

# **White Light Emission in Water through Admixtures of Donor- $\pi$ -Acceptor Siblings: Experiment and Simulation**

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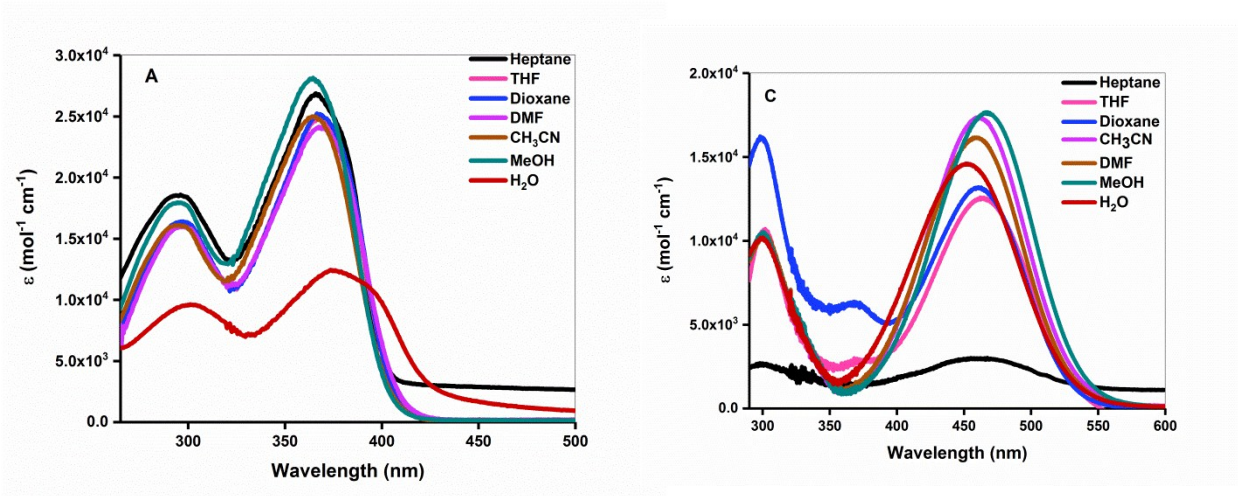


