

## **Electronic Supporting Information**

### **Tuning the Aggregation Performance by Varying the Substituent Position: Comparative Study of Neutral Bis-Urea Derivatives in Aqueous Medium**

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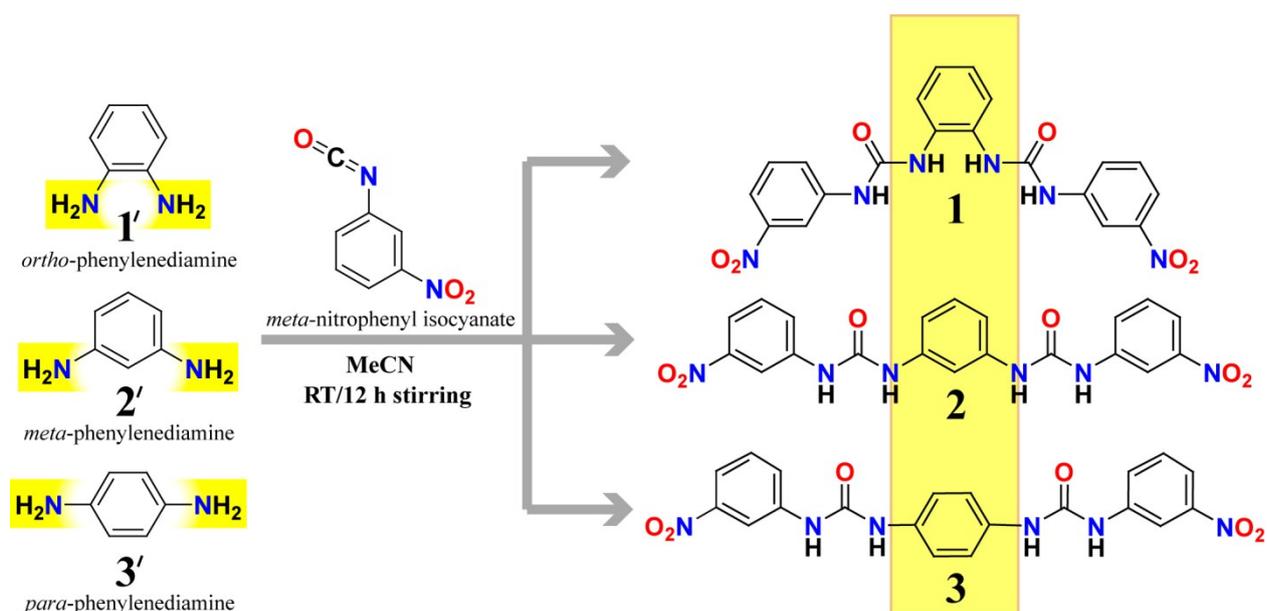
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**Materials and Experimental Methods:** All the materials for synthesis and experiments were purchased from commercial suppliers and used without further purification.

