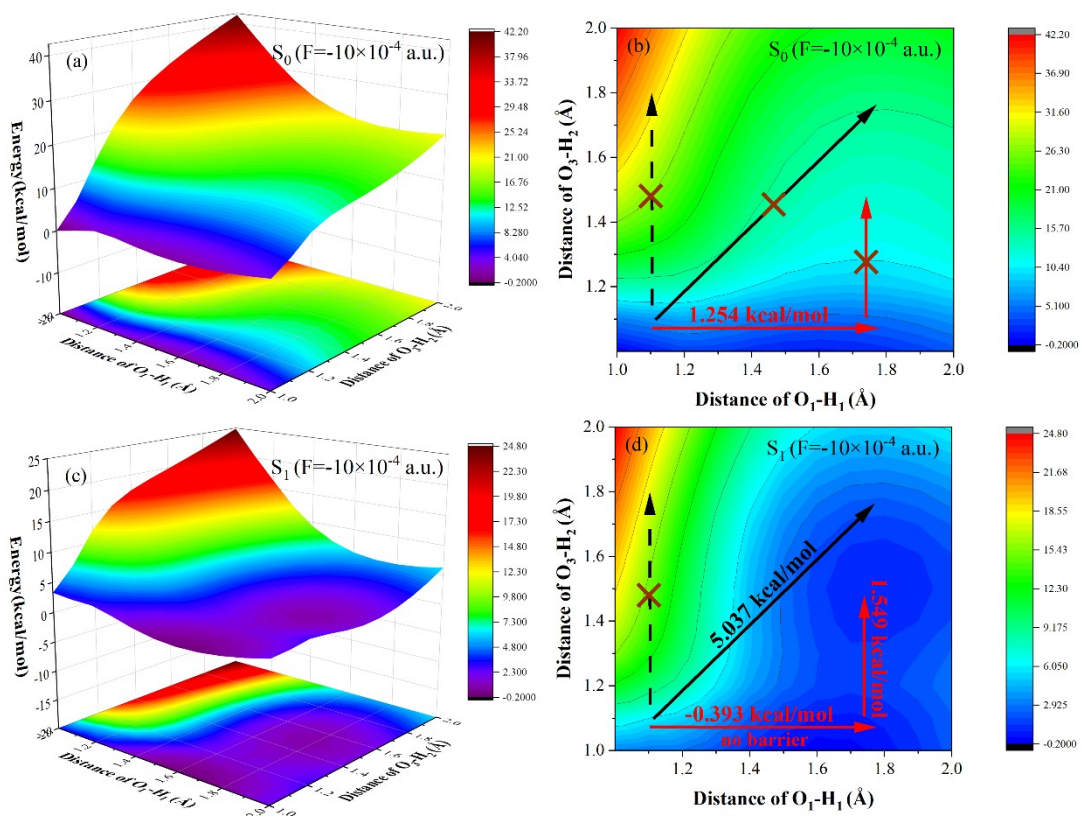# Electronic Supplementary Information for:

