

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

Ahmed El-Shafei<sup>1\*</sup>, Maqbool Hussain<sup>1</sup>, Aasim Atiq<sup>1</sup>, Ashraful Islam<sup>2\*</sup>, Liyuan Han<sup>2</sup>

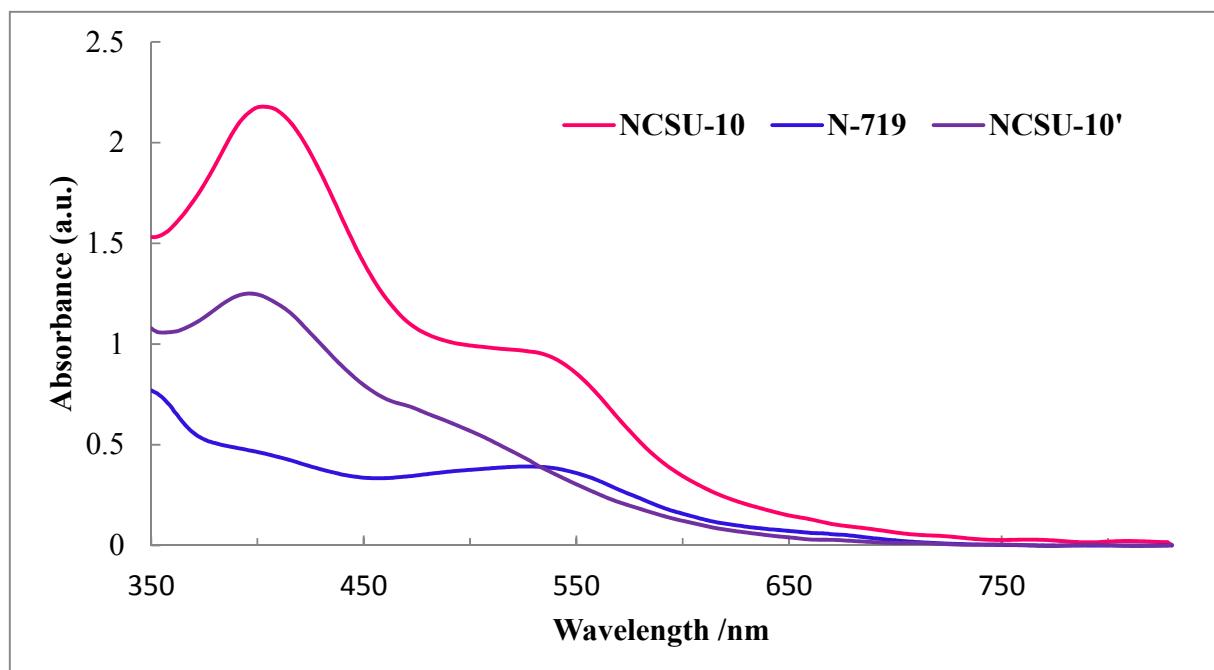
<sup>1</sup>Polymer and Color Chemistry Program, North Carolina State University, Raleigh, NC, 27695, USA

<sup>2</sup>Photovoltaic Materials Unit, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.

