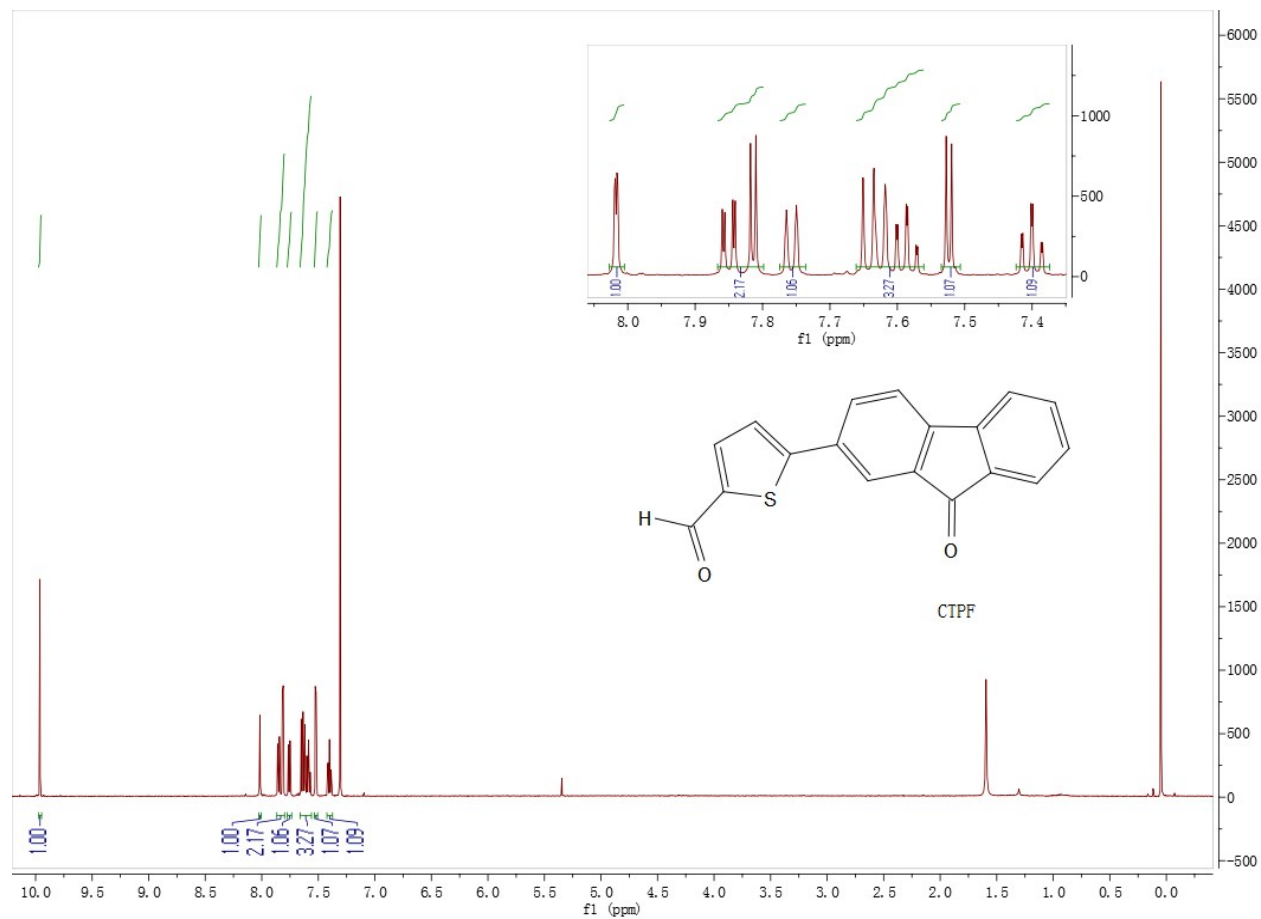
**Table S2.** The graphic representations of the frontier molecular orbits of **ATPF single-molecule**.

<b>ATPF single-molecule</b>		Excited State 1: Singlet-A 2.8624 eV 433.14 nm $f=0.0969$ 79 → 80 0.67617 79 → 81 0.16283
<b>LUMO+1</b> No.81 -0.07190 au		Excited State 2: Singlet-A 3.1201 eV 397.38 nm $f=0.0002$ 76 → 80 0.25725 77 → 80 0.61396 77 → 81 0.20303
<b>LUMO</b> No.80 -0.09260 au		Excited State 3: Singlet-A 3.5296 eV 351.27 nm $f=0.0074$ 78 → 80 -0.46549 78 → 81 0.47593 78 → 82 -0.18960
<b>HOMO</b> No.79 -0.21924 au		Excited State 4: Singlet-A 3.6165 eV 342.83 nm $f=0.5596$ 74 → 80 0.11681 76 → 80 0.13770 79 → 80 -0.14466 79 → 81 0.65138
<b>HOMO-1</b> No.78 -0.25309 au		

