Supporting information for

Deciphering Swift Reversal of Multifaceted Photodynamics of a Novel Pyrene Appended Unsymmetrical Salicylaldehyde Azine Derivative in Aqueous and Protein Environments

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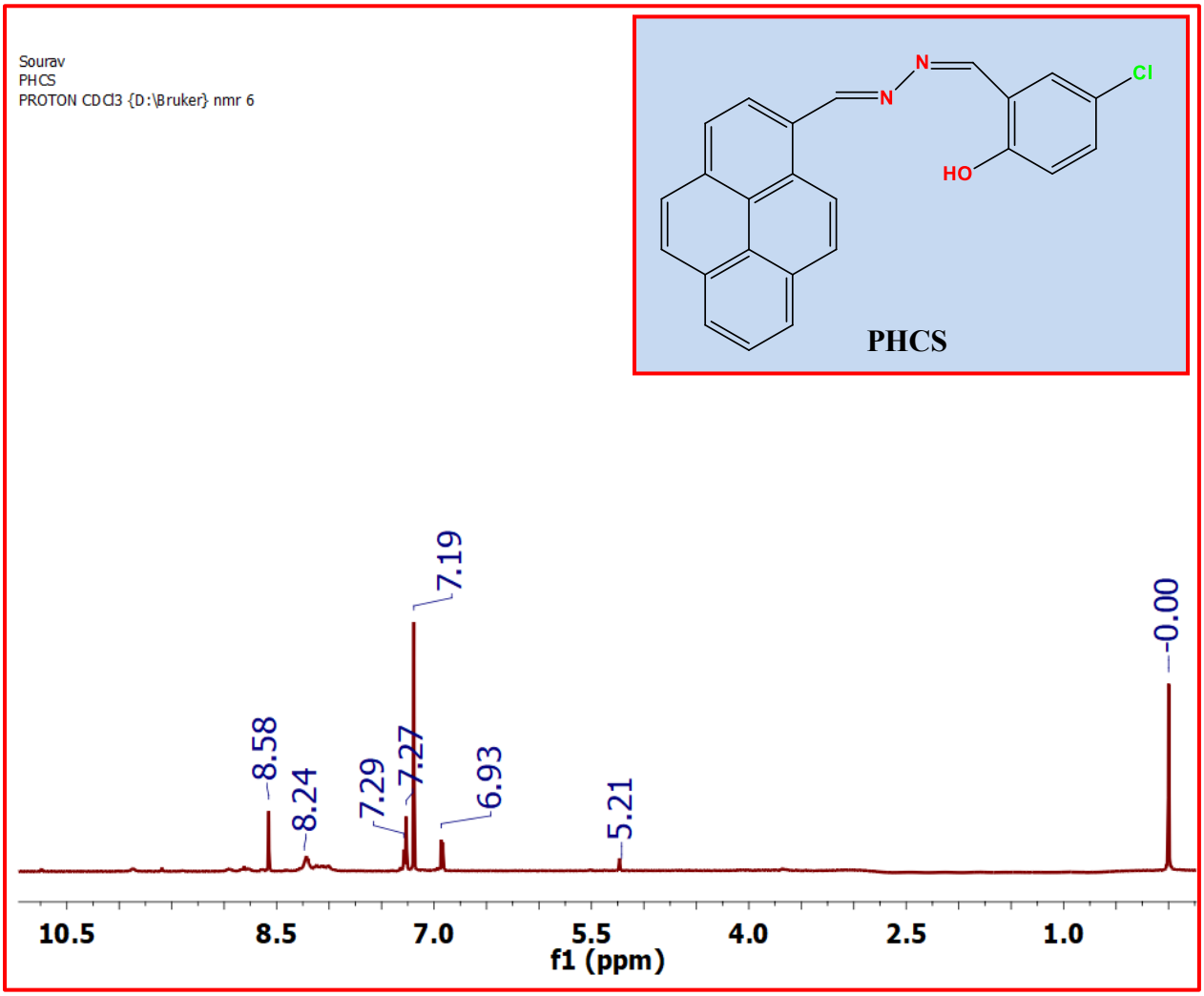

Fig. S1 ^{1}H NMR spectrum of **PHCS**.

