Supporting Information for

Unraveling the effect of solvents on the excited state dynamics of C540A by experimental and theoretical study

Jing Ge,[a] Xue-Dong Zhang,[a] Yue Peng,[a] and Xi-Lin Bai*[a]

[a] *School of Physics and Information Engineering, Key Laboratory of Spectral Measurement and Analysis of Shanxi Province, Shanxi Normal University, Taiyuan 030031, China.*

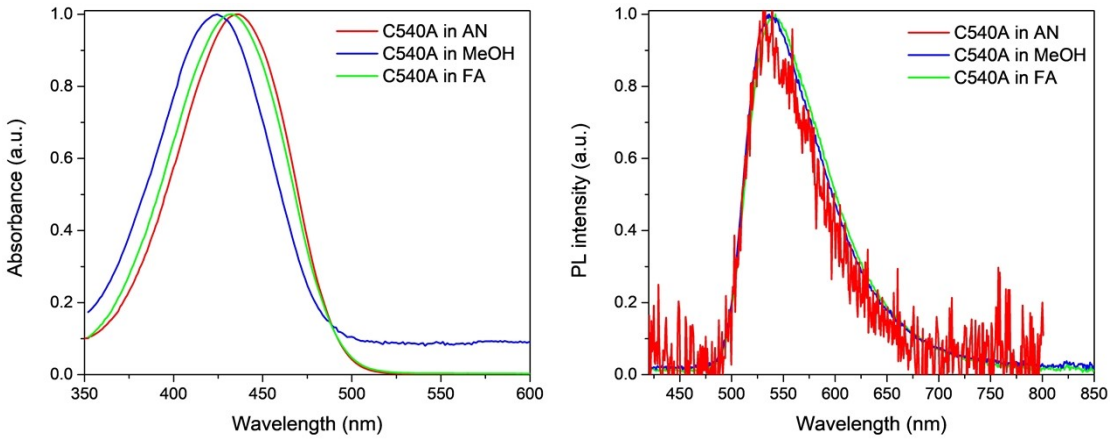

Figure S1 Normalized steady-state absorption (left) and fluorescence (right) spectra of C540A in AN, MeOH, and FA solvents.

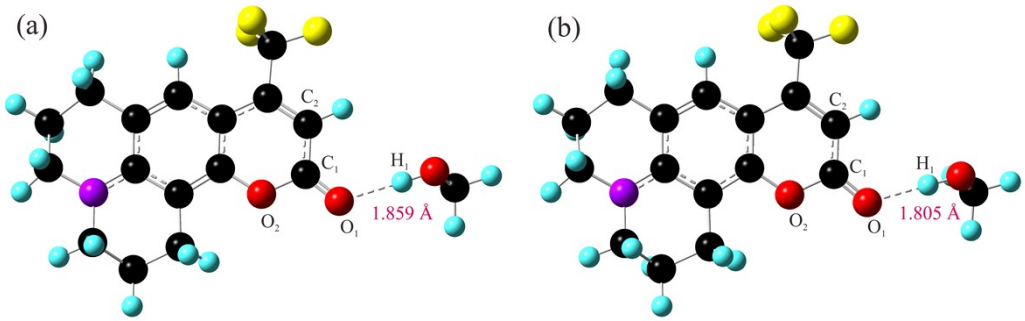

Figure S2 Optimized geometric structures for the C540A-MeOH complex in S_0 (a) and S_1 (b) at the B3LYP/TZVP/IEF-PCM (MeOH) level.

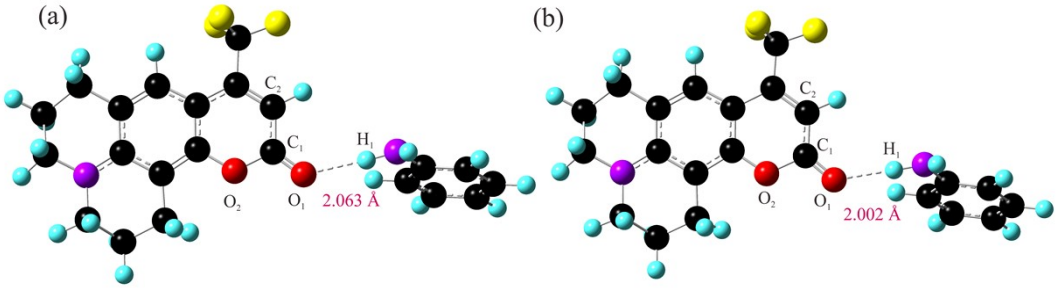

Figure S3 Optimized geometric structures for the C540A-AN complex in S_0 (a) and S_2 (b) at the B3LYP/TZVP/IEF-PCM (AN) level.

