Supplementary Material for "Solvent polarity dependent excited state behavior and thermally active delayed fluorescence for triquinolonobenzene"

Jinfeng Zhao, Hao Dong, Huan Yang,* and Yujun Zheng*

School of Physics, Shandong University, Jinan 250100, China

E-mail: h.yang@foxmail.com; yzheng@sdu.edu.cn

*To whom correspondence should be addressed

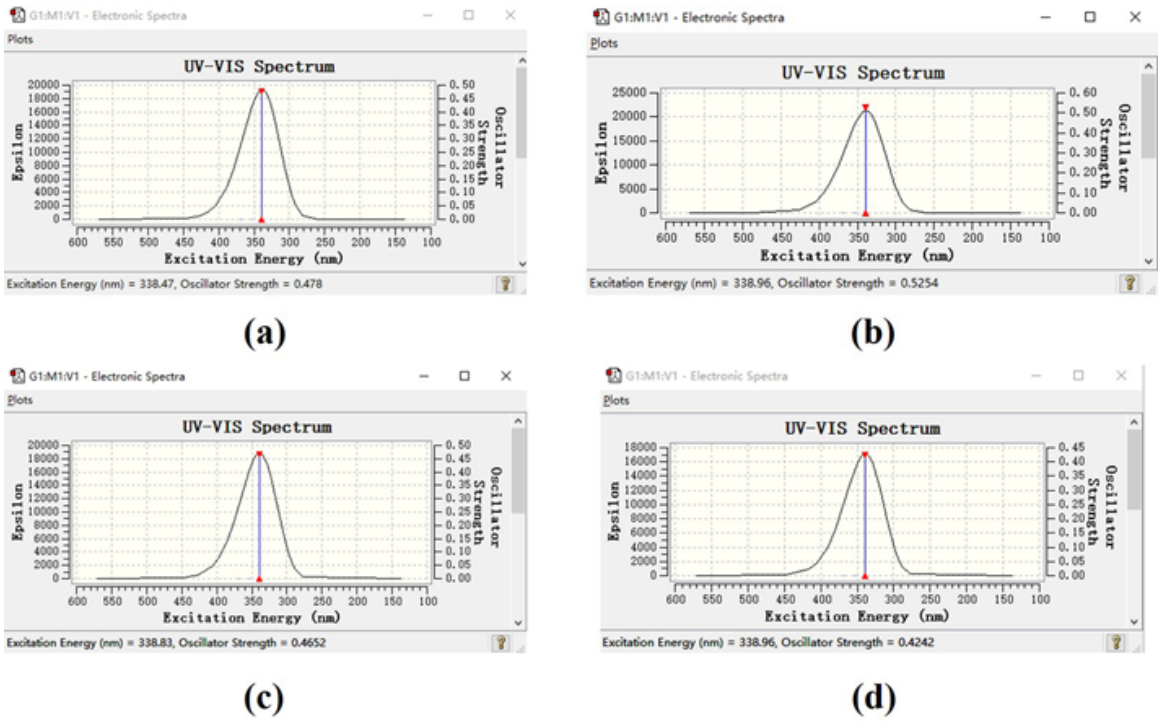

Figure S1: The theoretical absorption spectra of TQB-TA form in CYH (a), Tol (b), $CHCl_3$ (c) and DMF (d) solvents. Herein, the peaks in each figures indicate the $S_0 \rightarrow S_3$ transition since the oscillator strengths of $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ are almost 0.

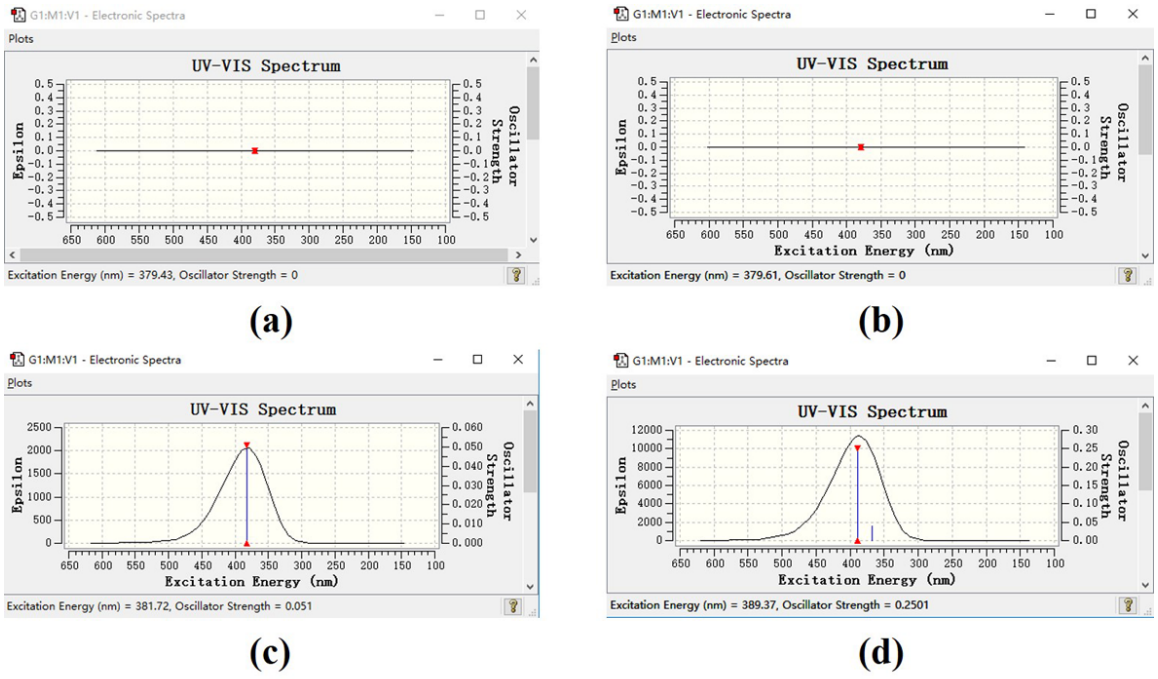

Figure S2: The theoretical S_1-state fluorescence spectra of TQB-TA form in CYH (a), Tol (b), $CHCl_3$ (c) and DMF (d) solvents.