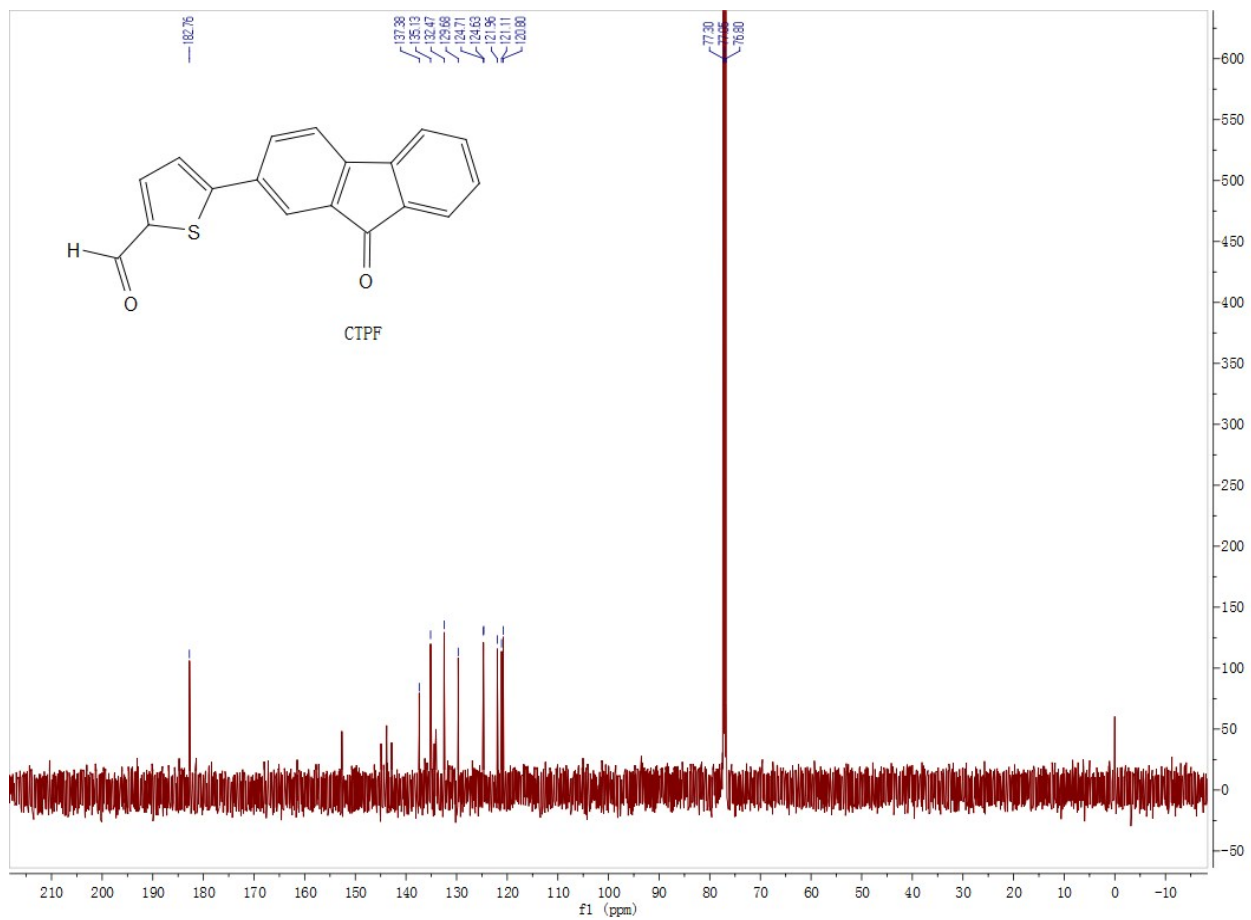
**Table S3.** The graphic representations of the frontier molecular orbits of **ATPF Dimer**.

