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Electronic Supplementary Information for:

Increasing the Anti-Stokes Shift in TTA Upconversion with Photosensitizers Showing Red-shifted Spin-Allowed Charge Transfer Absorption but Non-Compromised Triplet State Energy Level

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Contents

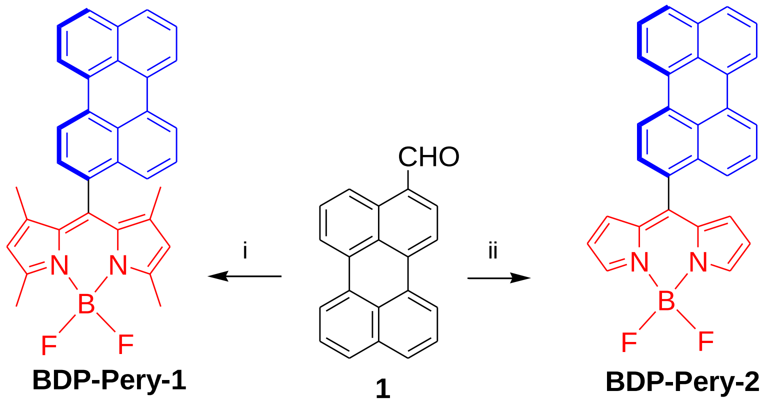
1.0 General Information

Analytical Measurements. All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before being used for synthesis. ^1H and ^{13}C NMR spectra were recorded on the Bruker Avance spectrometers (400 MHz or 500 MHz). The mass spectra were measured by HRMS (MALDI-TOF). UV–Vis absorption spectra were taken on a HP8453 UV–Vis spectrophotometer. The triplet lifetime was recorded by nanosecond transient absorption spectroscopy in deareated solution.

TTA Upconversion. A continuous diode pumped solid-state laser (589 nm) was used as the excitation source for the upconversion. The diameter of the laser spot was 2 mm, and power of the laser beam was measured with VLP-2000 pyroelectric laser power meter. For the upconversion experiments, the mixed solution of the triplet photosensitizer and triplet acceptor was degassed with N_2 for at least 15 min, and gas flow was kept on during the measurement. The solution was excited with the laser, and the upconverted fluorescence was recorded with a RF 5301PC spectrofluorometer. In order to repress the laser scattering, a small black box was put behind the fluorescent cuvette to dump the laser.

DFT calculation. The structure of the dyads BDP-Pery to simulate the absorption spectra have been obtained at the DFT level, by using the M062X[1] exchange and correlation functional coupled with the 6-31+G** basis set for all the atoms. The electronic spectra have been computed at the same level by means of the time-dependent extension of DFT (TDDFT). The solvent environment, toluene, has been simulated, with a dielectric constant of 2.37, with the integral equation formalism polarizable continuum model (IEFPCM),[2] which corresponds to a linear response in equilibrium and nonequilibrium solvation, in geometries optimization of the excited and ground states, respectively. All the calculations have been performed with Gaussian 09.[3]

2.0 Synthesis and Molecular Structure Characterization Data



Scheme S1. Synthesis route of compounds **BDP-Pery-1** and **BDP-Pery-2**.

Synthesis of the compound **BDP-Pery-1.** A mixture of **1** (126 mg, 0.45 mmol) and 2,4-dimethylpyrrole (0.2 mL, 94.5 mg, 0.9 mmol) in dry CH_2Cl_2 (100 mL) was stirred at room temperature (RT) under N_2. Trifluoroacetic acid (TFA. 0.01 mL) was added. After 1.5 h of stirring, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ. 100.0 mg) was added in one portion to the mixture. The solution was then stirred for 0.5 h at RT. With ice-bath cooling, triethylamine (1.4 mL) was added dropwise, then the mixture was stirred for 0.5 h. Afterward, $BF_3{\cdot}Et_2O$ (1.4 mL) was added dropwise. The reaction mixture was stirred overnight. The solution was concentrated under reduced pressure, the residual was mixed with water (20 mL), and the mixture was stirred for 24 h. Then the solution was extracted with CH_2Cl_2 (3 × 50 mL) and the organic layers were combined, dried over anhydrous $MgSO_4$ and evaporated under reduced pressure. The crude product was further purified using column chromatography (silica gel, CH_2Cl_2/hexane = 1:1, v/v) to give **BDP-Pery-1** as orange powder. Yield: 40 mg (18 %). Mp: > 250 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.30–8.22 (m, 4H), 7.74 (t, 2H, *J* = 8.0 Hz), 7.65 (d, 1H, *J* = 8.0 Hz), 7.55–7.39 (m, 4H), 5.96 (s, 2H), 2.60 (s, 6H), 1.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.74, 142.99, 140.04, 134.75, 133.17, 132.52, 131.95, 131.89, 131.49, 130.91, 130.62, 128.90, 128.61, 128.30, 127.81, 126.81, 126.76, 126.68, 124.85, 121.21, 120.88, 120.78, 120.08, 29.71, 26.93, 14.68, 14.20. MALDI-HRMS ($C_{33}H_{25}BF_2N_2$): calcd. $m/z = 498.2079$; found $m/z = 498.2050$. Anal. Calcd for [$C_{33}H_{25}BF_2N_2$ + $0.2CH_2Cl_2$]: C, 77.37; H, 4.97; N, 5.44. Found: C, 77.51; H, 4.70; N, 5.22.

Synthesis of the compound **BDP-Pery-2.** The synthesis procedures are similar to that for compound **BDP-Pery-1**. Mp: > 250 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.29–8.22 (m, 4H), 7.97 (s, 2H), 7.79–7.70 (m, 3H), 7.56–7.52 (m, 3H), 7.43 (t, 1H, *J* = 8.0 Hz), 6.81 (d, 2H, *J* = 4.0 Hz), 6.48 (d, 2H, *J* = 4.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.03, 144.46, 135.99, 134.64, 134.06, 133.59, 131.32, 131.16, 130.73, 130.36, 130.33, 128.99, 128.96, 128.77, 128.51, 128.38, 127.33, 126.85, 126.72, 126.04, 121.12, 121.03, 120.80, 118.98, 118.61. MALDI-HRMS ($C_{29}H_{17}BF_2N_2$): calcd. $m/z = 442.1453$; found $m/z = 442.1483$. Anal. Calcd for [$C_{29}H_{17}BF_2N_2$]: C, 78.76; H, 3.87; N, 6.33. Found: C, 78.59; H, 3.78; N, 6.15.

*Compound **1***: ^1H NMR ($CDCl_3$, 400 MHz): δ 10.29 (s, 1H), δ 9.15 (d, 1H, *J* = 8.0 Hz), 8.28–8.23 (m, 4H), 7.90 (d, 1H, *J* = 4.0 Hz), 7.84–7.79 (m, 1H), 7.73–7.64 (m, 1H), 7.55–7.50 (m, 2H). EI-HRMS ($C_{21}H_{12}O$): calcd. $m/z = 280.0888$; found $m/z = 280.0884$.