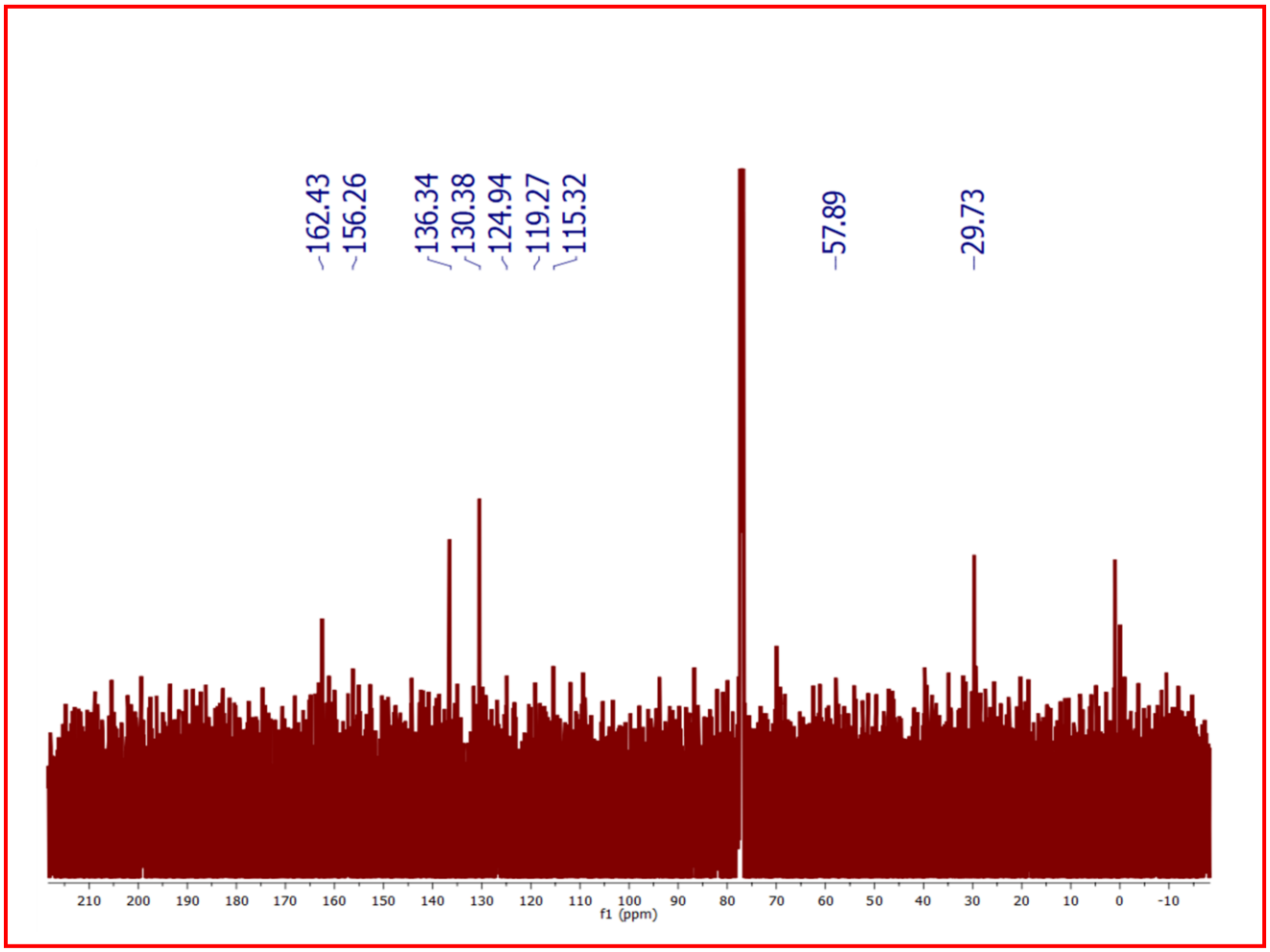

Fig. S2 ^{13}C NMR spectrum of **PHCS**.

