Supporting Information for:

Electronic Coupling and Spin Orbit Charge Transfer Intersystem Crossing (SOCT-ISC) in Phenothiazine-Perylene Compact Electron Donor/Acceptor Dyads

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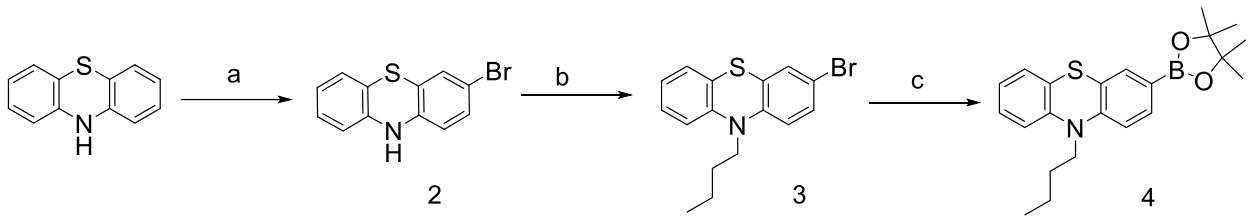
Contents

1. General Information

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before used for synthesis. ^{1}H and ^{13}C chemical shifts are reported in parts per million (ppm) relative to TMS, with the residual solvent peak used as an internal reference. The mass spectra were measured by TOF MS MALDI, ESI and TOF-MS EI spectrometer.

2. Synthesis of Compounds

Synthesis scheme S1[a]



[a] Key: (a) NBS, dry DMF, stirred at 0 °C for 1 h, under N_2, yield: 24%; (b)1-Bromobutane, KOH, dry DMF, overnight, under N_2, yield: 83%; (c) Bis(pinacolato)diboron, Pd(dppf)$Cl_2CH_2Cl_2$, CH_3COOK, dry 1,4-dioxane, stirred at 80 °C for 18 h, under N_2, yield: 52 %.

2.1. Compound 1 (3-Bromoperylene). Compound **1** (see the main text) was synthesized according to modified method.[1] In a 250 mL flask, perylene (1.0 g, 3.96 mmol) and DMF (20 mL) were stirred at room temperature until all perylene solid was dissolved. Then (20 mL) solution of NBS (706.0 mg, 3.96 mmol) was added dropwise. Stirred the reaction mixture at RT for 20 hrs. After that water (50 mL) was added to give golden solid which was collected by filtration and purified by column chromatography (silica gel, DCM/ PE = 1:4, v/v) to give

yellowish golden solid. (1.10 g, yield 84%). Mp: 243–245 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.24 – 8.15 (m, 3H), 8.10 (d, 1H, *J* = 8.0 Hz), 8.0 (d, 1H, *J* = 8.0 Hz), 7.77 – 7.67 (m, 3H), 7.60 (t, 1H, *J* = 8.0 Hz), 7.51 – 7.46 (m, 2H). TOF MS EI+: Calcd ($[C_{20}H_{11}Br]^+$), *m/z* = 330.0044; found, *m/z* = 330.0055.

2.2. Compound 2. Compound **2** was synthesized according to modified method.[2] under N_2 atmosphere, 10H-phenothiazine (2.98 g, 15.0 mmol) was mixed in dry DMF (20 mL), a solution of NBS (2.66 g, 15.0 mmol) in 10 mL DMF was added dropwise within 40 minutes, by monitoring the temperature at 0 °C. The reaction mixture was allowed to stir for 1h at this temperature. After completion of the reaction, water (50 mL) was added immediately. The organic layer was extracted with DCM (4 × 50 mL), and dried over anhydrous Na_2SO_4. Solvent was removed under reduced pressure, and residue was purified with column chromatography (silica gel, EA/ PE = 1:10, v/v) to give a greenish solid (1.0 g, yield 24 %). Mp: 174–176 ºC. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.72 (s, 1H), 7.15 – 7.10 (m, 2H), 7.02 (t, 1H, *J* = 10.0 Hz), 6.92 (d, 1H, *J* = 5.0 Hz), 6.78 (t, 1H, *J* = 5.0 Hz), 6.68 (d, 1H, *J* = 5.0 Hz), 6.62 (d, 1H, *J* = 10.0 Hz) . TOF ESI$^+$–MS: Calcd ($[C_{12}H_8BrNS]^+$), *m/z* = 278.9561; found, *m/z* = 278.9544.

2.3. Compound 3. Compound **3** was synthesized according to modified method,[3] under N_2 atmosphere, in a 20 mL flask KOH (303.0 mg, 5.4 mmol) was stirred in dry DMF (5 mL) at 0 °C for 15 minutes. Then add compound **2** (1.0 g, 3.6 mmol) and after 10 minutes 1-bromobutane (0.47 mL, 1.27 mmol) was added dropwise by a syringe. The reaction mixture was allowed to stir overnight. After completion of the reaction, the organic layer was extracted with DCM (4 × 50 mL) by washing with brine and dried over anhydrous Na_2SO_4. Solvent was removed under reduced pressure, and the residue was purified with

column chromatography (silica gel, *n*-hexane) to give a greenish oily product (1.0 g, yield 83 %). Mp: 60–64 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.24 – 7.21 (m, 2H), 7.18– 7.11 (m, 2H), 6.94 (t, 1H, *J* = 8.0 Hz), 6.87 (d, 1H, *J* = 8.0 Hz), 6.71– 6.68 (m, 1H), 3.83 (t, 2H, *J* = 8.0 Hz), 1.80 – 1.73 (m, 2H), 1.49– 1.40 (m, 2H), 0.95 (t, 3H, *J* = 4.0 Hz). TOF ESI$^+$–MS: Calcd ($[C_{16}H_{16}BrNS]^+$), *m/z* = 334.0187; found, *m/z* = 334.0260.

2.4. Compound 4. Under N_2 atmosphere, compound **3** (333.0 mg, 1.0 mmol), potassium acetate (245.3 mg, 2.50 mmol), bis(pinacolato)diboron (381.0 mg, 1.50 mmol) and dry 1,4 dioxane (10 mL) were mixed together and purged with N_2 gas for 30 minutes. After that $Pd(dppf)Cl_2.CH_2Cl_2$ (24.5 mg, 0.03 mmol) was added. The reaction mixture was stirred at 80 ^{o}C for 18 h, after completion of the reaction the organic layer was extracted with DCM (4 × 50 mL) and dried over anhydrous Na_2SO_4. Solvent was removed under reduced pressure, and the residue was purified with column chromatography (silica gel, DCM/ PE = 1:2, v/v) to give a yellowish oily product (200 mg, yield 52 %). Mp: 180–182 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.57 – 7.56 (m, 2H), 7.14 – 7.10 (m, 2H), 6.89 – 6.83 (m, 3H), 3.85 (s, 2H), 1.81 – 1.74 (m, 2H), 1.50 – 1.42 (m, 2H), 1.32 (s, 12H), 0.95 (t, 3H, *J* = 8.0 Hz). TOF ESI$^+$–MS: Calcd ($[C_{22}H_{28}BNO_2S]^+$), *m/z* = 382.1934; found, *m/z* = 382.2013.

3. Molecular Structure and Characterization Data

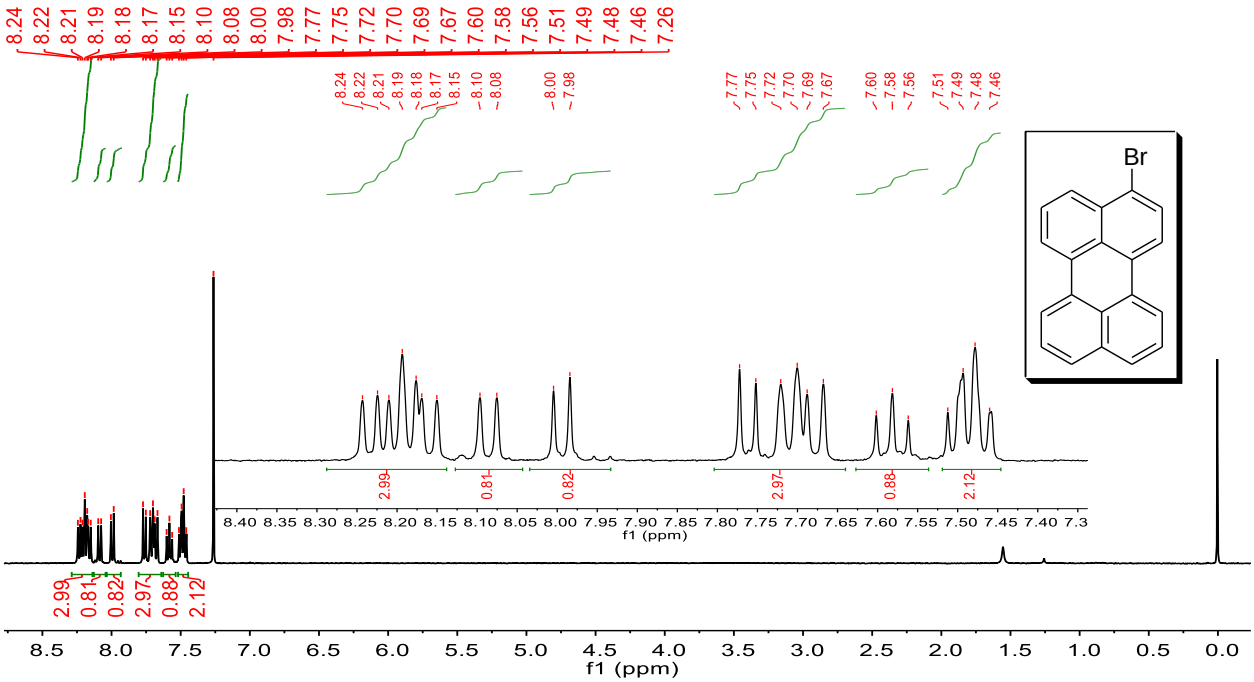


Figure S1. ^{1}H NMR spectrum of **1** ($CDCl_3$, 400 MHz).

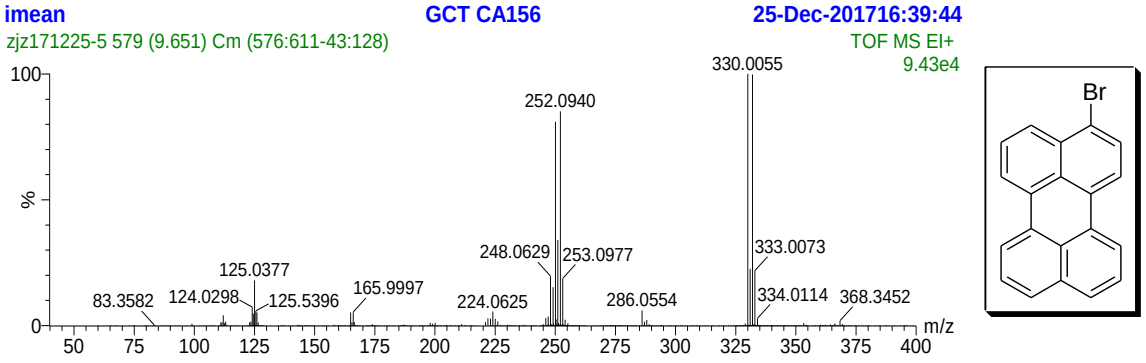


Figure S2. TOF-MS EI^{+} spectrum of **1.**

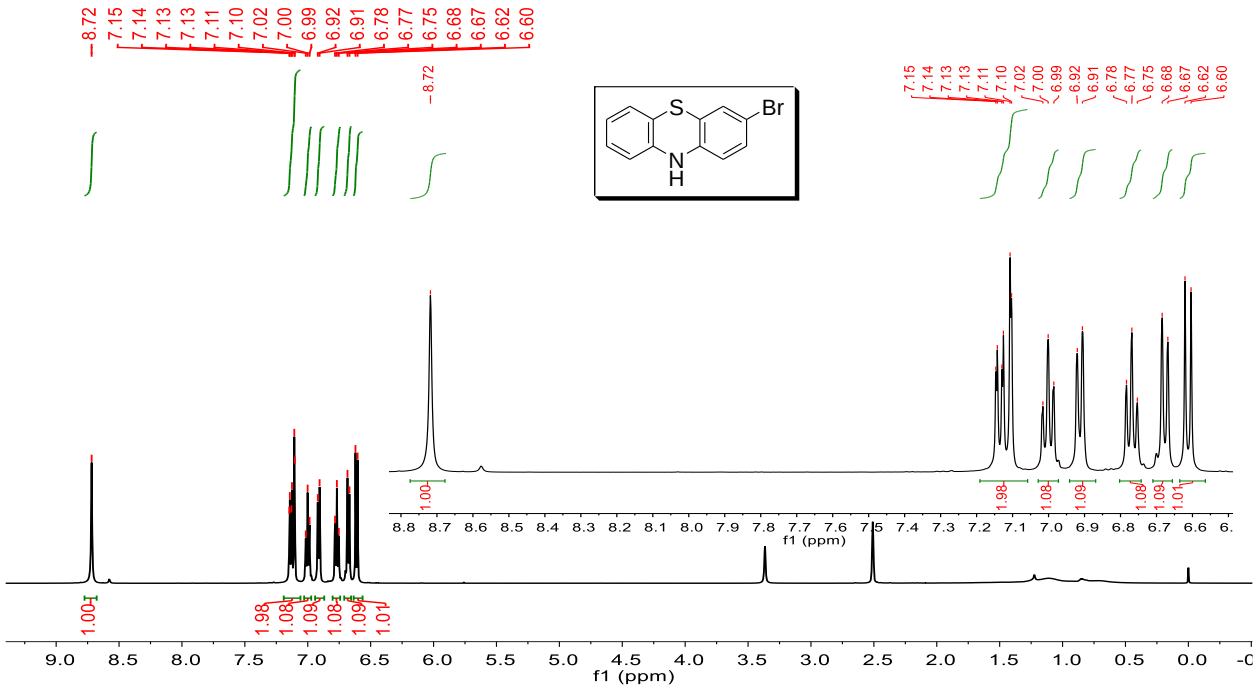


Figure S3. ^{1}H NMR spectrum of **2** (DMSO-d_6, 500 MHz).