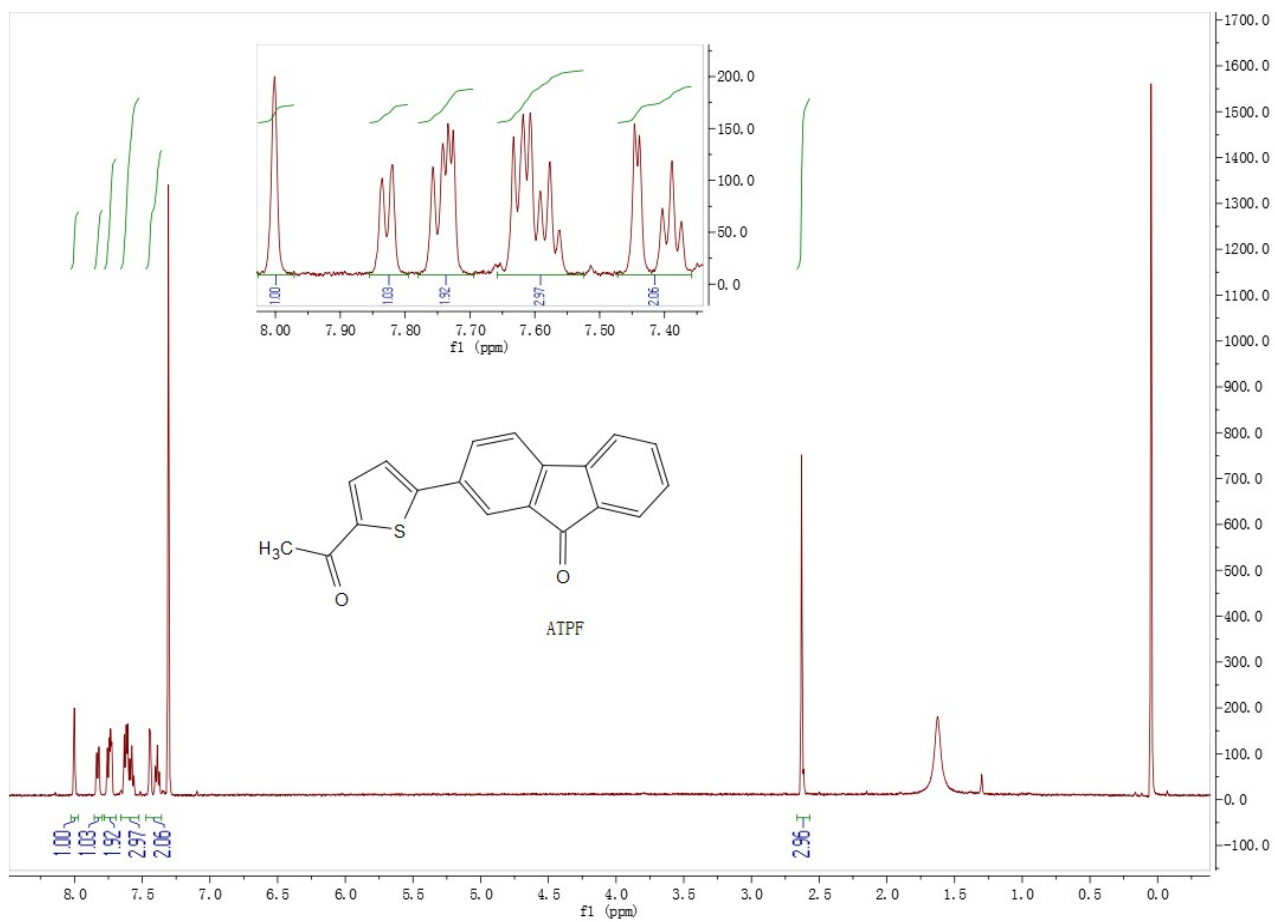
<b>ATPF Dimer<sup>-</sup></b>		Excited State 1: Singlet-A 2.5338 eV 489.31 nm f=0.0725 158 ->159 0.69393
<b>LUMO+1</b>		Excited State 2: Singlet-A 2.7157 eV 456.55 nm f=0.0000 158 ->160 0.68739 158 ->161 0.11667
No.160	-0.08993 au	
<b>LUMO</b>		Excited State 3: Singlet-A 2.9084 eV 426.30 nm f=0.0000 157 ->159 0.68538
No.159	-0.09861 au	
<b>HOMO</b>		Excited State 4: Singlet-A 3.0151 eV 411.22 nm f=0.0002 151 ->159 -0.10268 152 ->160 0.37633 152 ->161 0.14694 153 ->159 0.51728 153 ->162 0.12183 154 ->160 0.10303
No.158	-0.20216 au	
<b>HOMO-1</b>		
No.157	--0.21476 au	