Fig S1. Absorption spectra of stilbenes 1 and 3 in various solvents

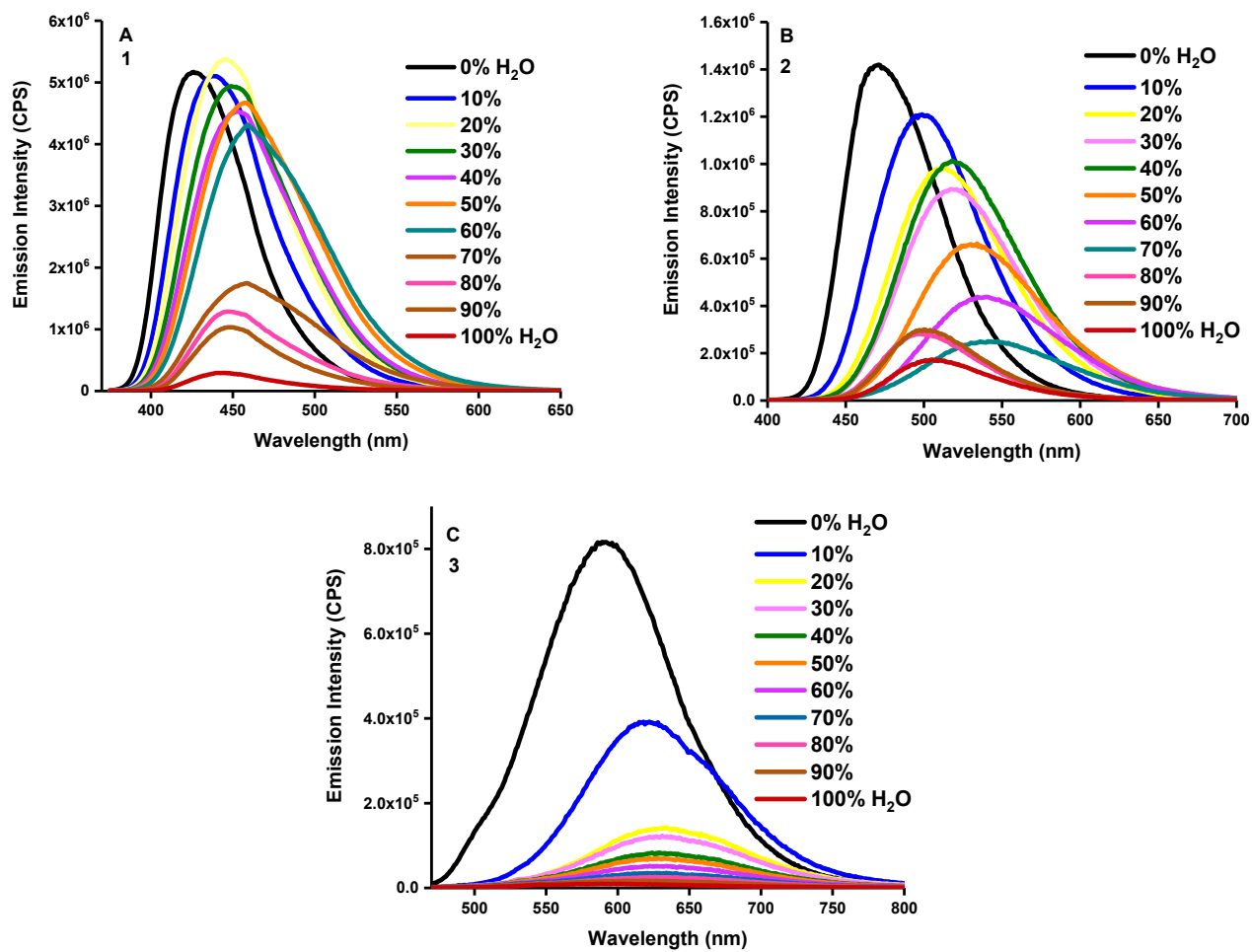


Fig S2. Emission spectra of Stilbenes 1-3 in dioxane-water binary mixture: Water fraction is gradually increased.

