

Supporting Information for

Remarkable Isomeric Effects on Mechanofluorochromism of Tetraphenylethylene-
based D- π -A Derivatives

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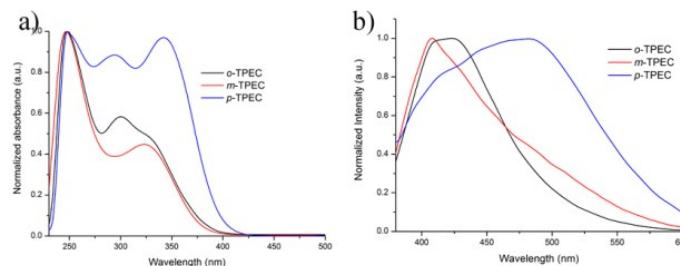


Fig.S1 Normalized absorption spectra (a) and fluorescence spectra (b, $\lambda_{\text{ex}} = 380$ nm) of *o*-TPEC, *m*-TPEC, and *p*-TPEC in THF ($c = 10^{-5}$ M).

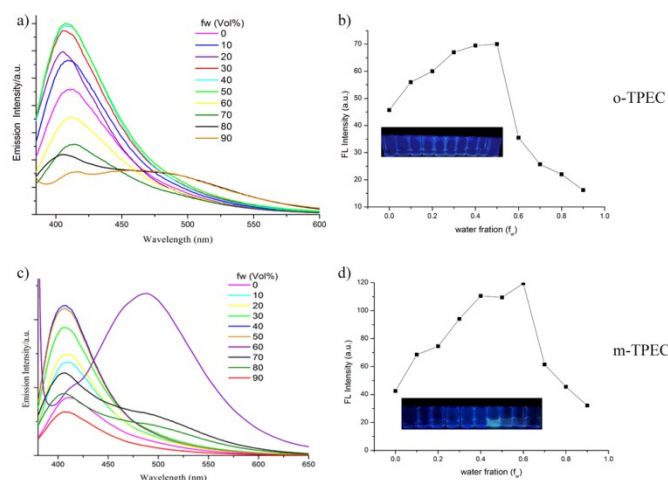


Fig.S2 Fluorescence spectra of *o*-TPEC and *m*-TPEC in the mixtures of THF and water with different volume ratios (a and c); the plots of the intensities vs. water contents (b and d); the insets are corresponding images of *o*-TPEC and *m*-TPEC under 365 nm light.

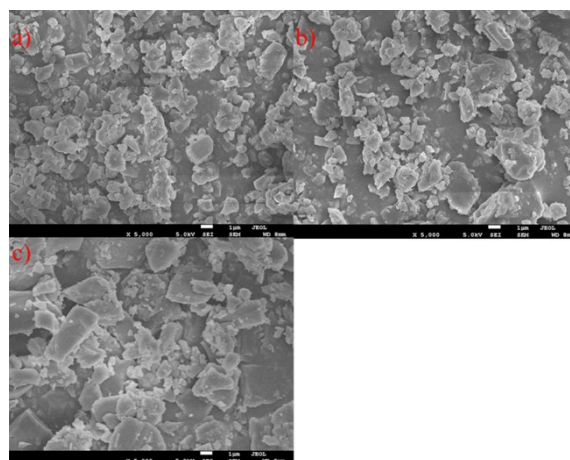


Fig.S3 FESEM images of (a) *o*-TPEC ($f_w=0.5$), (b) *m*-TPEC ($f_w=0.6$), and (c) *p*-TPEC ($f_w=0.9$).

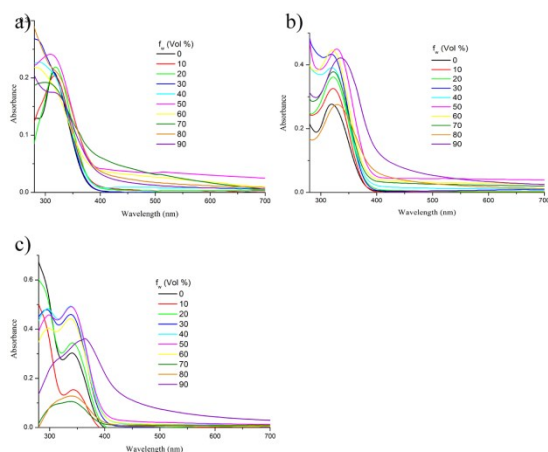


Fig.S4 Absorption spectra of *o*-TPEC (a), *m*-TPEC (b), and *p*-TPEC (c) in the mixtures of THF and water with different volume ratios ($c = 10^{-5}$ M).