## Supporting Information and Experimental Section

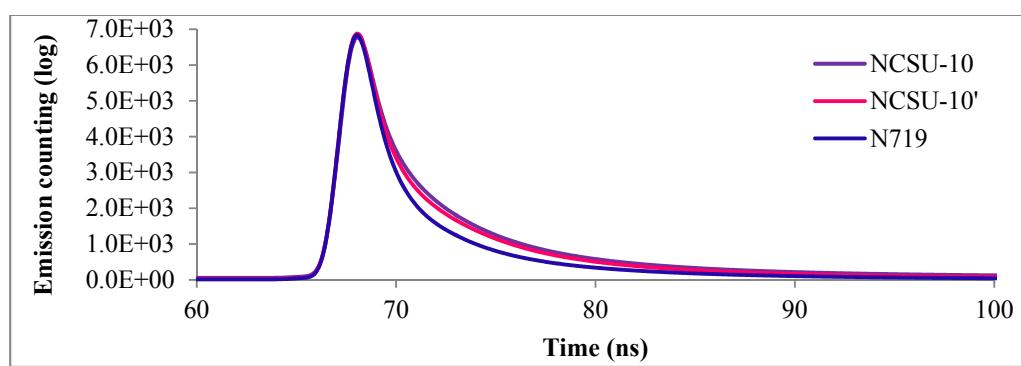
### 1.1. Analytical Measurements

#### 1.1.1. UV-Vis absorption of NCSU-10, NCSU-10', and N719 adsorbed on TiO<sub>2</sub>



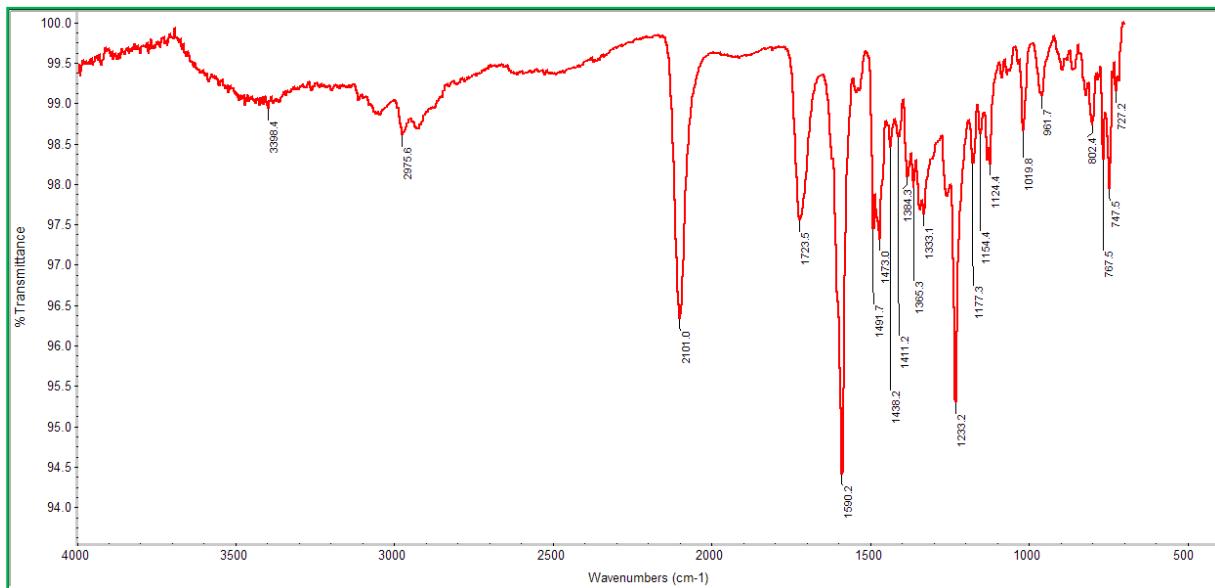
**Figure S1** Absorption spectrum of NCSU-10, NCSU-10', and N719 adsorbed on TiO<sub>2</sub>.