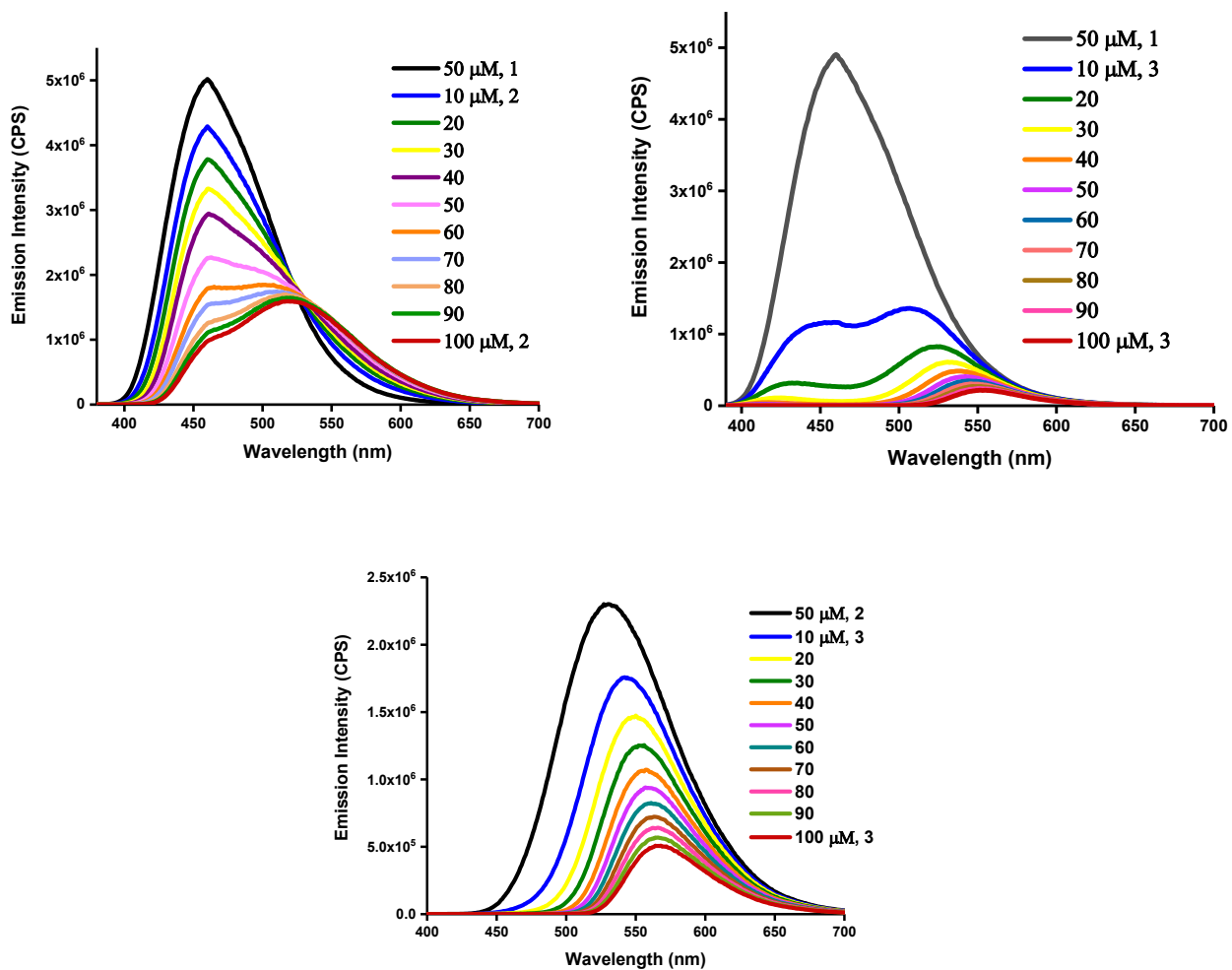


Fig S3. Emission spectra of binary mixtures of stilbenes (1-2, 1-3 and 2-3) in acetonitrile.

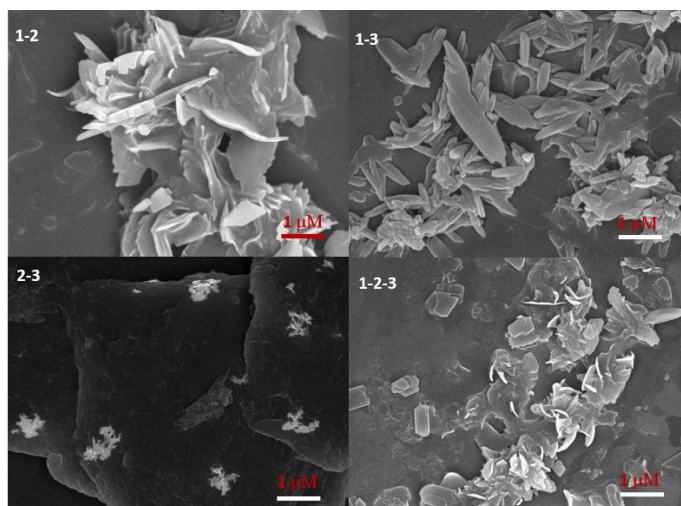


Fig S4. SEM images of mixtures of stilbenes (1-2, 1-3, 2-3 and 1-2-3) in water.

Table S1: Concentrations of samples used and their CIE coordinates obtained.

	Water: 1+3 ( $\mu\text{M}$ )	CIE Coordinates	CH <sub>3</sub> CN: 1+2 ( $\mu\text{M}$ )	CIE Coordinates
1	50 $\mu\text{M}$ & 10 $\mu\text{M}$	0.40,0.42	50 $\mu\text{M}$ & 10 $\mu\text{M}$	0.18,0.22
2	50 & 20	0.38,0.37	50 $\mu\text{M}$ & 20 $\mu\text{M}$	0.19, 0.28
3	50 & 30	0.37,0.35	50 $\mu\text{M}$ & 30 $\mu\text{M}$	0.20,0.36
4	50 & 40	0.35,0.33	50 $\mu\text{M}$ & 40 $\mu\text{M}$	0.22,0.40
5	50 & 50	0.34,0.33	50 $\mu\text{M}$ & 50 $\mu\text{M}$	0.49, 0.32
6	50 & 60	0.31, 0.32	50 $\mu\text{M}$ & 60 $\mu\text{M}$	0.60, 0.41
7	50 & 70	0.28,0.30	-	-

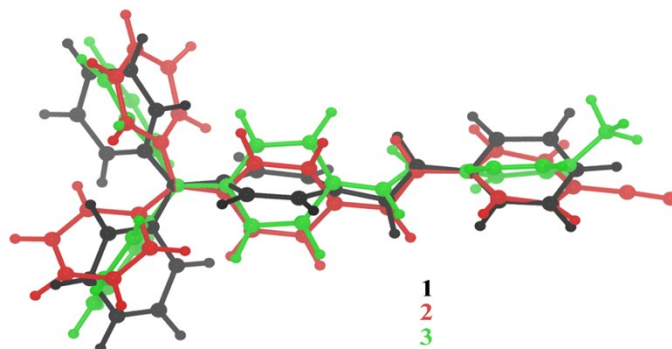


Fig S5. Figure showing superimposition of atomic coordinates of all three molecules obtained after 100 ns equilibrated run from single molecule MD simulation. (1 in black, 2 in red and 3 in green)