3.0 NMR and HRMS Spectra

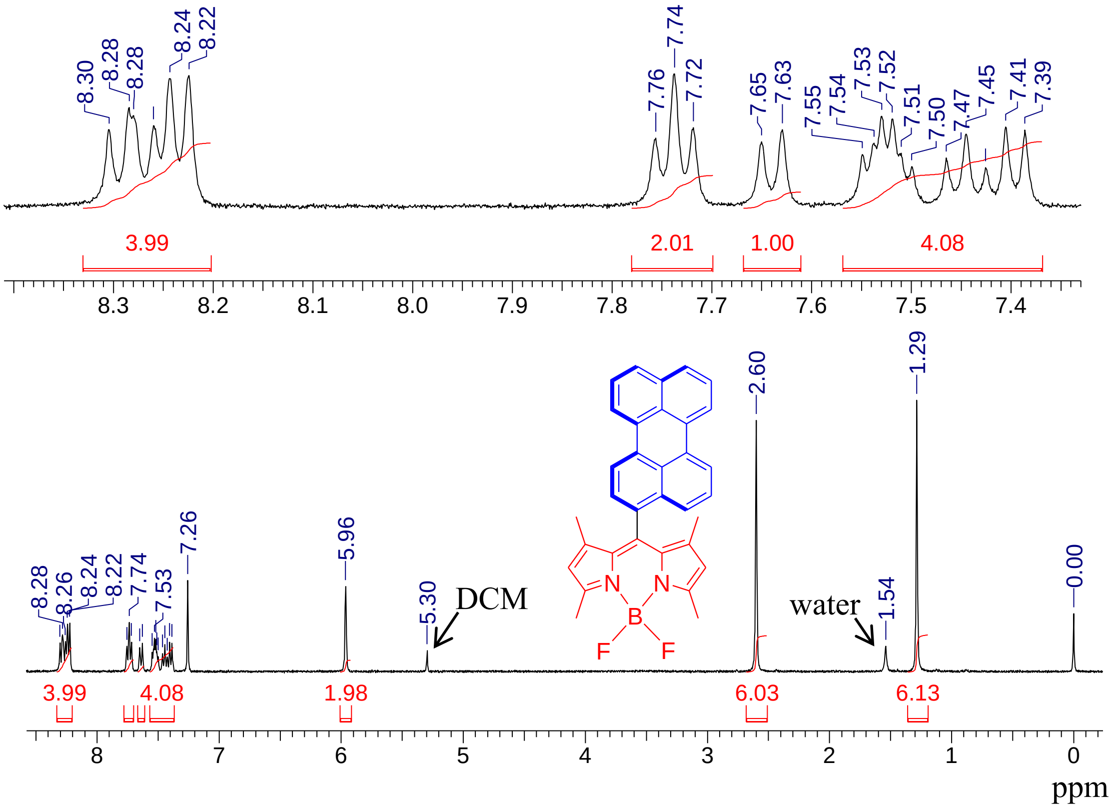


Figure S1. ^{1}H NMR spectrum of compound **BDP-Pery-1** (400 MHz, $CDCl_3$), 25°C.

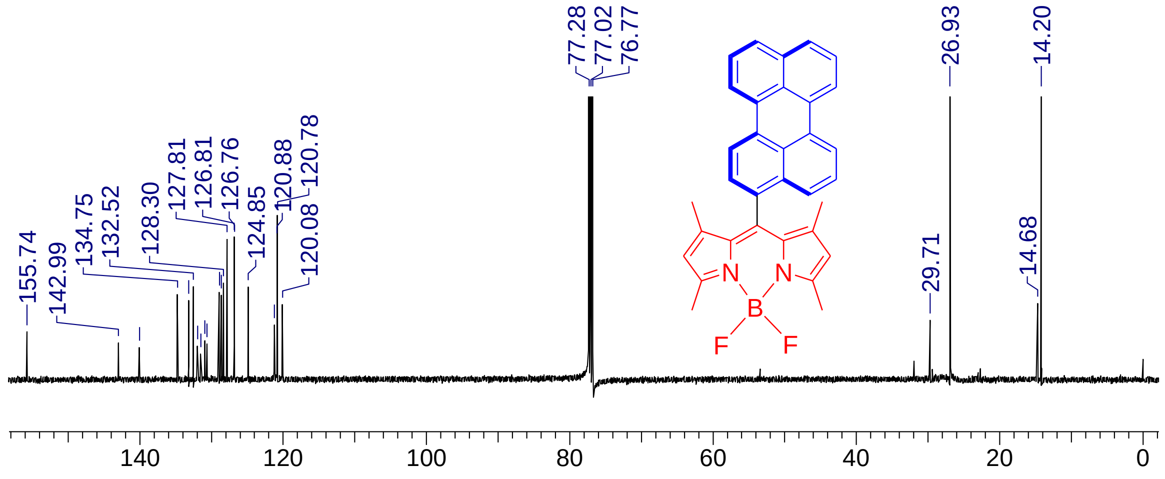


Figure S2. ^{13}C NMR spectrum of compound **BDP-Pery-1** (125 MHz, $CDCl_3$), 25°C.

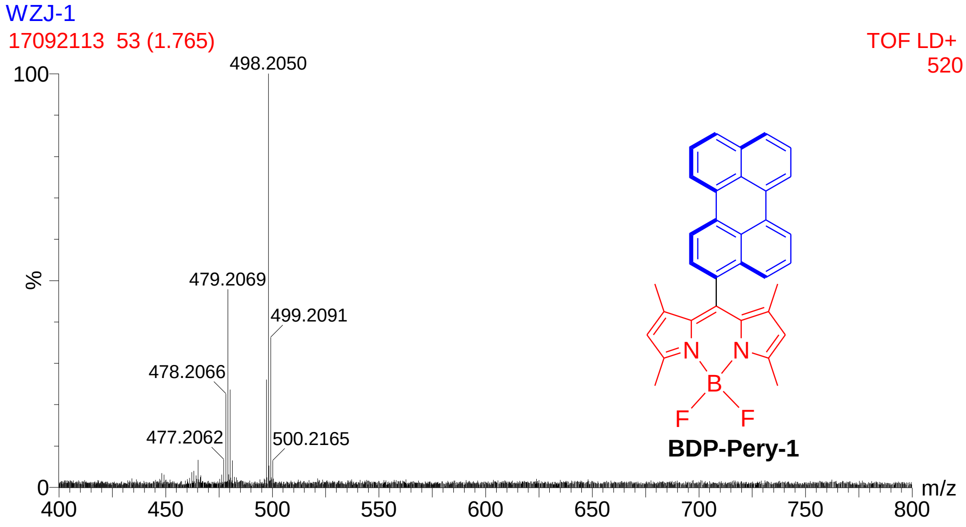


Figure S3. MALDI HR MS spectrum of **BDP-Pery-1**. 25°C.

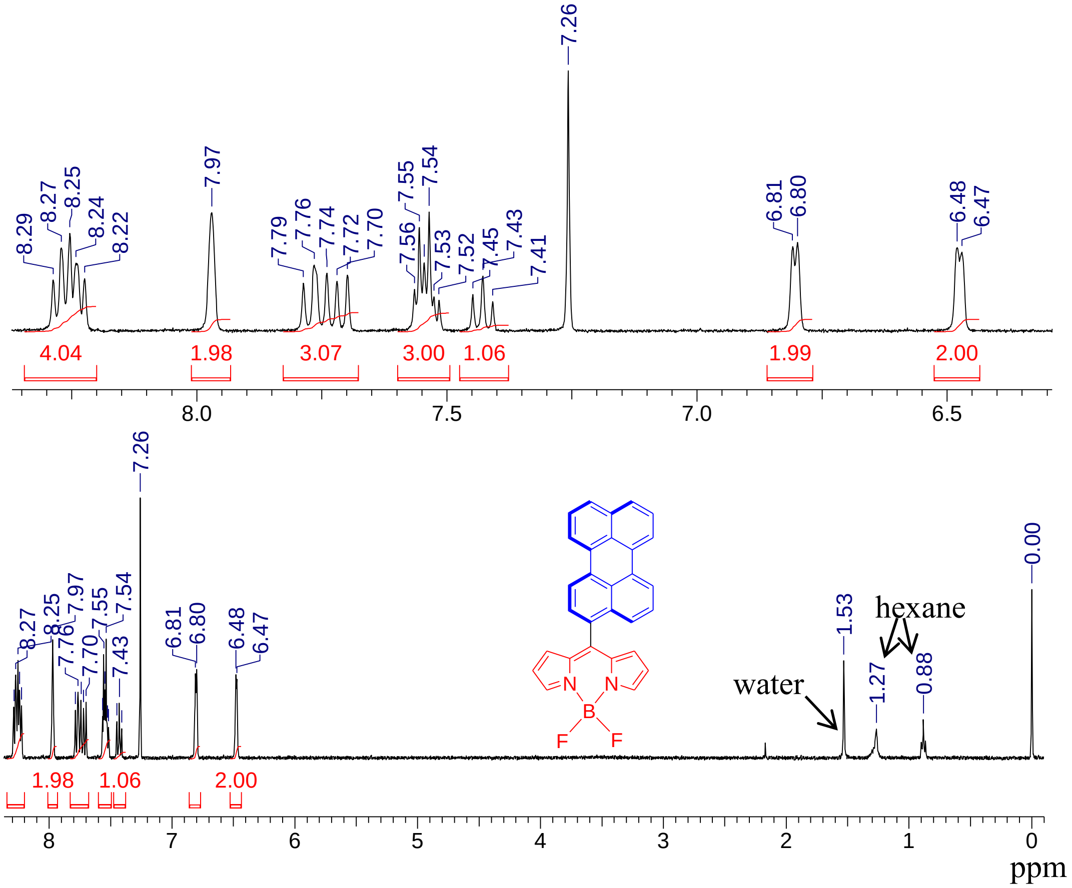


Figure S4. ^{1}H NMR spectrum of compound **BDP-Pery-2** (400 MHz, CDCl$_3$), 25°C.

