Electronic Supplementary Information (ESI):

Tetraphenylethene end-capped [1,2,5]thiadiazolo[3,4-c]pyridine with aggregation -induced emission and large two-photon absorption cross-sections

Tao Jiang[a], Yi Qu[*b], Bo Li[c], Yuting Gao[a] and Jianli Hua[*a]

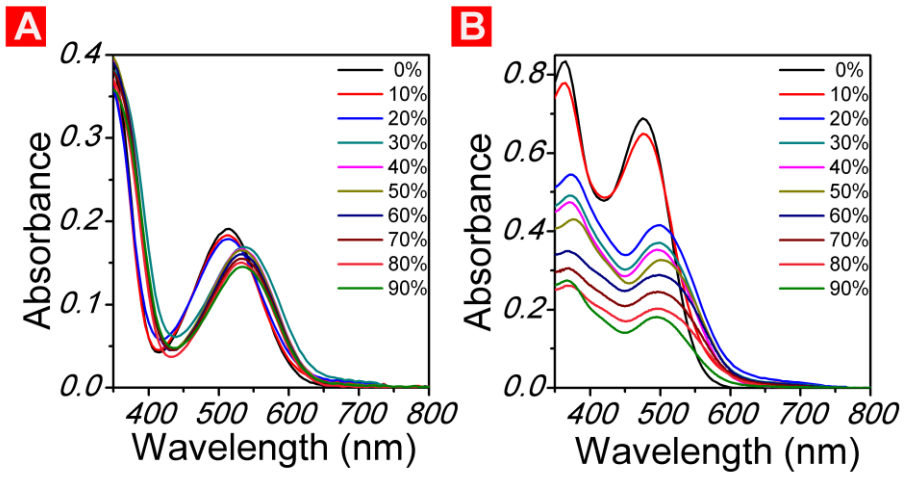

Figure S1 Absorption spectra of (A) **TPEPT1** and (B) **TPEPT2** versus water fraction (f_w) of aqueous at the concentration of 10^{-5} M.

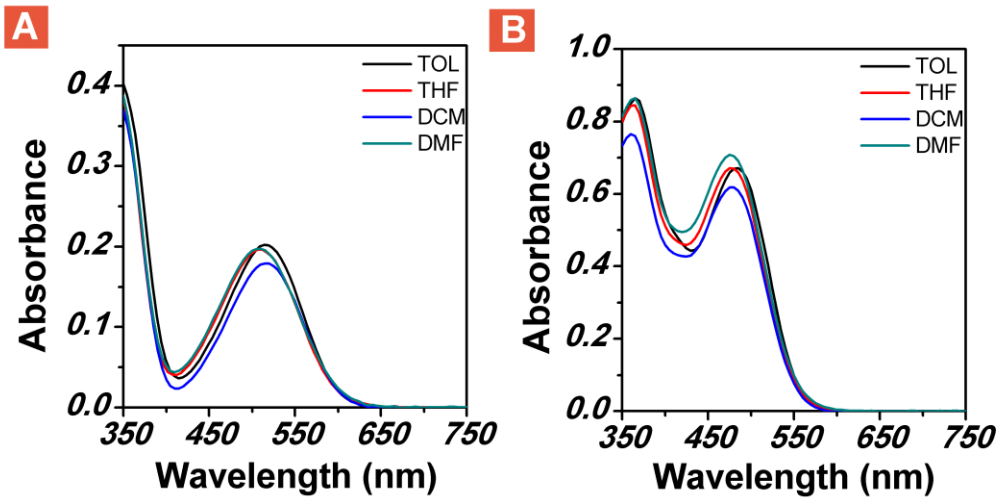

Figure S2 one-photon absorption spectra of (A) **TPEPT1** and (B) **TPEPT2** in different solvents at the concentration of 1×10^{-5} M.