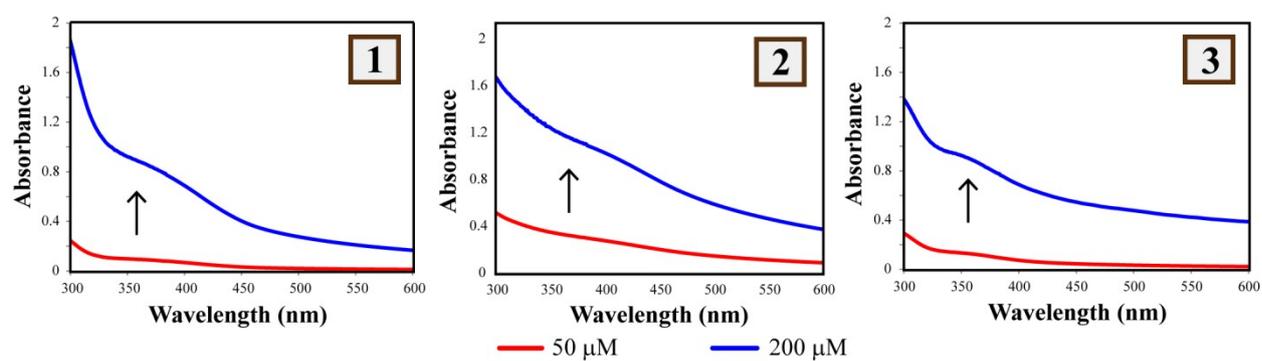
Stock solutions of **1**, **2** and **3** ( $5 \times 10^{-3}$  mol L<sup>-1</sup>) was prepared in DMF and then diluted to  $10 \times 10^{-6}$  mol L<sup>-1</sup> for various spectral studies for aggregation phenomenon in Millipore water and acetonitrile. The absorption measurements were recorded on a PerkinElmer Lambda-25 UV-Vis spectrophotometer using 10 mm path-length quartz cuvettes in the wavelength range of 300–700 nm, while the fluorescence spectra were recorded on a Horiba Fluoromax-4 Spectrofluorometer using 10 mm path length quartz cuvettes with a slit width of 3 nm at 298 K. The particle sizes were measured by dynamic light scattering (DLS) experiments on Malvern Zetasizer Nano ZS instrument equipped with a 4.0 mW He-Ne laser operating at a wavelength of 633 nm. The samples and the background were measured at room temperature (25 °C). The solution was equilibrated for 60 minutes before taking the measurements. The FT-IR spectra of air-dried compounds and their aggregated form were recorded on a PerkinElmer-Spectrum One FT-IR spectrometer with KBr disks in the range 4000–450 cm<sup>-1</sup>. The morphology of the aggregated species were investigated by using FESEM imaging studies by drop (1 mM/ 2  $\mu$ l) cast method on glass plates covered with Al-foil using Gemini 300 FESEM (Carl Zeiss).

To investigate the effect of external factor on aggregation behavior of all three compounds individually, the concentration of the respective compound was maintained at 50  $\mu$ M in final solutions of **1**, **2** and **3** for all spectral studies.

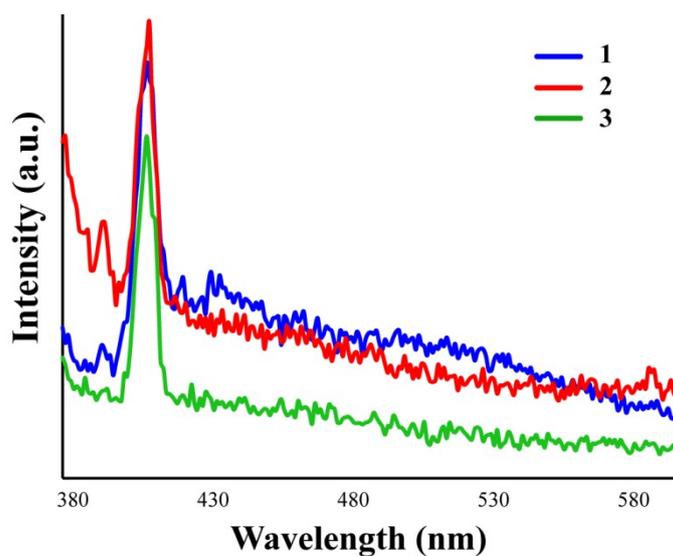
DFT optimizations of all three derivatives were carried out with the RB3LYP/ 6-31G method basis set using the Gaussian 09 program and the results are given in the **Table S1**.