Effect of the External Electric Field on the ESDPT Process and Photophysical

Properties of 1,8-Dihydroxy-2-Naphthalaldehyde
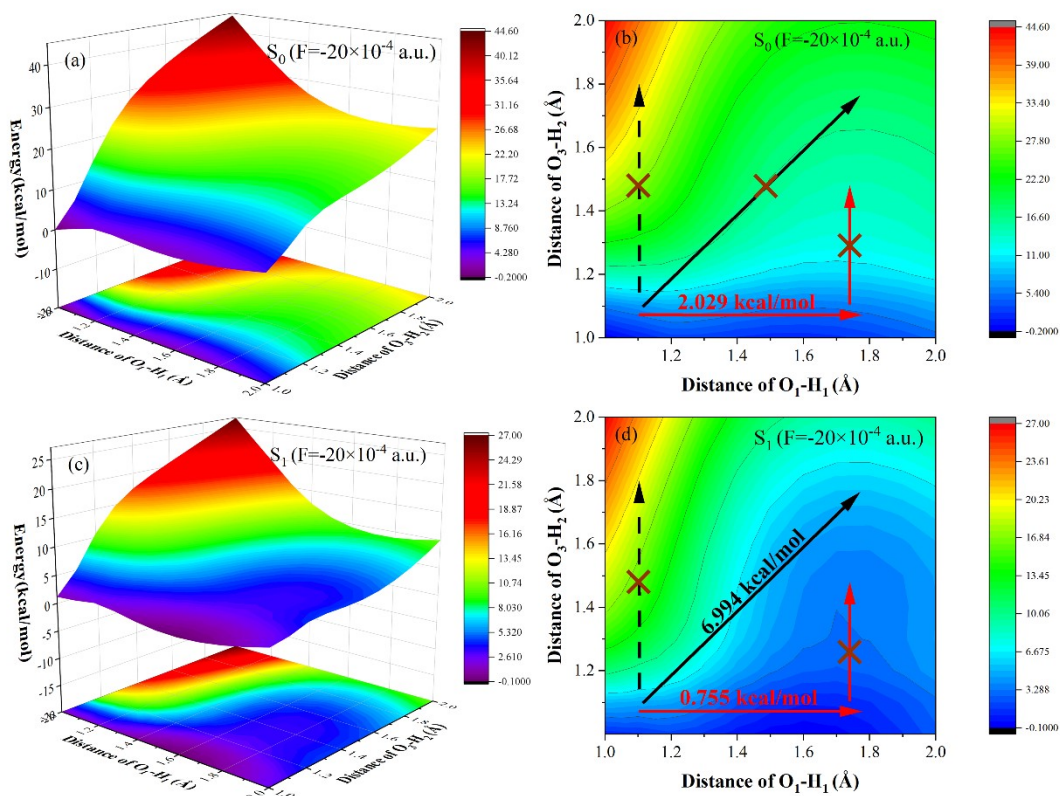
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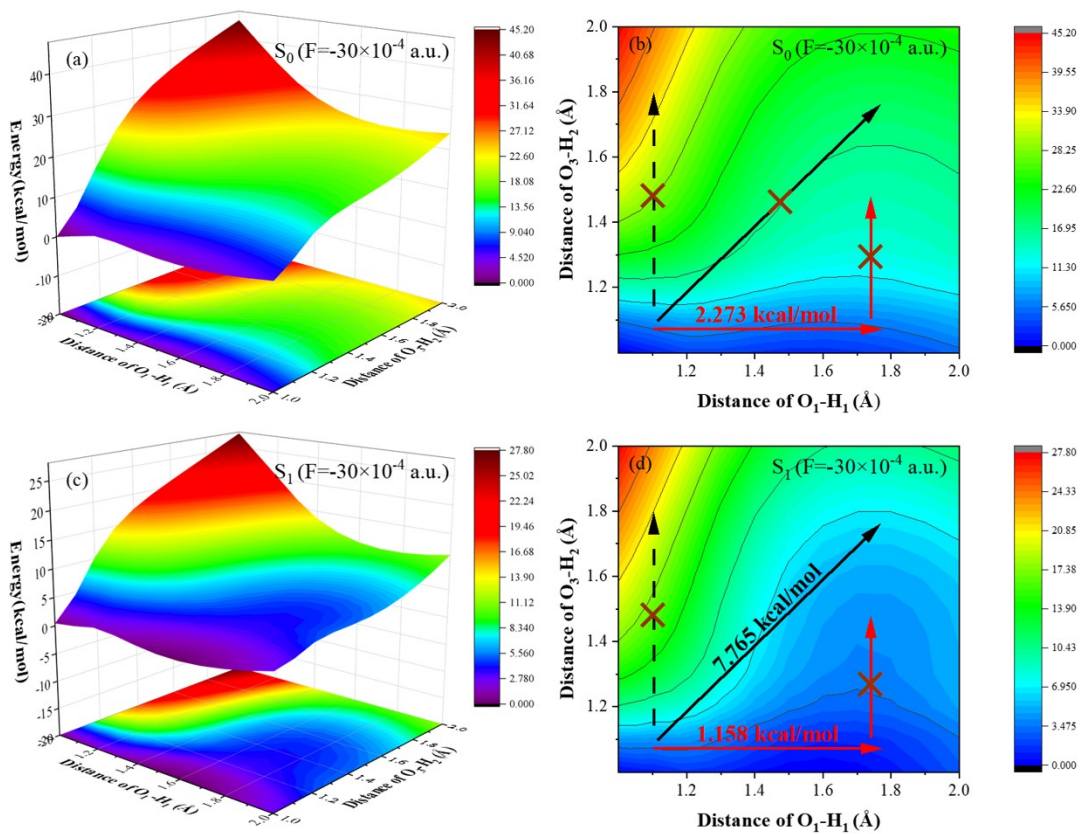
China. E-mail: cfsun@nefu.edu.cn

Figure S1(a). The scanned PESs in S_0 (a)-(b) and S_1 (c)-(d) states with a negetive EEF of -10×10^{-4} a.u.. Here, the arrows and numbers represent the direction of PT and the energy barrier, respectively.

Figure S1(b). The scanned PESs in S_0 (a)-(b) and S_1 (c)-(d) states with a negetive EEF of -20×10⁻⁴ a.u.. Here, the arrows and numbers represent the direction of PT and the energy barrier, respectively.