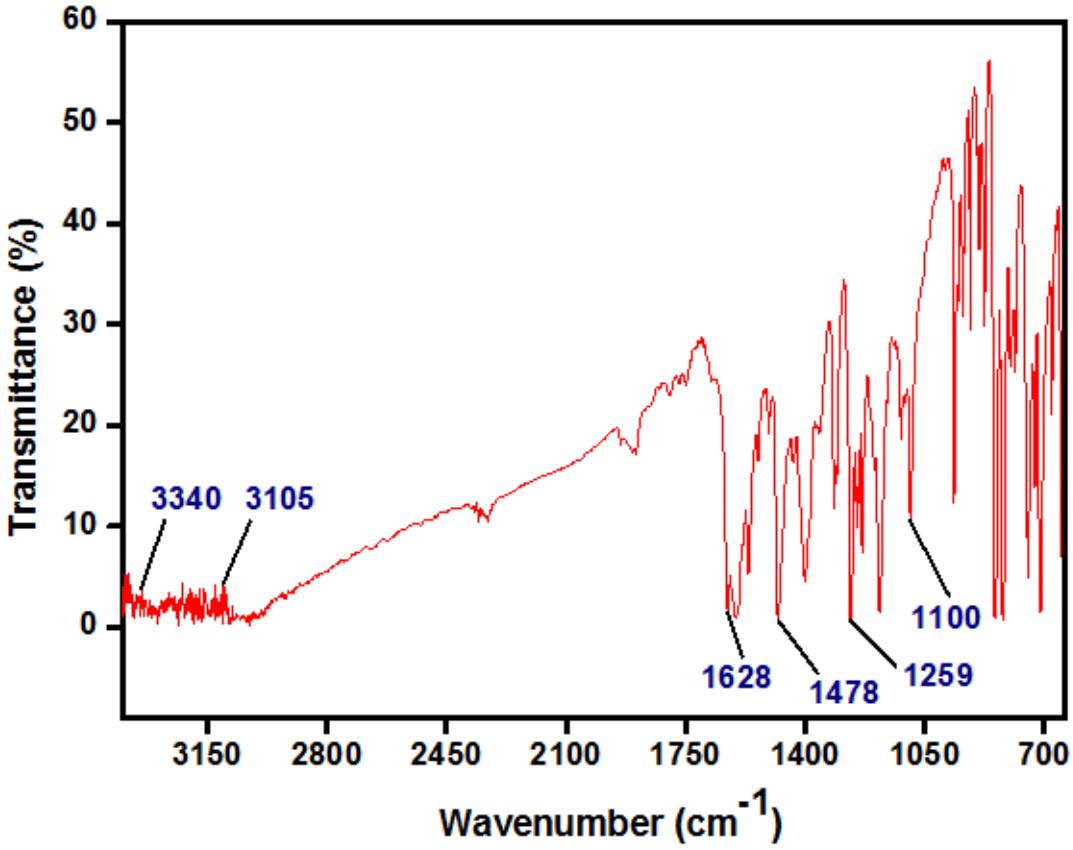

Fig. S3 FT-IR spectrum of **PHCS**.