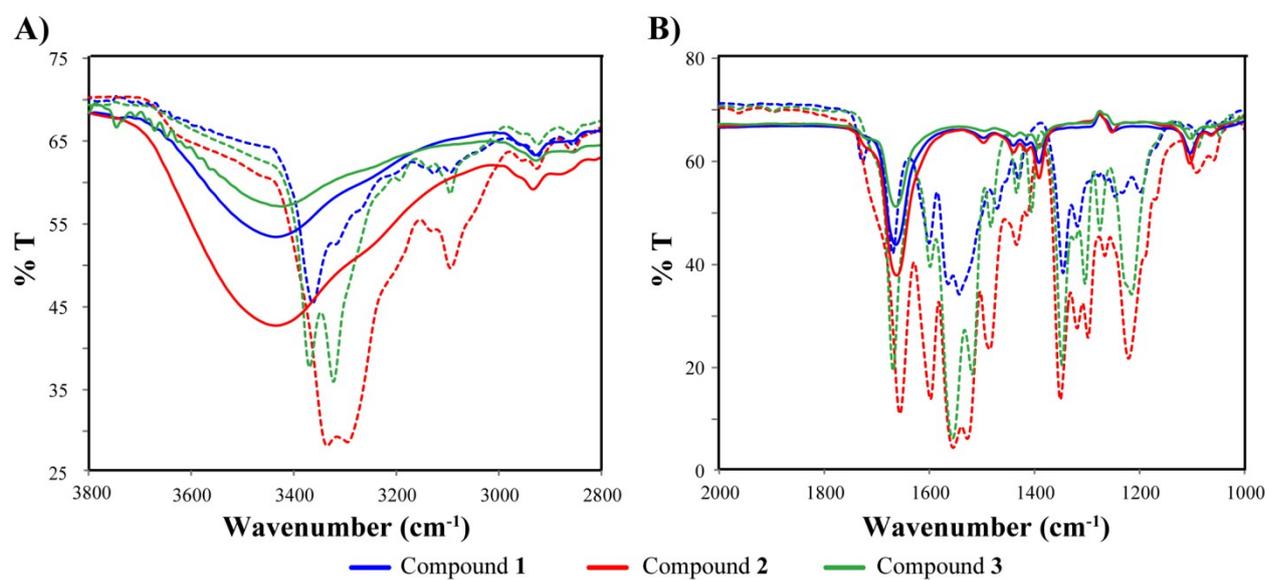
**Scheme S1:** Schematic representation of synthetic strategy of **1**, **2** and **3**.



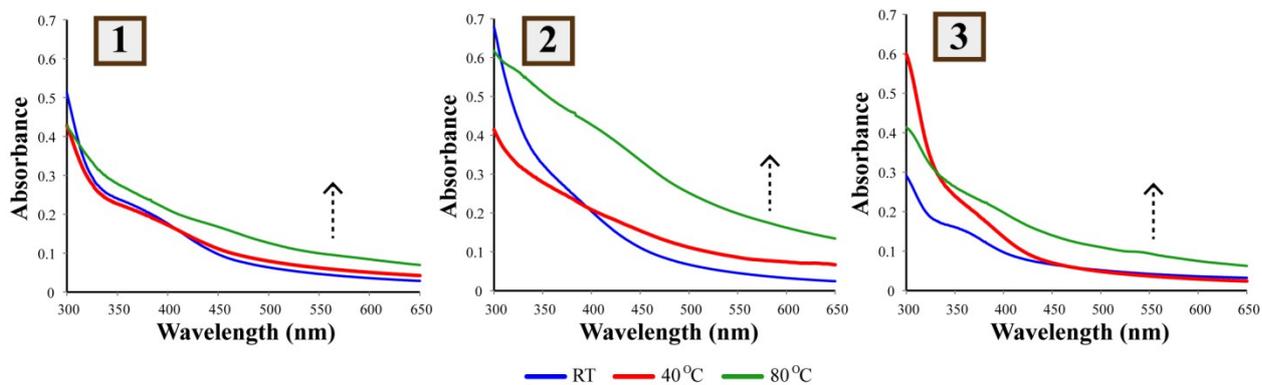
**Figure S1:** UV-Vis spectra of **1**, **2** and **3** in aqueous medium at higher concentration.



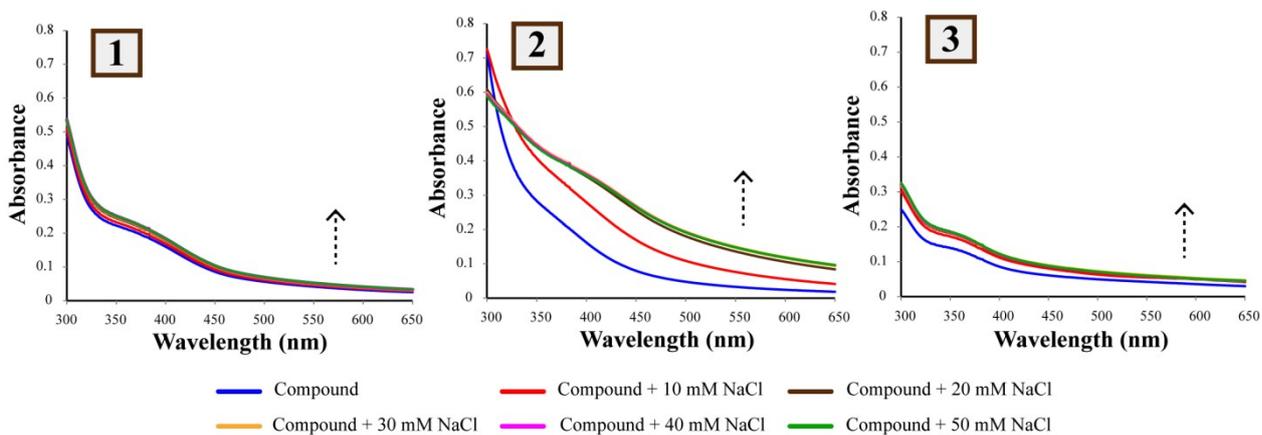
**Figure S2:** Fluorescence spectra of **1**, **2** and **3** in aqueous medium.