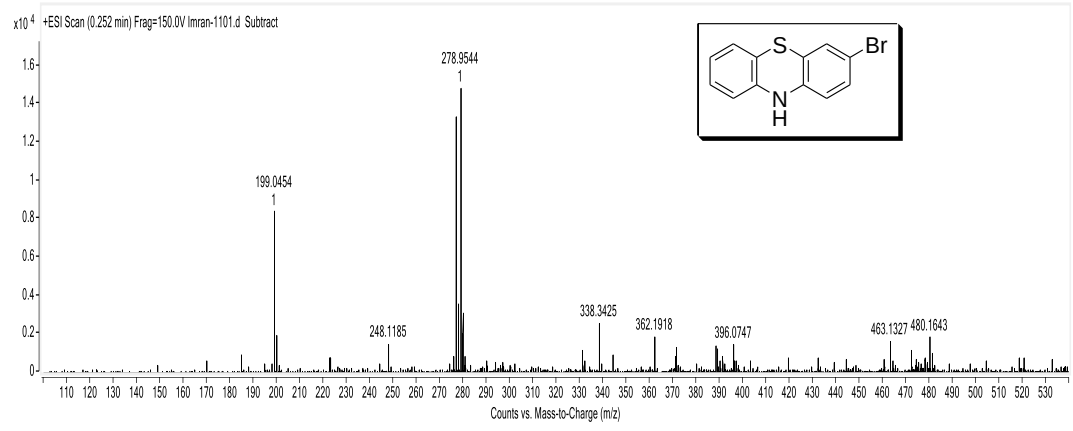


Figure S4. TOF-ESI^{+} spectrum of **2**.

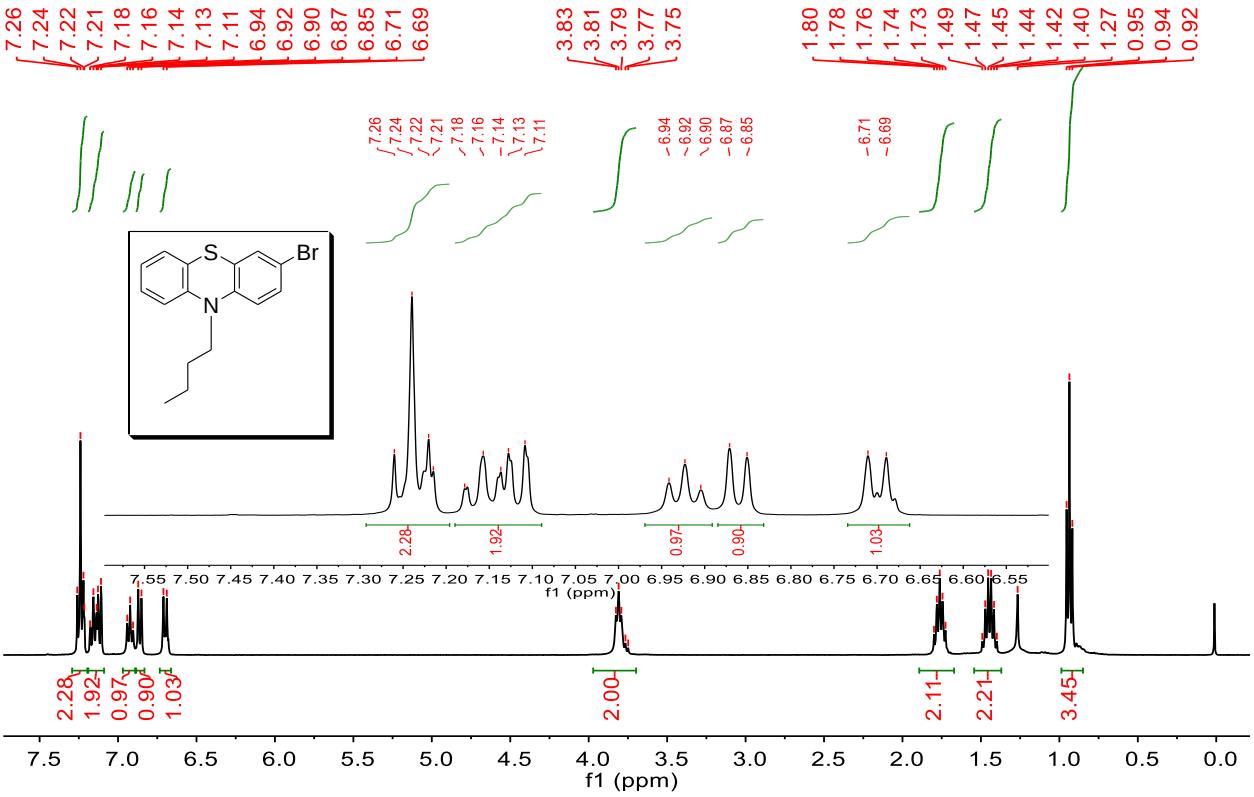


Figure S5. ^{1}H NMR spectrum of **3** ($CDCl_3$, 400 MHz).

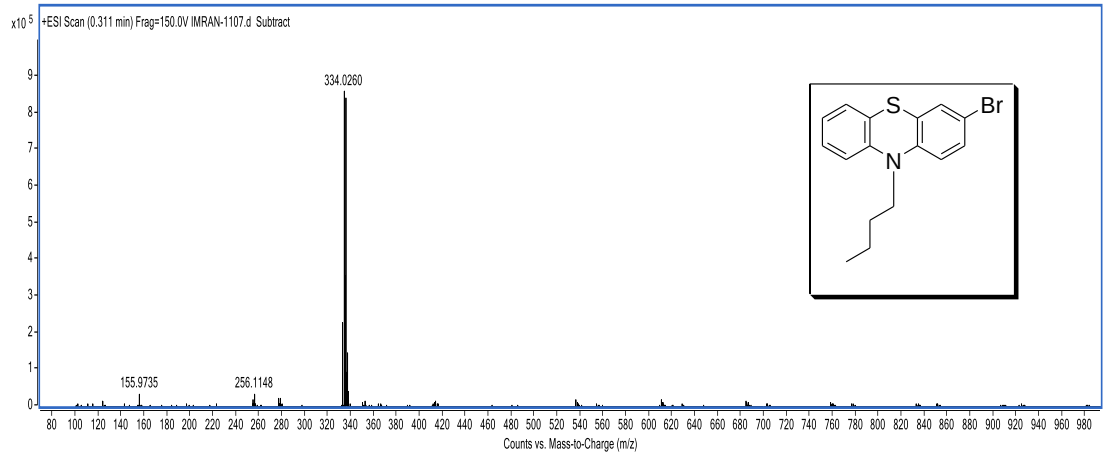


Figure S6. TOF-ESI^{+} spectrum of **3**.

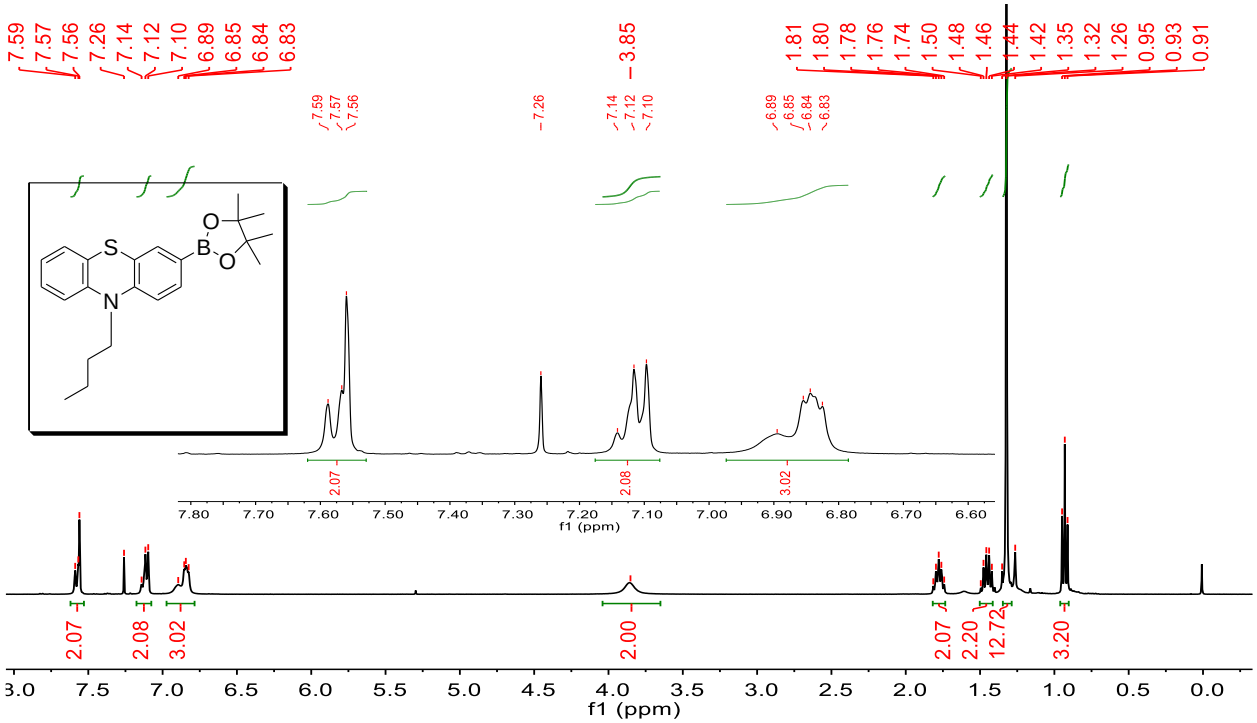


Figure S7. ^{1}H NMR spectrum of **4** ($CDCl_3$, 400 MHz).

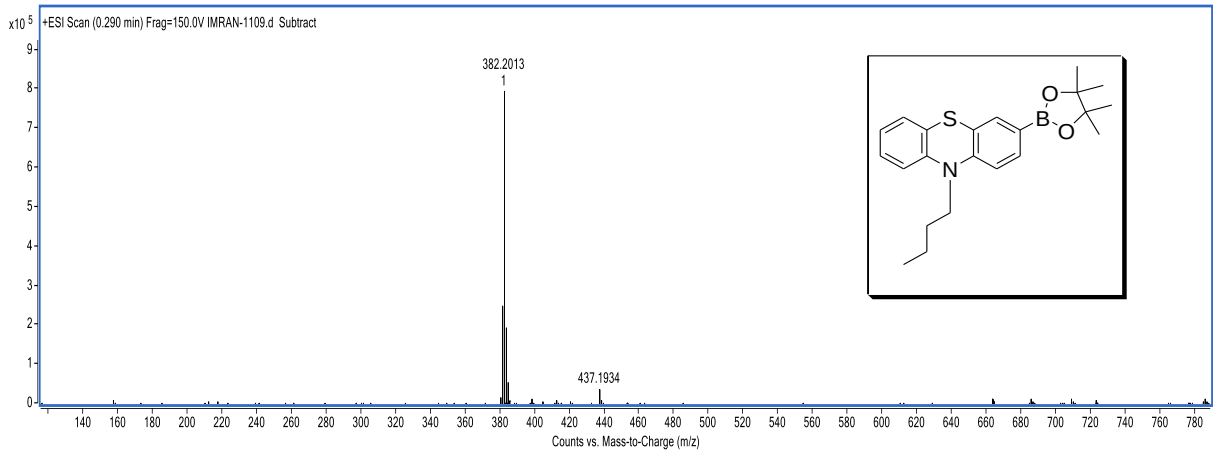


Figure S8. TOF-ESI^{+} spectrum of **4**.

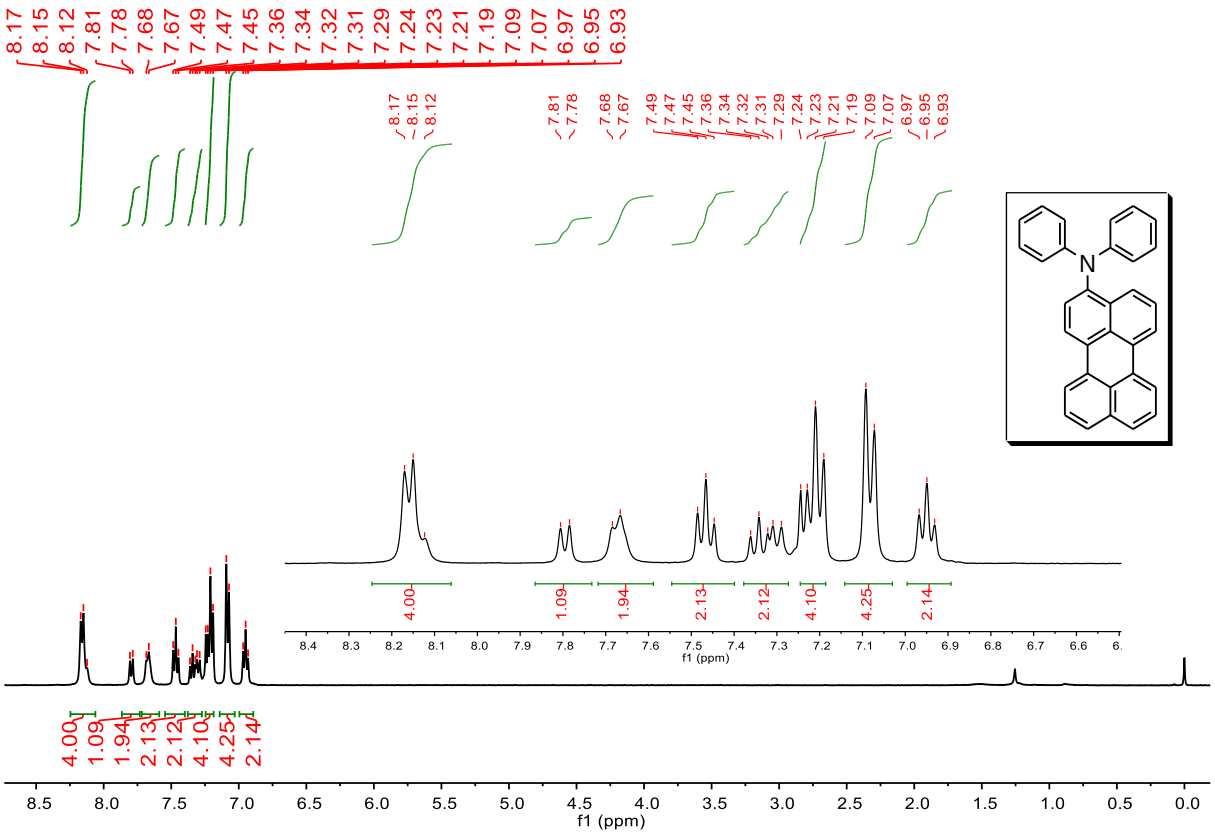


Figure S9. ^{1}H NMR spectrum of **Pery-DPA** ($CDCl_3$, 500 MHz).