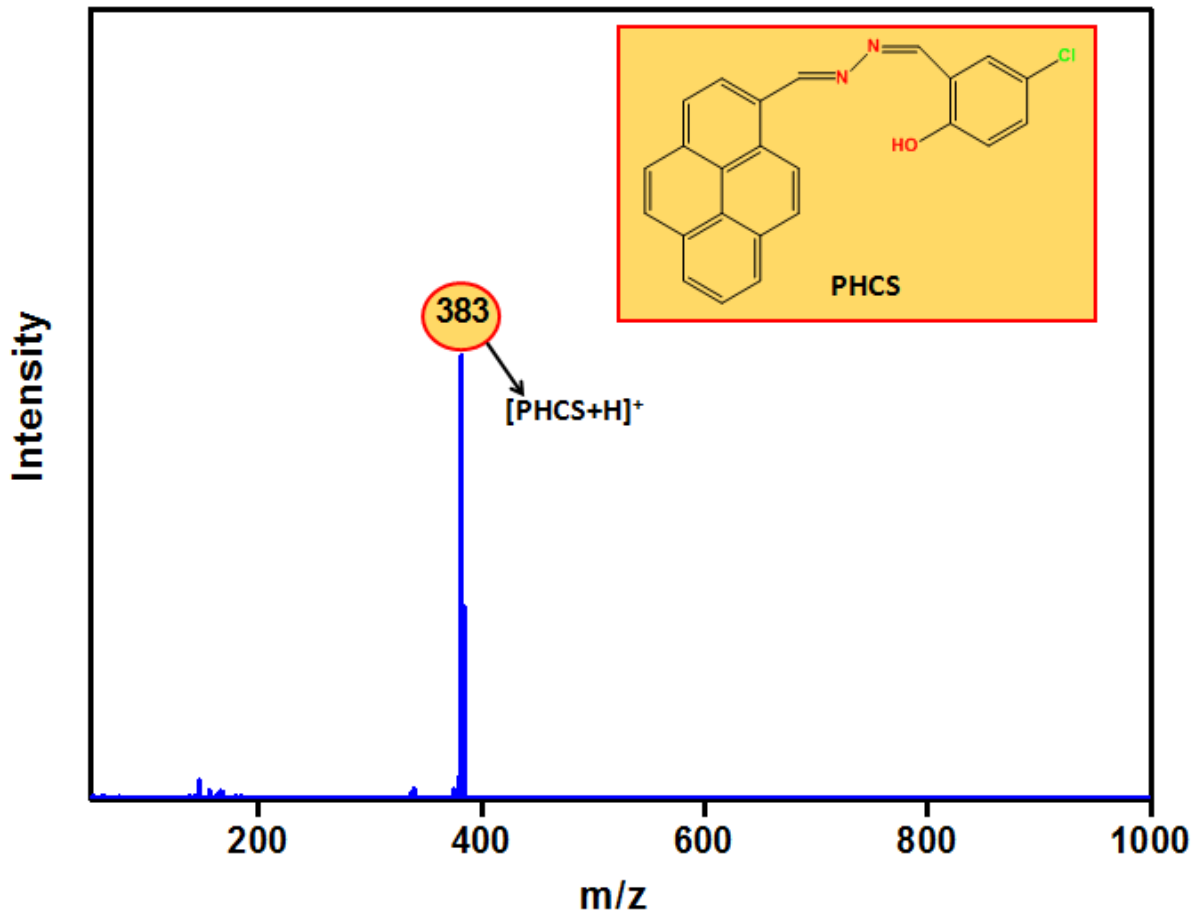

Fig. S4 ESI-MS spectrum of **PHCS**.