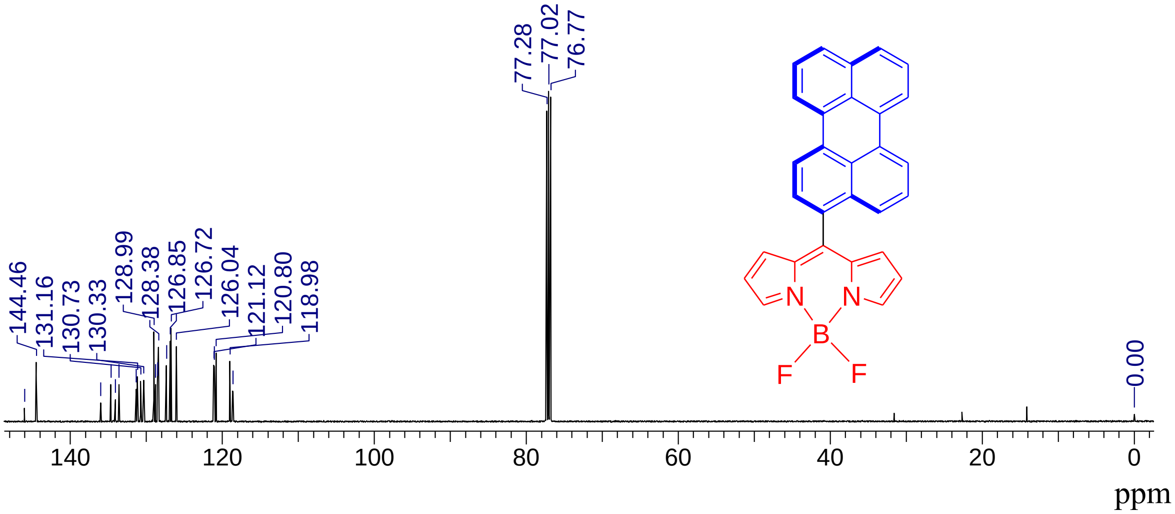


Figure S5. ^{13}C NMR spectrum of compound **BDP-Pery-2** (125 MHz, $CDCl_3$), 25°C.

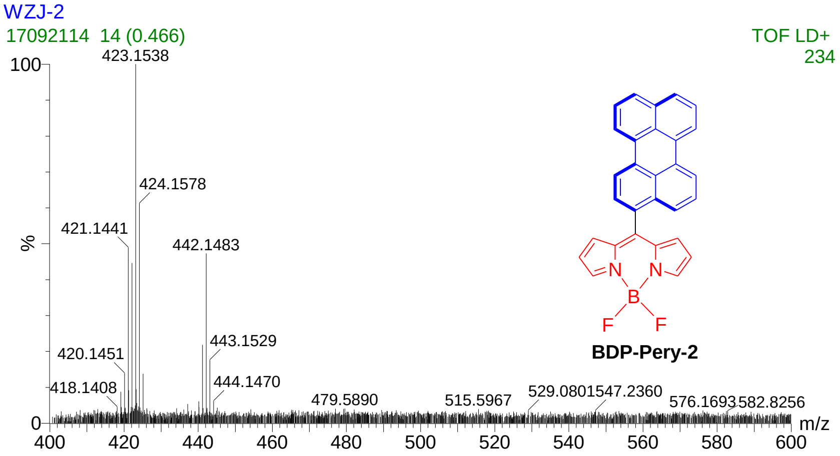


Figure S6. MALDI HR MS spectrum of **BDP-Pery-2**. 25°C.

4.0 Triplet-Triplet Annihilation Upconversion

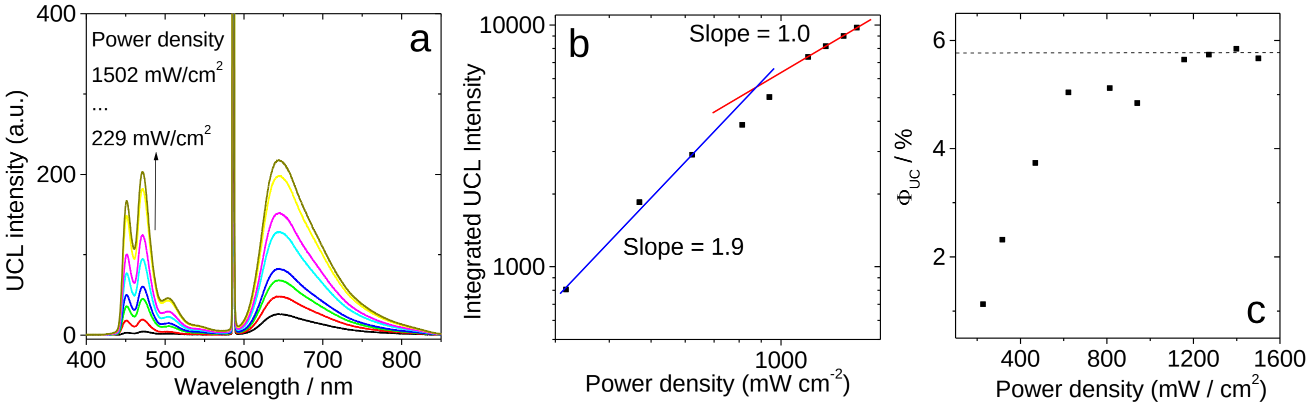


Figure S7. (a) Upconversion luminescence (UCL) spectra of **BDP-Pery-2** and perylene, ([**BDP-Pery-2**] = 1.0 × 10^{-5} M and [perylene] = 2.8 × 10^{-4} M) upon excitation with a 589 nm CW-laser at different incident power densities. (b) Integrated UCL intensity from (a) plotted as a function of incident power density. (c) Upconversion quantum yield plotted as a function of incident laser power density. In deaerated toluene, 20 °C.