Fig.S5 the optimized geometries of *o*-TPEC, *m*-TPEC, and *p*-TPEC.

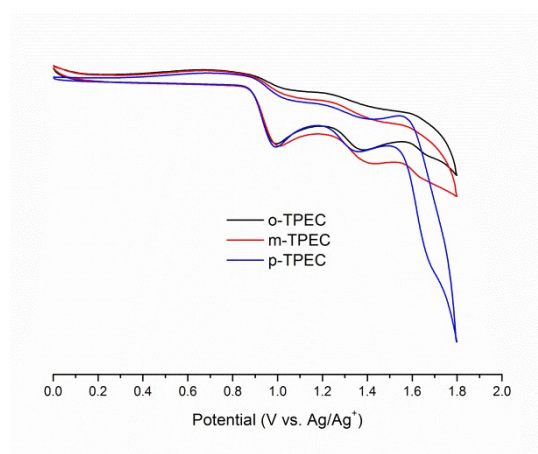


Fig. S6 Cyclic voltammetry (CV) plots of *o*-TPEC, *m*-TPEC, and *p*-TPEC.

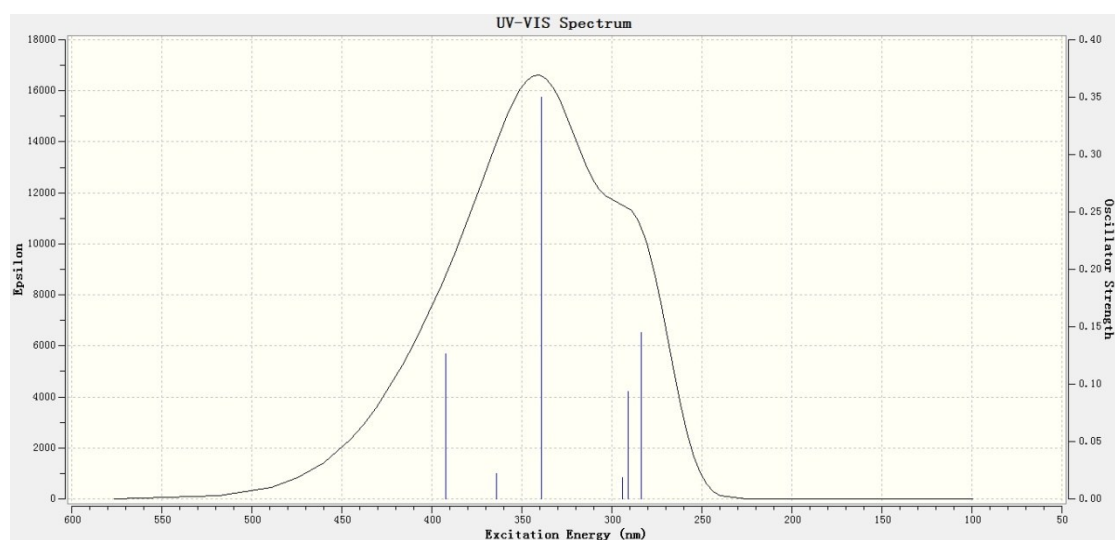


Fig. S7 Stimulated UV-vis absorption spectrum of *o*-TPEC.

Table. S1 Electronic transition data obtained by the TD/DFT-B3LYP/6-31G (d, p) calculation for *o*-TPEC.