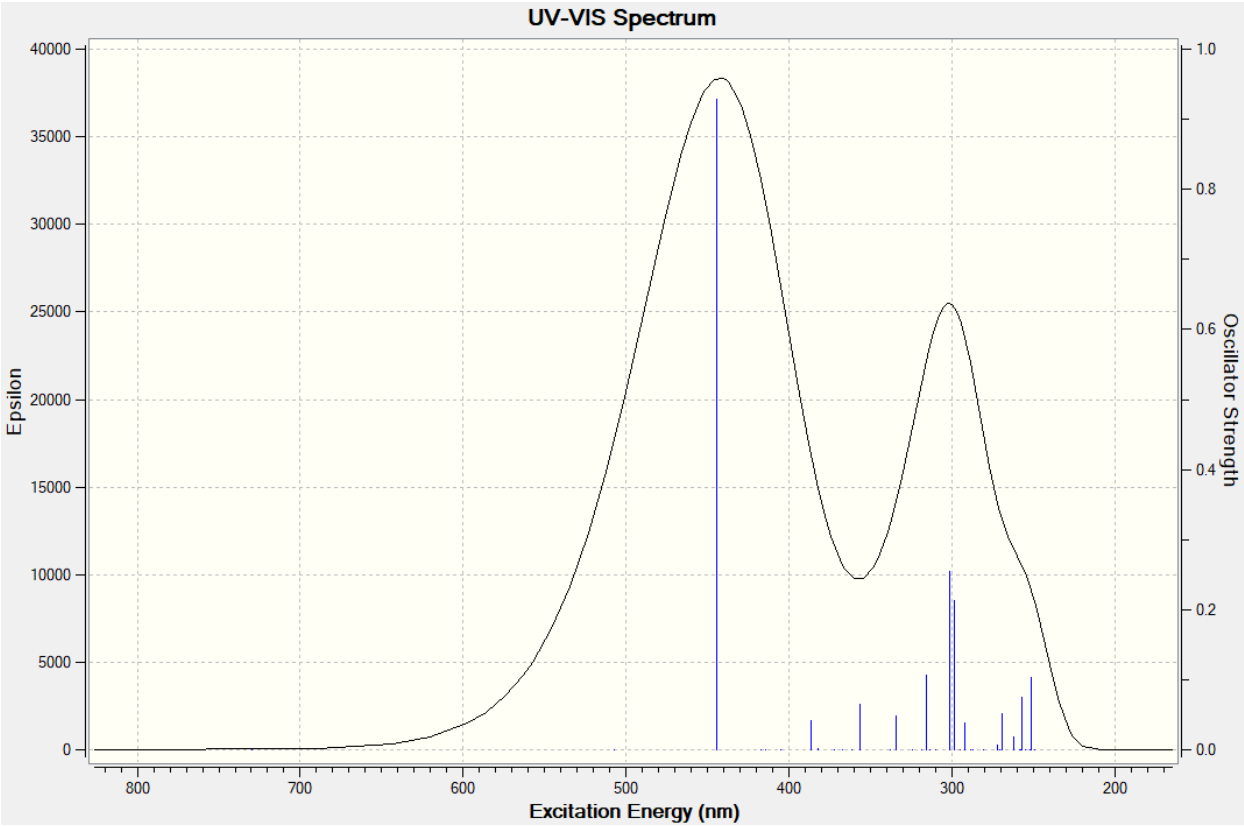

Fig. S5 Simulated UV-visible absorption spectrum of **PHCS** obtained by TD-DFT method (in gas phase medium).