#### 1.1.2. Fluorescence Spectra and time-resolved photoluminescence spectroscopy

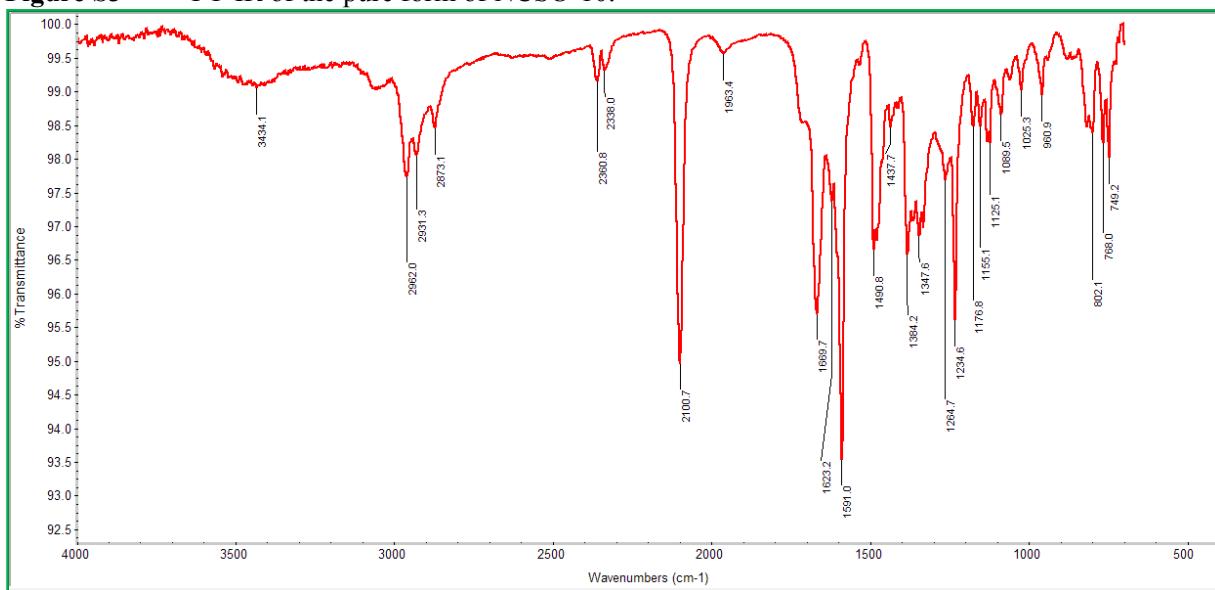


**Figure S2** Time-resolved emission decays for NCSU-10, NCSU-10', and N719 measured in DMF.

### 1.1.3. Infra Red Spectroscopy



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

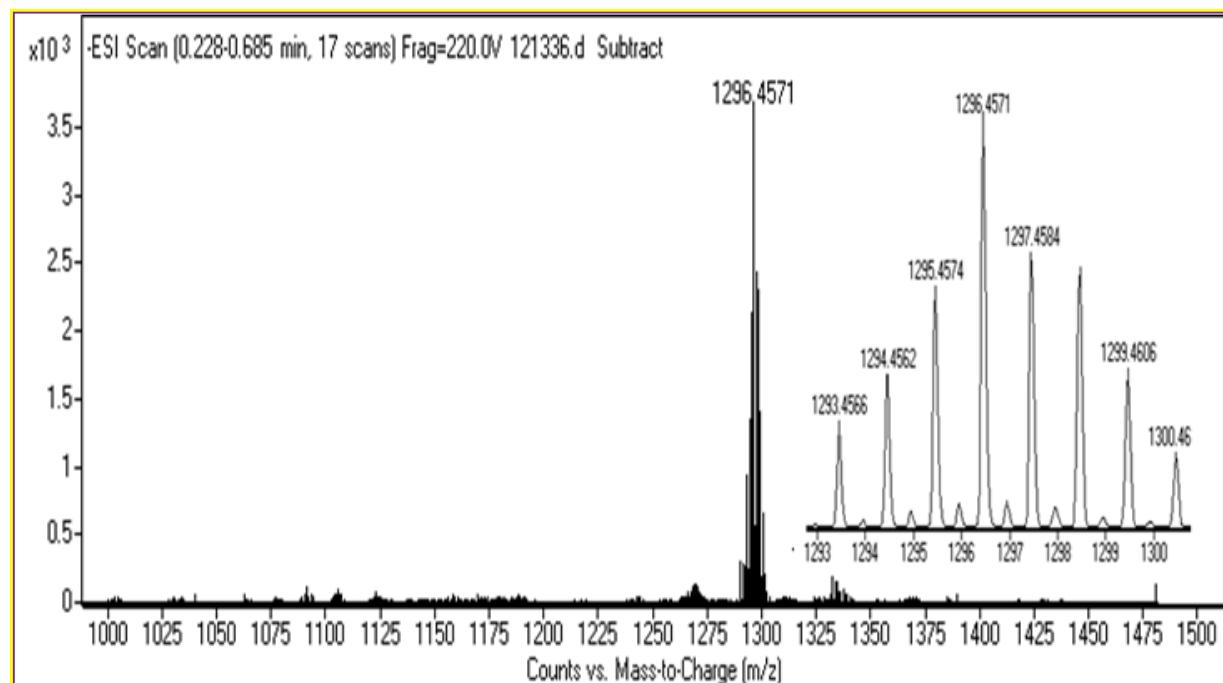


**Figure S4** FT-IR of the pure form of NCSU-10'.

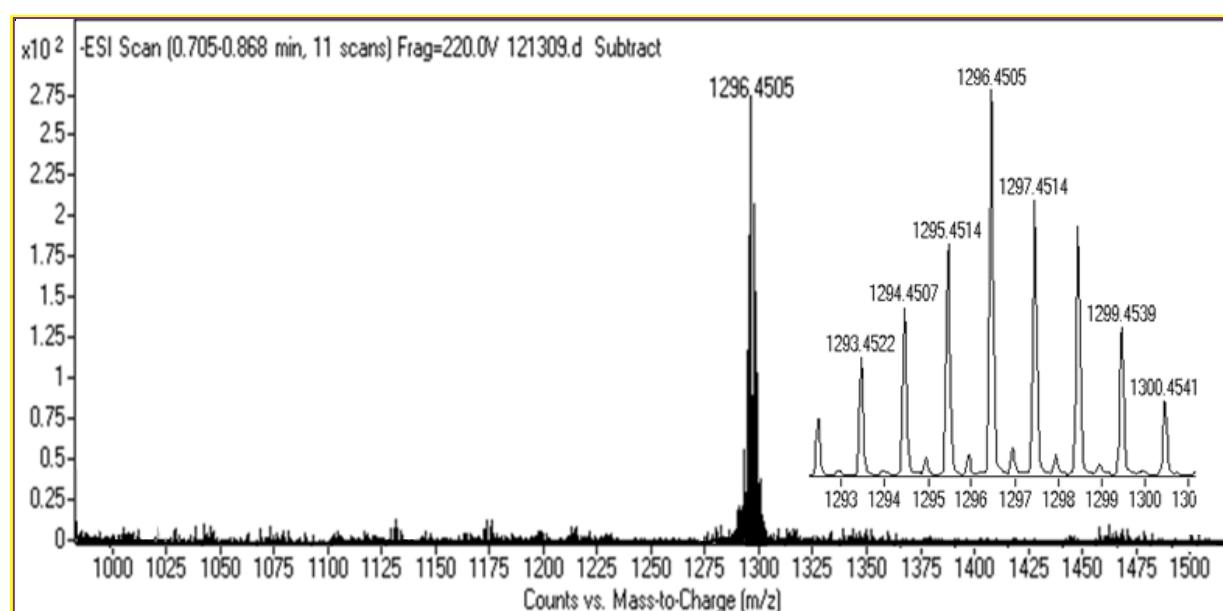
#### 1.1.4. Mass Spectrometry

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.