Transition assignment	E(eV)	$\lambda_{\text{abs}}(\text{nm})$	Oscillator strength
HOMO→LUMO (89%)	3.16	392.4	0.1265
HOMO-1→LUMO(24%)	3.41	364.1	0.0220
HOMO-2→LUMO(23%)			
HOMO-5→LUMO(18%)			
HOMO-3→LUMO(10%)			
HOMO→LUMO(10%)			
HOMO→LUMO +1(98%)	3.66	338.9	0.3502
HOMO-1→LUMO(51%)	4.22	294.0	0.0185
HOMO→LUMO+2(15%)			
HOMO-5→LUMO(11%)			
HOMO-2→LUMO(7%)			
HOMO-3→LUMO(7%)			
HOMO→LUMO+2(66%)	4.26	290.8	0.0934
HOMO→LUMO+3(7%)			
HOMO-1→LUMO(7%)			
HOMO-2→LUMO(7%)			
HOMO→LUMO+3(24%)	4.37	283.5	0.1453
HOMO-5→LUMO(20%)			
HOMO→LUMO+2(13%)			
HOMO-2→LUMO(9%)			
HOMO-7→LUMO(7%)			

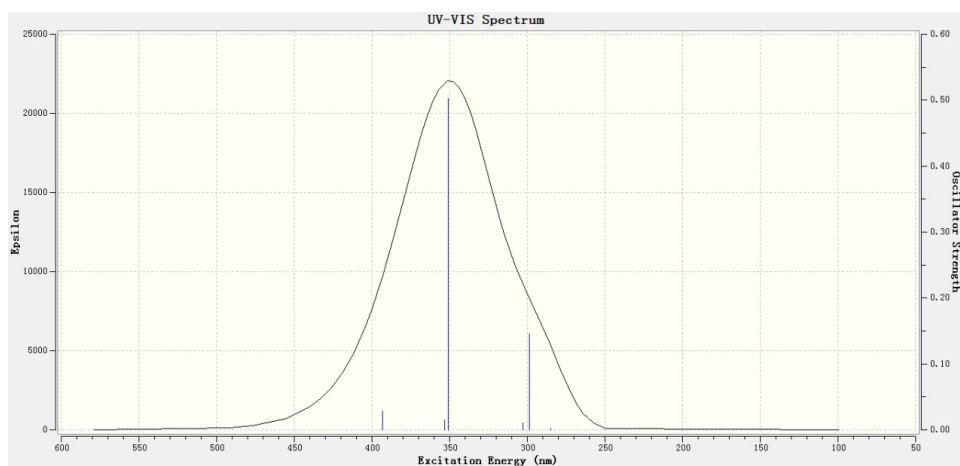


Fig. S8 Stimulated UV-vis absorption spectrum of *m*-TPEC.

Table. S2 Electronic transition data obtained by the TD/DFT-B3LYP/6-31G (d, p)
calculation for *m*-TPEC.

Transition assignment	E(eV)	λ_{abs} (nm)	Oscillator strength
HOMO→LUMO (99%)	3.15	393.3	0.0289
HOMO-6→LUMO(91%)	3.51	353.0	0.0155
HOMO→LUMO +1(96%)	3.53	350.8	0.5026
HOMO-1→LUMO(56%)	4.09	302.8	0.0107
HOMO→LUMO+2(34%)			
HOMO→LUMO+2(59%)	4.26	290.8	0.0934
HOMO-1→LUMO(32%)			
HOMO→LUMO+3(48%)	4.35	284.9	0.0023
HOMO-1→LUMO+1(13%)			
HOMO-3→LUMO(12%)			
HOMO-4→LUMO(7%)			