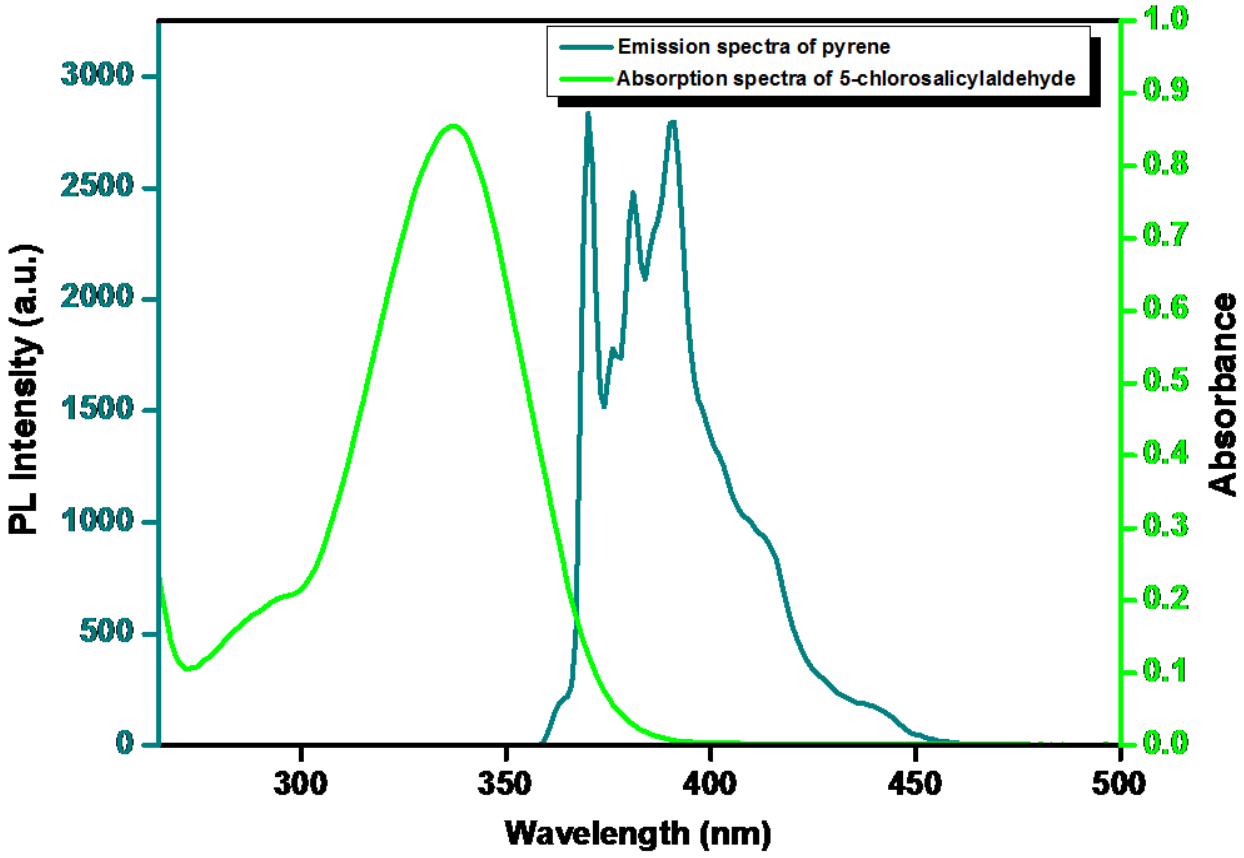

Fig. S6 Spectral overlap study between donor (pyrene) and acceptor (5-chlorosalicylaldehyde).