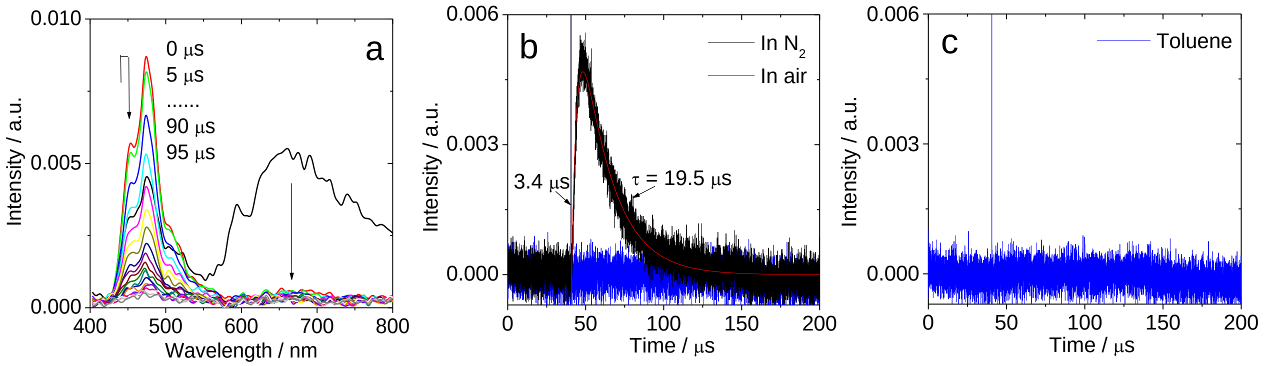


Figure S8. (a) The upconverted emission (delayed fluorescence) recorded with the nanosecond transient absorption spectrometer in the emission measurement mode. **BDP-Pery-2** (c = 1.0 × 10^{-5} M) mixed with perylene (c = 3.3 × 10^{-4} M), upon excitation at 589 nm. (b) The corresponding decay curves by monitoring the emission at 450 nm, under N_2 and air atmosphere, respectively. In toluene. (c) The corresponding blank decay trace of toluene alone by monitoring the emission at 450 nm (only scaterred light was recorded). 20 °C.

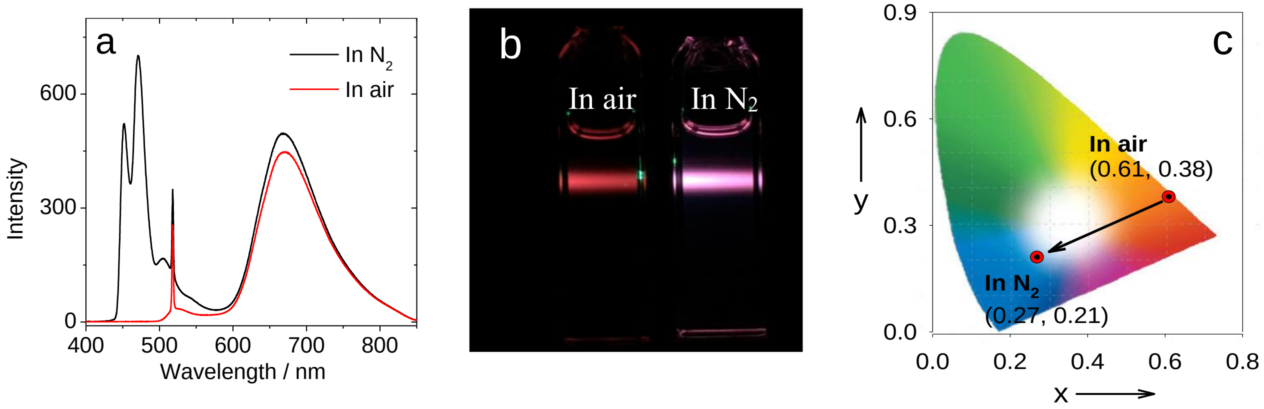


Figure S9. (a) Upconversions with sensitizers **BDP-Pery-2,** $c = 1.0 \times 10^{-5}$ M**.** Excited with 520 nm laser (380 mW cm^{-2}). c[perylene] = 3.3×10^{-4} M, in deaerated toluene. (b) The photographs and (c) CIE diagram of **BDP-Pery-2** mixed with perylene in air and in N_2 atmosphere. 20 °C.

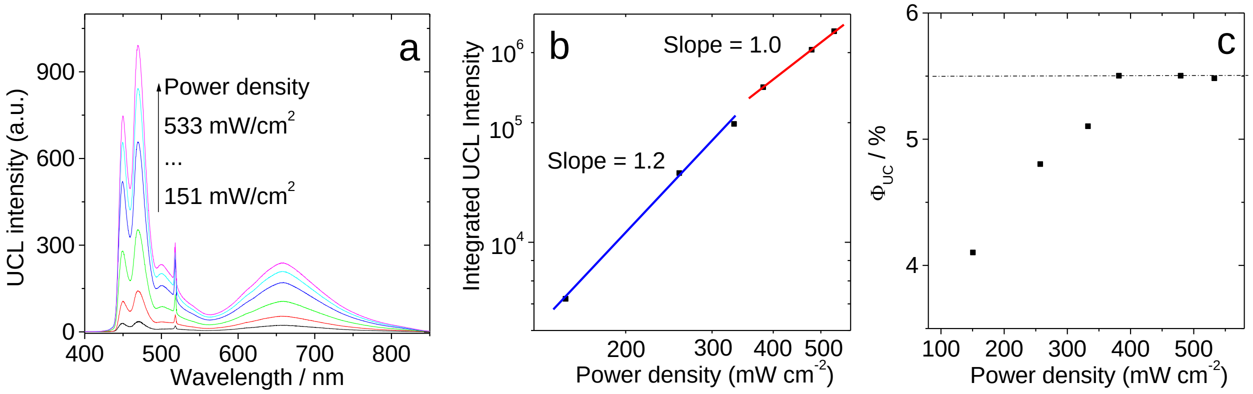


Figure S10. (a) Upconversion luminescence (UCL) spectra of **BDP-Pery-2** and perylene, ([**BDP-Pery-2**] = 1.0×10^{-5} M and [perylene] = 3.3×10^{-4} M) upon excitation with a CW 520 nm laser at different incident power densities. (b) Integrated UCL intensity data from part (a) plotted as a function of incident power density. (c) Upconversion quantum yield plotted as a function of incident power density. In deaerated toluene, 20 °C.

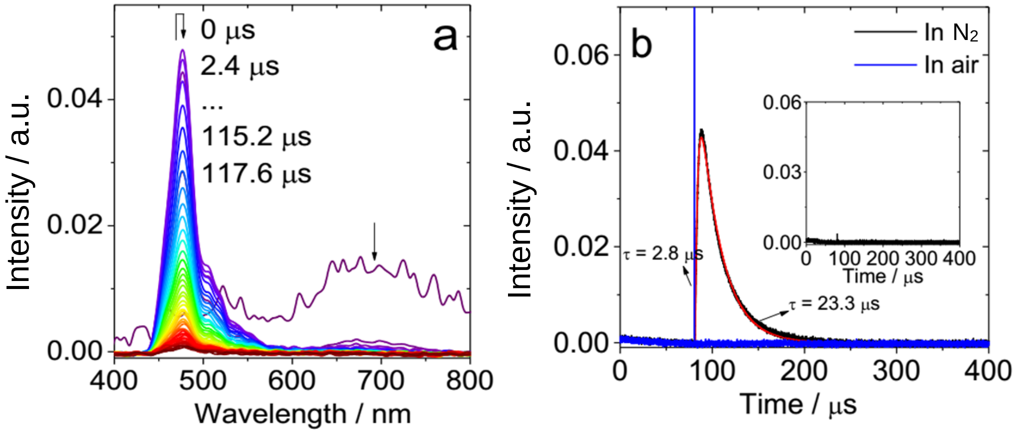


Figure S11. (a) The upconverted emission (delayed fluorescence) recorded with the nanosecond transient emission spectrometer. **BDP-Pery-2** (c = 1.0 × 10^{-5} M) mixed with perylene (c = 3.3 × 10^{-4} M), upon excitation at 520 nm. (b) The corresponding decay curves by monitoring the emission at 477 nm, under N_2 and air atmosphere, respectively. Inset: The corresponding decay curves of toluene solvent alone monitored at 477 nm. In deaerated toluene, 20 °C.