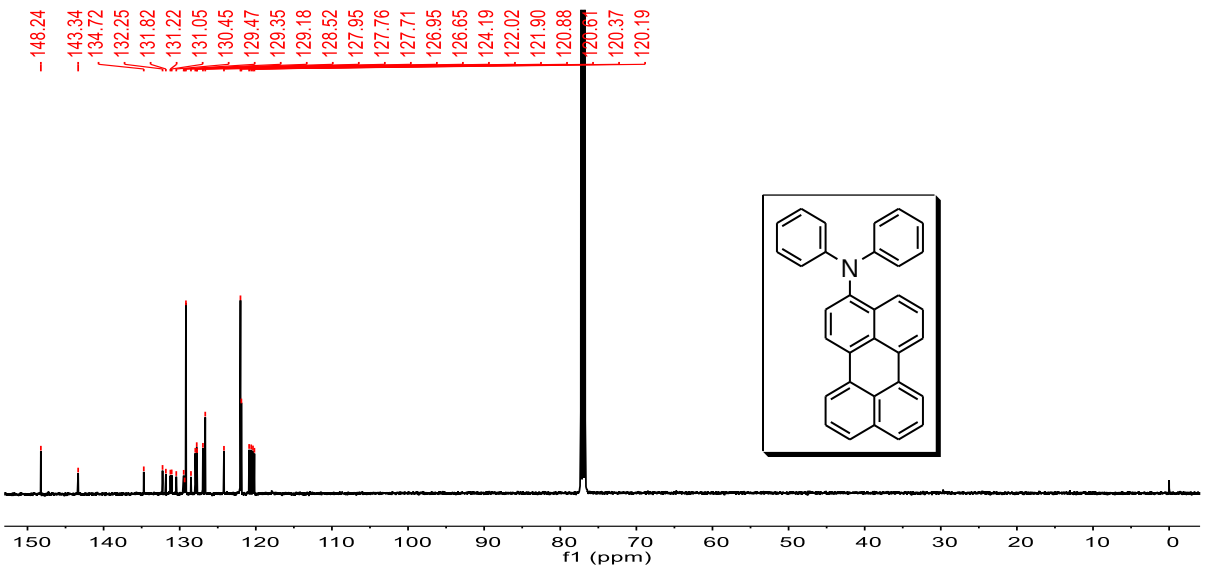


Figure S10. ^{13}C NMR spectrum of **Pery-DPA** ($CDCl_3$, 126 MHz).

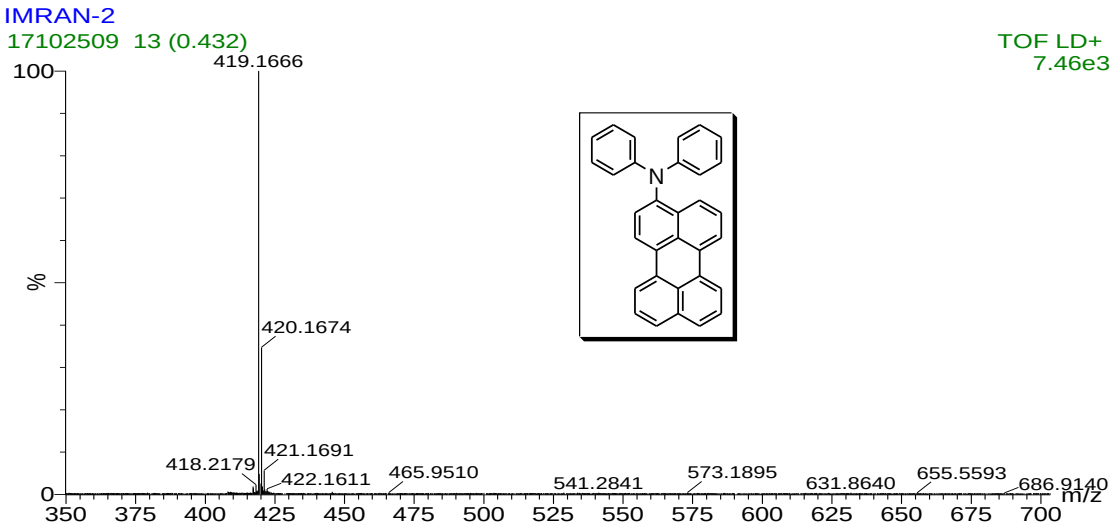


Figure S11. MALDI-HRMS spectrum of **Pery-DPA**.

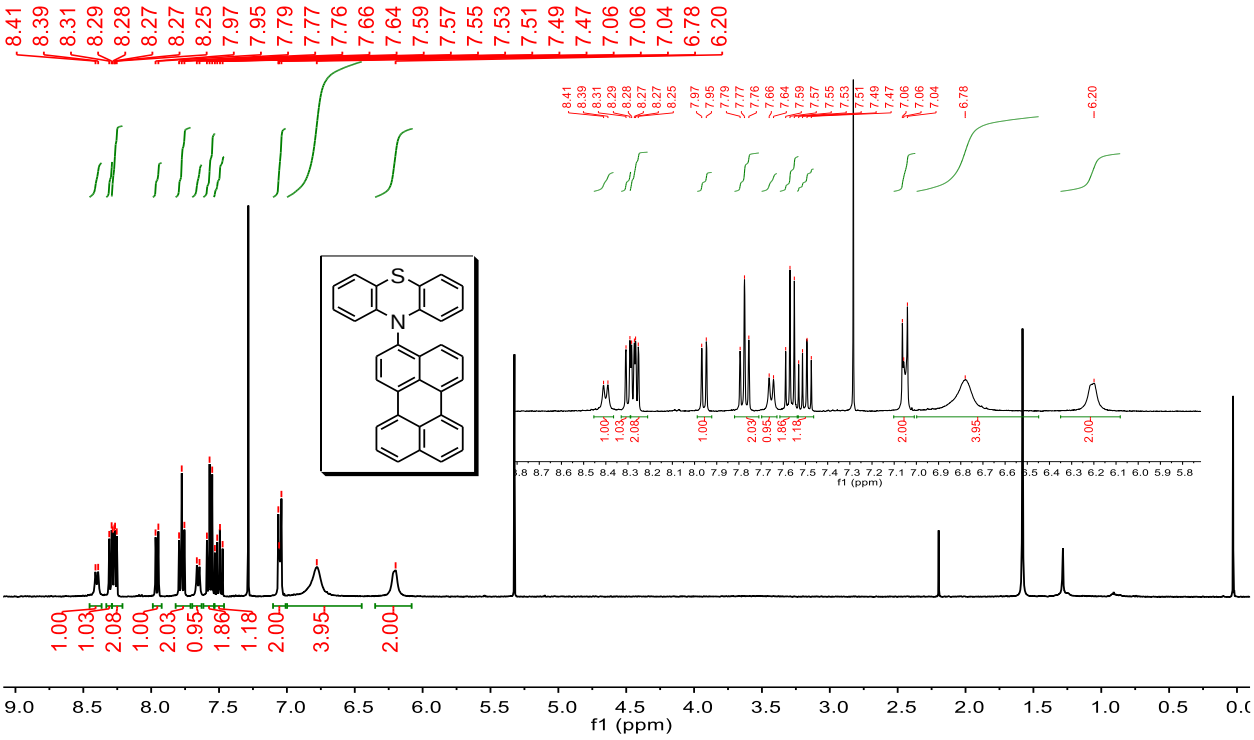


Figure S12. ^{1}H NMR spectrum of **Pery-N-PTZ** ($CDCl_3$, 500 MHz).

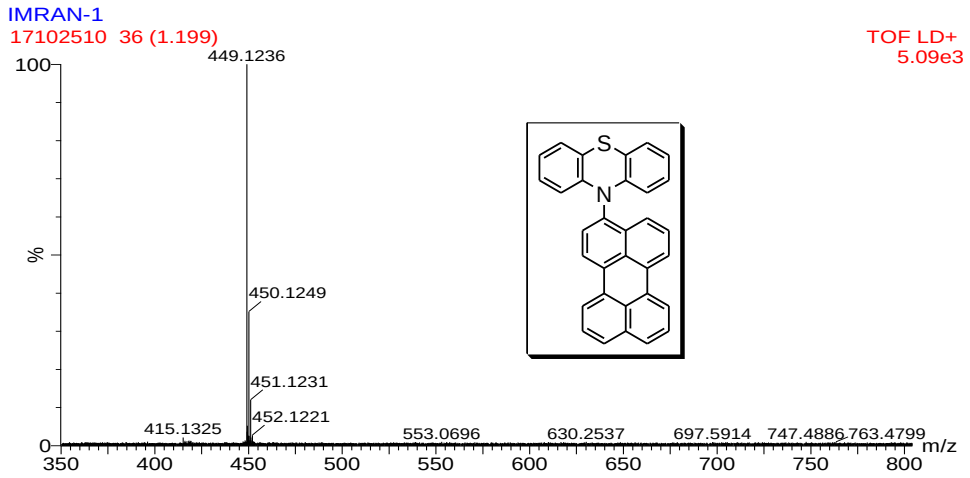


Figure S13. MALDI-HRMS spectrum of **Pery-N-PTZ**.

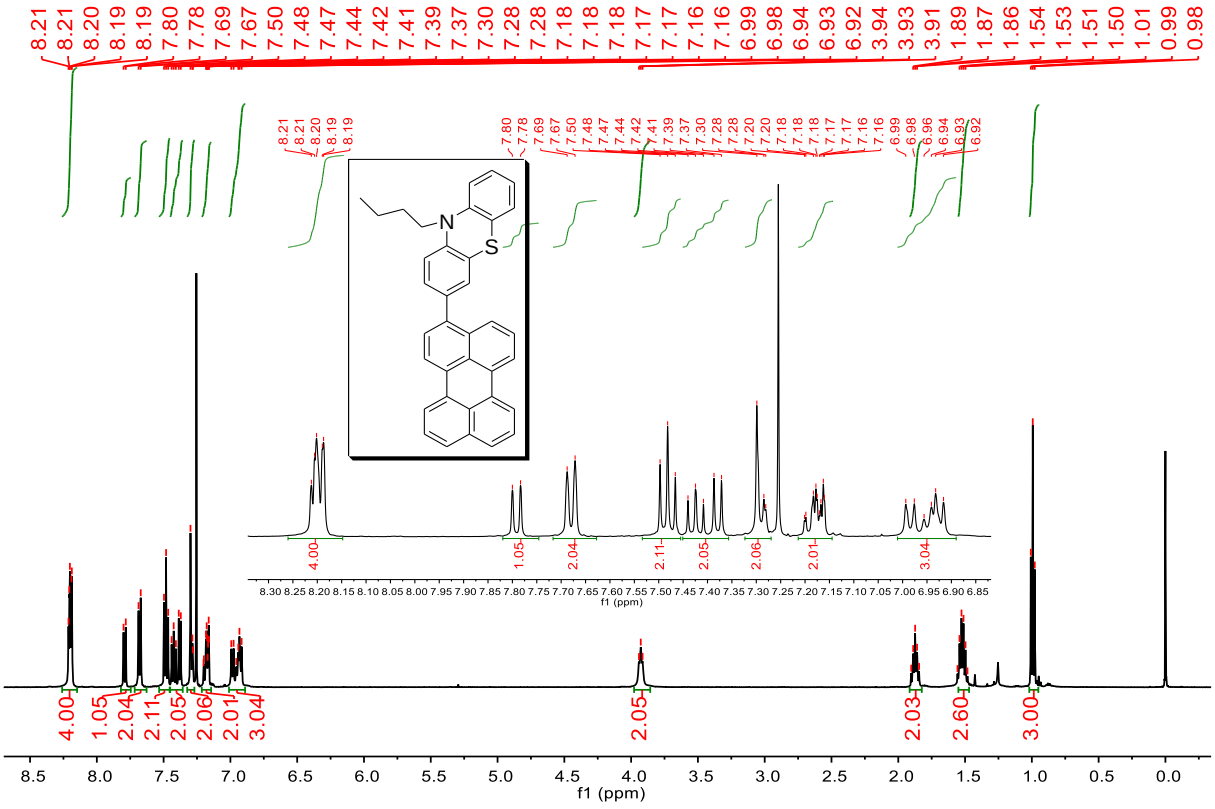


Figure S14. ^{1}H NMR spectrum of **Pery-C-PTZ** ($CDCl_3$, 500 MHz).

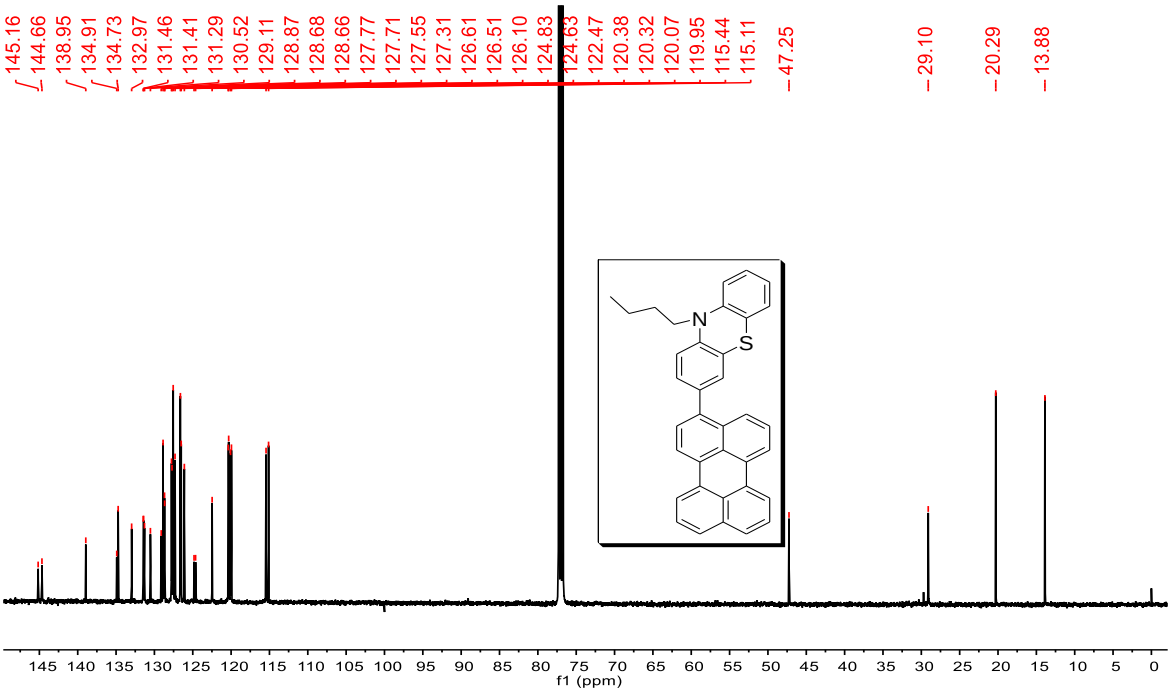


Figure S15. ^{13}C NMR spectrum of **Pery-C-PTZ** ($CDCl_3$, 126 MHz).