### 3. $^1\text{H}$ NMR and $^{13}\text{C}$ NMR of CTPF, ATPF, BTPF and ETPF

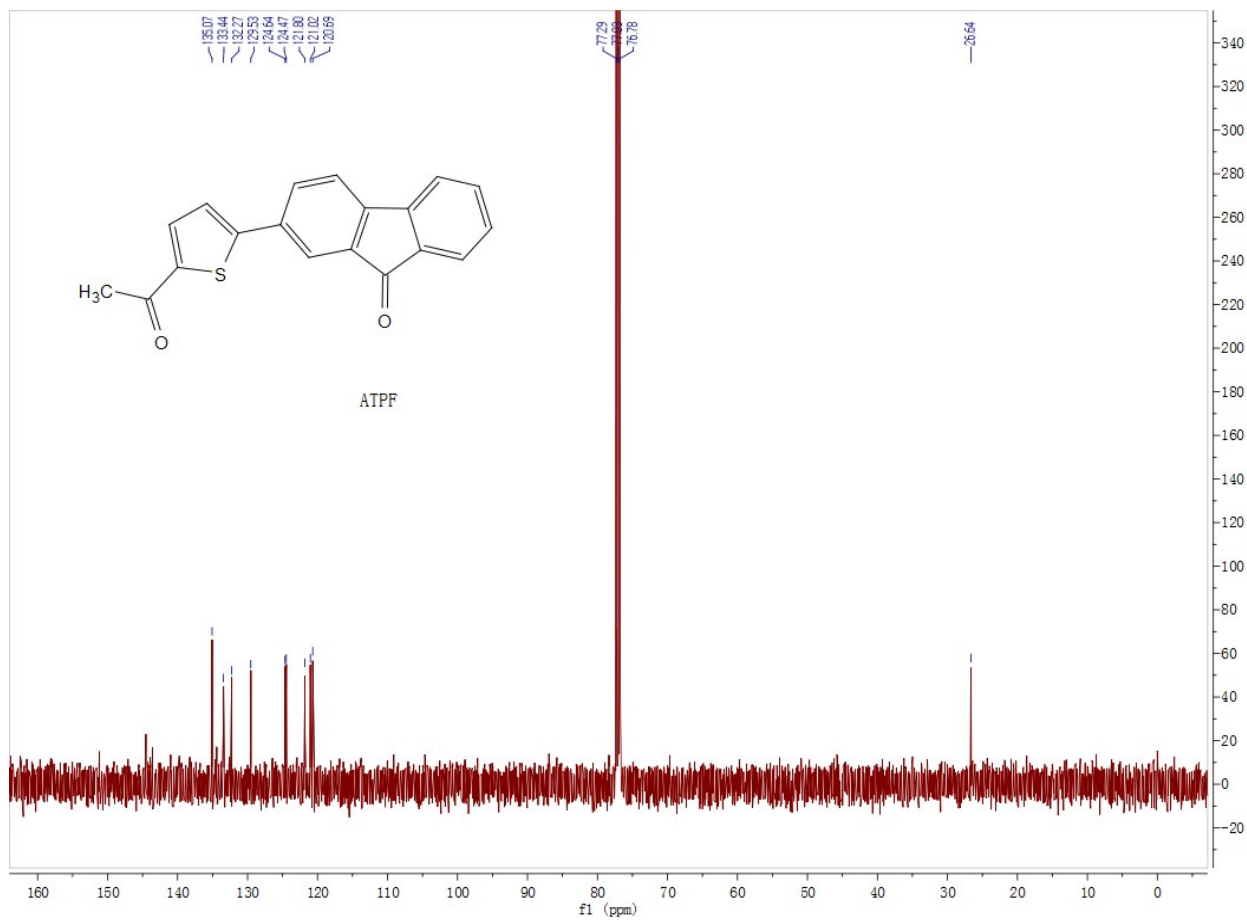


**Figure S1.