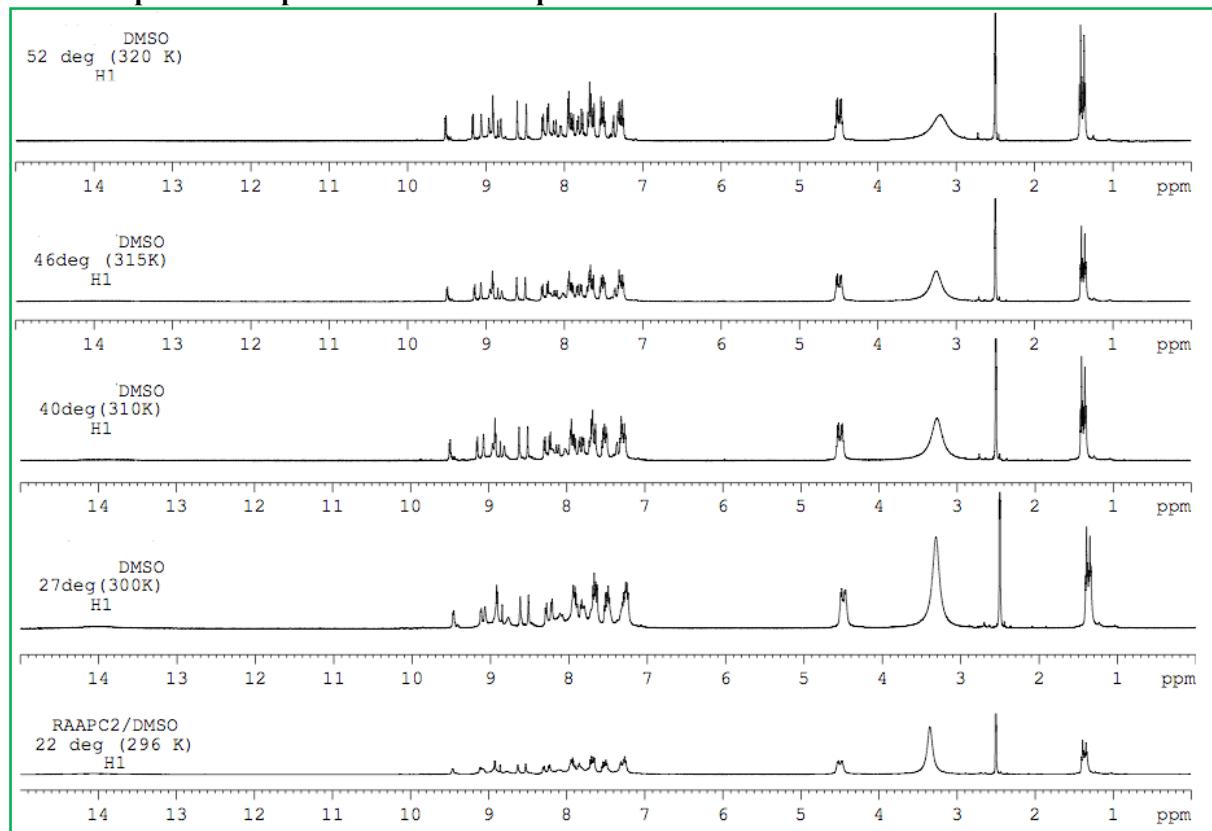


**Figure S5** ESI mass spectrum of **NCSU-10**, Mass 1056.18139;  $[M - 2H + TBA]^{-1}$ ; Theo. M/Z = 1296.4505, Found. M/Z = 1296.4571, Error = 5.09 ppm.