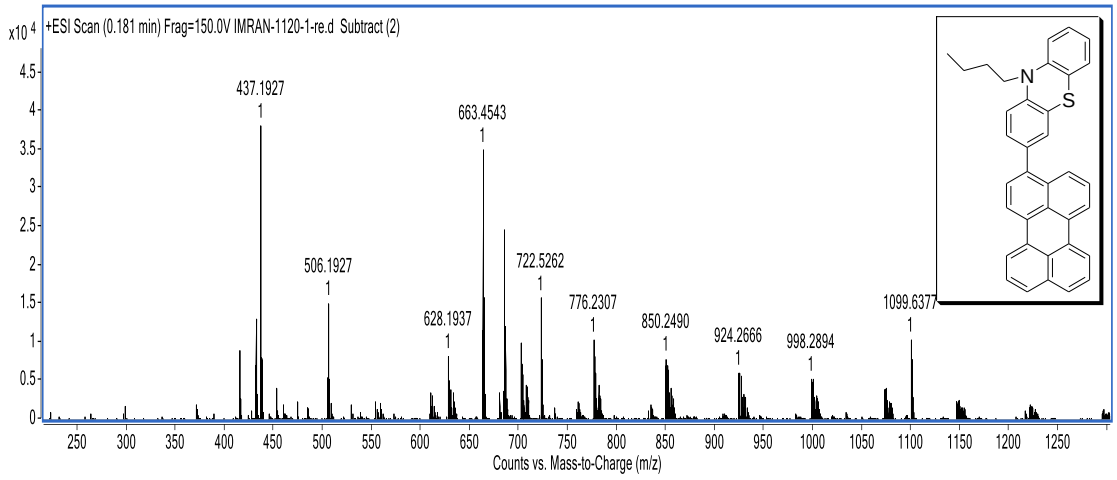


Figure S16. TOF-ESI MS spectrum of **Pery-C-PTZ**.

4. UV–Vis Absorption Spectra

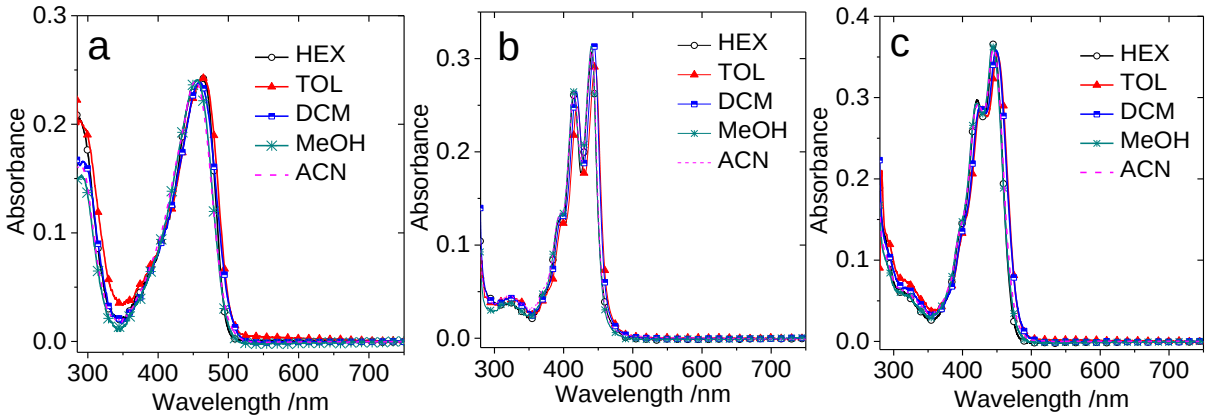


Figure S17. UV–Vis absorption spectra of compounds in different solvents, (a) **Pery-DPA**, (b) **Pery-N-PTZ** (c) **Pery-C-PTZ**, $c = 1.0 \times 10^{-5}$ M. 20 °C.

5. Fluorescence Emission Spectra

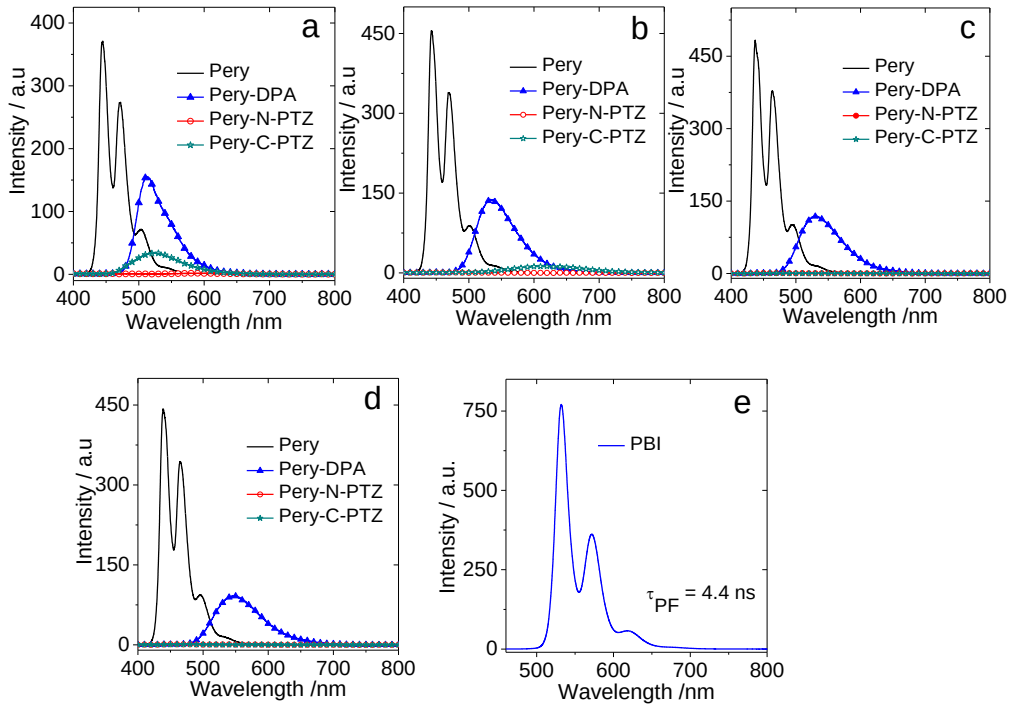


Figure S18. Fluorescence emission spectra of compounds (a) in toluene (λ_{ex} = 390 nm, A = 0.101); (b) in DCM (λ_{ex} = 394 nm, A = 0.107); (c) in MeOH (λ_{ex} = 389 nm, A = 0.105); (d) in ACN (λ_{ex} = 390 nm, A = 0.108). Optically matched solutions were used. (e) Prompt fluorescence of **(PBI)** triplet acceptor. In deaerated DCM, c = ca.1.0 × 10^{-5} M, 20 °C.

6. Fluorescence Lifetime

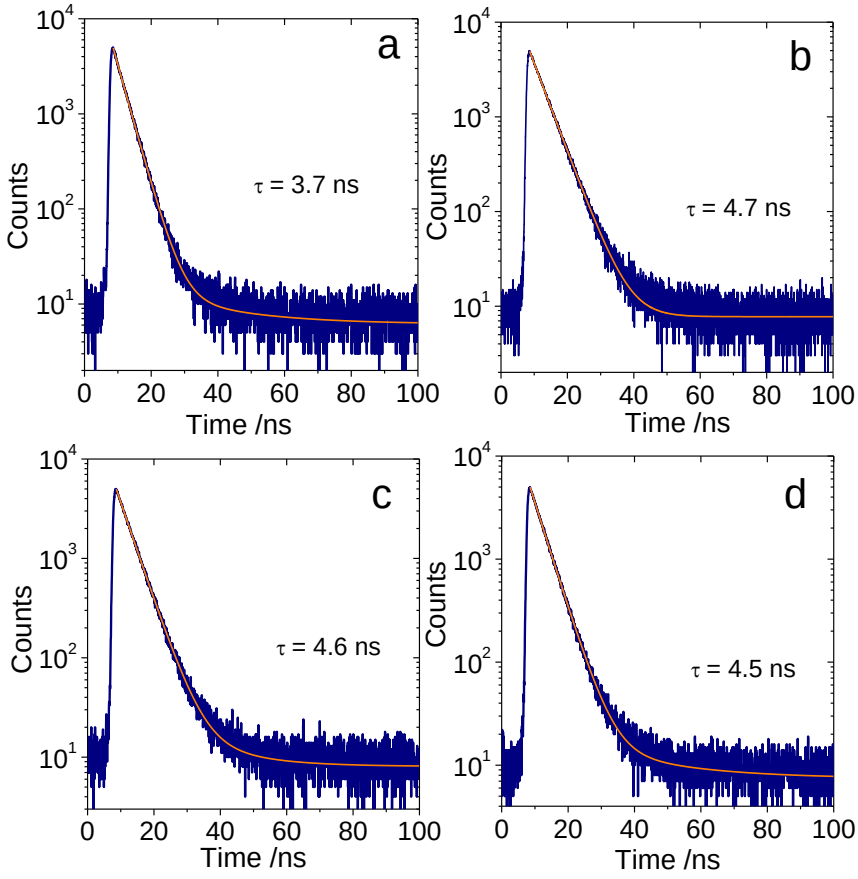


Figure S19. Fluorescence decay curves of perylene (a) In *n*-hexane at 436, (b) In toluene at 441 nm, (c) In DCM at 444, and (d) In ACN at 439 nm Excited with a picosecond pulsed laser (405 nm). $c = 1.0 \times 10^{-5}$ M. 20 °C.

Table S1. Fluorescence lifetime of the fluorescence emission in different solvents.

Compounds	τ_F [ns] [c]
Pery [a]	3.7 [d]/4.7 [e]/4.6 [f]/4.5 [g]
Pery-DPA [b]	3.9 [d]/4.4 [e]/6.5 [f]/7.0 [g]
Pery-N-PTZ [b]	4.5 [d] /7.4 [e]/3.8 [f]/3.8 [g]
Pery-C-PTZ [b]	1.6 [d] /1.4 [e]/4.3 [f]/1.9 [g]

[a] λ_{ex} = 400 nm for fluorescence lifetime measurements, [b] λ_{ex} = 445 nm for fluorescence lifetime measurements. [c] Fluorescence lifetimes, [d] In *n*-hexane. [e] In toluene. [f] In DCM. [g] In ACN. $c = 1.0 \times 10^{-5}$ M. 20 °C.

7. Redox Properties of the Compounds

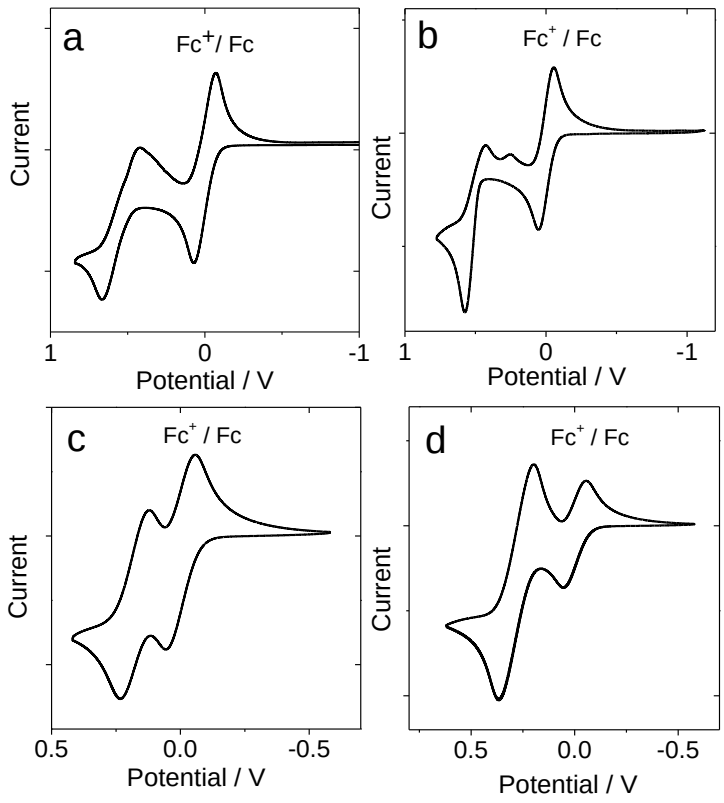


Figure S20. Cyclic voltammogram of the compounds (a) **Pery,** (b) **diphenylamine,** (c) **phenothiazine,** (d) **10-butyl-10*H*-phenothiazine**. Ferrocene was used as internal reference. Condition: in deaerated DCM containing 0.10 M $Bu_4N[PF_6]$ as supporting electrolyte, $Ag/AgNO_3$ as reference electrode. Scan rates: 50 mV/s. $c = 1.0 \times 10^{-5}$ M. 20 °C.

8. Nanosecond Transient Absorption Spectroscopy

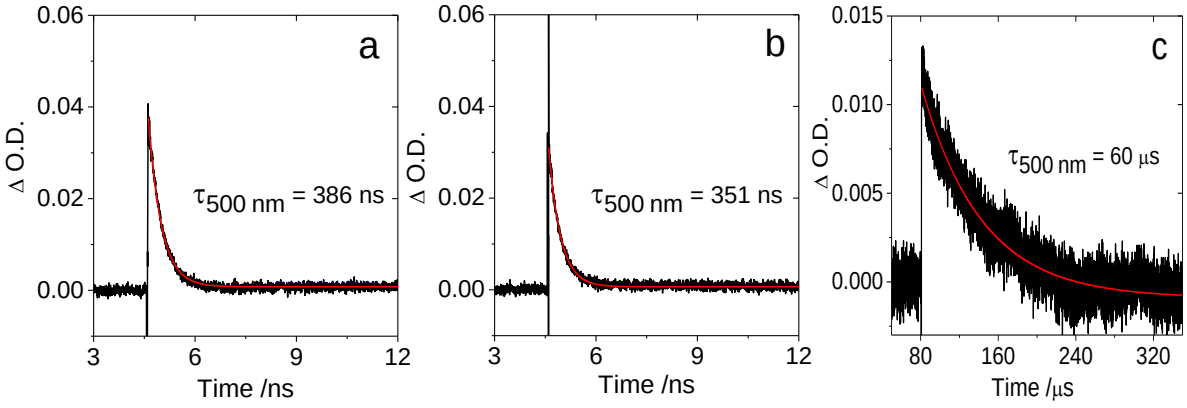


Figure S21. Decay traces of compounds (a) **Pery-N-PTZ,** (b) **Pery-C-PTZ.** In aerated DCM. $c = 1.0 \times 10^{-5}$ M and (c) **3-bromoperylene.** In deaerated toluene. $c = 5.0 \times 10^{-6}$ M. 20 °C.

