## **Electronic Supplementary Information**

## A new class of triphenylamine based novel sensitizers for DSSC: A comparative study of three different anchoring groups

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**Scheme S1** Synthesis of TPA sensitizers: (a) acetyl chloride, ZnCl<sub>2</sub>, DCM, rt, (b) DMF, POCl<sub>3</sub>, DCM, reflux. (c) Cyanoacetic acid, acetonitrile, piperidine, reflux. (d) Rhodanine 3-acetic acid, ammonium acetate, acetic acid, reflux. (e) p-aminosalicylic acid, ethanol, reflux.



**Figure S1.** The optimized geometries of the all three sensitizers, obtained at the B3LYP/6-31G(d) level in vacuum.



Figure S2. Chemical structures of TPACA, TPARN, and TPASA compared with reported analogue 2a.



Figure S3. HOMO energy of TPACA sensitizer.



Figure S4. HOMO energy of TPARN sensitizer.



Figure S5. HOMO energy of TPASA sensitizer.



**Figure S6.** <sup>1</sup>H NMR spectrum of compound 1.



Figure S7. <sup>13</sup>C NMR spectrum of compound



**Figure S8.** <sup>1</sup>H NMR spectrum of compound 2.



Figure S9. <sup>13</sup>C NMR spectrum of compound



Figure S10. <sup>1</sup>H NMR spectrum of compound TPACA



Figure S11. <sup>13</sup>C NMR spectrum of compound TPACA



Figure S12. <sup>1</sup>H NMR spectrum of compound TPARN



Figure S13. <sup>13</sup>C NMR spectrum of compound TPARN



Figure S14. <sup>1</sup>H NMR spectrum of compound TPASA



Figure S15. <sup>13</sup>C NMR spectrum of compound TPASA



Figure S16: MS spectrum of compound TPACA



Figure S17: MS spectrum of compound TPARN



Figure S18: MS spectrum of compound TPASA

Table S1 Optical properties of TPACA, TPARN and TPASA in acetonitrile.

Sensitizer	$\lambda_{abs} \left( \mathbf{nm} \right)$	€(M <sup>-1</sup> cm <sup>-1</sup> ) x10 <sup>4</sup>	λ <sub>em</sub> (nm)	Δv(cm <sup>-1</sup> )	Δv(nm)	ф (%)
TPACA	462	23.5	621	5541.96	159	2.97
TPARN	488	11.8	637	4793.22	149	3.54
TPASA	369	7.03	484	6439.11	115	5.64

**Table S2.** Vertical excitation energy and oscillator strength and orbital contributions of **TPACA**, **TPARN**, and **TPASA** with help of TD-B3LYP 6-31G(d) level in acetonitrile.

Sensitizers	Sate	$\lambda_{max}$	eV	Main configurations	f
TPACA	S <sub>0</sub> -S <sub>1</sub>	533	2.32	H-L (99.84%)	1.048
TPARN	S <sub>0</sub> -S1	581	2.13	H-L (99.88%)	1.131
TPASA	$S_0-S1$	482	2.56	H-L (99.02%)	1.157