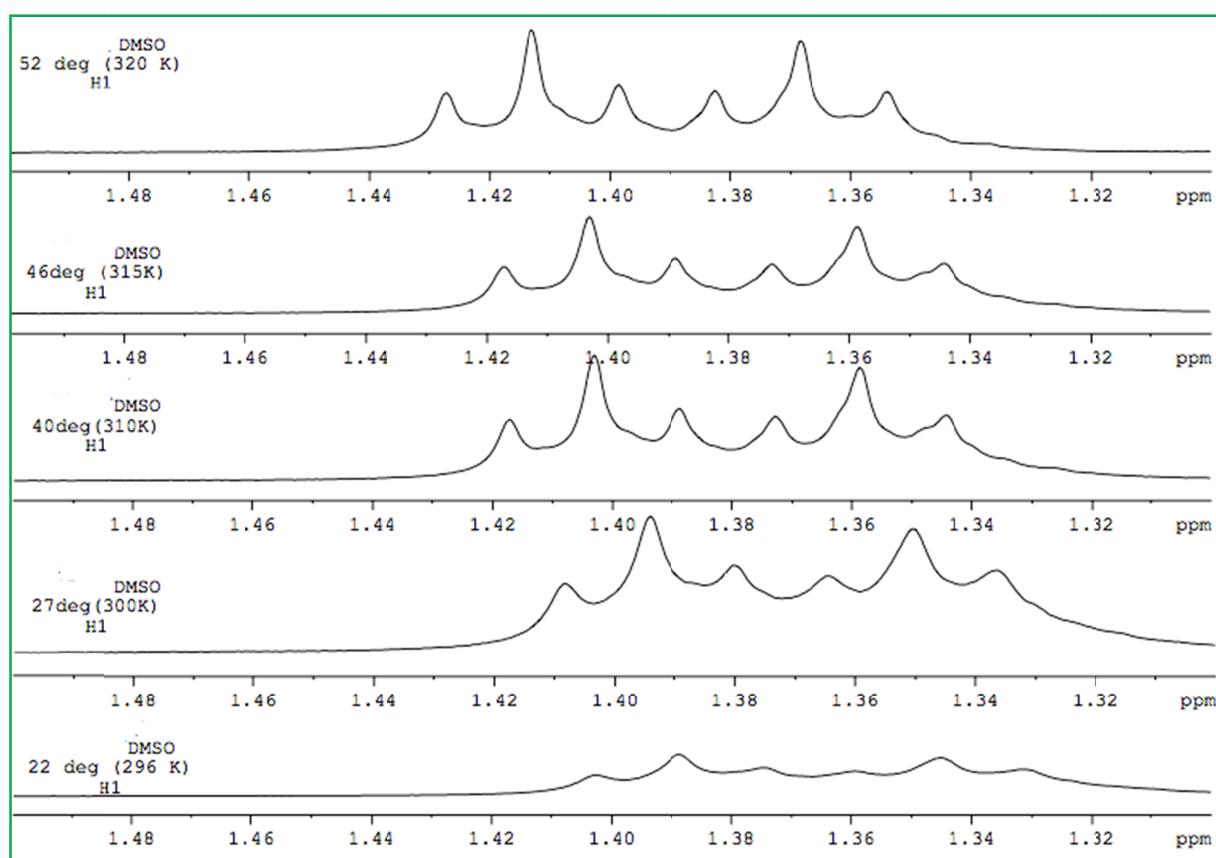


**Figure S6** ESI mass spectrum of **NCSU-10'**, Mass 1056.18139;  $[M - 2H + TBA]^{-1}$ ; Theo. M/Z = 1296.4505, Found. M/Z = 1296.4505, Error = 0.00 ppm.

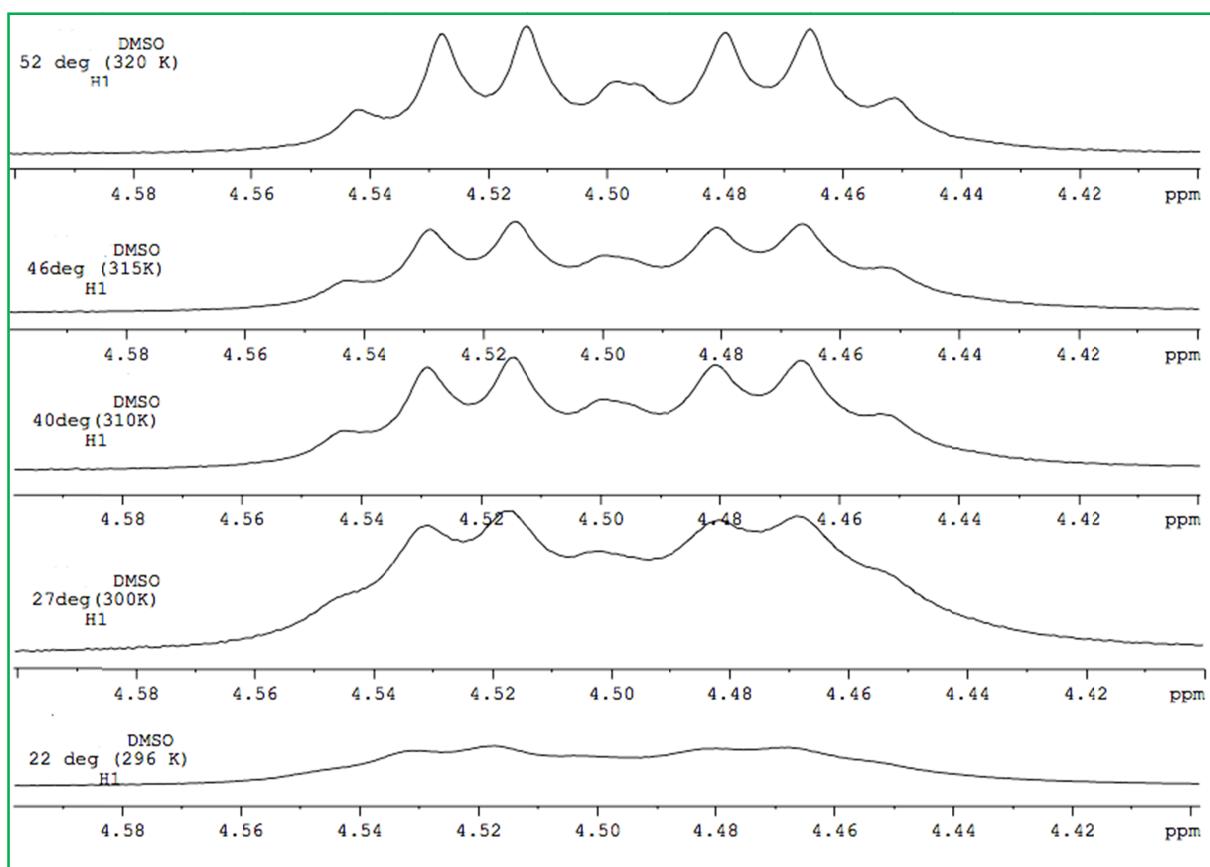
### 1.1.5. Temperature Dependent $^1\text{H}$ -NMR Experiments