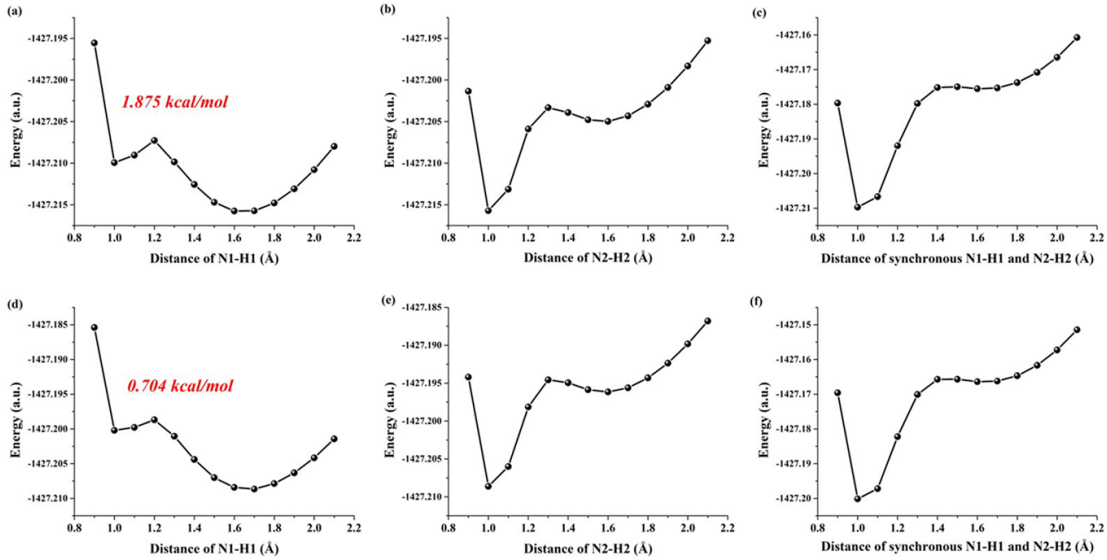

Figure S3: The constructed potential energy curves using Cam-B3LYP functional along with A $\rightarrow$ B, B $\rightarrow$ D and A $\rightarrow$ D paths in CYH (a-c) and DMF (d-f) solvents .

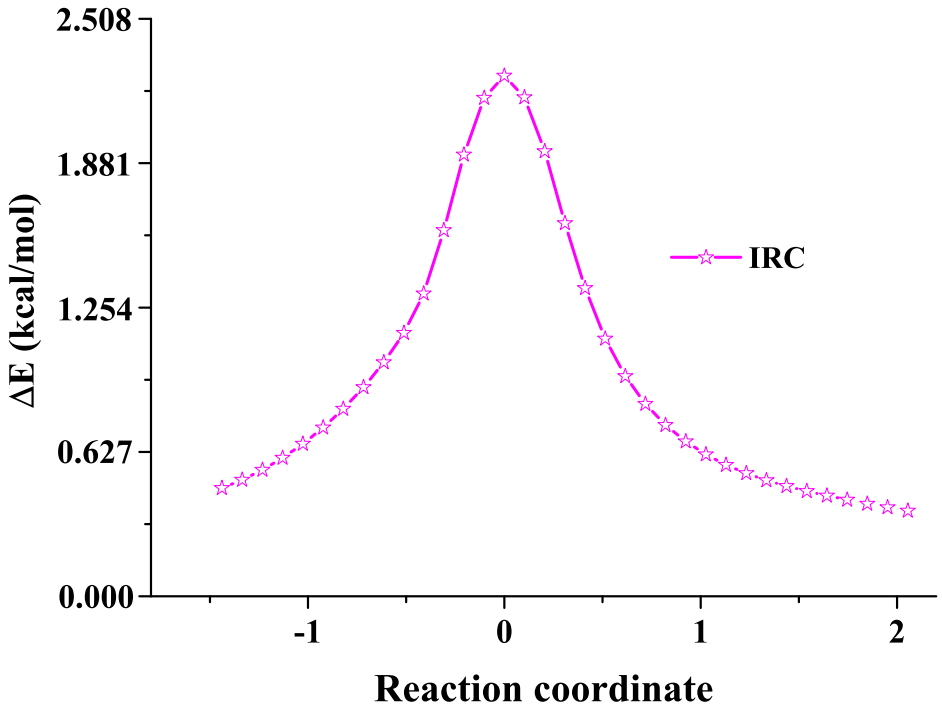

Figure S4: The energy profile along with the S_1-state IRC for the ESIPT path (A $\rightarrow$ B or C) based on TDDFT/B3LYP/TZVP theoretical level.