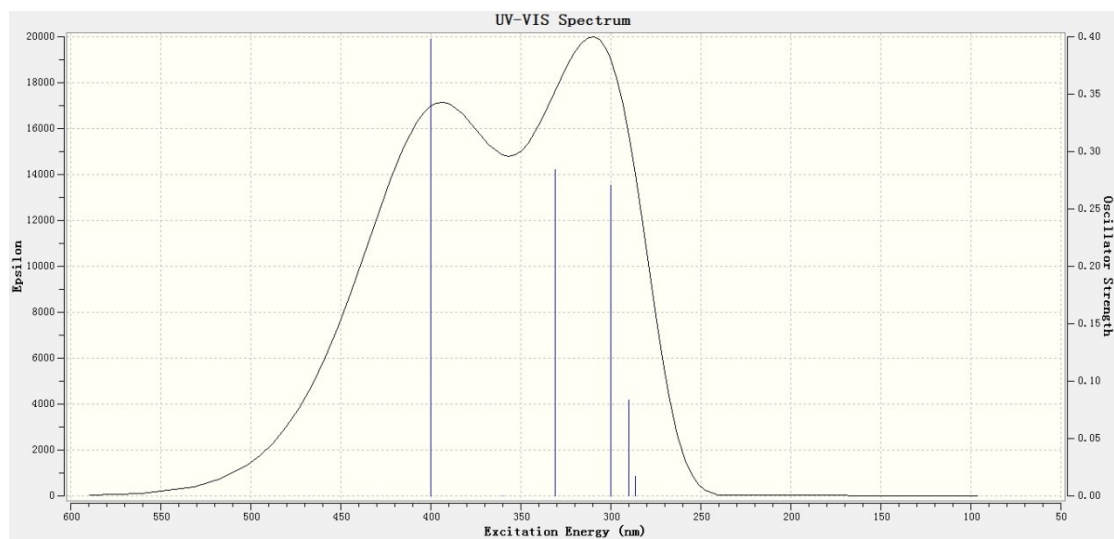


Fig. S9 Stimulated UV-vis absorption spectrum of *p*-TPEC.

Table. S3 Electronic transition data obtained by the TD/DFT-B3LYP/6-31G (d, p) calculation for *p*-TPEC.

Transition assignment	E(eV)	λ_{abs} (nm)	Oscillator strength
HOMO→LUMO (99%)	3.10	399.9	0.3977
HOMO-5→LUMO(83%)	3.45	359.8	0.0000
HOMO-5→LUMO+1(7%)			
HOMO→LUMO +1(97%)	3.74	331.1	0.2843
HOMO-1→LUMO(86%)	4.14	299.8	0.2710
HOMO-3→LUMO(49%)	4.27	290.1	0.0835
HOMO→LUMO+2(17%)			
HOMO→LUMO+3(6%)			
HOMO-1→LUMO(5%)			
HOMO-2→LUMO(82%)	4.33	286.2	0.0169
HOMO-2→LUMO+1(5%)			