Figure S1(c). The scanned PESs in S_0 (a)-(b) and S_1 (c)-(d) states with a negetive EEF of -30×10^{-4} a.u.. Here, the arrows and numbers represent the direction of PT and the energy barrier, respectively.
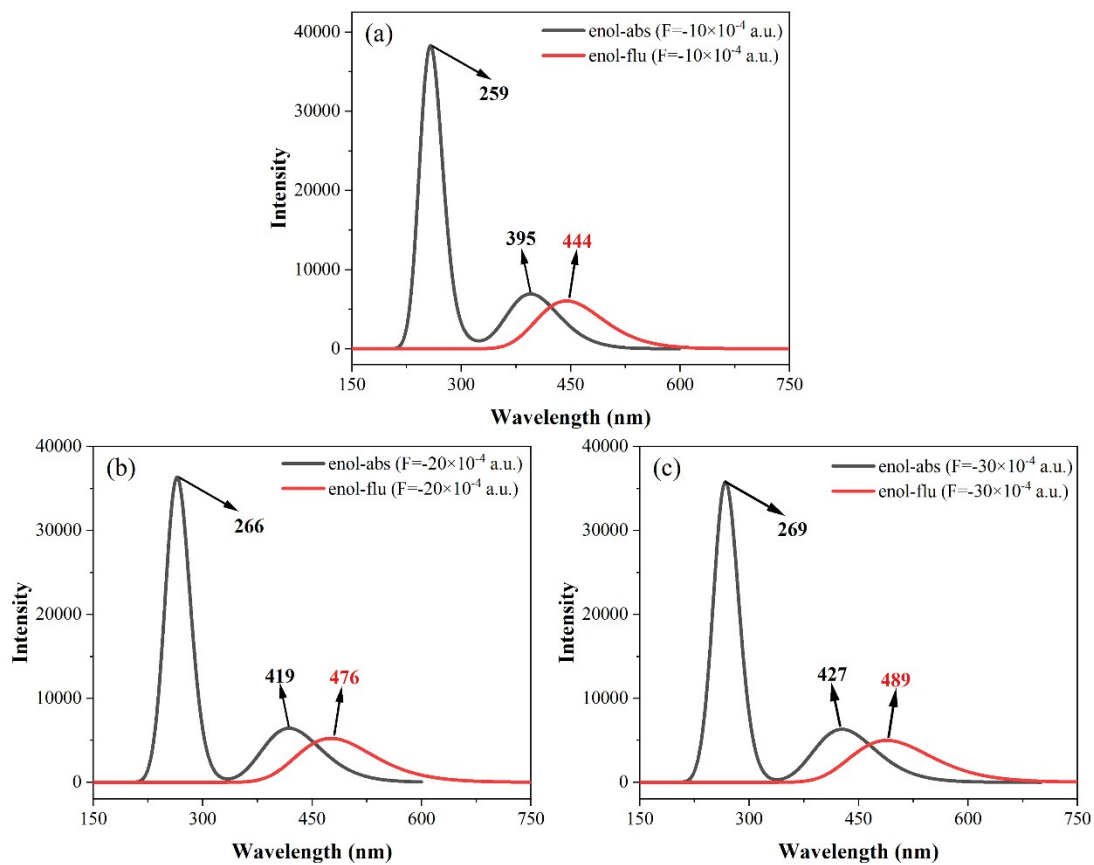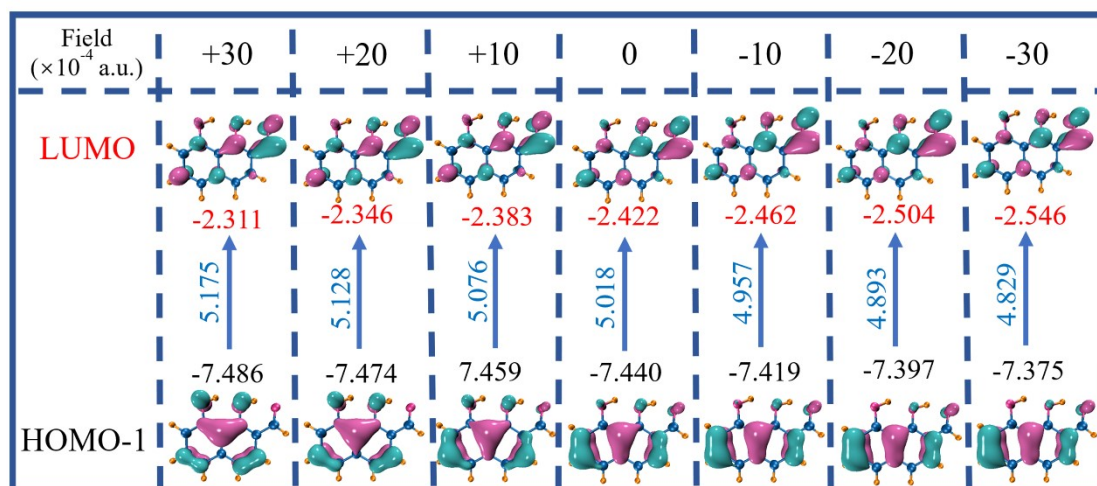
Figure S2. Absorption and fluorescence spectra of DHNA in the distinct external electric fields: (a) -10×10^{-4} a.u.; (b) -20×10^{-4} a.u.; (d) -30×10^{-4} a.u..

Figure S3. HOMO-1, LUMO energies and energy gaps of DHNA in the distinct EEFs (eV).