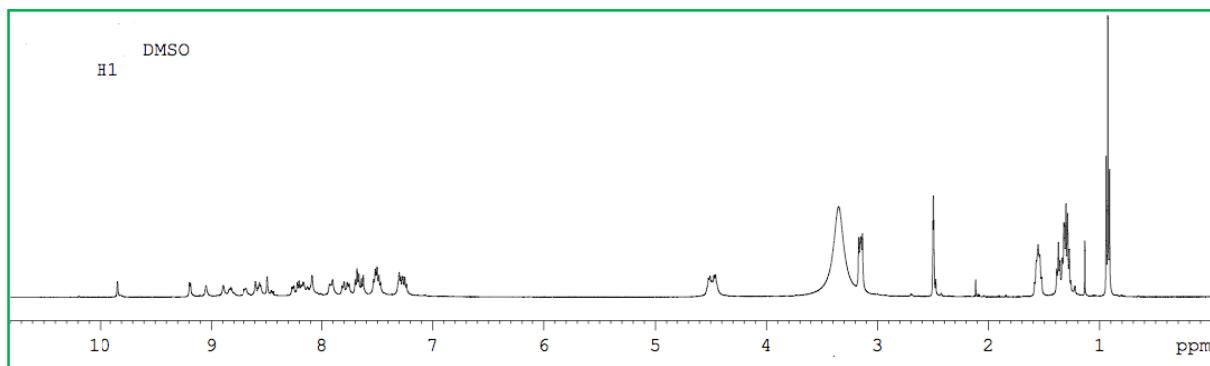
**Figure S7** Temperature dependent  $^1\text{H}$ -NMR for NCSU-10.



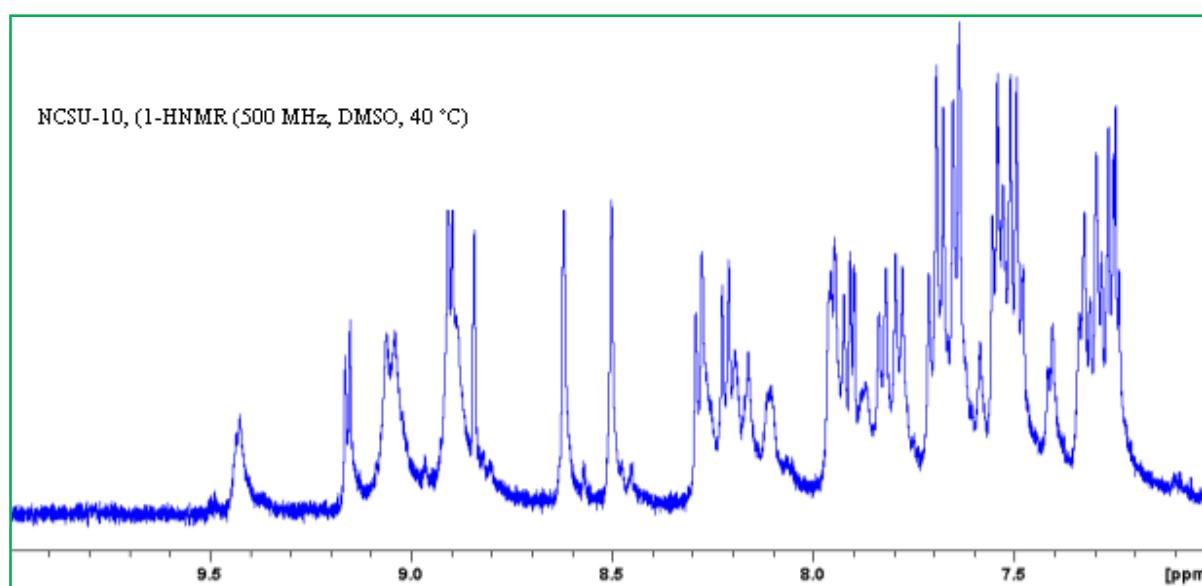
**Figure S8** Zoom-in on the  $2 \text{CH}_3$ , showing two triplets well resolved at 52 °C, for NCSU-10.