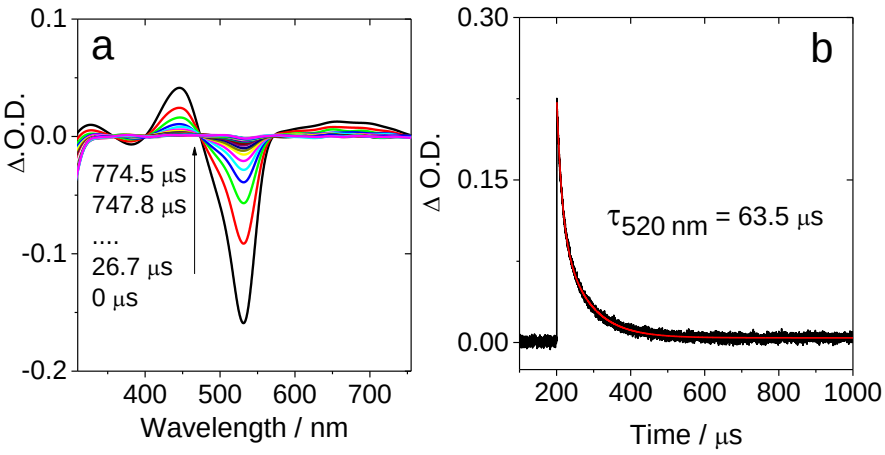


Figure S22. Nanosecond transient absorption spectra of (a) triplet photosensitizer (2,6-diiodobodipy) (b) decay trace at 520 nm. In deaerated DCM. 20 °C.

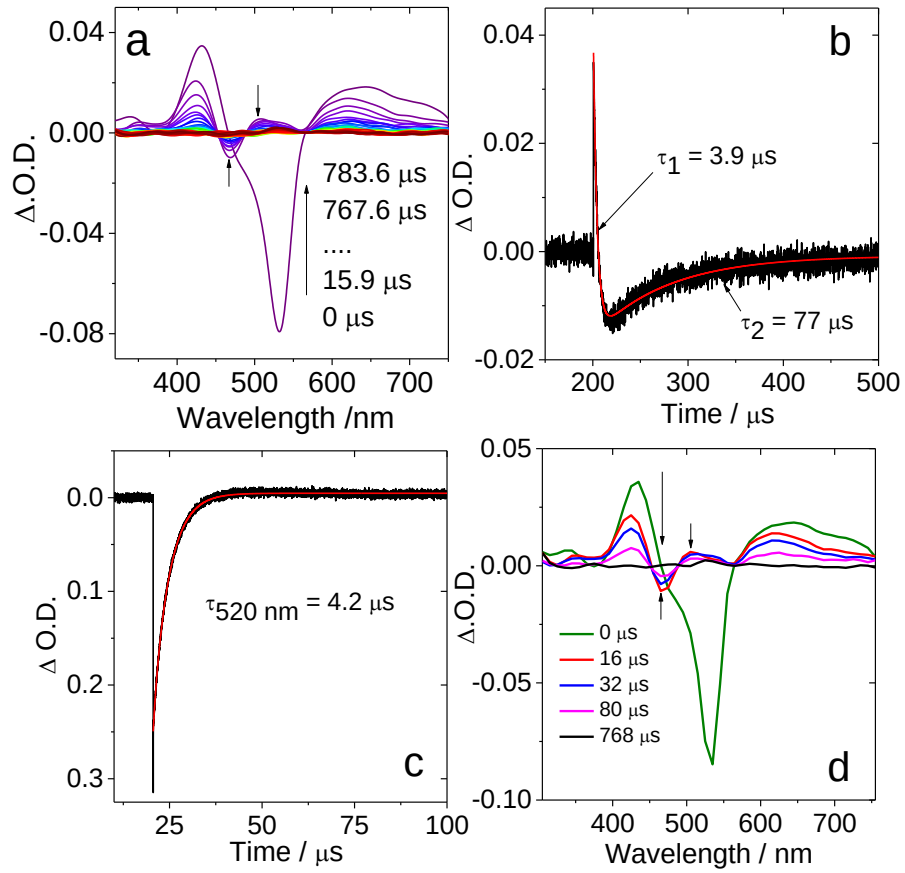


Figure S23. (a) Intermolecular triplet-triplet energy transfer (TTET) from 2,6-diiodobodipy to **Pery-DPA**, monitored by nanosecond transient absorption spectra of the mixture of 2,6-diiodobodipy and **Pery-DPA**. *c* [Diiodobodipy] = 1.0 × 10^{-5} M, *c* [**Pery-DPA**] = 4.0 ×10^{-5} M. (b) Decay trace of the mixture at 465 nm, (c) decay trace of the mixture at 520 nm. (d) Transient absorption spectra of the mixture with different delay time. The triplet energy donor 2,6-diiodoBodipy was selectively excited at 532 nm with OPO pulsed laser. In deaerated DCM. 20 °C.

9. Femtosecond Transient Absorption Spectroscopy.

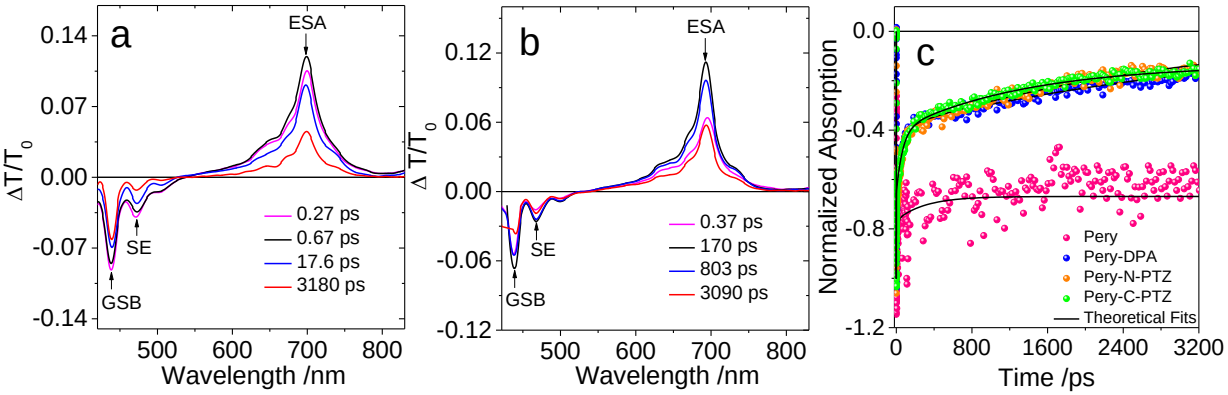


Figure S24. Femtosecond time-resolved transient absorption spectra of **Perylene** at different time delays. (a) In DCM, (b) In ACN and (c) Comparison of the decay traces of the compounds at 450 nm. GSB; Ground state bleach, ESA; S_1 excited state absorption. λ_{ex} = 400 nm, c = 1.0 × 10^{-3} M. 20 °C.

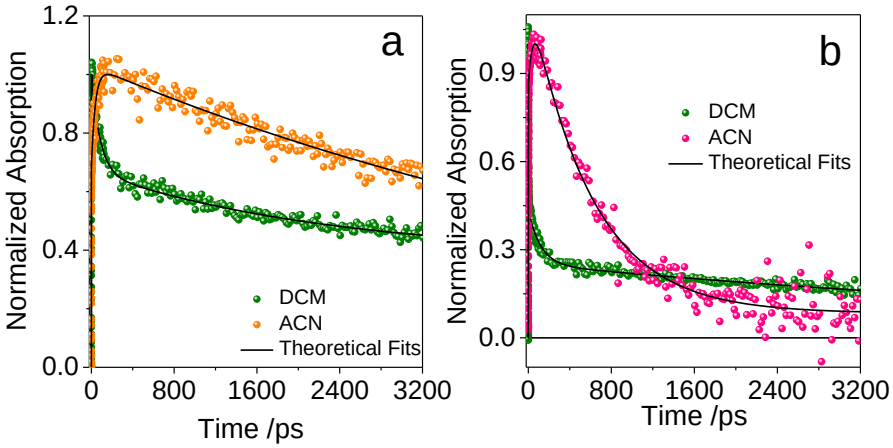


Figure S25. Decay traces of the compounds in different solvents at 650 nm. (a) **Pery-DPA,** (b) **Pery-C-PTZ**.

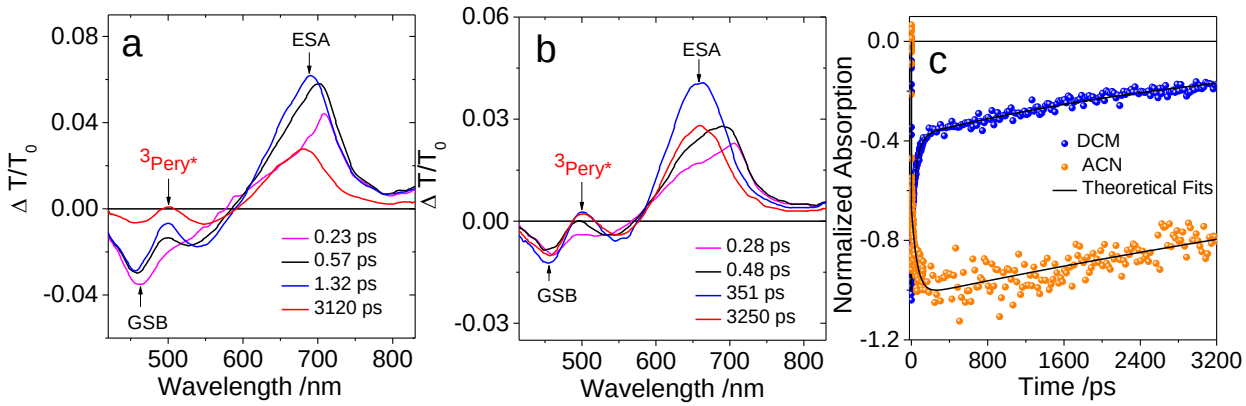


Figure S26. Femtosecond time-resolved transient absorption spectra of **Pery-DPA** at different time delays (a) in DCM, (b) in ACN and (c) decay traces at 450 nm in both solvents. GSB; Ground state bleach, ESA; S_1 excited state absorption. λ_{ex} = 400 nm, c = 1.0 × 10^{-3} M. 20 °C.

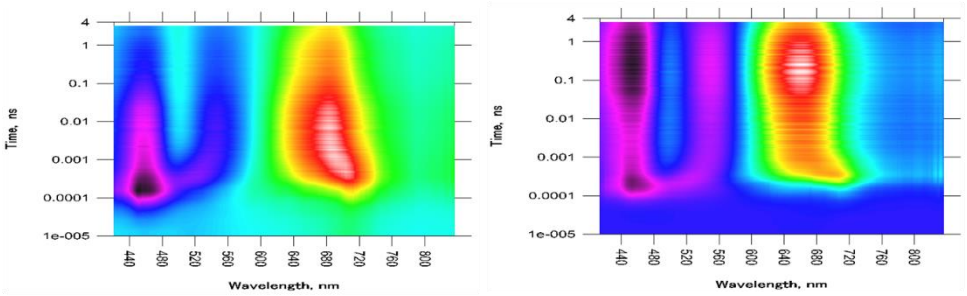


Figure S27. Transient absorption contour maps of **Pery-DPA** (left) DCM and (right) ACN, λ_{ex} = 400 nm.

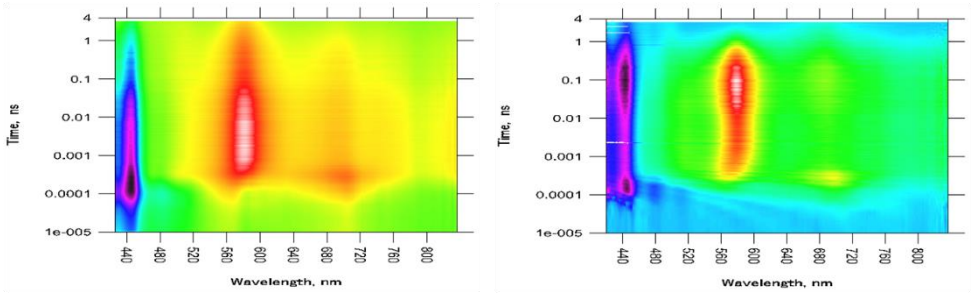


Figure S28. Transient absorption contour maps of **Pery-N-PTZ** (left) DCM and (right) ACN**,** λ_{ex} = 400 nm.

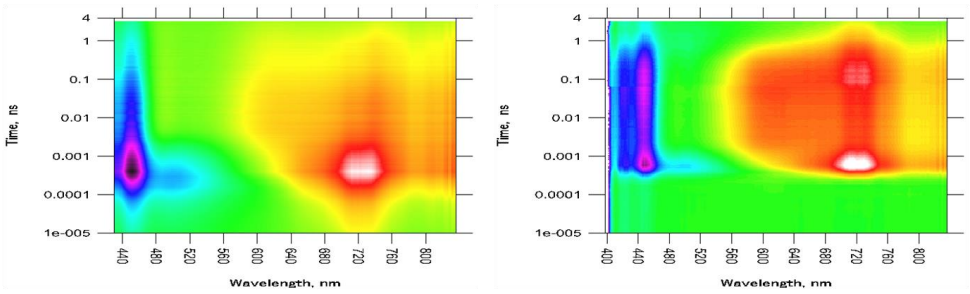


Figure S29. Transient absorption contour maps of **Pery-C-PTZ** (left) DCM and (right) ACN**,** λ_{ex} = 400 nm.

10. TTET/TTA-Induced Delayed Fluorescence

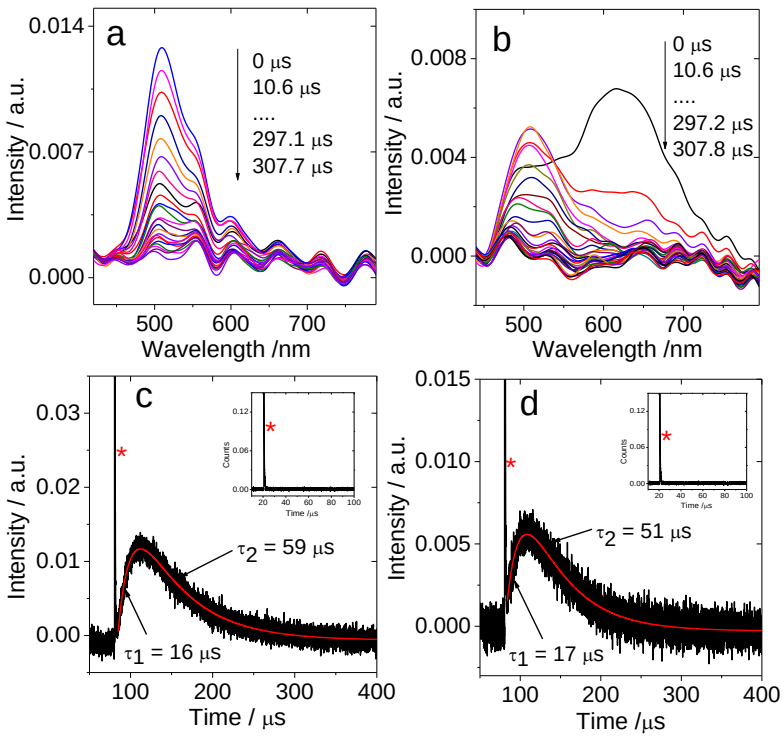


Figure S30. Delayed fluorescence with (a) **Pery-N-PTZ**, (b) **Pery-C-PTZ** as triplet photosensitizer and Solvent Green 5 triplet accepter. The decay traces (c) **Pery-N-PTZ** (d) **Pery-C-PTZ.** Insets in (c) and (d): only accepter, note there is no signal observed. Excited at 445 nm and emission was monitored at 510 nm. In deaerated DCM; The asterisks indicated the scattered laser. *c* [photosensitizer] and [accepter] = 1.0×10^{-5} M, 20 °C.