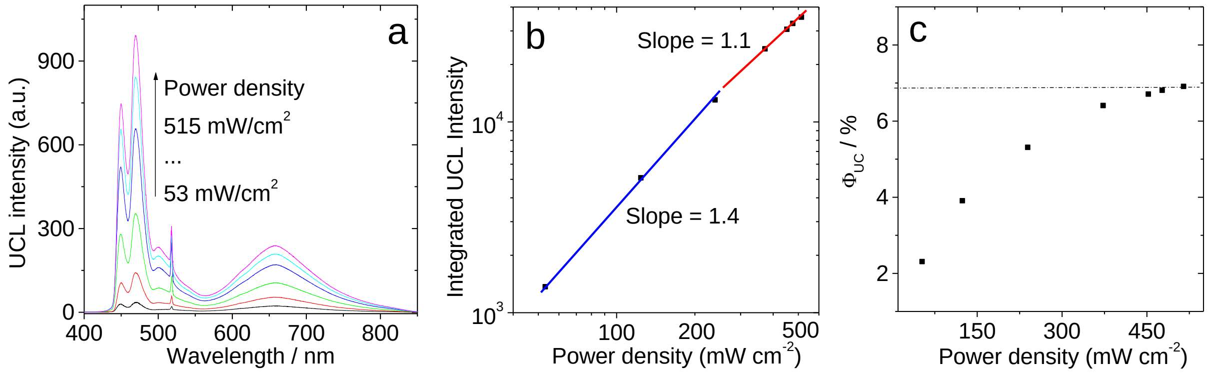


Figure S12. (a) Upconversion luminescence (UCL) spectra of **BDP-Pery-1** and perylene, ([**BDP-Pery-1**] = 1.0 × 10^{-5} M and [perylene] = 2.5 × 10^{-4} M) upon excitation with a CW 520 nm laser at different incident power densities. (b) Integrated UCL intensity data from part (a) plotted as a function of incident power density. (c) Upconversion quantum yield plotted as a function of incident power density. In deaerated dichloromethane, 20 °C.

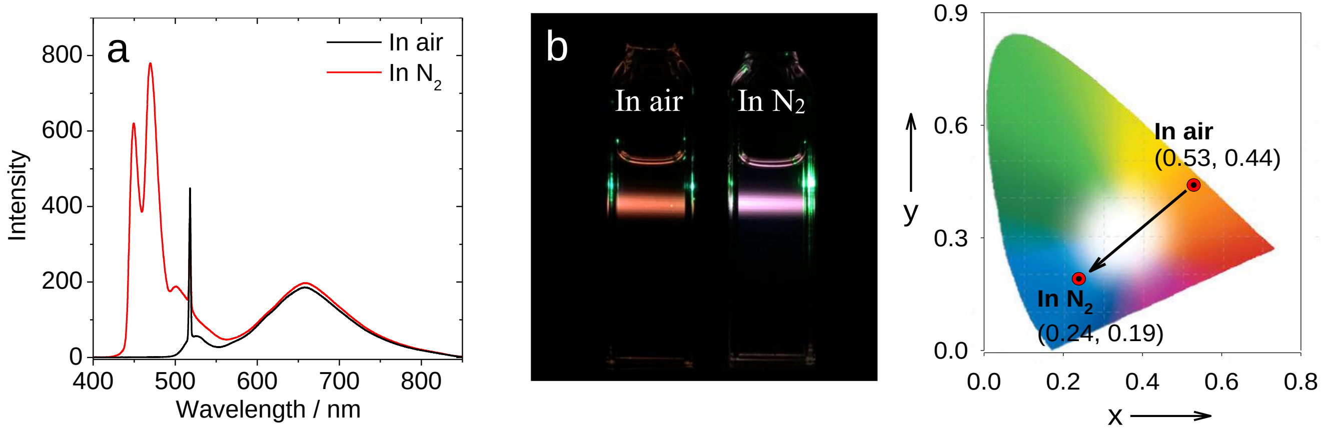


Figure S13. (a) Upconversions with sensitizers **BDP-Pery-1,** $c = 1.0 \times 10^{-5}$ M**.** Excited with 520 nm laser (478 mW cm^{-2}). c[perylene] = 2.5×10^{-4} M, in deaerated dichloromethane, 20 °C. (b) The photographs and (c) CIE diagram of **BDP-Pery-1** mixed with perylene in air and in N_2.

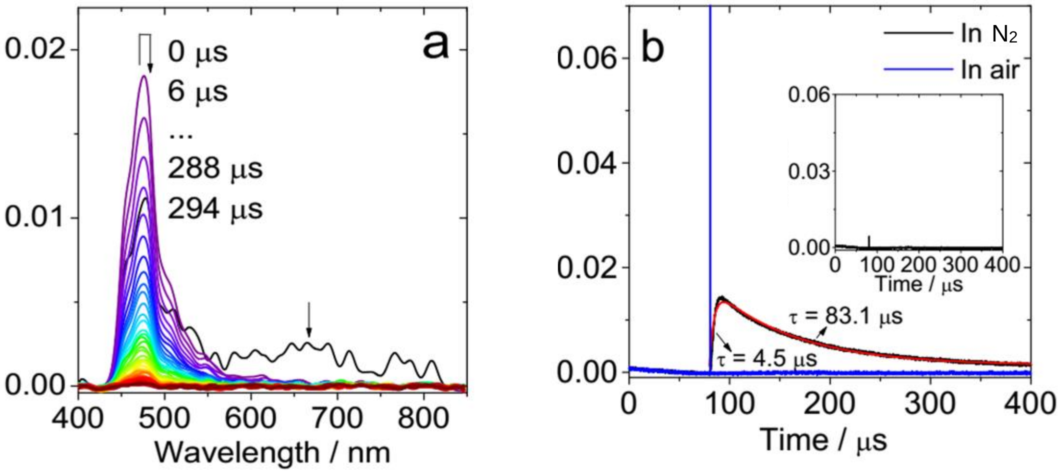


Figure S14. (a) Nanosecond transient emission spectra of **BDP-Pery-1** ($c = 1.0 \times 10^{-5}$ M) mixed with perylene ($c = 2.5 \times 10^{-4}$ M), upon excitation at 520 nm in deaerated dichloromethane, 20 °C. (b) The corresponding decay curves monitored at 477 nm, in N_2 and in air. Inset: The corresponding decay curves of dichloromethane monitored at 477 nm.

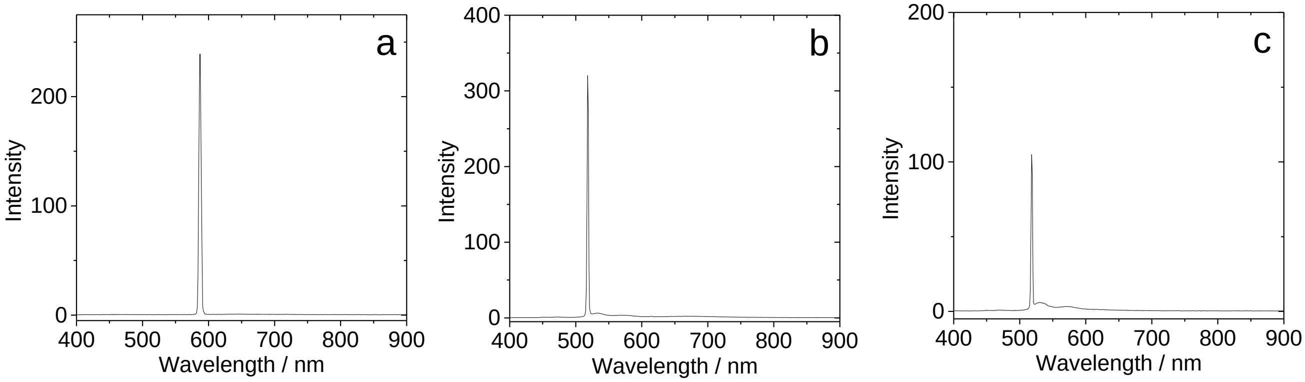


Figure S15. Fluorescence emission spectra of (a) perylene in deareated toluene, $c = 2.8 \times 10^{-4}$ M, excited with 589 nm laser (1.2 W cm^{-2}). (b) perylene in deareated toluene, $c = 3.3 \times 10^{-4}$ M, excited with 589 nm laser (380 mW cm^{-2}). (c) perylene in deareated DCM, $c = 2.5 \times 10^{-4}$ M, excited with 520 nm laser (478 mW cm^{-2}). The spectra are measured in the same condition of TTA upconversion.