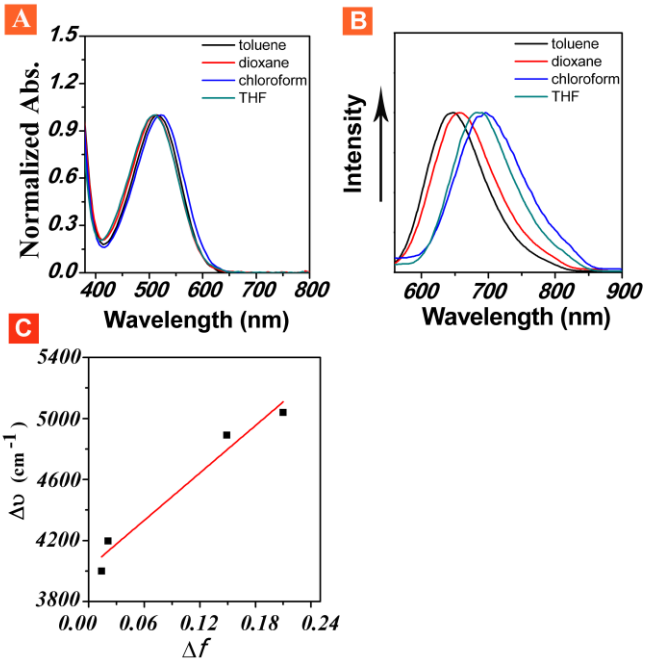

Figure S3 (A) Normalized absorption spectra of **TPEPT1** in different solvents at the concentration of 1 × 10^{-5} M. (B) Emission spectra of **TPEPT1** in different solvents at the concentration of 1 × 10^{-5} M, λ_{ex} = 510 nm. (C) Plot of Stokes shift (Δυ) of **TPEPT1** vs solvent polarity parameter (Δf) of its solution at the concentration of 1 × 10^{-5} M.[1]

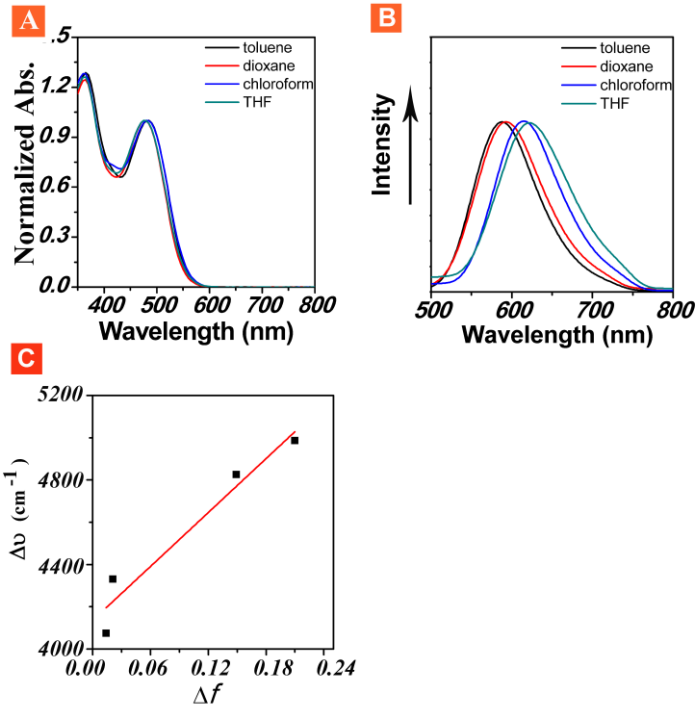

Figure S4 (A) Normalized absorption spectra of **TPEPT2** in different solvents at the concentration of 1 × 10^{-5} M. (B) Emission spectra of **TPEPT2** in different solvents at the concentration of 1 × 10^{-5} M, λ_{ex} = 475 nm. (C) Plot of Stokes shift (Δυ) of **TPEPT2** vs solvent polarity parameter (Δf) of its solution at the concentration of 1 × 10^{-5} M.[1]

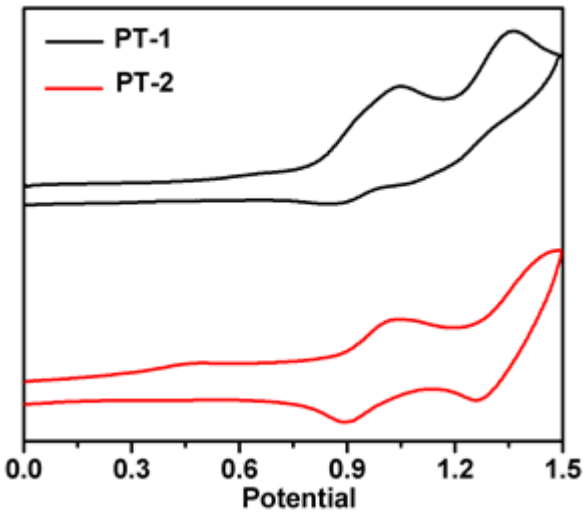

Figure S5. Cyclic voltammograms of **TPEPT1** and **TPEPT2** using 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as electrolyte in DCM with platinum button working electrodes, a platinum wire counter electrode, and an SCE reference electrode.