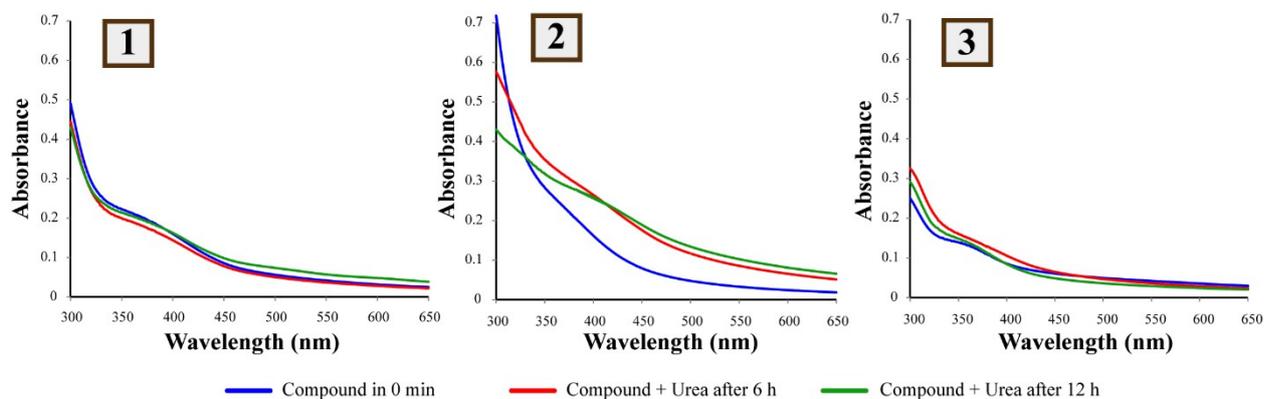
**Figure S3:** IR spectra of **1**, **2** and **3** and their aggregated form (A) region 3800-2800  $\text{cm}^{-1}$  and (B) region 1000-2000  $\text{cm}^{-1}$  (Dotted line - compound and Solid line - aggregated form).



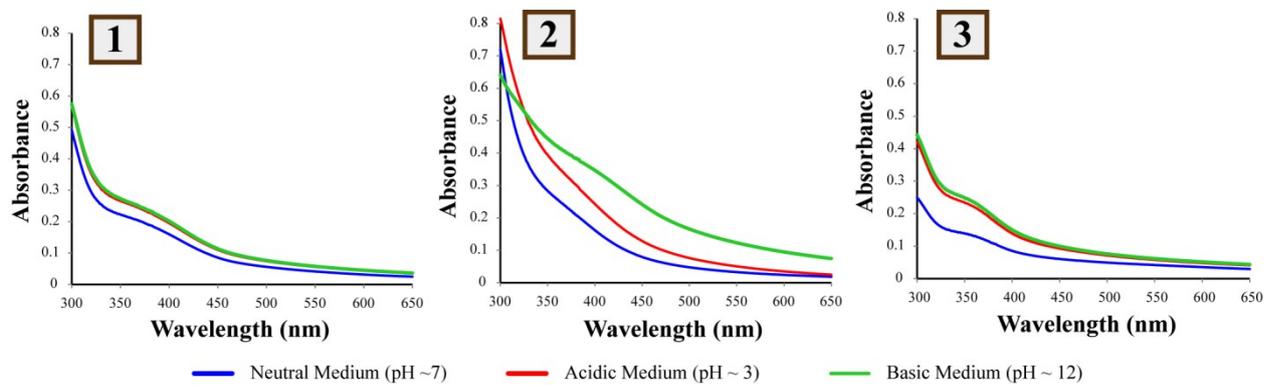
**Figure S4:** Effect of temperature on UV-Vis spectra of **1**, **2** and **3**.