11. Crystallographic Data

Table S2. Crystal Data and Structure Refinement for **Pery-N-PTZ.**

Compound	**Pery-N-PTZ**
Empirical formula	$C_{32}H_{24.50}NO_{2.75}S$
Formula weight	499.09
Colour	yellow
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system,	monoclinic
Space group	$P2_1/c$
a (Å)	17.192 (14)
b (Å)	11.141 (09)
c (Å)	14.656 (11)
α (deg)	90
β (deg)	110.892(12)
γ (deg)	90
Volume (Å^3)	2623 (4)
Z	4
Density calculated (Mg/m^3)	1.264
Absorption coefficient (mm^{-1})	0.156
F (000)	1046
Crystal size (mm)	0.51 × 0.42 × 0.33
θ (deg)	2.22 – 27.23
Limiting indices	-18<=h<=2, -14<=k<=13, -16<=l<=18
Reflections collected / unique	15329 / 5710 [R(int) = 0.0747]
Completeness to θ = 27.23	97.3 %
Absorption correction	none
Max. and min. transmission	0.9503 and 0.9246
Refinement method	full matrix least squares on F^2
Data / restraints / parameters	5710 / 0 / 343
Goodness of fit on F^2	1.293
Largest peak	1.512,
Deepest hole	-0.423
R_1	0.1365
R_1 (all data)	0.2124
wR_2	0.3722
wR_2 (all data)	0.4263

Table S3. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Pery-N-PTZ**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O4	9368(8)	743(12)	616(11)	58(3)
O3	554(6)	9489(13)	1413(8)	133(5)
O2	-939(3)	9382(4)	1901(4)	99(2)
C1	5051(5)	6394(5)	2571(5)	77(2)
C2	4235(6)	6194(5)	2047(6)	89(2)
C3	3833(4)	5273(5)	2325(4)	72(2)
C4	4220(4)	4530(4)	3098(4)	59(1)
C5	5066(3)	4717(4)	3630(4)	57(1)
C6	5489(4)	5654(5)	3348(5)	68(2)
C7	6335(5)	5843(6)	3885(6)	80(2)
C8	6750(4)	5117(6)	4636(6)	83(2)
C9	6337(4)	4208(5)	4916(5)	69(2)
C10	5504(3)	3974(4)	4433(4)	56(1)
C11	5060(3)	3015(4)	4727(4)	52(1)
C12	4225(3)	2811(4)	4193(4)	51(1)
C13	3779(3)	3539(4)	3371(4)	54(1)
C14	2956(3)	3297(5)	2866(4)	64(1)
C15	2540(4)	2334(5)	3095(4)	70(2)
C16	2963(3)	1629(4)	3904(4)	62(1)
C17	3799(3)	1841(4)	4466(4)	54(1)
C18	4228(4)	1140(4)	5271(4)	61(1)
C19	5034(4)	1367(5)	5797(4)	68(2)
C20	5447(4)	2301(5)	5515(4)	65(2)
C21	2463(3)	-420(5)	3577(4)	65(2)
C22	2709(4)	-468(5)	2794(5)	78(2)
C23	2614(5)	-1496(6)	2247(6)	102(2)
C24	2278(6)	-2496(7)	2461(6)	103(2)
C25	2013(5)	-2488(6)	3260(5)	89(2)
C26	2116(4)	-1454(5)	3832(4)	69(2)
C27	1670(4)	-41(6)	5022(5)	75(2)
C28	1138(4)	219(8)	5505(5)	88(2)
C29	976(5)	1391(8)	5709(6)	100(2)
C30	1380(5)	2287(7)	5406(5)	90(2)
C31	1905(4)	2027(6)	4901(5)	74(2)
C32	2044(3)	880(5)	4685(4)	62(1)
N1	2555(3)	619(4)	4151(4)	66(1)
O1	212(3)	11162(5)	2688(5)	147(3)
S1	1916(1)	-1553(2)	4905(2)	92(1)

Table S4. Anisotropic Displacement Parameters ($\times 10^3$) for **Pery-N-PTZ.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	59(3)	58(3)	58(3)	0(1)	22(2)	1(1)
O3	74(5)	228(13)	115(9)	47(8)	58(6)	51(7)
O2	113(3)	69(3)	117(4)	-2(3)	43(3)	-48(2)
C1	124(5)	51(3)	75(5)	3(3)	59(4)	-17(3)
C2	143(7)	59(4)	79(5)	8(3)	56(5)	-7(4)
C3	109(4)	54(3)	60(4)	6(3)	38(3)	-3(3)
C4	91(4)	44(3)	53(3)	-6(2)	41(3)	-1(2)
C5	83(3)	46(3)	54(3)	-12(2)	41(3)	-7(2)
C6	99(4)	56(3)	65(4)	-19(3)	51(3)	-21(3)
C7	107(5)	63(4)	91(5)	-19(4)	61(4)	-27(3)
C8	88(4)	74(4)	104(6)	-27(4)	53(4)	-29(3)
C9	87(4)	56(3)	71(4)	-8(3)	35(3)	-7(3)
C10	75(3)	45(3)	56(3)	-12(2)	34(3)	-5(2)
C11	67(3)	42(2)	50(3)	-7(2)	25(2)	-2(2)
C12	71(3)	38(2)	49(3)	-4(2)	28(2)	-3(2)
C13	75(3)	38(2)	55(3)	-4(2)	31(3)	-1(2)
C14	72(3)	54(3)	66(4)	5(3)	23(3)	3(2)
C15	72(3)	70(4)	70(4)	9(3)	26(3)	-4(3)
C16	70(3)	52(3)	67(4)	2(3)	30(3)	-10(2)
C17	70(3)	45(3)	50(3)	-5(2)	26(3)	-2(2)
C18	83(4)	45(3)	61(4)	4(3)	31(3)	-9(2)
C19	76(4)	61(3)	61(4)	8(3)	17(3)	-8(3)
C20	72(3)	63(3)	56(4)	-2(3)	17(3)	-6(3)
C21	73(3)	62(3)	57(4)	2(3)	21(3)	-8(3)
C22	111(5)	62(4)	70(4)	-1(3)	44(4)	0(3)
C23	160(7)	80(5)	77(5)	-4(4)	56(5)	-8(5)
C24	159(7)	80(5)	79(5)	-17(4)	52(5)	-11(5)
C25	112(5)	60(4)	82(5)	-3(3)	19(4)	-26(3)
C26	83(4)	57(3)	62(4)	1(3)	19(3)	-10(3)
C27	76(3)	87(4)	58(4)	0(3)	22(3)	-21(3)
C28	81(4)	114(6)	80(5)	5(4)	43(4)	-19(4)
C29	95(5)	125(6)	95(6)	-11(5)	51(4)	-14(4)
C30	103(5)	91(5)	83(5)	-6(4)	39(4)	-2(4)
C31	85(4)	69(4)	71(4)	2(3)	31(3)	-5(3)
C32	65(3)	70(3)	49(3)	-4(3)	19(3)	-16(3)
N1	75(3)	60(3)	67(3)	-7(2)	31(2)	-22(2)
O1	80(3)	127(4)	169(6)	-55(4)	-37(3)	-22(3)
S1	131(2)	72(1)	82(1)	9(1)	49(1)	-21(1)

Table S5. Bond Lengths in Å for **Pery-N-PTZ.**

Atom	Atom	Length/ Å
O4	H4A	0.8500
O4	H4B	0.8501
O3	H3A	0.8499
O3	H3B	0.8500
O2	H2A	0.9600
O2	H2C	0.9599
C1	C2	1.356(10)
C1	C6	1.390(9)
C1	H1	0.9300
C2	C3	1.376(8)
C2	H2	0.9300
C3	C4	1.369(8)
C3	H3	0.9300
C4	C5	1.399(8)
C4	C13	1.474(7)
C5	C6	1.415(7)
C5	C10	1.415(8)
C6	C7	1.401(9)
C7	C8	1.348(10)
C7	H7	0.9300
C8	C9	1.381(8)
C8	H8	0.9300
C9	C10	1.377(8)
C9	H9	0.9300
C10	C11	1.464(7)
C11	C20	1.364(7)
C11	C12	1.387(7)
C12	C13	1.427(7)
C12	C17	1.440(7)
C13	C14	1.370(8)
C14	C15	1.395(7)
C14	H14	0.9300
C15	C16	1.392(8)
C15	H15	0.9300
C16	C17	1.399(8)
C16	N1	1.439(6)
C17	C18	1.388(7)
C18	C19	1.348(8)
C18	H18	0.9300
C19	C20	1.402(8)
C19	H19	0.9300
C20	H20	0.9300

Atom	Atom	Length/ Å
C21	C22	1.359(8)
C21	N1	1.406(7)
C21	C26	1.407(7)
C22	C23	1.374(9)
C22	H22	0.9300
C23	C24	1.343(10)
C23	H23	0.9300
C24	C25	1.399(11)
C24	H24	0.9300
C25	C26	1.399(8)
C25	H25	0.9300
C26	S1	1.729(7)
C27	C28	1.373(9)
C27	C32	1.391(8)
C27	S1	1.760(7)
C28	C29	1.390(10)
C28	H28	0.9300
C29	C30	1.377(10)
C29	H29	0.9300
C30	C31	1.386(9)
C30	H30	0.9300
C31	C32	1.358(8)
C31	H31	0.9300
C32	N1	1.400(7)
O1	H1A	0.9600
O1	H1C	0.9600

Table S6. Bond Angles in ° for **Pery-N-PTZ.**

Atom	Atom	Atom	Angle/°
H4A	O4	H4B	109.5
H3A	O3	H3B	109.5
H2A	O2	H2C	109.5
C2	C1	C6	121.0(6)
C2	C1	H1	119.5
C6	C1	H1	119.5
C1	C2	C3	118.8(7)
C1	C2	H2	120.6
C3	C2	H2	120.6
C4	C3	C2	123.3(7)
C4	C3	H3	118.4
C2	C3	H3	118.4
C3	C4	C5	118.2(5)

Atom	Atom	Atom	Angle/°
C3	C4	C13	122.2(5)
C5	C4	C13	119.5(5)
C4	C5	C6	119.1(5)
C4	C5	C10	121.0(5)
C6	C5	C10	119.9(5)
C1	C6	C7	121.4(6)
C1	C6	C5	119.5(6)
C7	C6	C5	119.0(6)
C8	C7	C6	120.7(6)
C8	C7	H7	119.7
C6	C7	H7	119.7
C7	C8	C9	120.2(6)
C7	C8	H8	119.9
C9	C8	H8	119.9
C10	C9	C8	122.5(6)
C10	C9	H9	118.8
C8	C9	H9	118.8
C9	C10	C5	117.6(5)
C9	C10	C11	122.8(5)
C5	C10	C11	119.6(5)
C20	C11	C12	118.5(5)
C20	C11	C10	121.8(5)
C12	C11	C10	119.7(5)
C11	C12	C13	121.3(4)
C11	C12	C17	119.5(5)
C13	C12	C17	119.2(5)
C14	C13	C12	119.0(5)
C14	C13	C4	122.2(5)
C12	C13	C4	118.8(5)
C13	C14	C15	122.7(5)
C13	C14	H14	118.7
C15	C14	H14	118.7
C16	C15	C14	118.9(5)
C16	C15	H15	120.6
C14	C15	H15	120.6
C15	C16	C17	121.4(5)
C15	C16	N1	120.2(5)
C17	C16	N1	118.4(5)
C18	C17	C16	121.9(5)
C18	C17	C12	119.4(5)
C16	C17	C12	118.8(5)
C19	C18	C17	120.4(5)
C19	C18	H18	119.8
C17	C18	H18	119.8

Atom	Atom	Atom	Angle/°
C18	C19	C20	119.7(5)
C18	C19	H19	120.2
C20	C19	H19	120.2
C11	C20	C19	122.5(5)
C11	C20	H20	118.7
C19	C20	H20	118.7
C22	C21	N1	122.4(5)
C22	C21	C26	118.7(5)
N1	C21	C26	118.9(5)
C21	C22	C23	121.2(6)
C21	C22	H22	119.4
C23	C22	H22	119.4
C24	C23	C22	121.8(7)
C24	C23	H23	119.1
C22	C23	H23	119.1
C23	C24	C25	119.1(7)
C23	C24	H24	120.5
C25	C24	H24	120.5
C26	C25	C24	119.8(6)
C26	C25	H25	120.1
C24	C25	H25	120.1
C25	C26	C21	119.4(6)
C25	C26	S1	117.9(5)
C21	C26	S1	122.3(5)
C28	C27	C32	120.3(6)
C28	C27	S1	118.6(5)
C32	C27	S1	121.0(5)
C27	C28	C29	122.0(7)
C27	C28	H28	119.0
C29	C28	H28	119.0
C30	C29	C28	116.7(7)
C30	C29	H29	121.7
C28	C29	H29	121.7
C29	C30	C31	121.4(7)
C29	C30	H30	119.3
C31	C30	H30	119.3
C32	C31	C30	121.5(6)
C32	C31	H31	119.3
C30	C31	H31	119.3
C31	C32	C27	118.1(6)
C31	C32	N1	121.5(5)
C27	C32	N1	120.4(5)
C32	N1	C21	123.1(4)
C32	N1	C16	116.0(4)

C21	N1	C16	117.0(5)
H1A	O1	H1C	109.5
C26	S1	C27	99.2(3)

Table S7. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Pery-N-PTZ**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	**x**	**y**	**z**	U_{eq}
H4A	9332	897	34	87
H4B	9861	883	1004	87
H3A	571	9594	845	199
H3B	1027	9652	1839	199
H2A	-847	9360	1293	149
H2C	-672	10077	2266	149
H1	5321	7036	2408	92
H2	3951	6671	1511	107
H3	3272	5149	1969	87
H7	6612	6477	3722	96
H8	7318	5228	4967	100
H9	6632	3736	5451	83
H14	2662	3796	2349	77
H15	1990	2166	2713	84
H18	3957	509	5448	74
H19	5315	906	6345	82
H20	6005	2440	5879	78
H22	2947	206	2625	93
H23	2787	-1500	1714	123
H24	2222	-3185	2084	124
H25	1768	-3169	3409	107
H28	878	-409	5703	105
H29	613	1562	6033	120
H30	1300	3082	5543	109
H31	2168	2653	4705	89
H1A	348	11977	2592	221
H1C	496	10938	3357	221