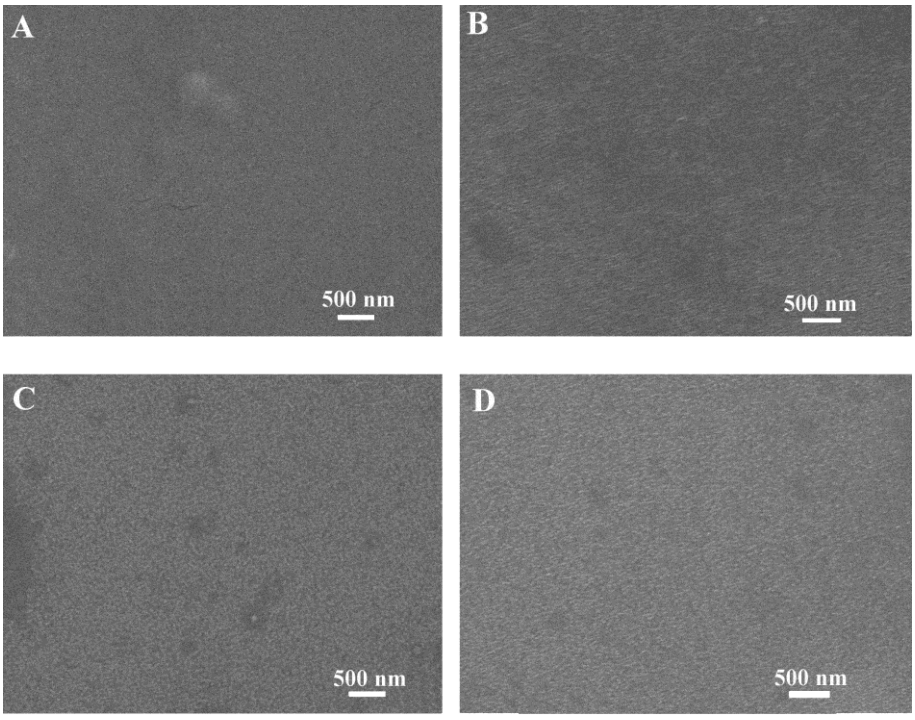

Figure S6 SEM images of **TPEPT1** in the different solvents (A) toluene, (B) THF, (C) DCM and (D) DMF. Concentration: 1×10^{-5} M.

Table S1. Photophysical properties of **TPEPT1** in different solvents[a]

Solvent	Δf	λ_{ab} (nm)	λ_{em} (nm)	$\Delta\upsilon$ (cm^{-1})
Toluene	0.014	514 nm	647 nm	3999
1,4-dioxane	0.021	515 nm	657 nm	4197
chloroform	0.149	522 nm	696 nm	4890
THF	0.210	512 nm	690 nm	5039

[a] Abbreviation: Δf = solvent polarity parameter taken from the ref. (Macromolecules, 2007, 40, 4879-4886), λ_{ab} = absorption maximum, λ_{em} = emission maximum, $\Delta\upsilon$ = stokes shift.

Table S2. Photophysical properties of **TPEPT2** in different solvents[a]

Solvent	Δf	λab (nm)	λem (nm)	Δυ (cm^{-1})
Toluene	0.014	475 nm	589 nm	4075
1,4-dioxane	0.021	475 nm	593 nm	4331
chloroform	0.149	479 nm	623 nm	4826
THF	0.210	473 nm	619 nm	4986

[a] Abbreviation: Δf = solvent polarity parameter taken from the ref. (Macromolecules, 2007, 40, 4879-4886), λ_{ab} = absorption maximum, λ_{em} = emission maximum, $\Delta\upsilon$ = stokes shift.

Table S3. Electrochemical properties of **TPEPT1** and **TPEPT2**

Compound	E_{HOMO}[a] (eV)	E_{LUMO}[b] (eV)	E_g[c] (eV)	λ_{cutoff}[d] (nm)
TPEPT1	-5.74	-3.86	1.88	650
TPEPT2	-5.74	-3.72	2.02	610

[a] HOMO = -e (Eox + 4.7) (eV). [b] E_g = energy band gap determined from the intercept of the normalized absorption and emission spectra. [c] ELUMO = E_g + E_{HOMO}. [d] Estimated from the absorption thresholds.

References

1 a) W. Z. Yuan, Y. Y. Gong, S. M. Chen, X. Y. Shen, J. W. Y. Lam, P. Lu, Y. W. Lu, Z. M. Wang, R. R. Hu, N. Xie, H. S. Kwok, Y. M. Zhang, J. Z. Sun and B. Z. Tang, *Chem. Mater*. 2012, **24**, 1518 – 1528. b) Y. J. Zhang, J. W. Sun, G. F. Bian, Y. Y. Chen, M. O. Yang, B. Hu and C. Zhang, *Photochem. Photobiol. Sci*., 2012, **11**, 1414 – 1421.