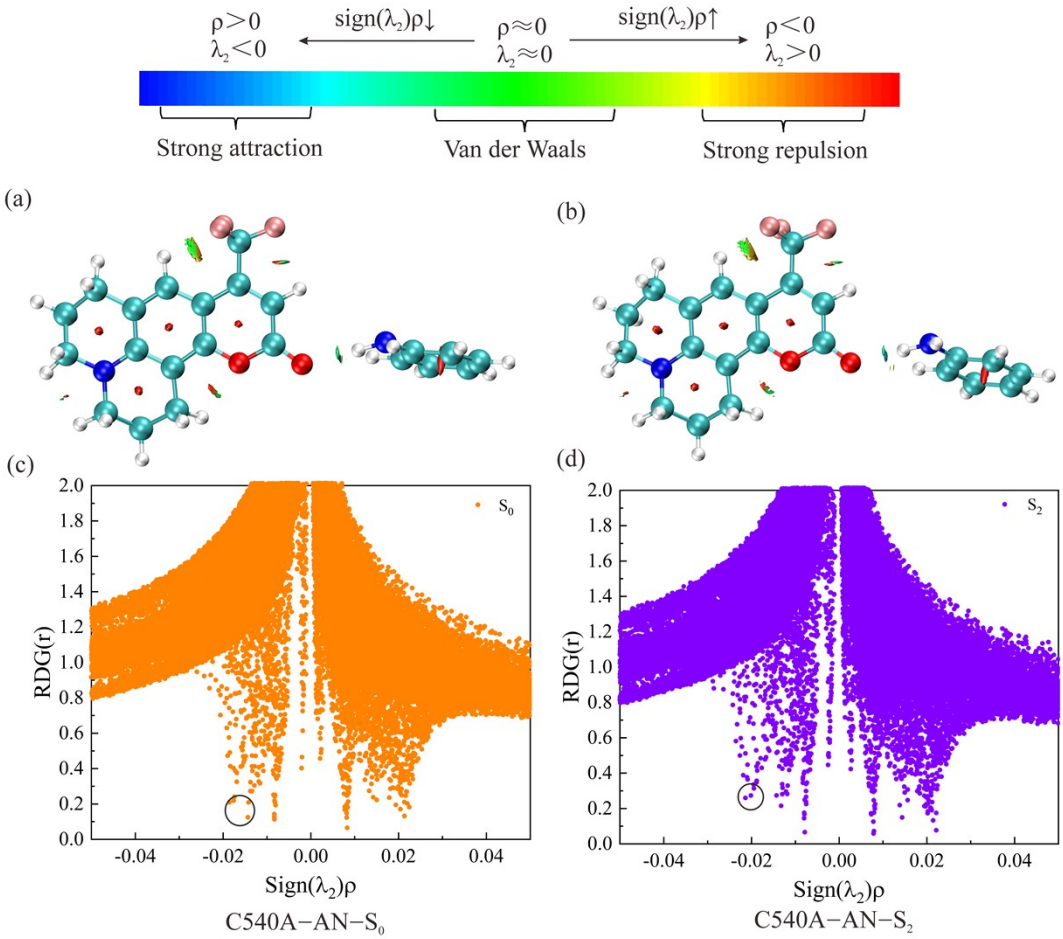

Figure S4 NCI isosurface of the C540A-AN complex in S_0 (a) and S_2 state (b). Plots of Sign(λ_2) versus RDG(r) for hydrogen-bonded complex C540A-AN in the S_0 (c) and S_2 state (d), respectively.

Table S1. Kinetic lifetimes of C540A fitted in FA, AN, and MeOH solvents.

solvent	τ_{rise} (ps)	τ_1 (ps)	τ_2 (ps)
FA	0.41 ± 0.02	163.50 ± 1.33	1688.42 ± 377.49
MeOH	0.58 ± 0.01	17.07 ± 0.83	7626.57 ± 1826.53
AN	0.65 ± 0.03	10.90 ± 2.03	110.97 ± 3.29

Table S2. Infrared spectra of hydrogen bond formation sites (cm^{-1}) of the isolated C540A and hydrogen-bonded complexes in three solvents in ground state and excited state.

Parameters	C540A		C540A-MeOH		C540A-FA		C540A-AN	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_2
C_1-O_1	1799	1797	1706	1702	1708	1704	1726	1721