**Supplementary Information** 

## Noncovalent Interactions Induced Self-Association in Anthraquinone-Iron Aqueous Redox Flow Batteries

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**Figure S1**. The anthraquinone-iron RFB was tested under 40 mA·cm<sup>-2</sup> without using glycine as the acid additive.



**Figure S2**. Images of (a) membrane and (b) carbon felt on the positive side after cycling in 0.1 M anthraquinone flow battery. Photographs of (c) membrane and (d) carbon felt on the positive side after cycling in 0.5 M anthraquinone flow battery.



**Figure S3.** <sup>1</sup>H NMR spectrum (500 MHz) of 28  $\mu$ L negative electrolyte in 0.55 mL D<sub>2</sub>O before cycle (bottom) and after 150 cycles (top). The chemical shifts moved downfield slightly after 150 cycles, suggesting the concentration decreased accordingly.



Figure S4. CV curves of 100  $\mu$ L negative electrolyte dissolving in 50 mL 1 M KCl before (black line) and after 150 cycles (red line).



Figure S5. CV curves of 1112  $\mu$ L positive electrolyte in 50 mL 1 M KCl before (black line) and after 150 cycles (red line).



**Figure S6**. Nyquist plot of the 0.5 M anthraquinone-iron RFB before (black dots) and after cycling (red dots). The frequency arranges from 500 kHz to 1 Hz.



Figure S7. <sup>1</sup>H DOSY (600 MHz) spectrum of 50 mM 1-DPAQC1 in D<sub>2</sub>O at 298 K.



**Figure S8**. Number-average molecular weight  $(M_n)$ , weight-average molecular weight  $(M_w)$ , and polydispersity index determined by GPC versus the concentration at 3.5, 12, 35 mg·mL<sup>-1</sup>.

**Figure S8** displayed that  $M_w$  increased with the concentration ranging from 3.5 to 35 mg·mL<sup>-1</sup>. However,  $M_n$  first increased to 4.10 kDa when the concentration was 12 mg·mL<sup>-1</sup>, and then decreased to 3.47 kDa as the concentration was 35 mg·mL<sup>-1</sup>. We attribute this trend to the polydispersity broadening.