Charaterization:

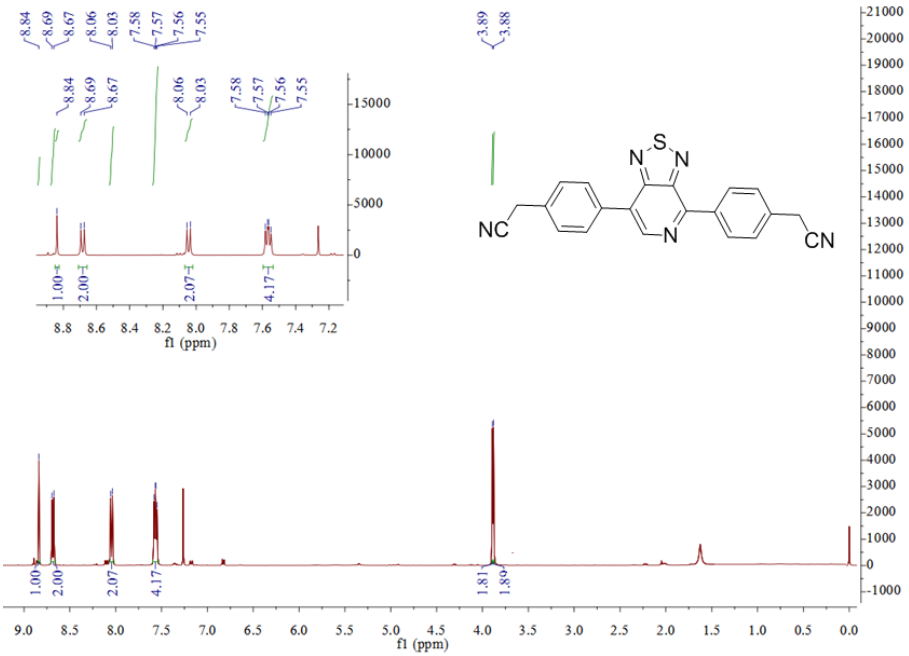

Figure S7. ^{1}H NMR spectrum of **3** in $CDCl_3$

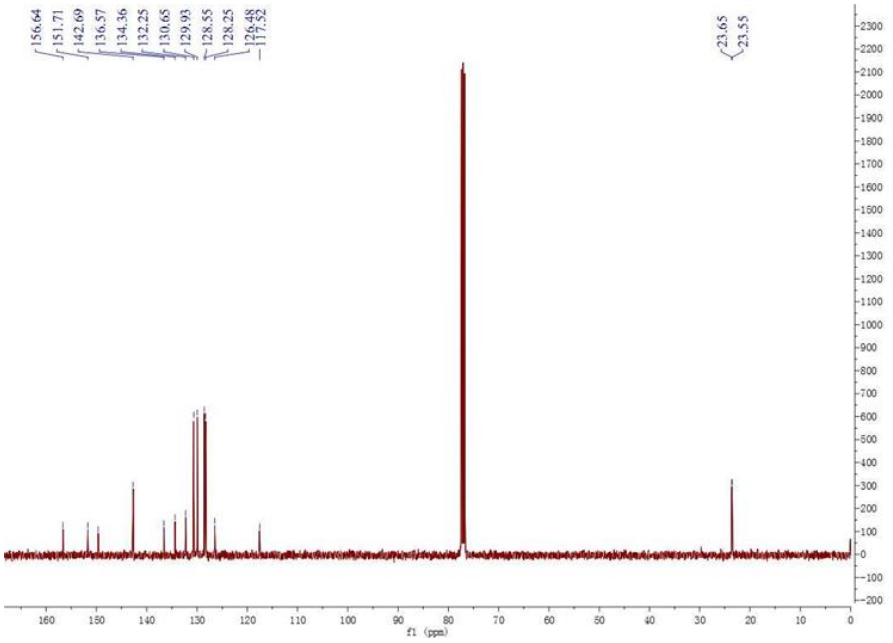

Figure S8. ^{13}C NMR spectrum of **3** in $CDCl_3$

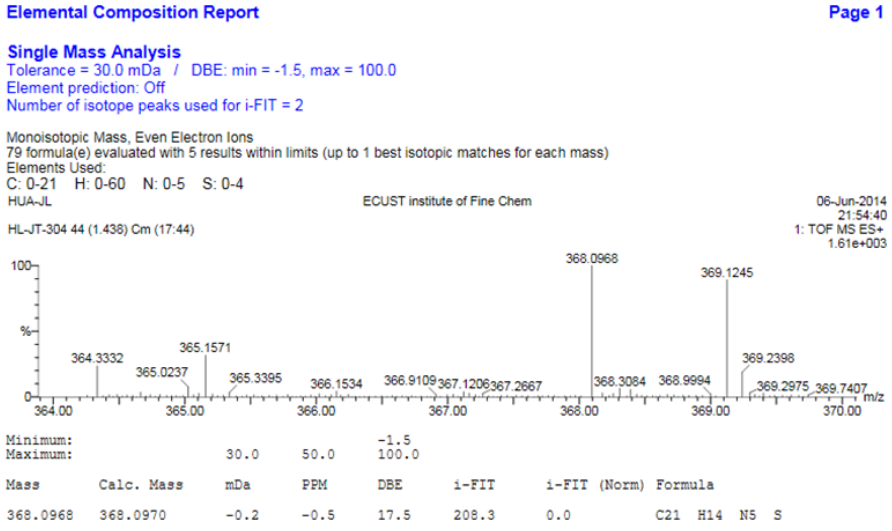

Figure S9. HR mass spectrum of **3**

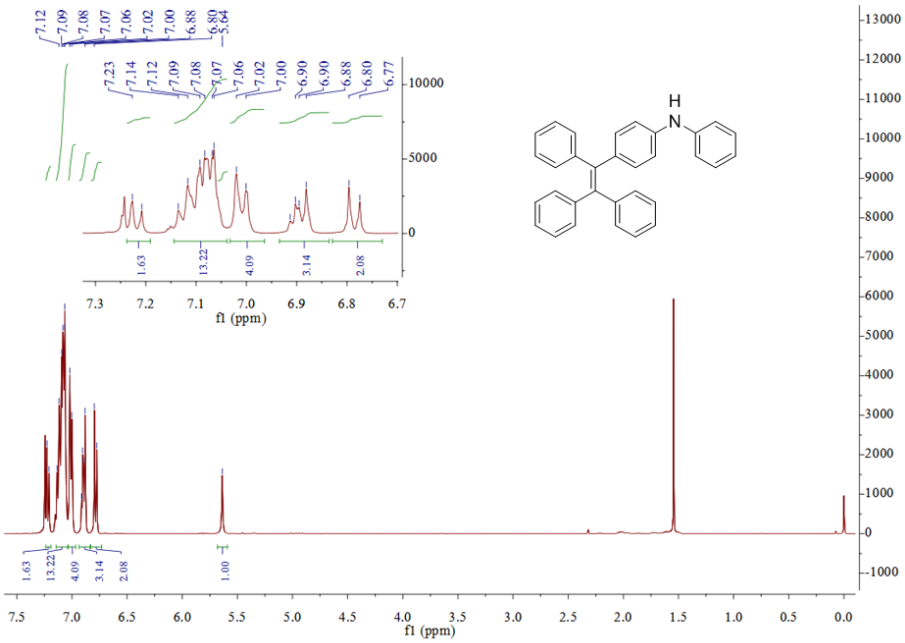