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of compound CTPF.



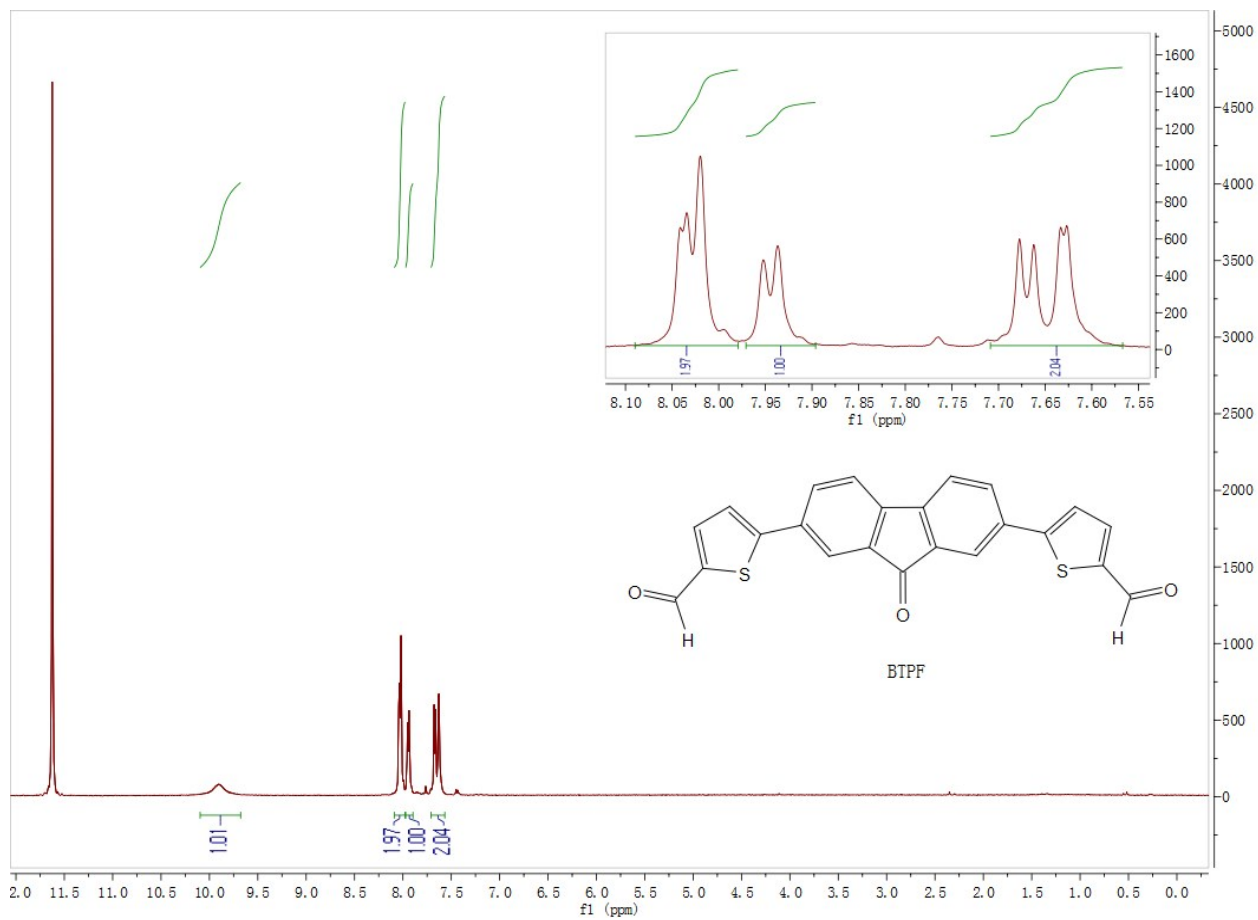


**Figure S3.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound ATPF.