5.0 Calculation of Triplet-Triplet Annihilation Upconversion Quantum Yield

The triplet triplet annihilation upconversion quantum yield of the triplet photosensitizers were calculated according to literature method.[4] The upconversion quantum yield (Φ_{UC}) was determined using the prompt fluorescence of **Methylene Blue** (**MB**, Φ_F = 3 % in MeOH) as the standard.[5] The upconversion quantum yield was calculated with following Eq S1, where Φ_{UC}, A_{sam}, I_{sam}, and η_{sam} represent the quantum yield, absorbance, integrated photoluminescence intensity, and refractive index of the sample. The subscripts sam and ref stand for sample and reference compound respectively. The equation is multiplied by a factor of 2 so as to set the maximum quantum yield to unity

$$\Phi_{\mathrm{UC}} = 2 \times \Phi_{\mathrm{F(ref)}} \times \frac{I_{\mathrm{sam}}}{I_{\mathrm{ref}}} \times \frac{1-10^{-A_{\mathrm{ref}}}}{1-10^{-A_{\mathrm{sam}}}} \times \left(\frac{\eta_{\mathrm{sam}}}{\eta_{\mathrm{ref}}}\right)^2 \qquad \text{(Eq. S1)}$$

The triplet triplet energy transfer efficiency of the upconversion system are calculated by Eq. S2.[6] The results are listed in Table S1. It shows that the TTET efficiency is high, due to the use of excess amount of the acceptor in the TTA upconversion system. The TTET kinetics are calculated by Eq. S3. The results are listed in Table S1.

$$\Phi_{\mathrm{TTET}} = 1 - \tau/\tau_0 \qquad \text{(Eq. S2)}$$

$$k_{\mathrm{TTET}} = \frac{1}{\tau} - \frac{1}{\tau_0} \qquad \text{(Eq. S3)}$$

Where τ_0 is the triplet state lifetime of the triplet energy donor in the absence of energy acceptor; τ is the triplet state lifetime of the triplet energy donor in the presence of energy acceptor.

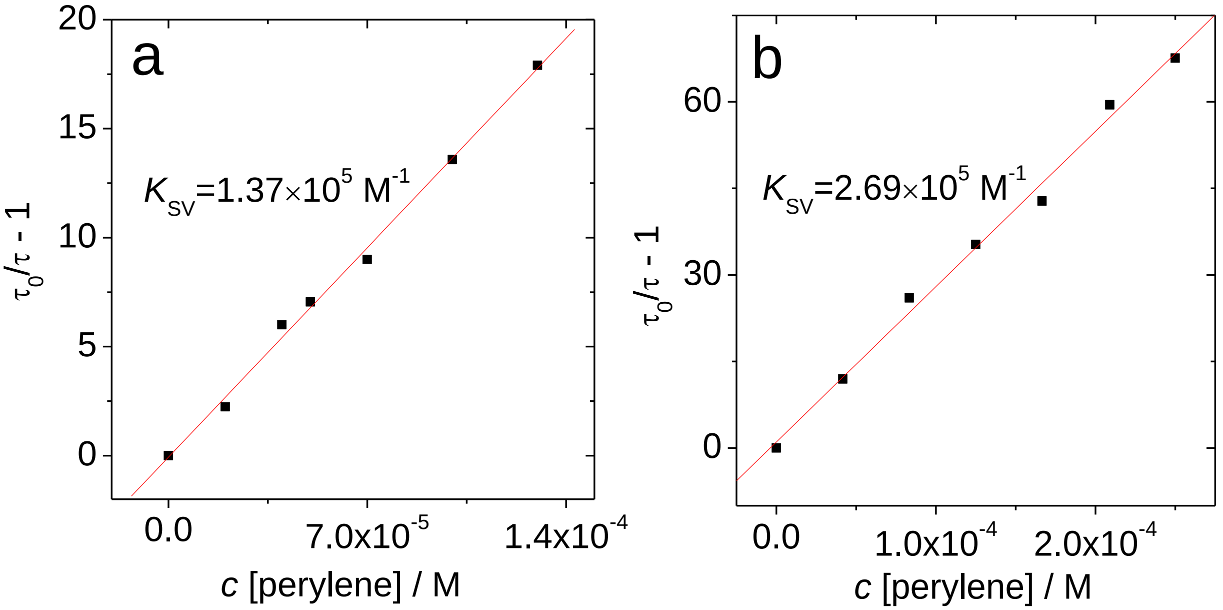


Figure S16. Stern–Volmer plots for lifetime quenching of (a) **BDP-Pery-2** (λ_{ex}=589 nm) in deaerated toluene and (b) **BDP-Pery-1** (λ_{ex}=520 nm) in deaerated DCM with increasing concentration of perylene. *c*[photosensitizers]=1.0×10^{-5} M. 20 °C.

The bimolecular quenching efficiency was also studied. Stern-Volmer quenching constant of perylene to **BDP-Pery-2** was calculated as $K_{SV} = 1.37 \times 10^5$ M^{-1}. The bimolecular quenching constant was calculated as $k_q = K_{SV}/\tau_0 = 1.96 \times 10^9$ M^{-1} s^{-1}. In order to study the quenching efficiency of the triplet state of **BDP-Pery-2** by perylene, which is given by $f_Q = k_q/k_0$, where k_0 is the diffusion-controlled bimolecular quenching rating constants, can be calculated with the Smoluchowski equation (Eq. S4),[7] D is the sum of the diffusion coefficients of the energy donor (D_f) and quencher (D_q), N is Avogadro's number. R is the collision radius, the sum of the molecule radii of the energy donor (R_f) and the quencher (R_q). Diffusion coefficients can be obtained from Stokes-Einstein equation:[8] k is Boltzmann's constant, η is the solvent viscosity, R is the molecule radius.

$$k_0 = 4\pi RND/1000 = \frac{4\pi N}{1000}\left(R_f + R_q\right)\left(D_f + D_q\right) \tag{S4}$$

$$D = k\mathrm{T}/6\pi\eta R \tag{S5}$$

The molecule radii of the energy donor **BDP-Pery-2** is 6.9 Å, and it is 4.7 Å for the quencher (perylene). According to Eq. S5 the diffusion coefficients of the energy donor (**BDP-Pery-2**) is 5.3×10^{-6} cm^2 s^{-1} and quencher (perylene) is 7.8×10^{-6} cm^2 s^{-1} (in toluene at 20 °C). Thus k_0 was calculated as 1.14×10^{10} M^{-1} s^{-1}. The quenching efficiency is $f_Q = k_q / k_0 = 17.2$ %.

It should be noted that the quenching efficiency (f_Q) and the TTET efficiency (Φ_{TTET}) are different. The quenching efficiency is the nature of the donor/acceptor pair in certain solvent, which is not dependent on the concentration of triplet acceptor. $f_Q = 17.2\%$ means that 17.2% of the collisional encounters are effective in quenching. This means not all the collisional encounters have quenching effect. [7] Although the quenching efficiency is low (maybe due to the barely matched triplet energy levels of triplet energy donor and acceptor), the TTET efficiency can be enhanced by increasing the concentration of the acceptor, which increases the possibility of collision. As such the TTET efficiency is dependent on the concentration of the acceptor. It should be noted that in the TTA upconversion experiment, the acceptor is in excessive amount. As such the TTET efficiency for the TTA upconversion system is calculated to be high (Table S1).

Table S1. Triplet excited state lifetimes (τ_0), Stern–Volmer quenching constant (K_{SV}), bimolecular quenching constants (k_q), quenching efficiency (f_Q) and TTET efficiency (Φ_{TTET}) of the BDP-Perylene sensitizers. 20 °C.