Figure S10. ^{1}H NMR spectrum of **5** in $CDCl_3$

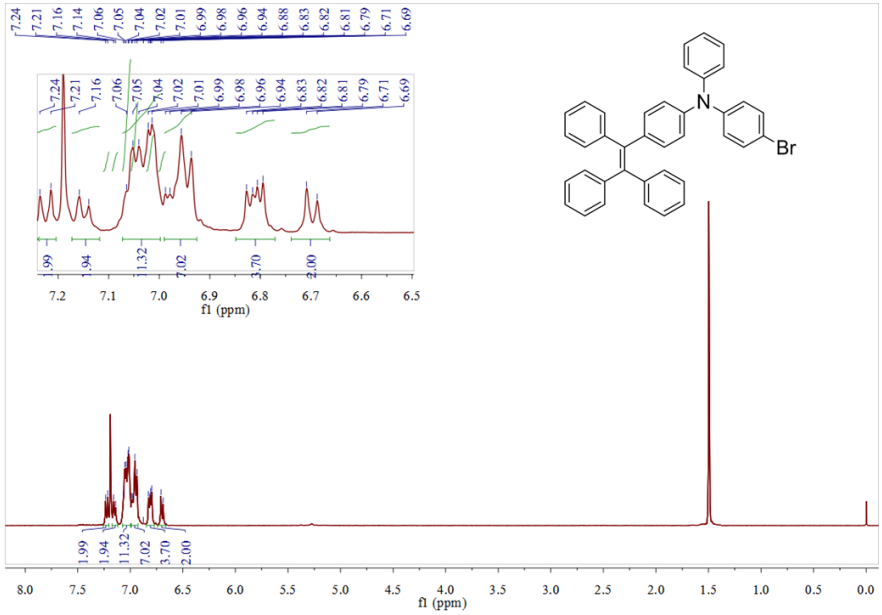

Figure S11. ^{1}H NMR spectrum of **6** in $CDCl_3$

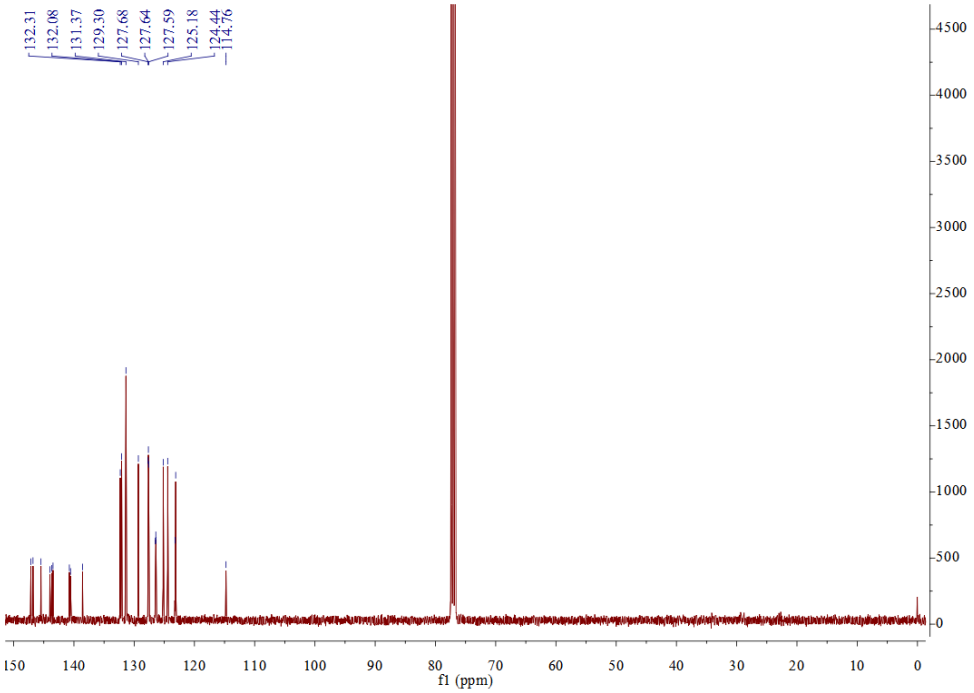

Figure S12. ^{13}C NMR spectrum of **6** in $CDCl_3$

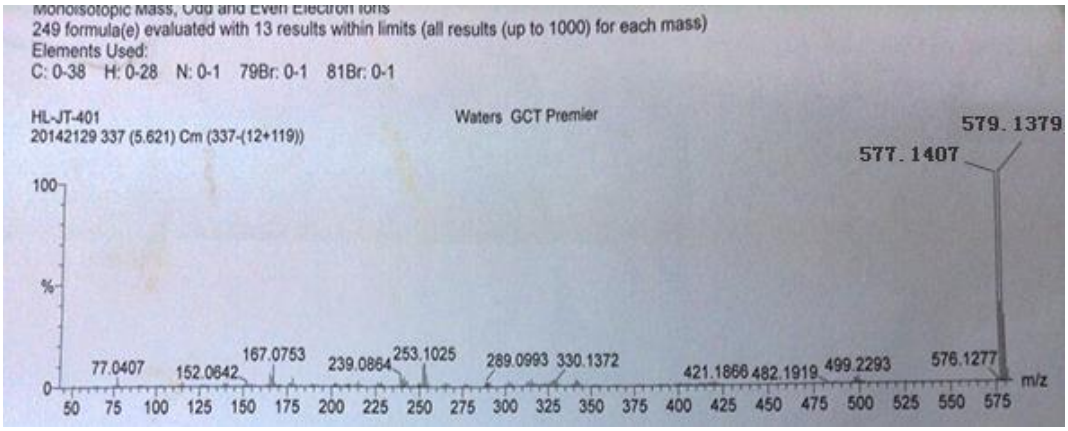