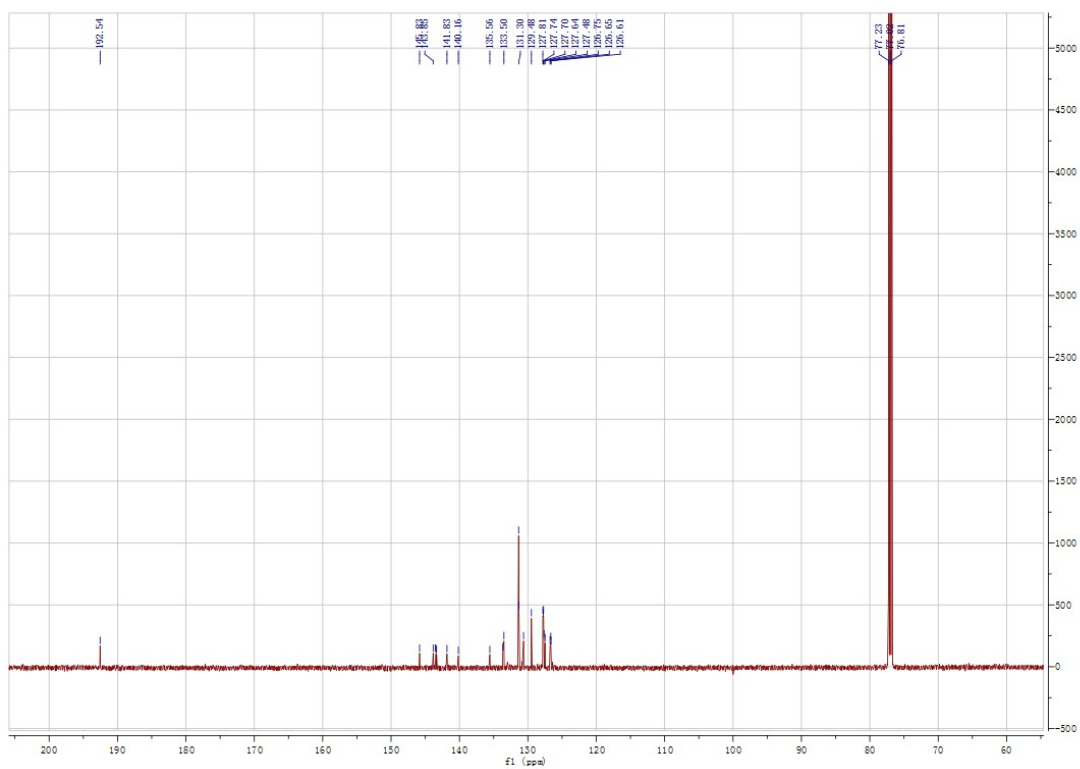


Fig. S12 ^{13}C NMR (151 MHz, CDCl_3) spectrum of compound *o*-TPEC.

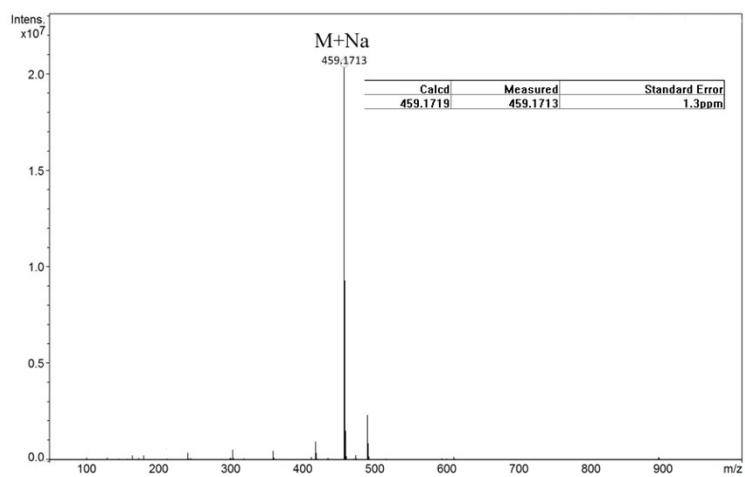


Fig.S13 HR-MS of compound *o*-TPEC.