**Figure S5:** UV-Vis spectra of **1**, **2** and **3** in presence of salt (NaCl).



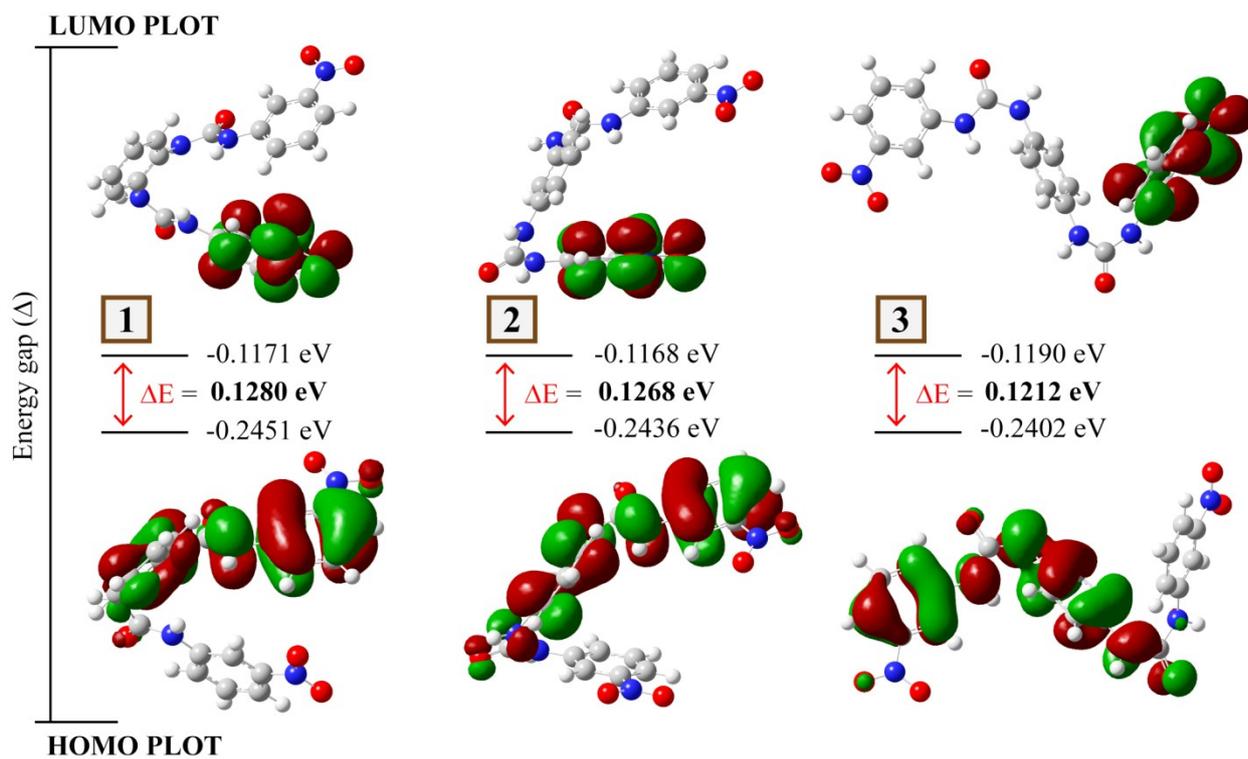
**Figure S6:** UV-Vis spectra of **1**, **2** and **3** in presence of urea.



**Figure S7:** UV-Vis spectra of **1**, **2** and **3** with the variation in pH of the medium.

**Table S1:** Summary of DFT data.

	Total Energy (a.u)	HOMO Energy (eV)	LUMO Energy (eV)	$\Delta E$ (eV)
<b>Compound 1</b>	-1551.013	-0.2451	-0.1171	0.1280
<b>Compound 2</b>	-1551.006	-0.2436	-0.1168	0.1268
<b>Compound 3</b>	-1551.006	-0.2402	-0.1190	0.1212



**Figure S8:** Frontier molecular orbital plots of **1**, **2** and **3** ( $\Delta E$  = energy gap between HOMO and LUMO).