	τ_0 [μs]	K_{SV} [10^5 M^{-1}]	k_q [10^9 M^{-1}s^{-1}]	Φ_{uc} ^{a} [%]	k_0 ^{b} [10^{10} M^{-1}s^{-1}]	f_Q ^{c} [%]	Φ_{TTET} ^{d} [%]	k_{TTET} ^{e} [10^5 s^{-1}]
BDP-Pery-1[f]	127	2.69	2.12	6.8	1.59	13.3	98.7	5.8
BDP-Pery-2[g]	70.0	1.37	1.96	5.7	1.14	17.2	97.7	3.6

[a] Upconversion quantum yields. [b] Diffusion-controlled bimolecular quenching rate constants. [c] Quenching efficiency. [d] Triplet triplet energy transfer (TTET) efficiency. [e] TTET kinetics. [f] In deareated DCM, excited with 520 nm. [g] In deareated toluene, excited with 589 nm.

6.0 Calculation of Triplet Quantum Yield

Due to the overlap of the ESA band and the bleaching band of perylene, the triplet quantum yield will be underestimated by the ground state depletion method.[9] Thus the triplet quantum yield of Bodipy-perylene dyads was determined by TTET method, use styryl-Bodipy as the triplet energy acceptor. Because both triplet of perylene and Bodipy moiety are observed in ns-TA, the original equation[10] (Eq S6) was deduced and revised as Eq S7:

$$\Phi_{\mathrm{T}}^{\mathrm{sam}} = \Phi_{\mathrm{T}}^{\mathrm{ref}} \times \frac{\Delta A_{\mathrm{sam}}}{\Delta A_{\mathrm{ref}}} \times \frac{f_{\mathrm{ref}}}{f_{\mathrm{sam}}} \qquad \text{(Eq. S6)}$$

$$\Phi_{\mathrm{T}}^{\mathrm{sam}} = \Phi_{\mathrm{T}}^{\mathrm{ref}} \times \frac{\frac{\Delta A_{\mathrm{sam}} \times X}{f_{1\mathrm{sam}}} + \frac{\Delta A_{\mathrm{sam}} \times (1 - X)}{f_{2\mathrm{sam}}}}{\Delta A_{\mathrm{ref}}} \times f_{\mathrm{ref}} \qquad \text{(Eq S7)}$$

Where superscripts sam and ref designate sample and reference compound, respectively. Φ_{T} is the triplet quantum yield, ΔA is the transient absorption of the acceptor triplet formed by energy transfer from the donor, *f* is the triplet-triplet energy transfer efficiency, X is the contribution percentage of one moiety to the transient absorption of the acceptor triplet.

Note that it is impossible to exactly determine the contribution (X) of the triplet of styryl-Bodipy from each moiety. Moreover, the TTET efficiency is high due to the TTET time constants (estimated by the growing kinetics of the ESA of styryl-BDP at 380 nm) is far more fast than the decay of PS (in the absence of acceptor), thus the TTET efficiency (*f*) is taken as

1 for all the triplet energy donor acceptor pairs. Thus the triplet quantum yield can be estimated by Eq S8:

$$\Phi_{\mathrm{T}}^{\mathrm{sam}} = \Phi_{\mathrm{T}}^{\mathrm{ref}} \times \frac{\Delta A_{\mathrm{sam}}}{\Delta A_{\mathrm{ref}}} \qquad \text{(Eq. S8)}$$

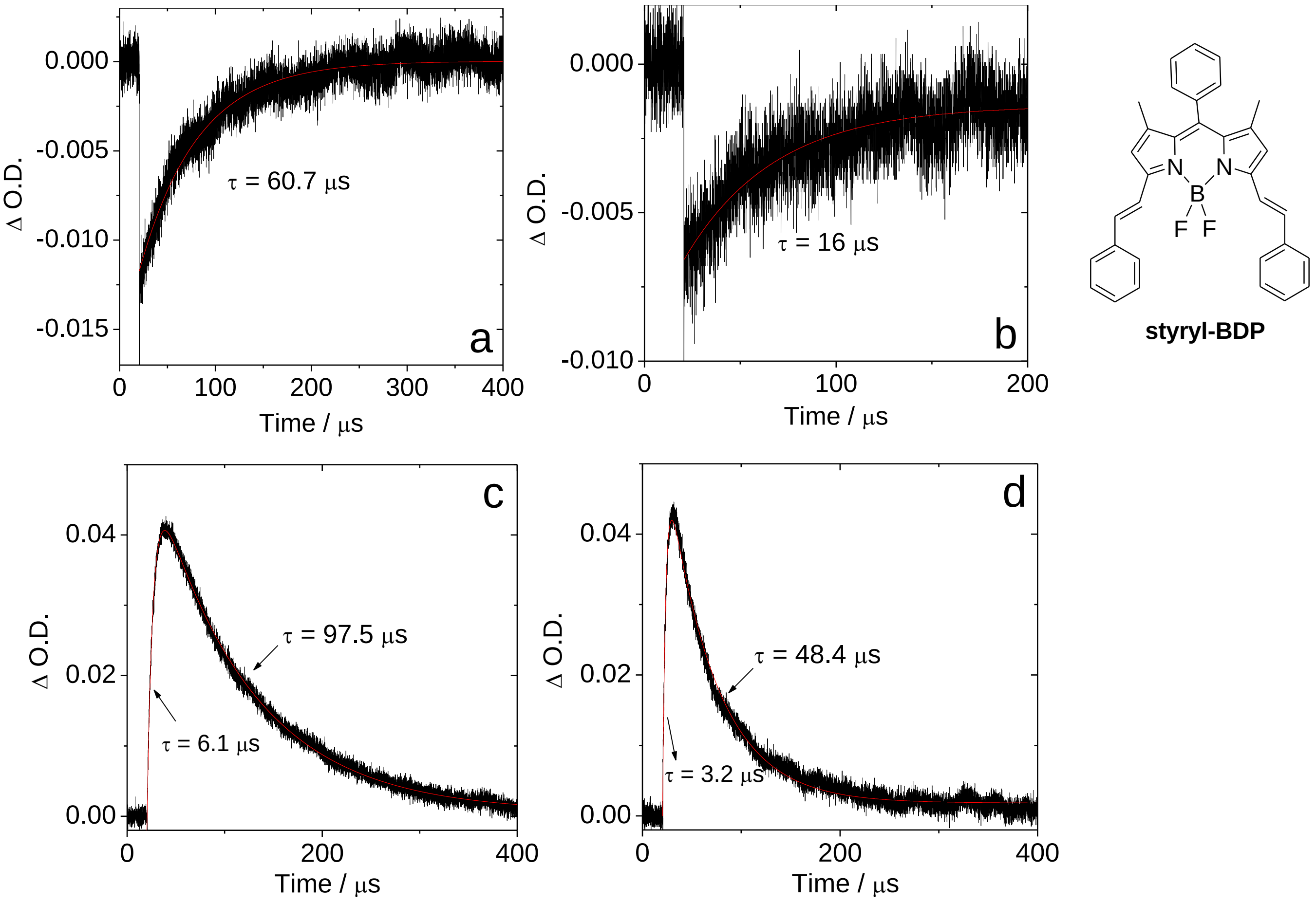


Figure S17. Nanosecond transient absorption spectra: (a) Decay trace of **BDP-Pery-2** at 515 nm in toluene. (b) Decay trace of Methyl Blue at 600 nm in methonal. (c) Decay trace at 380 nm for **BDP-Pery-2** mixed with styryl-BDP in toluene. (d) Decay trace at 380 nm for Methyl Blue mixed with styryl-BDP in methonal. The solutions in each figure show the same absorbance (0.16) at the excitation wavelength (λ_{ex} = 555 nm), and the styryl-BDP is of the same quantity. 20 °C.

