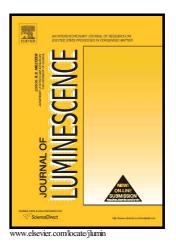
## Author's Accepted Manuscript

D- $\pi$ -A type Barbituric Derivatives: Aggregation induced emission, mechanofluorochromic and solvatochromic properties

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### **ACCEPTED MANUSCRIPT**

# $D-\pi$ -A type Barbituric Derivatives: Aggregation induced emission,

mechanofluorochromic and solvatochromic properties

Kai Li<sup>a</sup>, Xi Su<sup>a</sup>, Yixuan Wang<sup>b</sup>, Furong Tao<sup>a</sup>, Yuezhi Cui<sup>a</sup>\*, Huayong Zhang<sup>a</sup>, Tianduo Li<sup>a</sup>

<sup>a</sup>QiLu University of Technology (Shandong Academy of Sciences), College of Chemistry and Pharmaceutical Engineering, QiLu University of Technology, Shandong Provincial Key Laboratory of Fine Chemicals, Jinan 250353, China <sup>b</sup>Department of Chemistry and Forensic Science, Albany State University, Albany, Georgia 31705, USA

Tel: +86 13969083466; Fax: +86 531 89631760;

E-mail address: yuezhicui@163.com

#### **Abstract**

Four new barbituric derivatives that bears the furan and thiophene and the 1,3-dimethyl barbituric acid moiety, has been synthesized. These D- $\pi$ -A type conjugated compounds showed obvious intramolecular charge transfer (ICT) properties, which were evidenced by theoretical calculations and spectral analysis. The compounds exhibited Aggregation induced emission (AIE) characteristic. **TOB-1** and FTB-1 were quite weakly emission in pure THF, while a significant AIE effect was observed in water/THF ( $f_w = 70\%$  and 90%) mixtures with a large AIE factor of 40.5 and 46.8. Barbituric acid derivatives with thiophene electron donating group possess the distinct mechanofluorochromic (MFC) behavior. The original powder of FTB-1, BFTB-2 and TFTB-4 could emit strong orange-yellow (614 nm), orange-red (663 nm) and yellow (571 nm) light under UV irradiation, while the fluorescence color changed into orange (629 nm), red (691 nm) and orange yellow (583 nm) emission after grinding, respectively, a red shift of 15, 28 and 12 nm was observed, respectively. Among them, the emission color of compound BFTB-2 can be observed by naked eyes. Such mechanochromism was reversible upon the treatment of grinding and fuming with CH<sub>2</sub>Cl<sub>2</sub>. The XRD studies of the powders showed that the MFC

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