Figure S13. HR mass spectrum of **6**

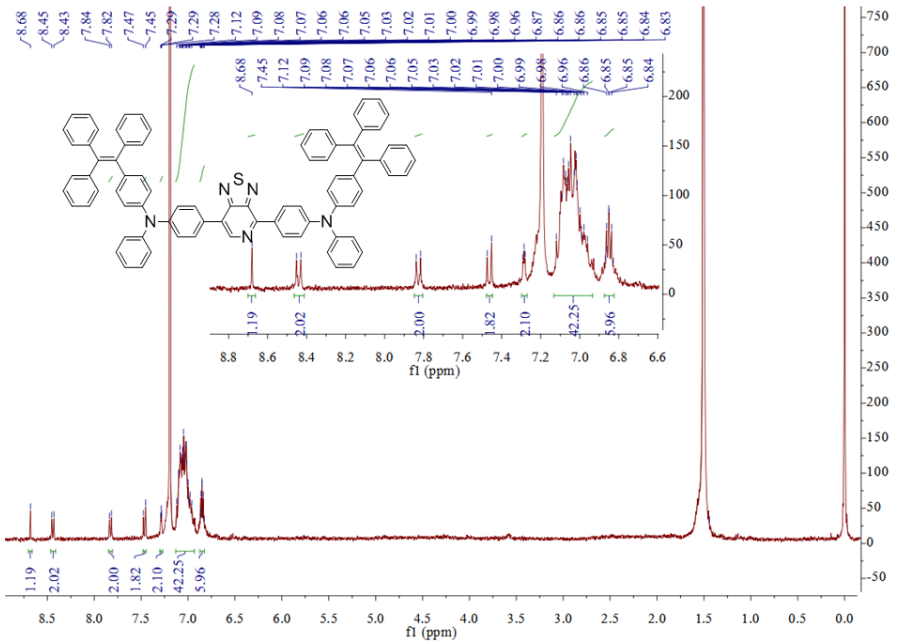

Figure S14. ^{1}H NMR spectrum of **TPEPT1** in $CDCl_3$

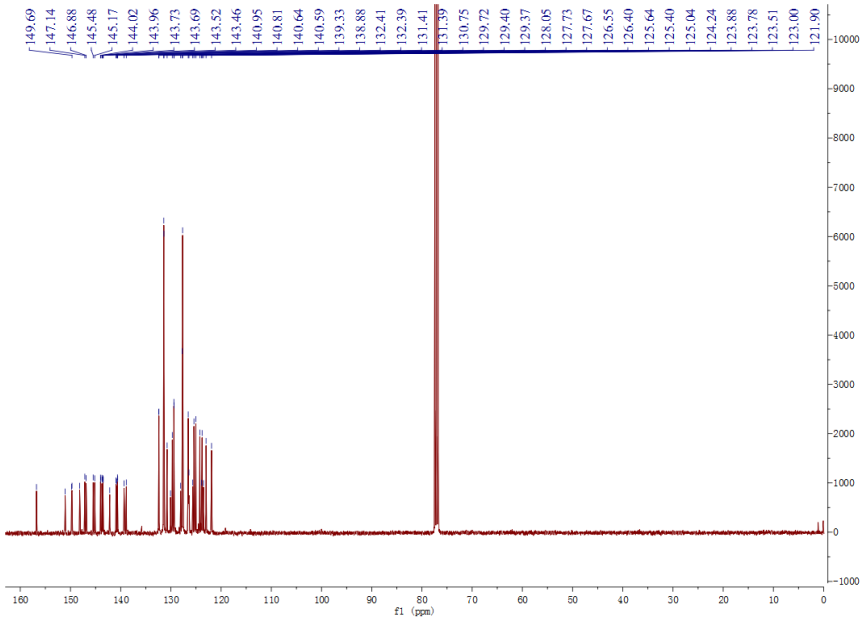

Figure S15. ^{13}C NMR spectrum of **TPEPT1** in $CDCl_3$

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
200 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-90 H: 0-60 N: 0-9 S: 0-3

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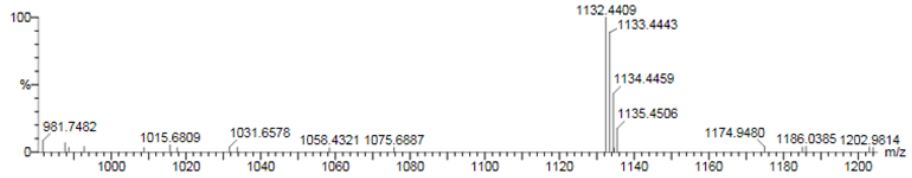
HL-JT-201 136 (0.934) Cm (136:165) 1: TOF MS ES+ 5.35e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1132.4409	1132.4413	-0.4	-0.4	55.5	10.5	0.0	C81 H58 N5 S