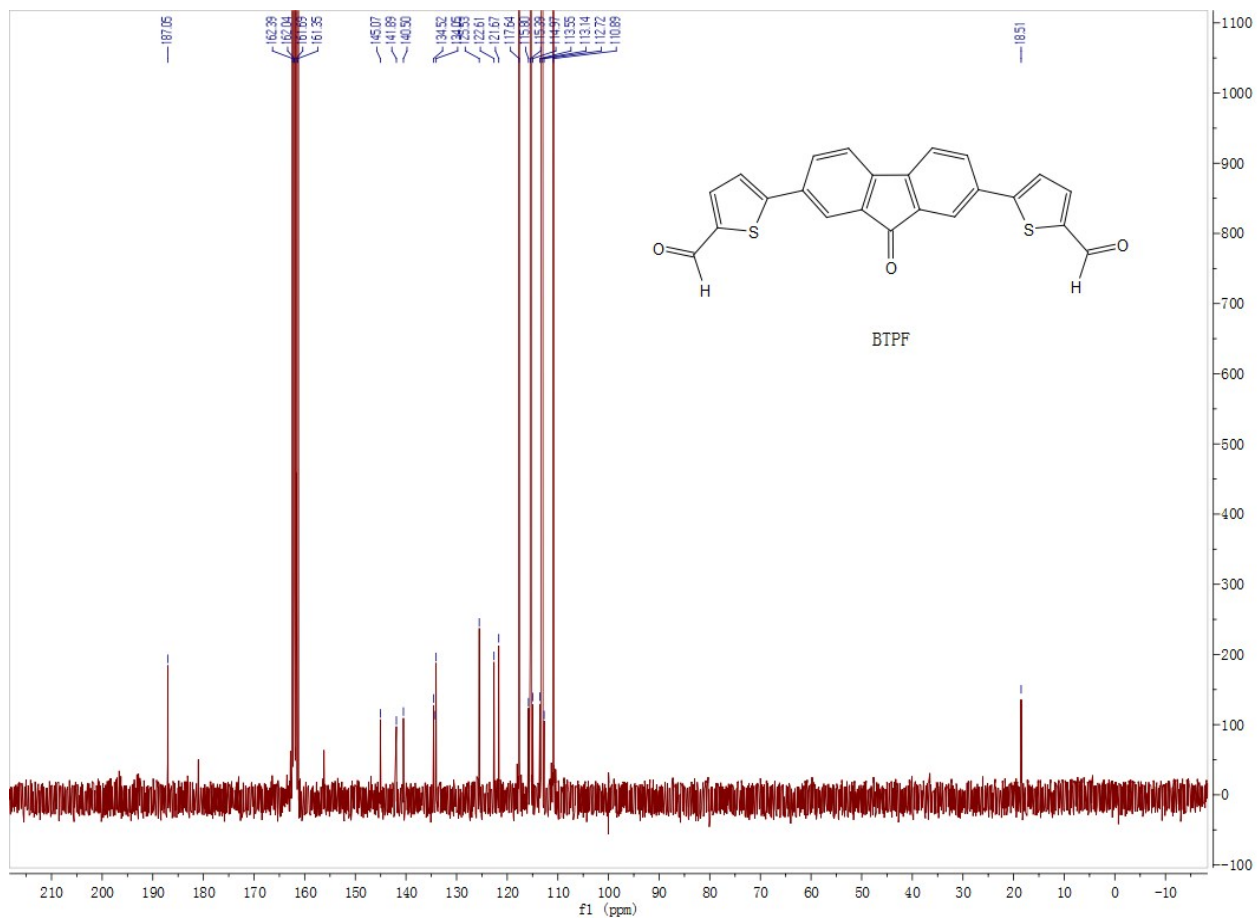


**Figure S4.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of compound ATPF.

