## Supporting Information

New D-D- $\pi$-A type organic dyes having carbazol-N-yl phenothiazine moiety as a donor (D-D) unit for efficient dye-sensitized solar cells: Experimental and theoretical studies
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Quantum chemical calculation

| CPhPA | Front view | Side view |
| :--- | :--- | :--- | :--- |
| CPhTPA |  |  |

Figure S1. Optimized structures of the dyes calculated by B3LYP/6-31G(d,p) in $\mathrm{CH}_{2} \mathrm{Cl}_{2}$ solvent.

Table S1 Excitation energy (eV), oscillator strength ( $f$ ) and transition composition of the dyes at the 20 lowest transitions $(f>0.200)$ were calculated by TD CAM-B3LYP/6-31G(d,p) in $\mathrm{CH}_{2} \mathrm{Cl}_{2}(\mathrm{C}-\mathrm{PCM}$ model).

| Dye |  | $\mathrm{E}_{\mathrm{ex}}$ <br> $[\mathrm{eV}, \mathrm{nm}]$ | $f$ | Transition contribution |
| :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |
| CPhPA | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{1}$ | $3.04(407)$ | 0.9708 | $0.61(\mathrm{H} \rightarrow \mathrm{L})+0.25(\mathrm{H} \rightarrow \mathrm{L}+1)$ |
|  | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{2}$ | $3.82(324)$ | 0.2670 | $0.54(\mathrm{H} \rightarrow \mathrm{L}+1)+0.24(\mathrm{H}-3 \rightarrow \mathrm{~L})$ |
|  | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{3}$ | $4.06(305)$ | 0.3284 | $0.52(\mathrm{H}-3 \rightarrow \mathrm{~L}+2)+0.21(\mathrm{H} \rightarrow \mathrm{L})$ |
| CPhTPA | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{1}$ | $3.00(413)$ | 1.7595 | $0.52(\mathrm{H} \rightarrow \mathrm{L})+0.27(\mathrm{H}-3 \rightarrow \mathrm{~L})$ |
|  | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{4}$ | $4.31(287)$ | 0.2981 | $0.35(\mathrm{H} \rightarrow \mathrm{L}+3)$ |
|  | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{10}$ | $4.81(257)$ | 0.2607 | $0.64(\mathrm{H}-2 \rightarrow \mathrm{~L}+2)$ |
| CPhT2PA | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{1}$ | $2.82(440)$ | 2.1499 | $0.51(\mathrm{H} \rightarrow \mathrm{L})+0.24(\mathrm{H} \rightarrow \mathrm{L}+1)$ |
|  | $\mathrm{S}_{0} \rightarrow \mathrm{~S}_{13}$ | $4.81(257)$ | 0.2505 | $0.57(\mathrm{H}-3 \rightarrow \mathrm{~L}+2)$ |

Note: H = HOMO, L = LUMO, L+1 = LUMO+1, ..


Figure S2. DPV curves measured in $\mathrm{CH}_{2} \mathrm{Cl}_{2}$ with $n$ - $\mathrm{Bu}_{4} \mathrm{NPF}_{6}$ as a supporting electrolyte at a scan rate of $50 \mathrm{mV} \mathrm{s}^{-1}$.

## ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$-NMR spectra

## Compound 3




## Compound 4




## Compound 5




## Compound 6




## Compound 7




## Compound 8




## Compound 9




## Compound 10




## CPhPA




## CPhTPA




## CPhT2PA







