## Evaluation of Fused Aromatic-Substituted

## Diketopyrrolopyrrole Derivatives for Singlet Fission Sensitizers

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## 1. Solvation effect on SF relevant excited state energies

The solvation effect was evaluated by polarizable continuum model (PCM). Two common solvents, namely toluene (Tol) and dichlorimethane (DCM), were considered. They show quite similar results for both  $E(S_1)$ ,  $E(T_1)$ , and  $E(T_2)$ , and the maximum difference of which is ~ 0.11 eV. As a result,  $E(S_1)$ ,  $E(T_1)$ , and  $E(T_2)$  were calculated with toluene taken as solvent for all DPP derivatives in this work.

Table S1. Adiabatic Excitation Energies [eV] of DPP derivatives in different solutions.

Compound	Solvent	<b>E(S</b> <sub>1</sub> )	<b>E</b> ( <b>T</b> <sub>1</sub> )	<b>E</b> ( <b>T</b> <sub>2</sub> )
1T-DPP	Tol	2.152	1.041	2.550
	DCM	2.047	1.051	2.529
F2T-DPP	Tol	1.958	0.971	2.319
	DCM	1.847	0.979	2.305
F3T-DPP	Tol	1.827	0.934	2.164
	DCM	1.714	0.942	2.153



Figure S1. Molecular Structures of *n***F**-**DPP** and *n***T**-**DPP**.



Figure S2  $y_1/y_0$  of *Fn*F-DPP and *Fn*T-DPP with respect of the number (*n*) of fused thiophene and furan rings.



Figure S3  $E(T_1)$  of fused and non-fused aromatic substituted DPP derivatives with respect to the number (n) of thiophene and furan rings on each sides.





Figure S4 (a)  $E(S_1)$ ,  $E(T_1)$  and  $E(T_2)$ , as well as (b)  $\Delta E_{SF}$  and  $\Delta E_{TTA}$  of **R-FBF'-DPP** and **R-TBT'-DPP**.