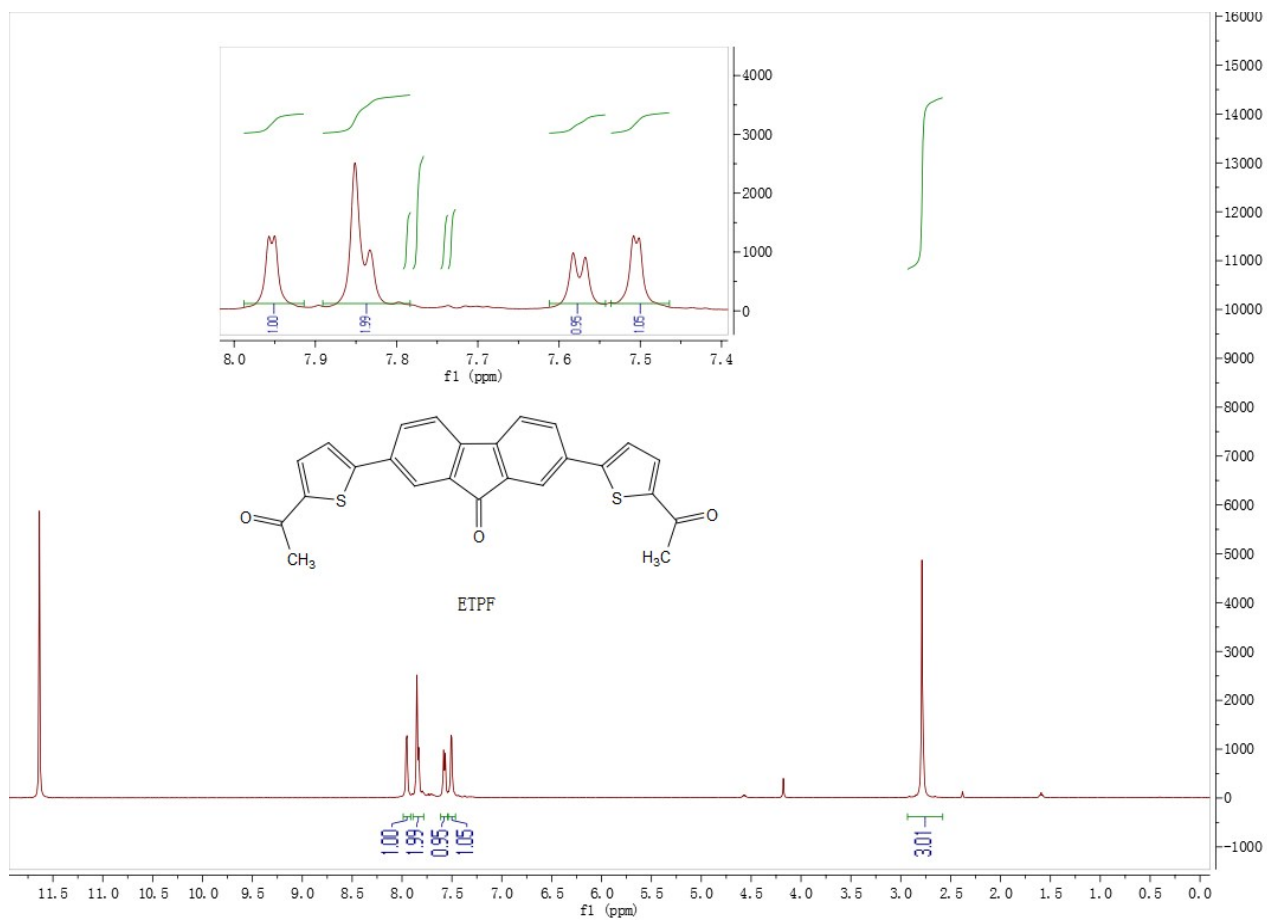




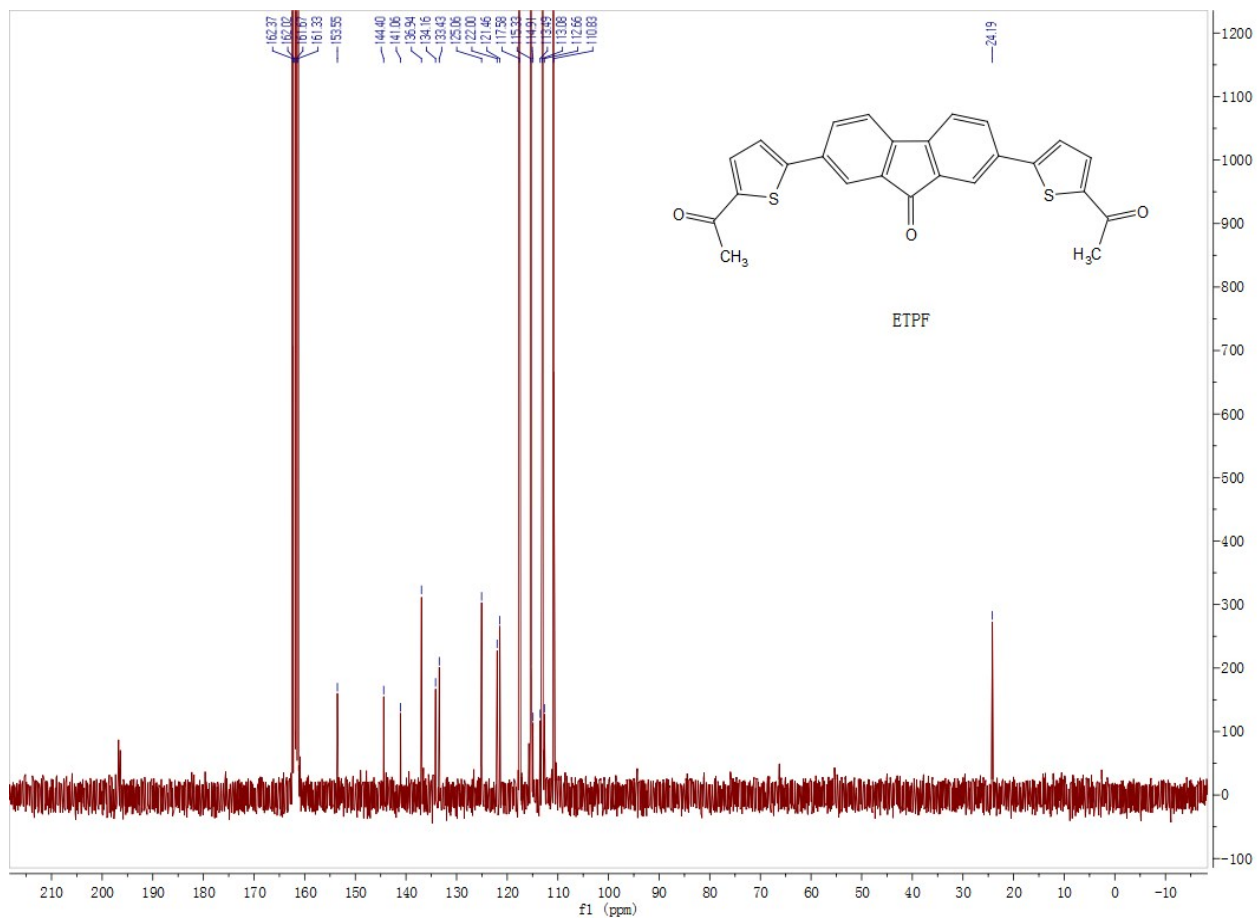
**Figure S5.** <sup>1</sup>H NMR spectrum (500 MHz, TFA) of compound **BTPF**.