7.0 DFT Calculations

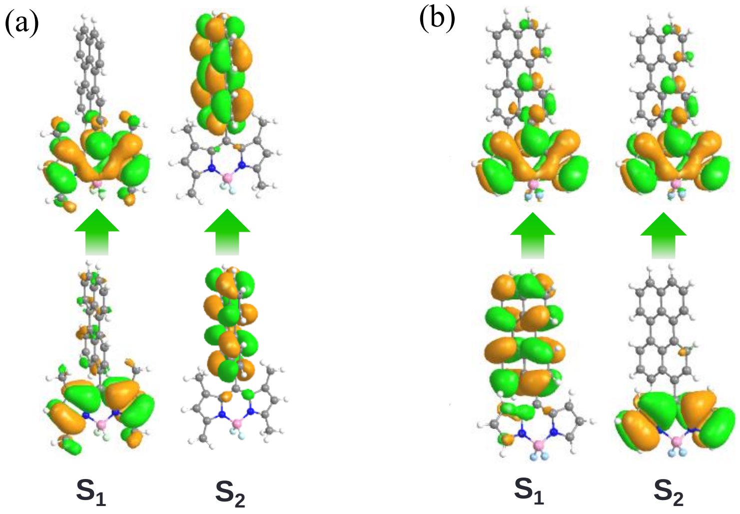


Figure S18. Natural Transition Orbital (NTO) pairs for selected singlet excited states of (a) **BDP-Pery-1** and (b) **BDP-Pery-2**. Hole and particle wave functions are placed at the start and the end of the arrows, respectively. Calculated at TDDFT//M06-2X//6-31+G** level with Gaussian 09W.

Table S2. M062X/6-31+G** Vertical Singlet and Triplet Energies for All the Investigated Molecules in Toluene by Using the IEFPCM Method.

Compound	**Excited State** [a]	**MO contribution** [b]	**Energy level (wavelength)**	***f*** [c]
BDP-Pery-1	$\mathbf{T_1}$	H-1 → L (90%)	1.51 eV (821 nm)	0
	$\mathbf{T_2}$	H → L+1 (56%)	1.93 eV (642 nm)	0
BDP-Pery-2	$\mathbf{T_1}$	H-1 → L (94%)	1.57 eV (790 nm)	0
	$\mathbf{T_2}$	H → L+1 (73%)	1.91 eV (649 nm)	0
	$\mathbf{T_3}$	H → L (65%)	2.56 eV (484 nm)	0

[a] Only selected excited states were considered. [b] Main transitions associated to each excited state, H stands for HOMO and L stands for LUMO. Only the main configurations are presented. [c] Oscillator strength.

Coordinates of the Optimized Geometries of the Compounds

BDP-Pery-1

E(RM062X) = -1606.3142418 a.u.
Dipole Moment = 6.0398 Debye
Imaginary Freq = 0

	X	Y	Z
C	4.254538	2.516093	0.004970
C	2.007075	2.566464	-0.297044
C	2.474417	1.216500	-0.282036
C	1.794646	-0.000483	-0.387699
C	2.473398	-1.218464	-0.286688
C	2.004944	-2.567904	-0.306801
C	4.252406	-2.520618	-0.004316
N	3.856766	1.240352	-0.092700
N	3.855700	-1.244135	-0.097295
B	4.784877	-0.002408	-0.052942
F	5.640317	-0.000726	-1.159934
F	5.540423	-0.004799	1.121319
C	3.131162	3.361024	-0.116598
C	3.128372	-3.364100	-0.129131
H	3.152314	-4.445102	-0.089574
H	3.156071	4.441850	-0.072994
C	0.319645	0.000604	-0.594284
C	-0.561831	-0.001643	0.525660
C	-0.193353	0.003935	-1.868328
C	-0.053420	-0.005180	1.850572
C	-1.972924	-0.000157	0.308111
C	-1.583173	0.005259	-2.082178
H	0.481371	0.005626	-2.720076
C	-0.915943	-0.007126	2.917365
H	1.020499	-0.006317	2.009621
C	-2.854393	-0.002094	1.437045
C	-2.482579	0.003339	-1.030113
H	-1.932144	0.007918	-3.107429
C	-2.307784	-0.005549	2.708799
H	-0.529714	-0.009849	3.931500
H	-2.948246	-0.007091	3.582279
C	-3.945330	0.004810	-1.252590
C	-4.823068	0.003100	-0.123192
C	-4.494404	0.007842	-2.523664
C	-4.317642	-0.000251	1.214924
C	-6.233531	0.004740	-0.336734

BDP-Pery-2

E(RM062X) = -1449.10369930 a.u.
Dipole Moment = 7.1554 Debye
Imaginary Freq = 0

	X	Y	Z
C	-5.014161	9.023148	-1.607077
C	-6.032441	8.273611	-1.006342
C	-6.799641	8.832761	0.024048
C	-3.716472	10.777804	-1.924383
C	-3.271844	9.782617	-2.818919
C	-4.083539	8.676621	-2.618038
C	-7.891534	8.304447	0.753192
C	-8.299333	9.287099	1.642980
C	-7.455091	10.396617	1.434396
N	-6.564778	10.125736	0.475207
N	-4.748214	10.326457	-1.206190
B	-5.507851	11.117756	-0.098055
F	-6.141151	12.225019	-0.650258
F	-4.625709	11.514322	0.898942
H	-2.450911	9.880241	-3.513547
H	-4.031850	7.716846	-3.113403
H	-3.335768	11.779506	-1.771796
H	-8.306558	7.314191	0.621626
H	-7.459958	11.362085	1.923858
H	-9.105820	9.233431	2.359102
C	-6.322030	6.906575	-1.503215
C	-6.148278	5.748767	-0.682271
C	-6.776263	6.762795	-2.796294
C	-6.502029	4.465185	-1.202713
C	-5.588795	5.843116	0.618834
C	-7.133691	5.501981	-3.298739
H	-6.890050	7.641094	-3.425133
C	-6.304340	3.299509	-0.393201
C	-7.033265	4.357194	-2.527785
C	-5.414065	4.714979	1.378921
H	-5.295226	6.812437	1.006917
C	-5.776979	3.451969	0.877151
C	-6.657129	1.967891	-0.934890
C	-7.450558	3.035947	-3.042551
H	-4.986727	4.791092	2.373510
C	-7.234939	1.873435	-2.239259

C	-5.887939	0.009384	-2.730671	C	-6.453948	0.803608	-0.213413
H	-3.855897	0.009084	-3.398861	C	-8.048803	2.889158	-4.282972
C	-5.218838	-0.001622	2.265903	C	-7.608913	0.595097	-2.748445
C	-7.113604	0.003194	0.775373	C	-6.812446	-0.459801	-0.724060
C	-6.744647	0.007911	-1.659520	C	-8.423732	1.625564	-4.780190
H	-6.274488	0.011771	-3.744697	C	-7.384464	-0.565937	-1.966293
C	-6.611415	0.000097	2.051653	C	-8.203764	0.496914	-4.032200
H	-4.867899	-0.004057	3.290717	H	-6.633414	-1.345538	-0.123045
H	-8.185023	0.004528	0.595940	H	-8.887371	1.554717	-5.758799
H	-7.821173	0.009089	-1.805421	H	-7.672583	-1.533125	-2.368451
H	-7.279946	-0.001051	2.906444	H	-8.484370	-0.483802	-4.406009
C	5.677518	-2.903810	0.214155	H	-7.498744	5.453271	-4.317009
H	6.333995	-2.363175	-0.472396	H	-5.621131	2.590947	1.515592
H	5.987218	-2.649446	1.232375	H	-8.249728	3.754378	-4.903303
H	5.802417	-3.977153	0.064498	H	-6.010030	0.839389	0.774150
C	0.602888	-3.071656	-0.468964				
H	-0.052779	-2.702971	0.326181				
H	0.165896	-2.754630	-1.420015				
H	0.601727	-4.163214	-0.434676				
C	0.605454	3.072081	-0.457193				
H	0.168753	2.760511	-1.410184				
H	-0.050916	2.699557	0.335565				
H	0.605067	4.163441	-0.417048				
C	5.679941	2.897465	0.224695				
H	5.989127	2.640725	1.242479				
H	6.336143	2.357775	-0.462843				
H	5.805816	3.971032	0.077434				

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