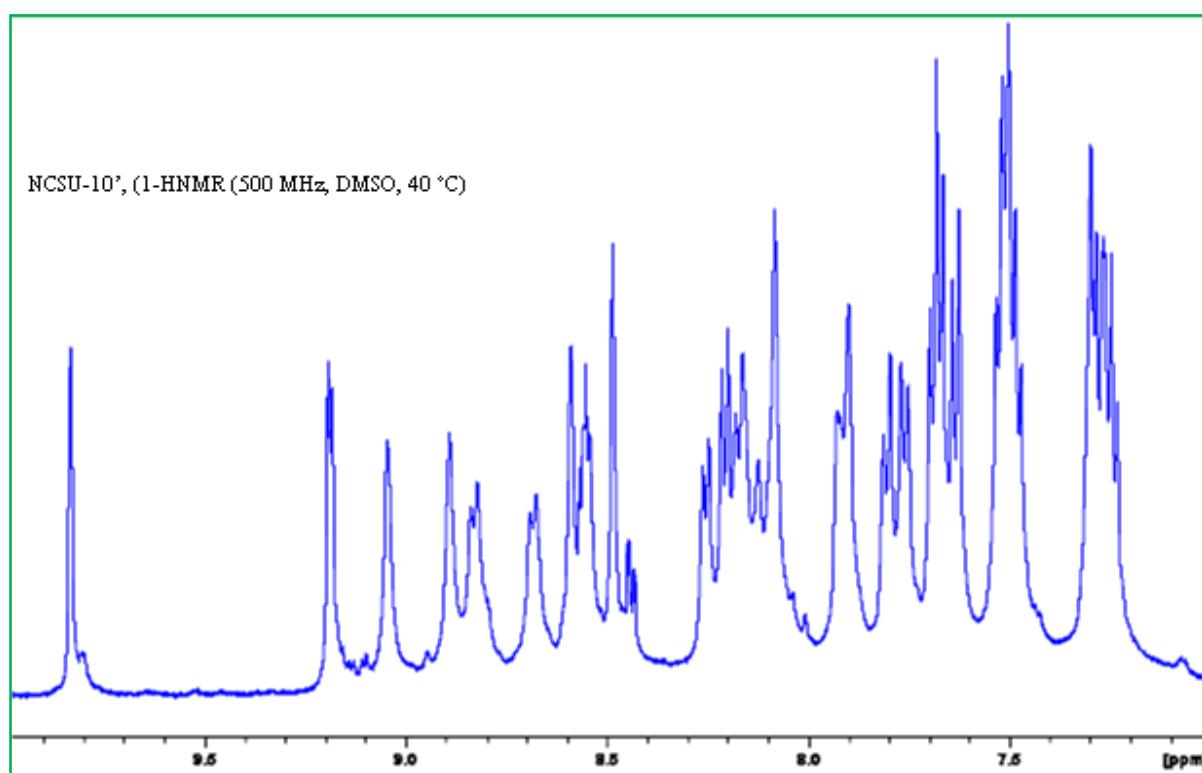
**Figure S9** Zoom-in on the  $2\text{CH}_2$ , showing two quartets well resolved at  $52\text{ }^{\circ}\text{C}$ , for NCSU-10.