Table S8. Crystal Data and Structure Refinement for **Pery-C-PTZ.**

Compound	**Pery-C-PTZ**
Empirical formula	$C_{35.50}H_{25.50}NO_0S$
Formula weight	498.13
Colour	yellow
Temperature (K)	296 (2)
Wavelength (Å)	0.71073
Crystal system,	triclinic
Space group	P-1
a (Å)	8.3216(11)
b (Å)	10.3887(13)
c (Å)	15.2001(19)
α (deg)	85.457(9)
β (deg)	84.712(9)
γ (deg)	78.669(8)
Volume ($Å^3$)	1280.4 (3)
Z	2
Density calculated (Mg/m^3)	1.304
Absorption coefficient (mm^{-1})	0.152
F (000)	523
Crystal size (mm)	0.42 × 0.37 × 0.30
θ (deg.)	1.35–25.99
Limiting indices	-10<=h<=10-12<=k<=12, -18<=l<=18
Reflections collected / unique	10140 / 4844 [R(int) = 0.0675]
Completeness to θ = 25.99	96.2 %
Absorption correction	none
Max. and min. transmission	0.9557, 0.9388
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	4844 / 0 / 341
Goodness of fit on F^2	1.038
Largest peak	0.827
Deepest hole	- 0.352
R_1	0.0884
R_1 (all data)	0.1311
wR_2	0.2689
wR_2 (all data)	0.3125

Table S9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **Pery-C-PTZ**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C36A	2800(30)	14020(20)	-335(14)	248(9)
C35A	3520(15)	13142(11)	424(7)	136(4)
C34A	3072(15)	13276(12)	1373(8)	140(4)
C34B	1680(20)	13422(15)	817(10)	92(5)
C35B	2780(30)	14610(20)	617(16)	141(8)
C36B	2490(30)	15090(30)	-259(17)	155(9)
S1	3085(1)	8681(1)	1145(1)	71(1)
C11	7980(4)	6410(3)	5333(2)	50(1)
C12	8679(4)	7465(3)	4880(2)	47(1)
C5	10402(5)	5844(3)	6247(2)	51(1)
C17	7808(4)	8259(3)	4200(2)	49(1)
C4	11067(5)	6914(4)	5807(2)	54(1)
C18	6238(5)	8059(4)	4024(2)	53(1)
C10	8867(5)	5589(3)	6031(2)	51(1)
C13	10231(4)	7689(3)	5071(2)	48(1)
C20	6504(5)	6208(4)	5090(2)	58(1)
C6	11260(5)	5059(4)	6927(2)	57(1)
C16	8600(5)	9192(4)	3703(2)	56(1)
N1	1980(4)	11375(3)	1686(2)	68(1)
C19	5635(5)	7028(4)	4454(2)	58(1)
C15	10102(5)	9356(4)	3869(2)	58(1)
C21	5209(5)	8949(4)	3388(2)	56(1)
C14	10925(5)	8612(4)	4552(2)	58(1)
C3	12476(5)	7182(4)	6098(3)	64(1)
C22	4679(4)	8471(4)	2669(2)	55(1)
C7	10597(6)	3997(4)	7356(3)	68(1)
C24	3092(5)	10591(4)	2255(2)	56(1)
C23	3662(4)	9290(4)	2094(2)	56(1)
C26	4648(5)	10273(4)	3535(3)	61(1)
C1	12717(5)	5354(4)	7170(3)	68(1)
C9	8260(5)	4569(4)	6497(2)	62(1)
C2	13329(5)	6392(4)	6768(3)	72(1)
C28	685(5)	10794(4)	1459(2)	65(1)
C25	3610(5)	11090(4)	2984(2)	61(1)
C8	9120(6)	3784(4)	7154(3)	72(1)
C27	1036(5)	9506(4)	1209(2)	65(1)
C29	-226(7)	8911(6)	994(3)	82(1)
C32	-959(6)	11470(5)	1505(3)	86(2)

Atom	x	y	z	U_{eq}
C30	-1795(7)	9576(7)	1016(3)	98(2)
C31	-2174(7)	10829(8)	1266(3)	101(2)
C33	1765(8)	12811(5)	1680(3)	35(1)

Table S10. Anisotropic Displacement Parameters ($\times 10^3$) for **Pery-C-PTZ.** The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$.

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	79(1)	80(1)	51(1)	-13(1)	-9(1)	-5(1)
C11	50(2)	59(2)	43(2)	-9(2)	3(2)	-16(2)
C2	49(2)	51(2)	42(2)	-10(1)	5(1)	-15(2)
C5	57(2)	51(2)	45(2)	-7(2)	3(2)	-12(2)
C17	54(2)	53(2)	43(2)	-6(2)	0(2)	-14(2)
C4	50(2)	61(2)	53(2)	-14(2)	3(2)	-14(2)
C18	54(2)	59(2)	47(2)	-7(2)	-1(2)	-13(2)
C10	61(2)	48(2)	45(2)	-5(1)	1(2)	-12(2)
C13	51(2)	51(2)	43(2)	-9(1)	4(2)	-13(2)
C20	55(2)	61(2)	62(2)	1(2)	0(2)	-27(2)
C6	60(2)	58(2)	50(2)	-8(2)	-3(2)	-5(2)
C16	57(2)	70(2)	44(2)	-1(2)	2(2)	-20(2)
N1	80(2)	68(2)	51(2)	4(2)	-5(2)	-3(2)
C19	50(2)	68(2)	61(2)	-3(2)	-4(2)	-23(2)
C15	64(3)	60(2)	52(2)	1(2)	6(2)	-25(2)
C21	52(2)	68(2)	51(2)	-5(2)	2(2)	-20(2)
C14	55(2)	61(2)	62(2)	-6(2)	2(2)	-20(2)
C3	60(3)	67(2)	68(2)	-7(2)	-6(2)	-20(2)
C22	57(2)	58(2)	51(2)	-7(2)	-1(2)	-10(2)
C7	79(3)	61(2)	59(2)	4(2)	-4(2)	-1(2)
C24	54(2)	63(2)	49(2)	3(2)	8(2)	-11(2)
C23	55(2)	59(2)	51(2)	-5(2)	3(2)	-9(2)
C26	62(3)	67(2)	56(2)	-12(2)	-1(2)	-19(2)
C1	69(3)	77(3)	57(2)	-4(2)	-15(2)	-4(2)
C9	64(3)	67(2)	56(2)	1(2)	2(2)	-22(2)
C2	61(3)	87(3)	68(2)	-9(2)	-13(2)	-11(2)
C28	63(3)	87(3)	39(2)	4(2)	0(2)	-6(2)
C25	66(3)	54(2)	62(2)	-5(2)	-1(2)	-15(2)
C8	90(3)	61(2)	63(2)	7(2)	0(2)	-15(2)
C27	70(3)	84(3)	38(2)	6(2)	-7(2)	-10(2)
C29	85(4)	110(4)	55(2)	20(2)	-21(2)	-33(3)
C32	72(3)	117(4)	52(2)	6(2)	-2(2)	14(3)

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C30	85(4)	147(5)	66(3)	23(3)	-19(3)	-38(4)
C31	59(3)	169(6)	66(3)	21(4)	-10(2)	-8(4)
C33	50(4)	17(2)	35(3)	8(2)	-3(2)	-1(2)

Table S11. Bond Lengths in Å for **Pery-C-PTZ**

Atom	Atom	Length/ Å
C36A	C35A	1.50(2)
C35A	C34A	1.466(14)
C34A	C33	1.308(12)
C34B	C33	1.413(15)
C34B	C35B	1.67(3)
C35B	C36B	1.41(3)
S1	C27	1.750(4)
S1	C23	1.762(4)
C11	C20	1.374(5)
C11	C12	1.440(4)
C11	C10	1.467(5)
C12	C13	1.416(5)
C12	C17	1.429(5)
C5	C6	1.421(5)
C5	C10	1.426(5)
C5	C4	1.430(5)
C17	C16	1.410(5)
C17	C18	1.415(5)
C4	C3	1.375(5)
C4	C13	1.472(5)
C18	C19	1.365(5)
C18	C21	1.491(5)
C10	C9	1.380(5)
C13	C14	1.374(5)
C20	C19	1.393(5)
C6	C1	1.395(6)
C6	C7	1.416(5)
C16	C15	1.343(5)
N1	C28	1.415(5)
N1	C24	1.417(5)
N1	C33	1.467(6)
C15	C14	1.393(5)
C21	C22	1.377(5)
C21	C26	1.392(5)
C3	C2	1.410(6)
C22	C23	1.392(5)
C7	C8	1.358(6)

Atom	Atom	Length/ Å
C24	C23	1.375(5)
C24	C25	1.396(5)
C26	C25	1.378(5)
C1	C2	1.360(6)
C9	C8	1.395(6)
C28	C27	1.388(6)
C28	C32	1.408(6)
C27	C29	1.393(6)
C29	C30	1.351(7)
C32	C31	1.403(8)
C30	C31	1.354(8)

Table S12. Bond Angles in ° for **Pery-C-PTZ.**

Atom	Atom	Atom	Angle/°
C34A	C35A	C36A	127.6(12)
C33	C34A	C35A	114.9(10)
C33	C34B	C35B	114.2(13)
C36B	C35B	C34B	104.3(19)
C27	S1	C23	97.18(19)
C20	C11	C12	118.4(3)
C20	C11	C10	122.5(3)
C12	C11	C10	119.1(3)
C13	C12	C17	120.0(3)
C13	C12	C11	121.2(3)
C17	C12	C11	118.8(3)
C6	C5	C10	120.0(3)
C6	C5	C4	119.3(3)
C10	C5	C4	120.7(3)
C16	C17	C18	122.5(3)
C16	C17	C12	117.5(3)
C18	C17	C12	120.0(3)
C3	C4	C5	118.0(3)
C3	C4	C13	122.4(3)
C5	C4	C13	119.6(3)
C19	C18	C17	119.3(3)
C19	C18	C21	118.8(3)
C17	C18	C21	121.9(3)
C9	C10	C5	118.2(3)
C9	C10	C11	122.1(3)
C5	C10	C11	119.7(3)
C14	C13	C12	118.8(3)
C14	C13	C4	121.9(3)

Atom	Atom	Atom	Angle/°
C12	C13	C4	119.2(3)
C11	C20	C19	122.1(3)
C1	C6	C7	121.3(4)
C1	C6	C5	119.9(4)
C7	C6	C5	118.9(4)
C15	C16	C17	121.8(3)
C28	N1	C24	115.9(3)
C28	N1	C33	119.8(4)
C24	N1	C33	118.8(4)
C18	C19	C20	121.2(4)
C16	C15	C14	120.6(3)
C22	C21	C26	117.5(4)
C22	C21	C18	121.2(3)
C26	C21	C18	121.2(3)
C13	C14	C15	121.2(4)
C4	C3	C2	122.3(4)
C21	C22	C23	121.3(4)
C8	C7	C6	120.3(4)
C23	C24	C25	118.8(3)
C23	C24	N1	119.0(4)
C25	C24	N1	122.2(4)
C24	C23	C22	120.6(4)
C24	C23	S1	118.7(3)
C22	C23	S1	120.7(3)
C25	C26	C21	121.9(4)
C2	C1	C6	120.9(4)
C10	C9	C8	121.7(4)
C1	C2	C3	119.5(4)
C27	C28	C32	118.9(5
C27	C28	N1	119.1(4)
C32	C28	N1	121.9(5)
C26	C25	C24	119.8(4)
C7	C8	C9	120.8(4)
C28	C27	C29	120.0(4)
C28	C27	S1	118.5(3)
C29	C27	S1	121.5(4)
C30	C29	C27	120.9(6)
C31	C32	C28	118.5(5)
C29	C30	C31	120.3(5)
C30	C31	C32	121.3(5)
C34A	C33	C34B	65.3(8)
C34A	C33	N1	114.1(7)
C34B	C33	N1	112.6(8)

Table S13. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Pery-C-PTZ.** U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H36A	3282	13662	-884	372
H36B	3030	14882	-307	372
H36C	1633	14064	-298	372
H35A	3382	12264	314	163
H35B	4693	13129	347	163
H34A	3992	12827	1697	167
H34B	2889	14201	1487	167
H34C	543	13789	723	110
H34D	2072	12758	392	110
H35C	2406	15305	1024	169
H35D	3937	14270	673	169
H36D	3086	15787	-426	232
H36E	1337	15418	-299	232
H36F	2857	14389	-649	232
H20	6071	5501	5358	69
H16	8067	9708	3249	68
H19	4626	6871	4319	70
H15	10598	9972	3524	70
H14	11962	8742	4659	70
H3	12881	7910	5843	76
H22	5008	7585	2564	67
H7	11177	3444	7779	82
H26	4983	10616	4019	73
H1	13278	4834	7613	82
H9	7252	4401	6371	74
H2	14302	6580	6934	86
H25	3256	11972	3098	73
H8	8675	3105	7457	86
H29	15	8044	834	98
H32	-1233	12324	1690	103
H30	-2620	9171	859	117
H31	-3260	11273	1280	121
H33	785	13344	1876	42

12. Theoretical Computations.

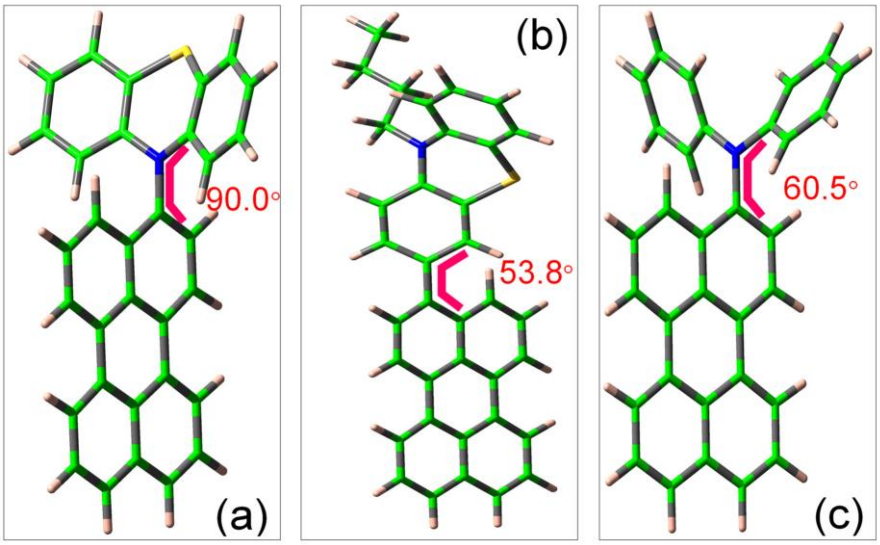


Figure S31. Optimized Conformations and the Dihedral Angles (degree) at C–N and C–C bonds of dyads (a) **Pery-N-PTZ**, (b) **Pery-C-PTZ**, and (c) **Pery-DPA** Calculated at (B3LYP/6-31G (d) level) with Gaussian 09W based on optimized ground state.