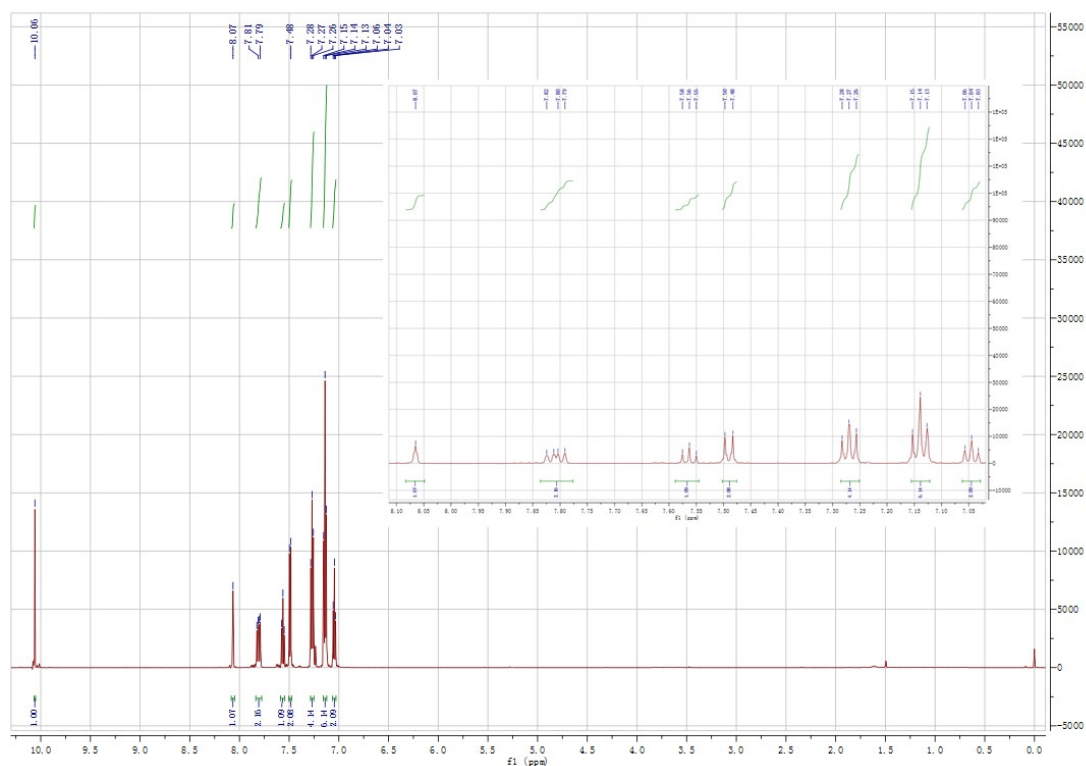


Fig.S14 ^1H NMR (600 MHz, CDCl_3) spectrum of compound *m*-TPEC.

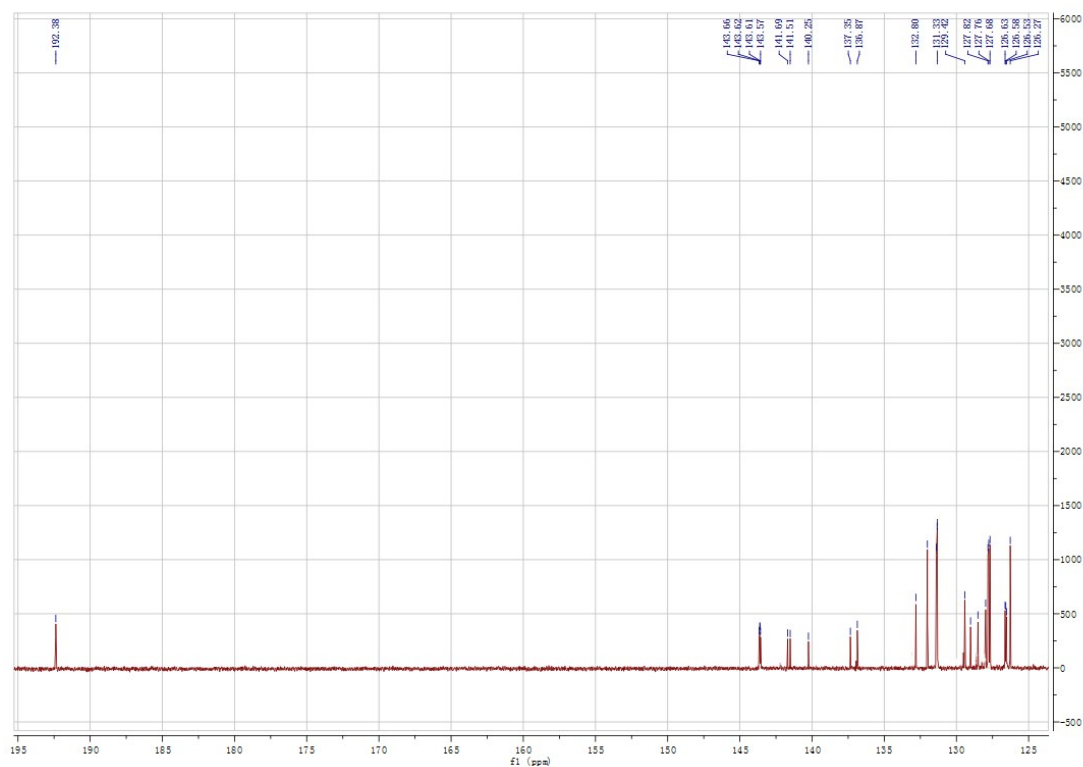


Fig. S15 ^{13}C NMR (151 MHz, CDCl_3) spectrum of compound *m*-TPEC.