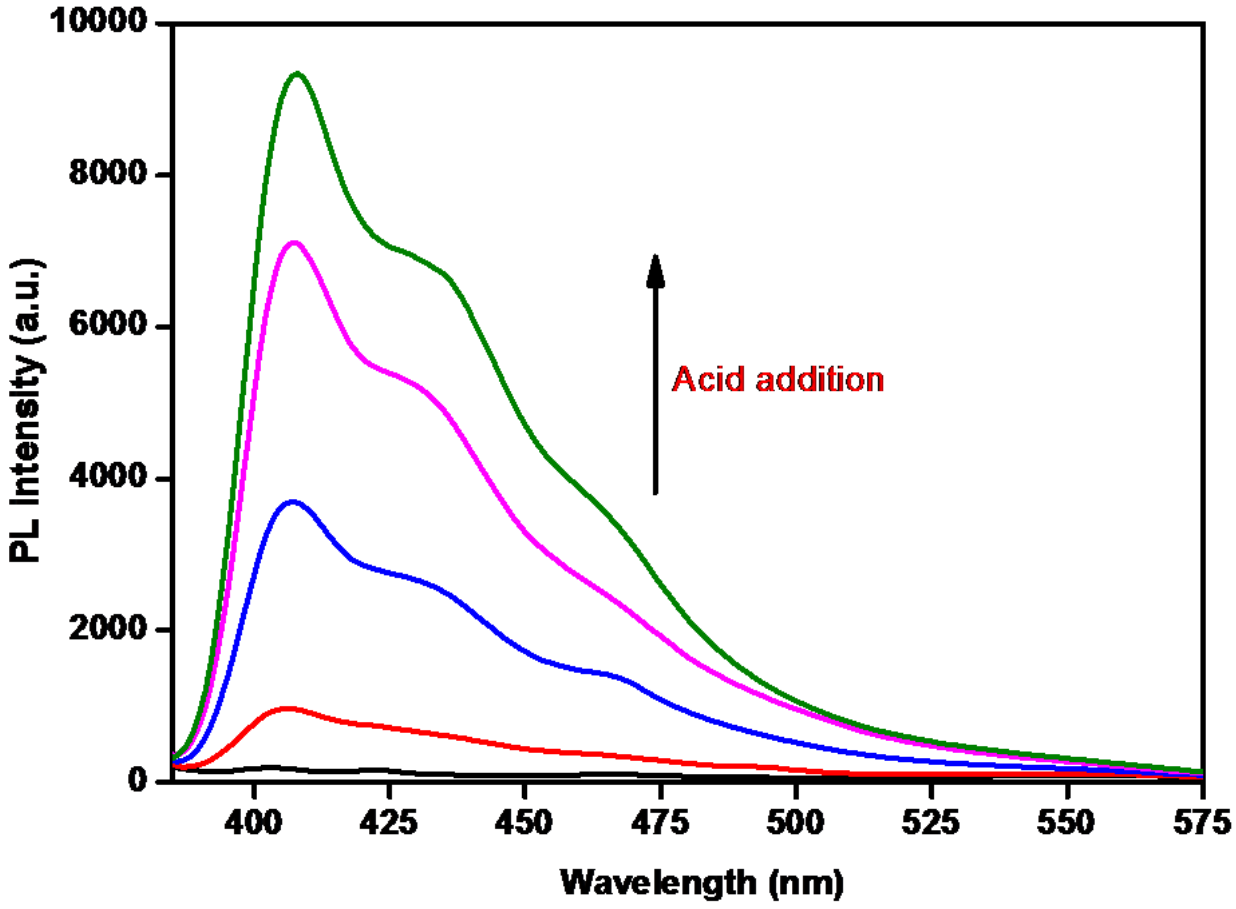

Fig. S7 Effect of addition of trifluoroacetic acid (5 μl) on fluorescence spectra of **PHCS** (15 μM) in THF. Ex = 375 nm, slit = 5/5 nm.