**Figure S10**  ${}^1\text{H-NMR}$  of NCSU-10'.

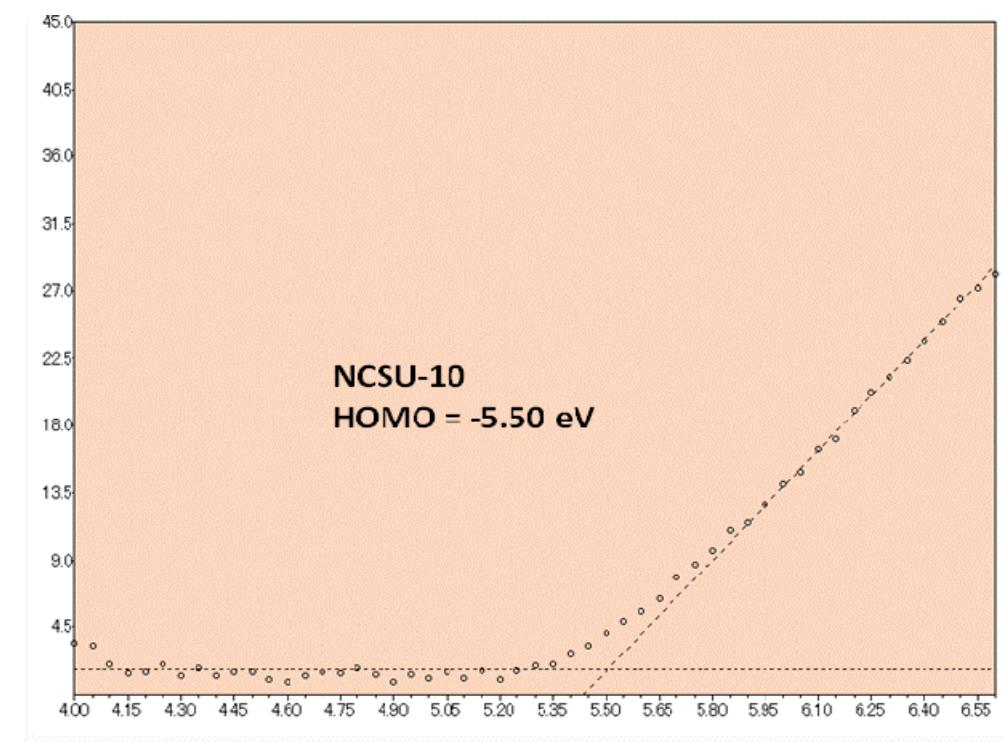


**Figure S11** Zoom-in on the aromatic region of NCSU-10.

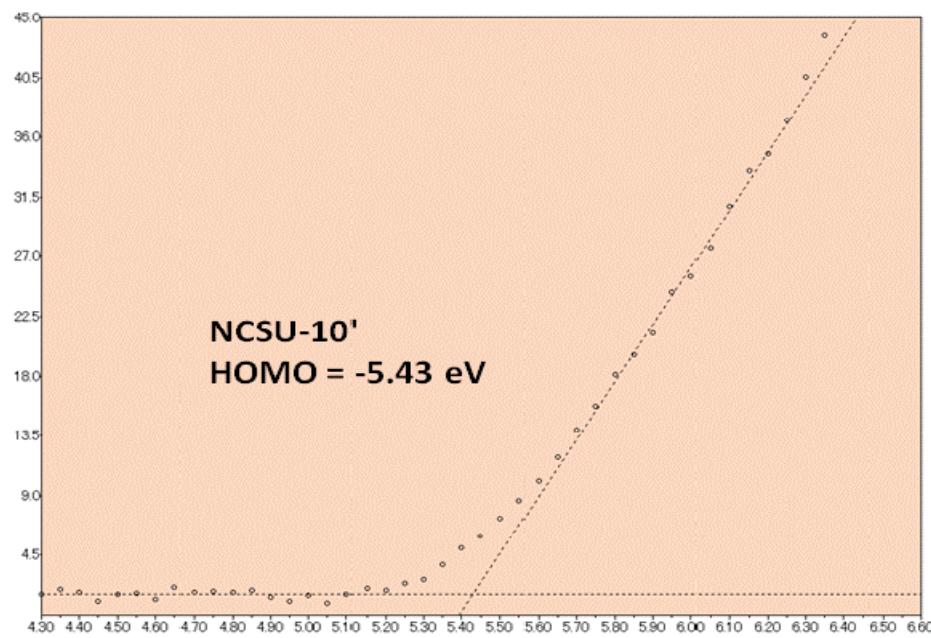


**Figure S12** Zoom-in on the aromatic region of NCSU-10'.

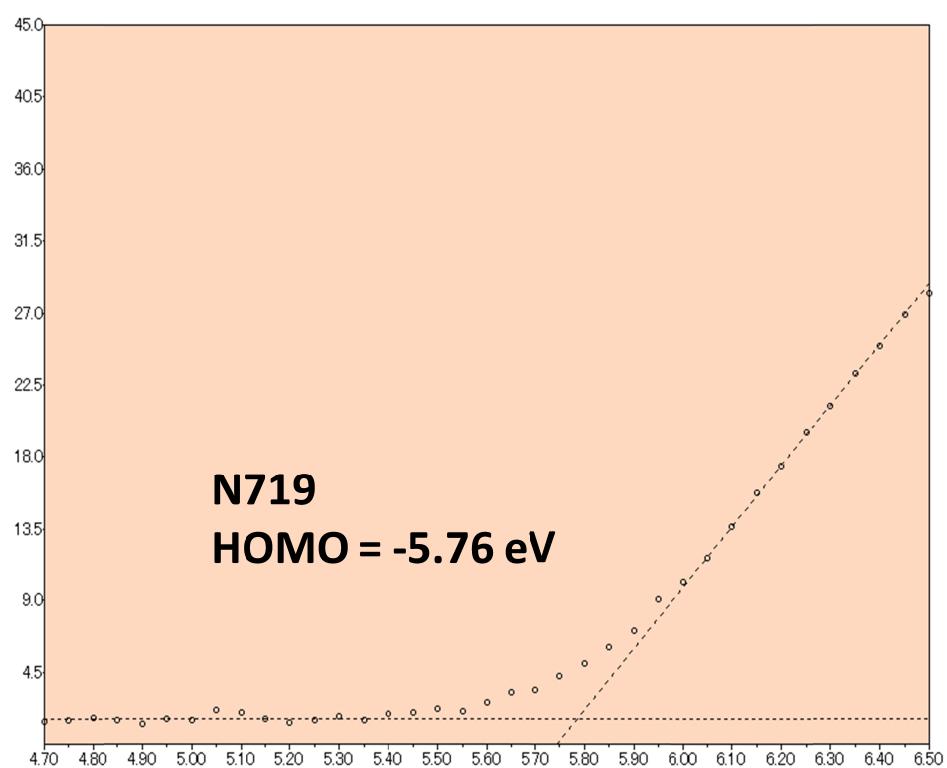
## 1.2. Photoemission Yield Spectrometer (AC3) and $E_{0-0}$ Measurements



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



**Figure S14** HOMO energy value of NCSU-10'



**Figure S15** HOMO energy value of N719.