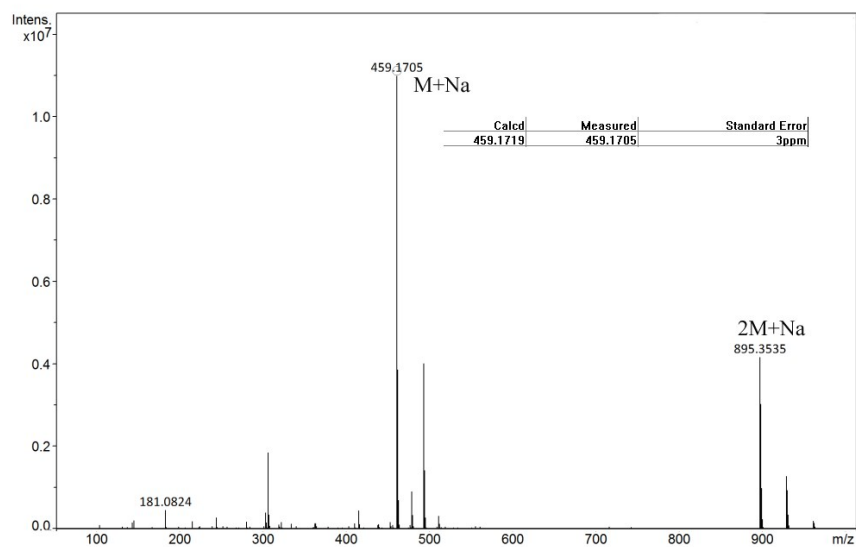


Fig.S16 HR-MS of compound *m*-TPEC.

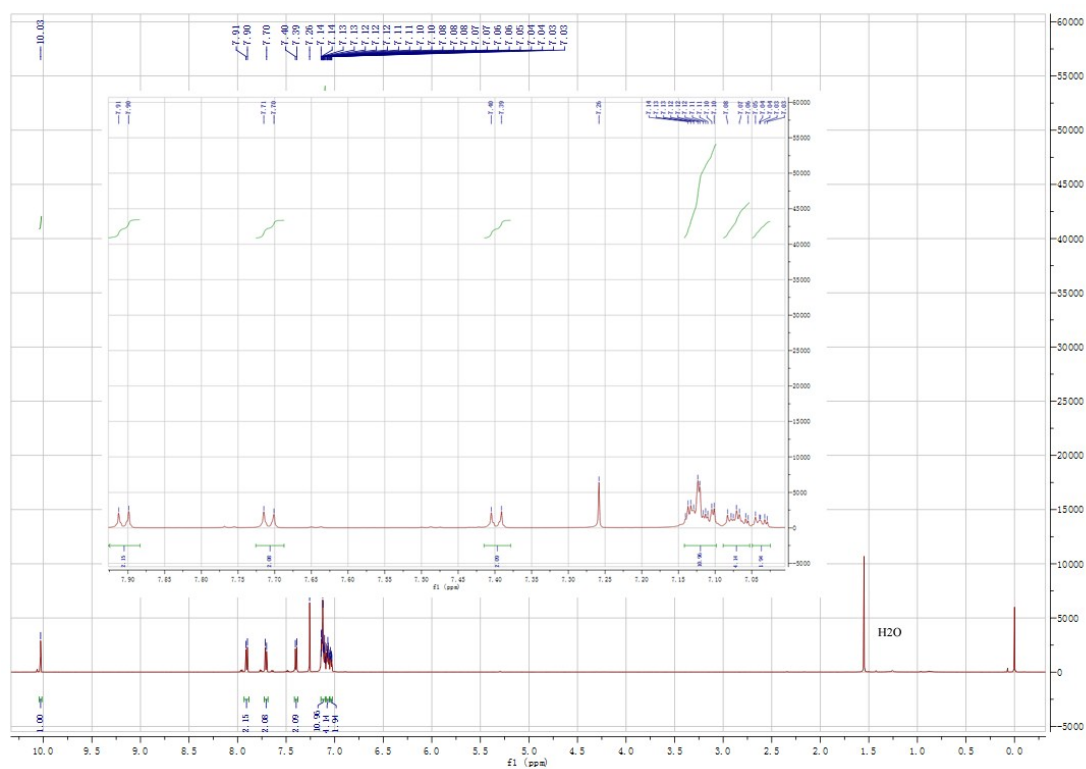


Fig.S17 1H NMR (600 MHz, $CDCl_3$) spectrum of compound *p*-TPEC.