Figure S16. HR mass spectrum of **TPEPT1**

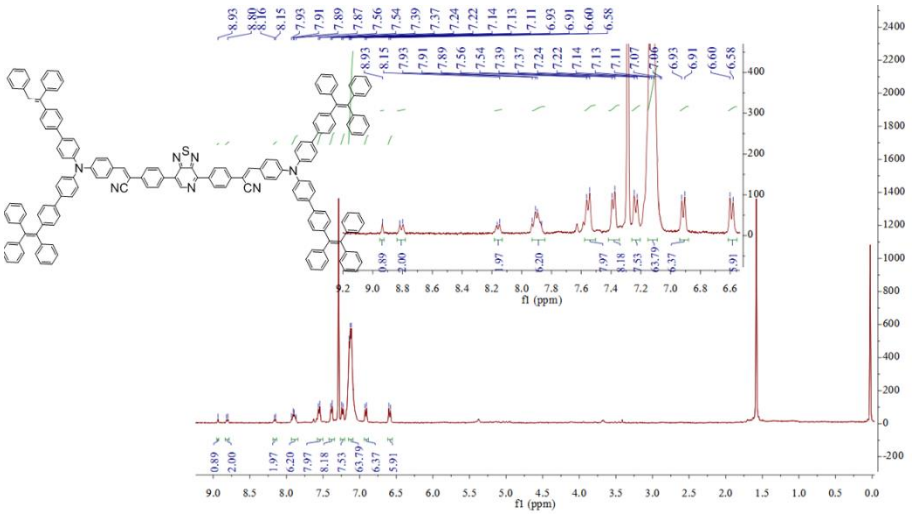


Figure S17. ^{1}H NMR spectrum of **TPEPT2** in $CDCl_3$

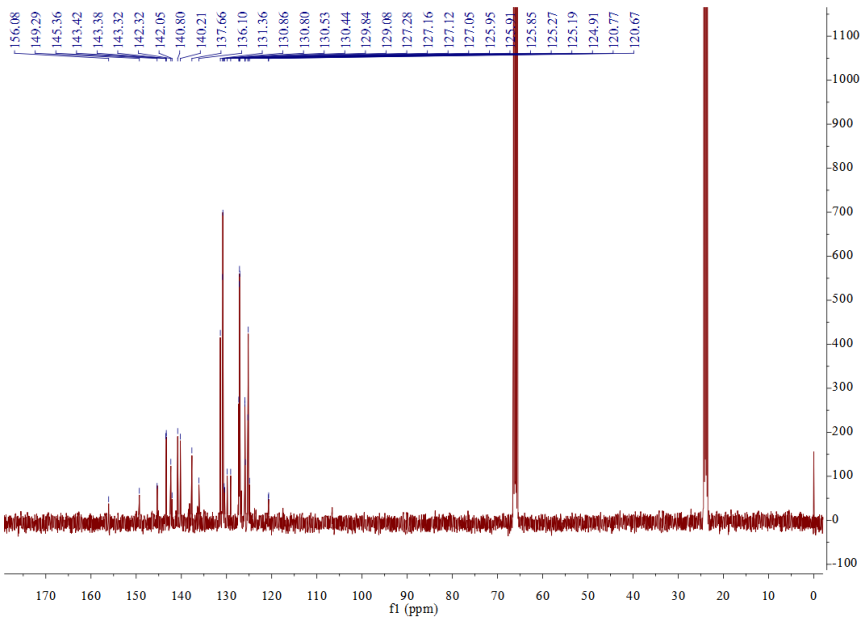


Figure S18. ^{13}C NMR spectrum of **TPEPT2** in THF-d_8

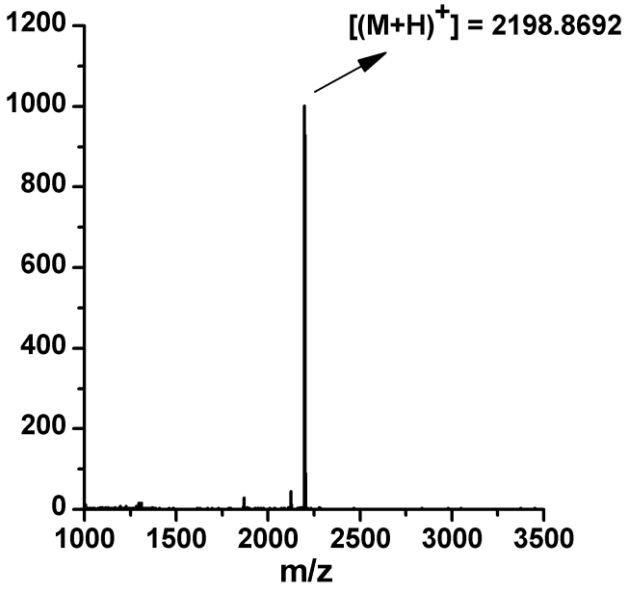


Figure S19. MALDI-TOF spectrum of **TPEPE2**