**Figure S6.**  $^{13}\text{C}$  NMR spectrum (125 MHz, TFA) of compound **BTPF**.



**Figure S7.** <sup>1</sup>H NMR spectrum (500 MHz, TFA) of compound **ETPF**.



**Figure S8.**  $^{13}\text{C}$  NMR spectrum (125 MHz, TFA) of compound **ETPF**.

## 4. TOF-MS-EI

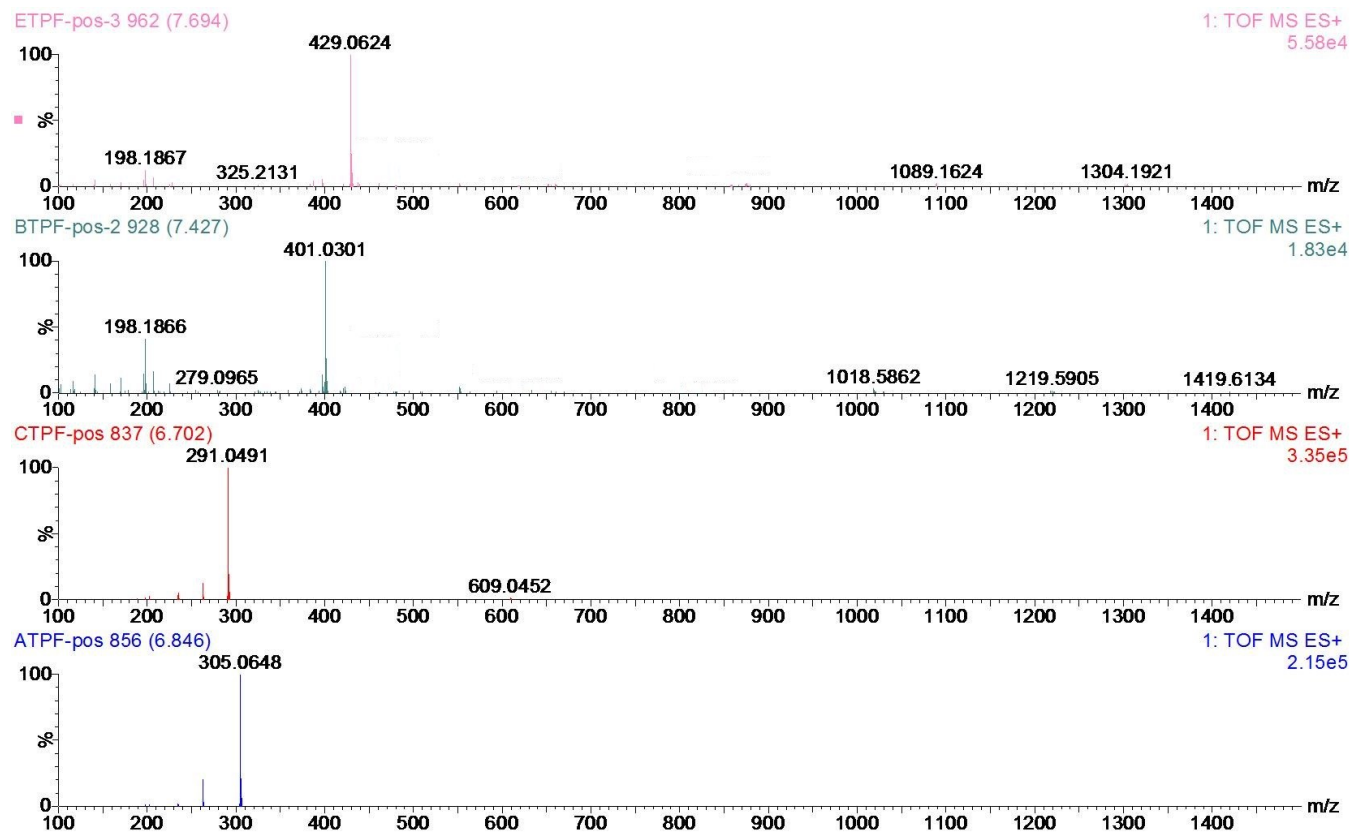


Figure S9. The TOF-MS-EI pictures of compounds CTPF, ATPF, BTPF and ETPF.