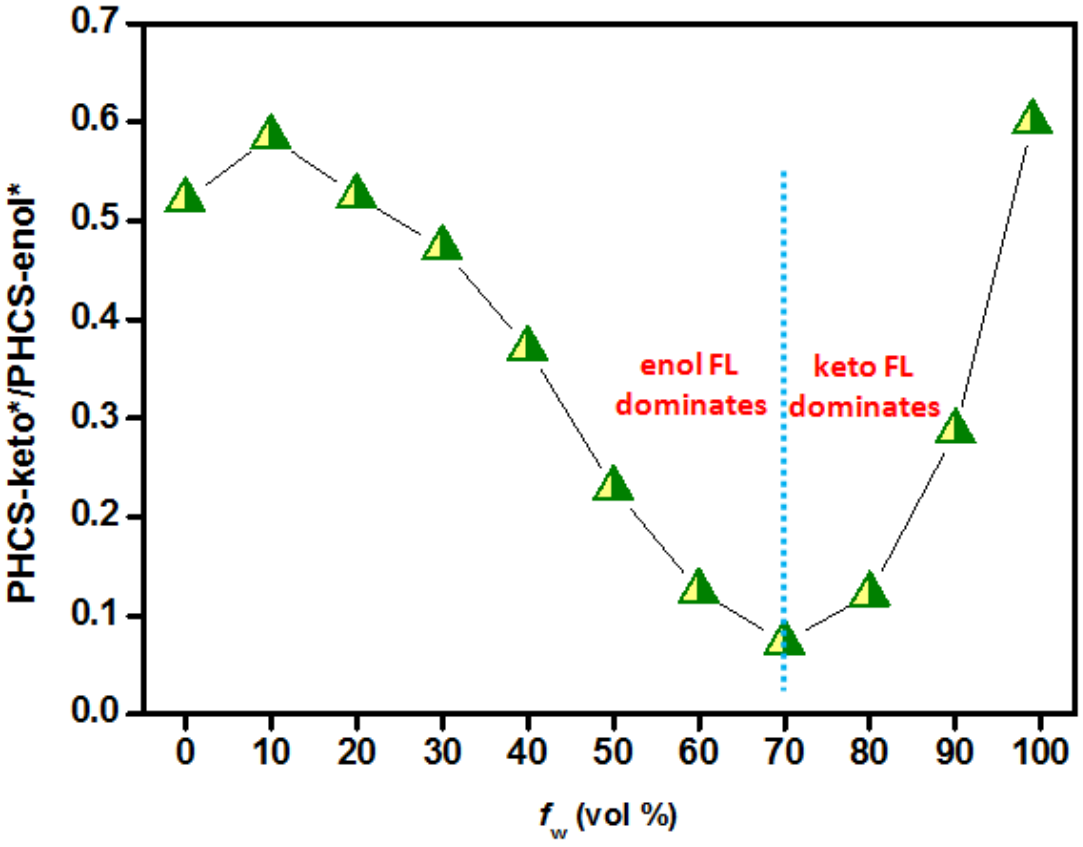

Fig. S8 Ratio of keto by enol isomer of **PHCS** with water variation in THF.

Table S1. Selected optimized geometrical parameters for **PHCS** in the ground state calculated at B3LYP levels.

Bond distance (Å)			
$C_{11}–C_{26}$	1.455	$N_{29}–C_{30}$	1.307
$C_{26}–N_{28}$	1.304	$C_{30}–C_{32}$	1.447
$N_{28}–N_{29}$	1.413	$C_{42}–C_{43}$	1.012
Bond Angle (°)			
$C_{11}–C_{26}–N_{28}$	126.5	$N_{29}–C_{30}–C_{32}$	121.3
$N_{28}–N_{29}–C_{30}$	114.4	$N_{29}–H_{43}–O_{42}$	144.5

Table S2. Electronic states involved in absorption, wavelength (nm), excitation energy (eV) and the corresponding oscillator strength (*f*) for the transitions of **PHCS** (obtained from TD-DFT calculations).

Excitation energy (eV)	**Wavelength (nm)**	**Oscillator strength (*f*)**	**MO contributions**
4.115	301.25	0.2552	HOMO-2 → LUMO
2.969	417.47	0.9284	HOMO → LUMO

Table S3. Fluorescence lifetime decay parameters of **PHCS** in THF.

Solvent	**τ_1 (ns)**	**α_1 (%)**	**τ_2 (ns)**	**α_2 (%)**	**τ_{av} (ns)**	**χ^2**	**k_{et} (10^9 s^{-1})**
THF	0.435	98.69	2.854	1.31	1.035	1.09	1.95

Table S4. Fluorescence lifetime decay parameters of **PHCS** (0-40 μM) in THF solvent. Excitation = 375 nm nanoLED source, emission = 450 nm, bandpass = 6 nm, peak preset = 2000.

Concentration of PHCS solution (μM)	τ_1 **(ns)**	τ_2 **(ns)**	α_1 **(%)**	α_2 **(%)**	τ_{av} **(ns)**	χ^2
1	0.039	0.915	96.41	3.59	0.039	1.14
5	0.069	1.327	91.31	8.69	0.075	1.01
10	0.077	1.609	85.82	14.18	0.089	1.1
15	0.435	2.854	98.69	1.31	1.035	1.09
40	1.145	5.716	30.41	69.59	2.581	1.16