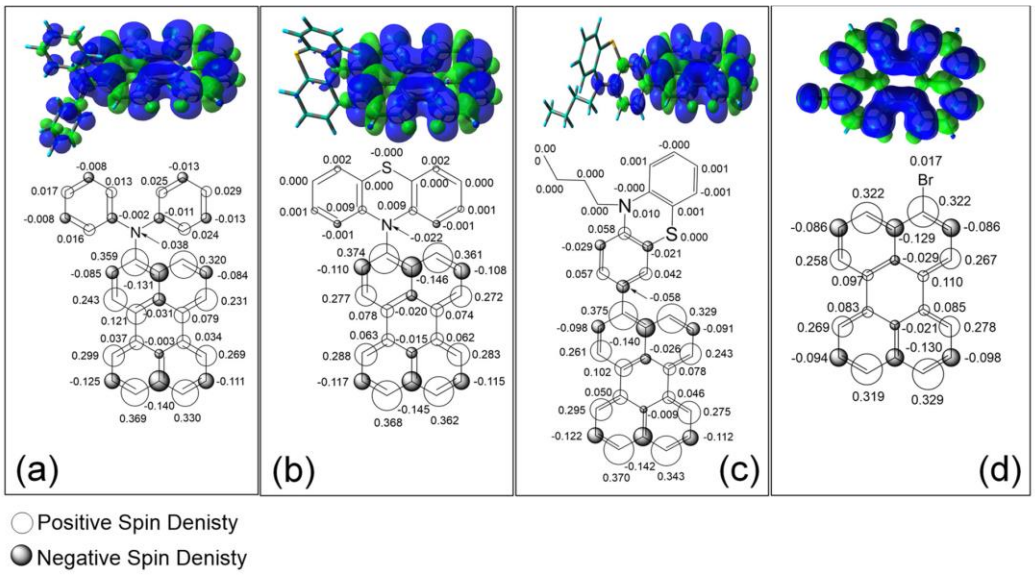


Figure S32. Spin density distribution of (a) **Pery-DPA**, (b) **Pery-N-PTZ**, (c) **Pery-C-PTZ,** (d) **3-Bromoperylene** obtained at (B3LYP/6-31G (d)) level using Gaussian 09W.

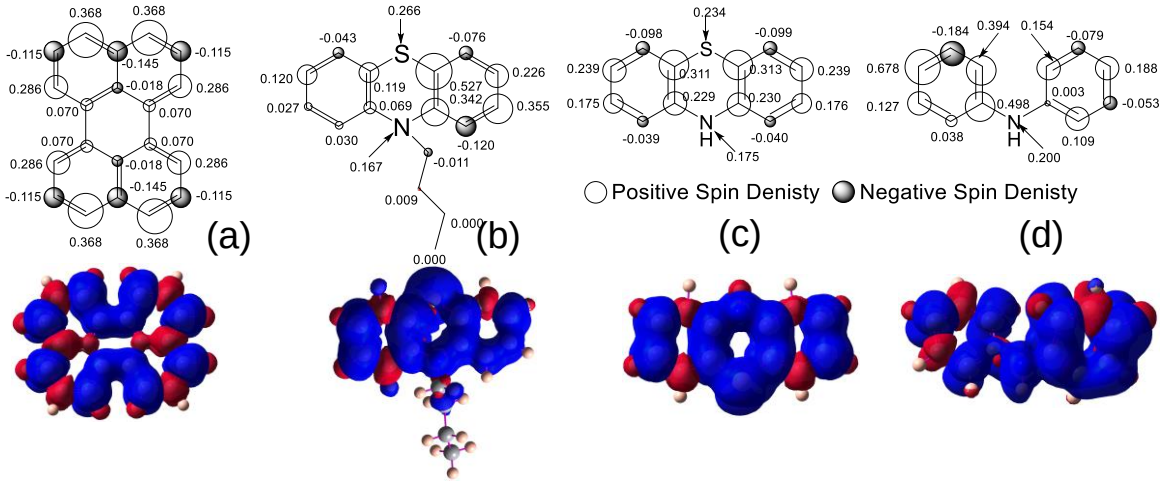


Figure S33. Spin density distribution of (a) **Perylene**, (b) **10-butyl-10H-phenothiazine,** (c) **Phenothiazine,** (d) **Diphenylamine** obtained at (B3LYP/6-31G (d)) level using Gaussian 09W.

13. X,y,z Coordinates of the Optimized Geometries

Pery-DPA

Charge = 0; Multiplicity = 1

Symbolic Z−Matrix:

C	-0.73002700	-1.40740200	0.96605300
C	0.64029600	-1.65349700	1.12617300
C	1.61014400	-0.84684400	0.53854300
C	1.17687400	0.25124600	-0.27500100
C	-0.22841600	0.49013600	-0.46719000
C	-1.17946600	-0.35112200	0.19621100
C	2.12852800	1.10721100	-0.92367800
C	1.65884200	2.12348500	-1.74972500
C	0.28550600	2.33104700	-1.95829000
C	-0.64520500	1.53588300	-1.32901100
C	3.05211200	-1.09391000	0.72569800
C	3.99941700	-0.21545300	0.10582200

C	3.57270900	0.88495900	-0.70588100
C	5.40307500	-0.44275700	0.30266300
C	6.34506600	0.42984200	-0.29987300
C	5.91708800	1.48918700	-1.06683500
C	4.54226200	1.71265400	-1.26580500
C	3.53046800	-2.15288800	1.49321300
C	4.90722200	-2.37511600	1.67854700
C	5.83114900	-1.53658700	1.09766800
N	-2.58170300	-0.11862300	0.05086500
C	-3.39815300	-1.19465000	-0.39593400
C	-3.15684400	1.05640300	0.60437800
C	-4.60806000	-1.51258600	0.24275000
C	-5.38741100	-2.57399500	-0.21646100
C	-4.97014000	-3.34721500	-1.30203200
C	-3.76066300	-3.04087900	-1.93129200
C	-2.98340600	-1.97149000	-1.49095200
C	-4.30385800	1.62959300	0.02512400
C	-4.85463700	2.79321200	0.55704200
C	-4.26859600	3.42090700	1.66007100
C	-3.12366600	2.86144300	2.22907400
C	-2.57368600	1.68673200	1.71532900
H	-1.45215900	-2.05033200	1.45996100
H	0.92768300	-2.49252300	1.74895500
H	2.35430000	2.77577100	-2.26487100
H	-0.03795000	3.12563000	-2.62485200
H	-4.93392400	-0.92892900	1.09739300
H	7.40499800	0.24757700	-0.14253700
H	6.63642600	2.16200400	-1.52537100
H	4.25216800	2.56166600	-1.87378900
H	2.83969000	-2.83783000	1.97123700
H	5.23255300	-3.21473600	2.28649600
H	6.89679700	-1.69852500	1.23751000
H	-1.70388300	1.69573700	-1.49338900
H	-6.32055400	-2.80502800	0.29078200
H	-5.57788100	-4.17641800	-1.65256600
H	-3.42310900	-3.62915900	-2.78054000
H	-2.05156800	-1.72922800	-1.99251200
H	-4.75760500	1.16014700	-0.84195400
H	-5.74135800	3.21925100	0.09481700
H	-4.69724500	4.33232100	2.06660000
H	-2.65556500	3.33321100	3.08912900
H	-1.69103400	1.25445500	2.17505300

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6−31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = −1286.8569 a.u.

RMS Gradient Norm = 0.000003292 a.u.

Imaginary Freq = 0

Dipole Moment = 0.39657446 Debye

Point Group = C1

Pery-N-PTZ

Charge = 0; Multiplicity = 1

Symbolic Z−Matrix:

C	0.53918900	0.00471600	2.96581900
C	1.91997500	0.00444600	2.70468400
C	2.42141800	0.00253400	1.40683600
C	1.49443300	0.00025900	0.31149000
C	0.08263000	0.00073000	0.58639100
C	1.95464200	-0.00243600	-1.04648800
C	1.00917800	-0.00382500	-2.06669700
C	-0.36873700	-0.00321000	-1.80068000
C	-0.83936400	-0.00109200	-0.50573200
C	3.87236400	0.00288200	1.12967200
C	4.32737300	-0.00054800	-0.22842800
C	3.40455100	-0.00363200	-1.32379400
C	5.73705200	-0.00088100	-0.49842300
C	6.19350100	-0.00472500	-1.84124000
C	5.29213600	-0.00818900	-2.88108500
C	3.90947700	-0.00760900	-2.62098300
C	4.82138300	0.00642800	2.14817000
C	6.20258300	0.00633800	1.87944800
C	6.65726800	0.00261700	0.58074300
H	0.19229100	0.00628000	3.99523700
H	2.59522600	0.00579000	3.55220000
H	1.31894400	-0.00534700	-3.10481400
H	-1.07912100	-0.00428900	-2.62159600
H	7.26362100	-0.00494500	-2.03134400

H	5.63943100	-0.01131500	-3.91035700
H	3.23633700	-0.01044600	-3.47037200
H	4.51024700	0.00946700	3.18635400
H	6.90493300	0.00916800	2.70819000
H	7.72203400	0.00237800	0.36284800
C	-2.85833200	-3.61066000	0.47827600
C	-2.20759900	-2.39247500	0.28085400
C	-2.92225600	-1.24168200	-0.09159200
C	-4.31543500	-1.35966000	-0.26652400
C	-4.96533500	-2.57186600	-0.02642600
C	-4.24137800	-3.70759800	0.33726400
C	-4.31499500	1.35935100	-0.27130700
C	-2.92184600	1.24156900	-0.09589200
C	-2.20693400	2.39347800	0.27242000
H	-1.13340800	2.33935500	0.40257500
C	-4.24031200	3.70942500	0.32388200
C	-4.96457700	2.57256800	-0.03576400
H	-2.27211800	-4.48219700	0.75565500
H	-1.13404600	-2.33813700	0.41069100
H	-6.04331900	-2.62418900	-0.15220900
H	-4.75353100	-4.65064500	0.50247300
H	-4.75221500	4.65321600	0.48557600
H	-6.04252500	2.62478000	-0.16187400
N	-2.26424200	-0.00049400	-0.29515300
S	-5.25603800	-0.00130800	-0.93270000
C	-0.36829500	0.00305500	1.93134900
H	-1.43409300	0.00338500	2.13053600
C	-2.85734800	3.61255500	0.46540000
H	-2.27085200	4.48489700	0.73966500

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6−31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = −1683.8444 a.u.

RMS Gradient Norm = 0.000010316 a.u.

Imaginary Freq = 0

Dipole Moment = 3.7823132 Debye

Point Group = C1

Pery-C-PTZ

Charge = 0; Multiplicity = 1

Symbolic Z–Matrix:

C	1.60915900	-0.87816700	-1.75370400
C	2.99537600	-1.04501700	-1.87542900
C	3.88719100	-0.47839600	-0.97188000
C	3.35614000	0.32713100	0.08828800
C	1.93250600	0.51604700	0.20063000
C	1.05060200	-0.13077700	-0.73005700
C	4.23046800	0.96362200	1.03209600
C	3.67611200	1.77699200	2.01513900
C	2.29138200	1.99103700	2.09938800
C	1.43493300	1.37658900	1.21432200
C	5.34462900	-0.68038200	-1.08169700
C	6.21151800	-0.06322300	-0.12283900
C	5.68939000	0.74969200	0.93457500
C	7.62922300	-0.26514700	-0.22293000
C	8.49155000	0.33854000	0.72756400
C	7.97245400	1.11068300	1.74139000
C	6.58347800	1.31189700	1.84193700
C	5.91232300	-1.45870700	-2.08719000
C	7.30271800	-1.65067800	-2.18402600
C	8.15037900	-1.06699900	-1.27036200
C	-0.43143900	-0.03396900	-0.63927000
C	-1.12703800	-0.39909800	0.52615800
C	-2.51678000	-0.33066700	0.58751700
C	-3.27700500	0.07300900	-0.52855900
C	-2.58456500	0.38775200	-1.70798500
C	-1.19163100	0.35196600	-1.75268900
S	-3.36641300	-0.69830200	2.11323600
C	-4.81669300	-1.46625100	1.41095000
C	-5.35025500	-0.93840400	0.21893100
N	-4.68712000	0.13602600	-0.42562200
C	-5.43289500	-2.53665800	2.06020500
C	-6.61645900	-3.07836300	1.55581000
C	-7.15562600	-2.56239500	0.37778200
C	-6.52246300	-1.51570000	-0.29454900
C	-5.43757200	0.98695400	-1.35699300
C	-6.58505000	1.74983300	-0.68035700
C	-7.33741300	2.64841300	-1.67085500
C	-8.47726000	3.43330900	-1.01364500
H	0.95583800	-1.37534300	-2.46518000
H	3.35668700	-1.65353000	-2.69635200

H	4.31206400	2.27952800	2.73449000
H	1.89935600	2.65237300	2.86708500
H	0.36904200	1.56064900	1.27690700
H	9.56308600	0.17822500	0.64087100
H	8.62992000	1.57146900	2.47341600
H	6.22164000	1.92398900	2.65987600
H	5.28374200	-1.94212800	-2.82611700
H	7.69919300	-2.26640000	-2.98661100
H	9.22571100	-1.21123000	-1.33572300
H	-0.57862800	-0.74490100	1.39727400
H	-3.13066800	0.66143900	-2.60391200
H	-0.68621100	0.62641000	-2.67415800
H	-4.98863200	-2.93295300	2.96886600
H	-7.10457300	-3.89702600	2.07604300
H	-8.06911800	-2.98123700	-0.03508600
H	-6.94768000	-1.14818400	-1.22182400
H	-5.81013300	0.41459900	-2.22095000
H	-4.73299500	1.72119000	-1.75221100
H	-6.16521900	2.35631500	0.13256300
H	-7.28998000	1.05067500	-0.21584200
H	-7.74105500	2.03280800	-2.48728800
H	-6.63171600	3.35015300	-2.13767100
H	-8.99823000	4.06344600	-1.74328400
H	-8.10062600	4.08596500	-0.21679400
H	-9.21669900	2.75754900	-0.56679400

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6−31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = −1841.1051 a.u.

RMS Gradient Norm = 0.000001982 a.u.

Imaginary Freq = 0

Dipole Moment = 2.9195663 Debye

Point Group = C1

14. References

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