A novel carbazole-based dye outperformed the benchmark dye N719 for high efficiency dye-sensitized solar cells (DSSCs)

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Supporting Information and Experimental Section

1.1. Analytical Measurements

1.1.1. UV-Vis absorption of NCSU-10, NCSU-10', and N719 adsorbed on TiO$_2$

Figure S1  Absorption spectrum of NCSU-10, NCSU-10', and N719 adsorbed on TiO$_2$.

1.1.2. Fluorescence Spectra and time-resolved photoluminescence spectroscopy

Figure S2  Time-resolved emission decays for NCSU-10, NCSU-10', and N719 measured in DMF.
1.1.3. Infra Red Spectroscopy

Figure S3 FT-IR of the pure form of NCSU-10.

Figure S4 FT-IR of the pure form of NCSU-10’.
1.1.4. Mass Spectrometry

ESI mass spectrum of **NCSU-10**, Mass 1056.18139; \([M - 2H + TBA]^{-1}\); Theo. m/z = 1296.4505, found. m/z = 1296.4571, Error = 5.00 ppm.

ESI mass spectrum of **NCSU-10′**, Mass 1056.18139; \([M - 2H + TBA]^{-1}\); Theo. m/z = 1296.4505, Found. m/z = 1296.4505, Error = 0.00 ppm.

![Figure S5](image1.png)

**Figure S5** ESI mass spectrum of **NCSU-10**, Mass 1056.18139; \([M - 2H + TBA]^{-1}\); Theo. M/Z = 1296.4505, Found. M/Z = 1296.4571, Error = 5.09 ppm.

![Figure S6](image2.png)

**Figure S6** ESI mass spectrum of **NCSU-10′**, Mass 1056.18139; \([M - 2H + TBA]^{-1}\); Theo. M/Z = 1296.4505, Found. M/Z = 1296.4505, Error = 0.00 ppm.
1.1.5. Temperature Dependent $^1$H-NMR Experiments

Figure S7  Temperature dependent $^1$H-NMR for NCSU-10.
Figure S8  Zoom-in on the 2 CH₃, showing two triplets well resolved at 52 °C, for NCSU-10.
Figure S9  Zoom-in on the 2 CH₂, showing two quartets well resolved at 52 °C, for NCSU-10.

Figure S10  ¹H-NMR of NCSU-10."
Figure S11  Zoom-in on the aromatic region of NCSU-10.

Figure S12  Zoom-in on the aromatic region of NCSU-10'.
1.2. Photoemission Yield Spectrometer (AC3) and E_{0,0} Measurements

**Figure S13**  HOMO energy value of NCSU-10.

**Figure S14**  HOMO energy value of NCSU-10'
Figure S15  HOMO energy value of N719.