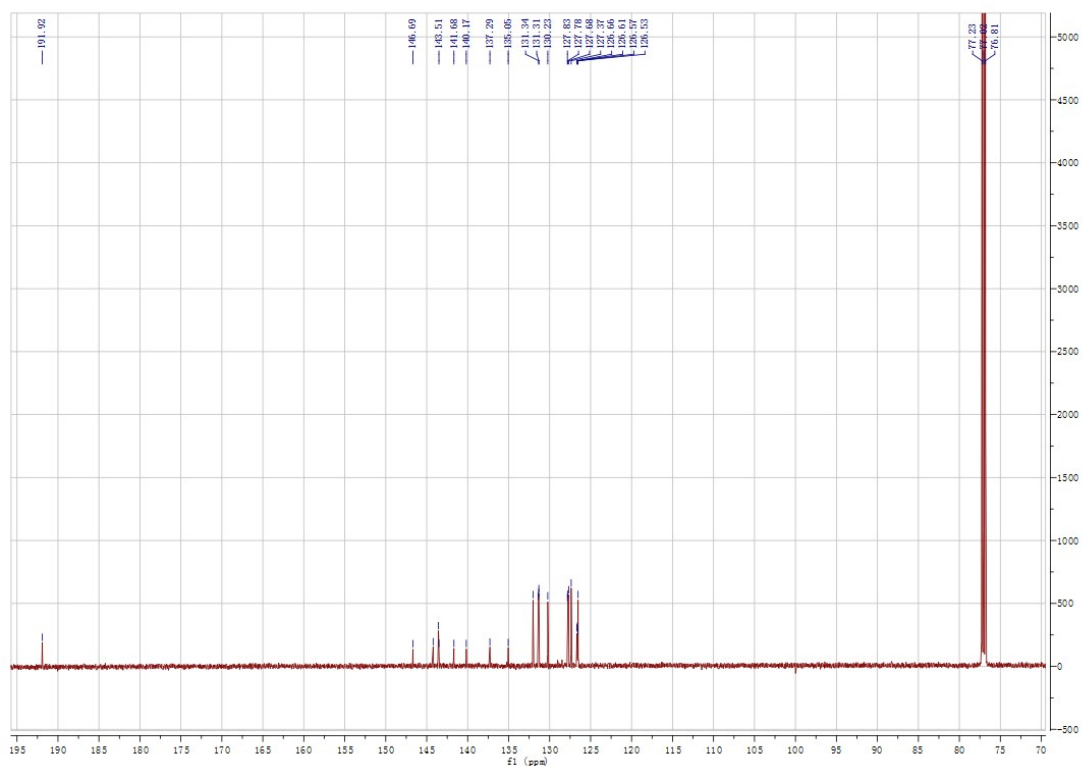


Fig. S18 ^{13}C NMR (151 MHz, CDCl_3) spectrum of compound *p*-TPEC.

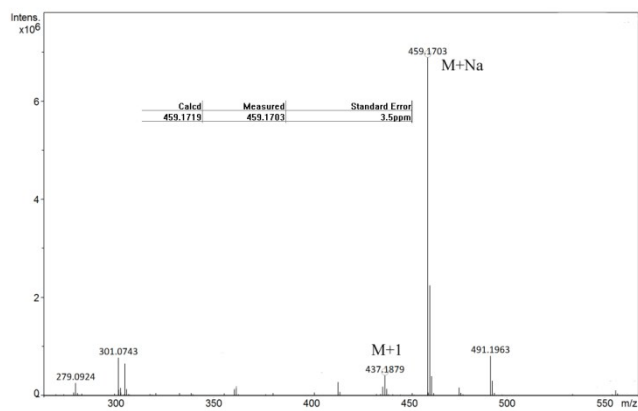


Fig.S19 HR-MS of compound *p*-TPEC.