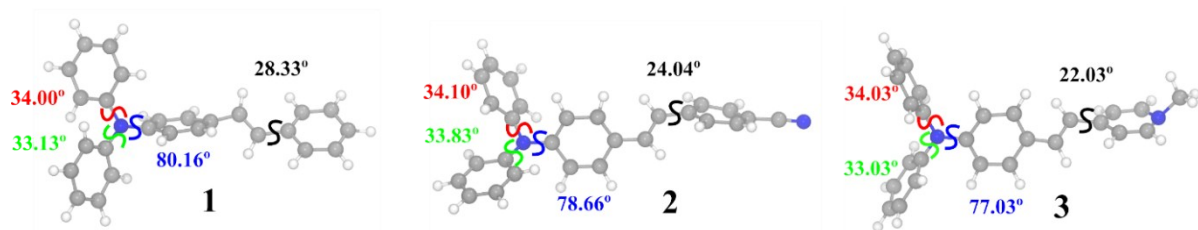


Fig S6. Geometry obtained from 100 ns equilibrated MD simulation with selected dihedral angles.

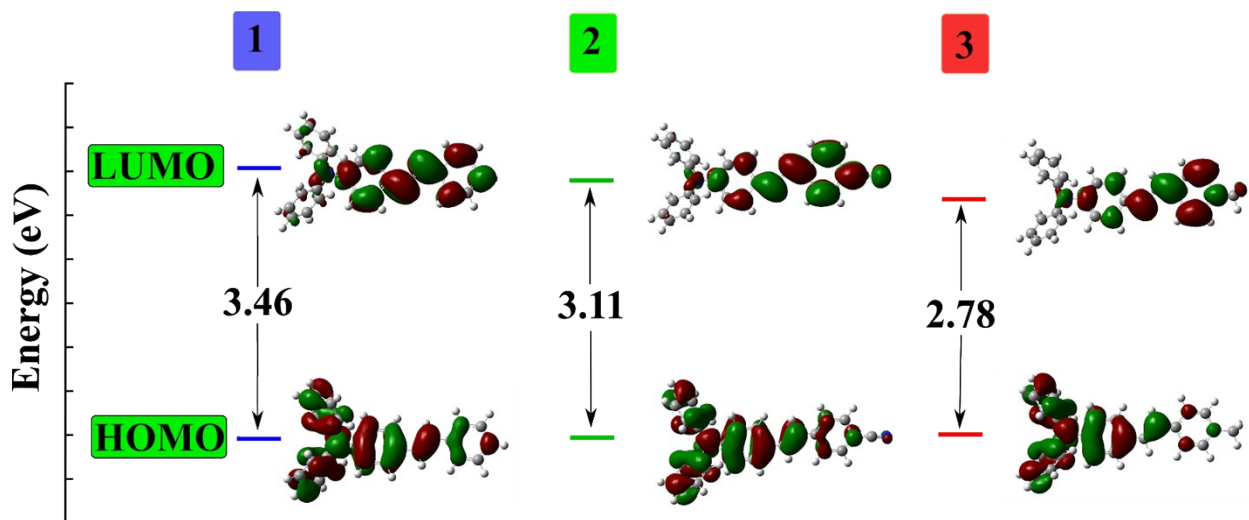


Fig S7. Schematic diagram shows the energy level comparison of the molecules estimated from DFT computation and the isodensity surface plots of the frontier molecular orbitals (FMOs).

Table-S2: Theoretically computed energy differences and their comparison with experimental data

Molecule	Energies (Hartrees)				XS <sub>0</sub> -GS <sub>0</sub>	XS <sub>1</sub> -GS <sub>1</sub>	Solvent Contribution (Abs) kcal/mol	Solvent Contribution (Em) kcal/mol	Absorption (nm)		Emission (nm)	
	Ground State (GS <sub>0</sub> )	Excited State (XS <sub>0</sub> )	Excited State (XS <sub>1</sub> )	Ground State (GS <sub>1</sub> )					Theor	Expt	Theor	Expt
1	-1058.02664159	-1057.89946191	-1057.91250700	-1058.01162921	3.46073714435619	2.69725410519141	-8.12	-0.016776206	358	377	460	451
2	-1150.2736002	-1150.15894980	-1150.171343275	-1150.2585301	3.11979789455581	2.372475569802	-12.95	-16.24	400	400	522.59	504
3	-1574.20239	-1574.10013	-1574.10781505	-1574.191210	2.78263776399694	2.26929334242881	-45.29	-48.99	445.67	450	548	670

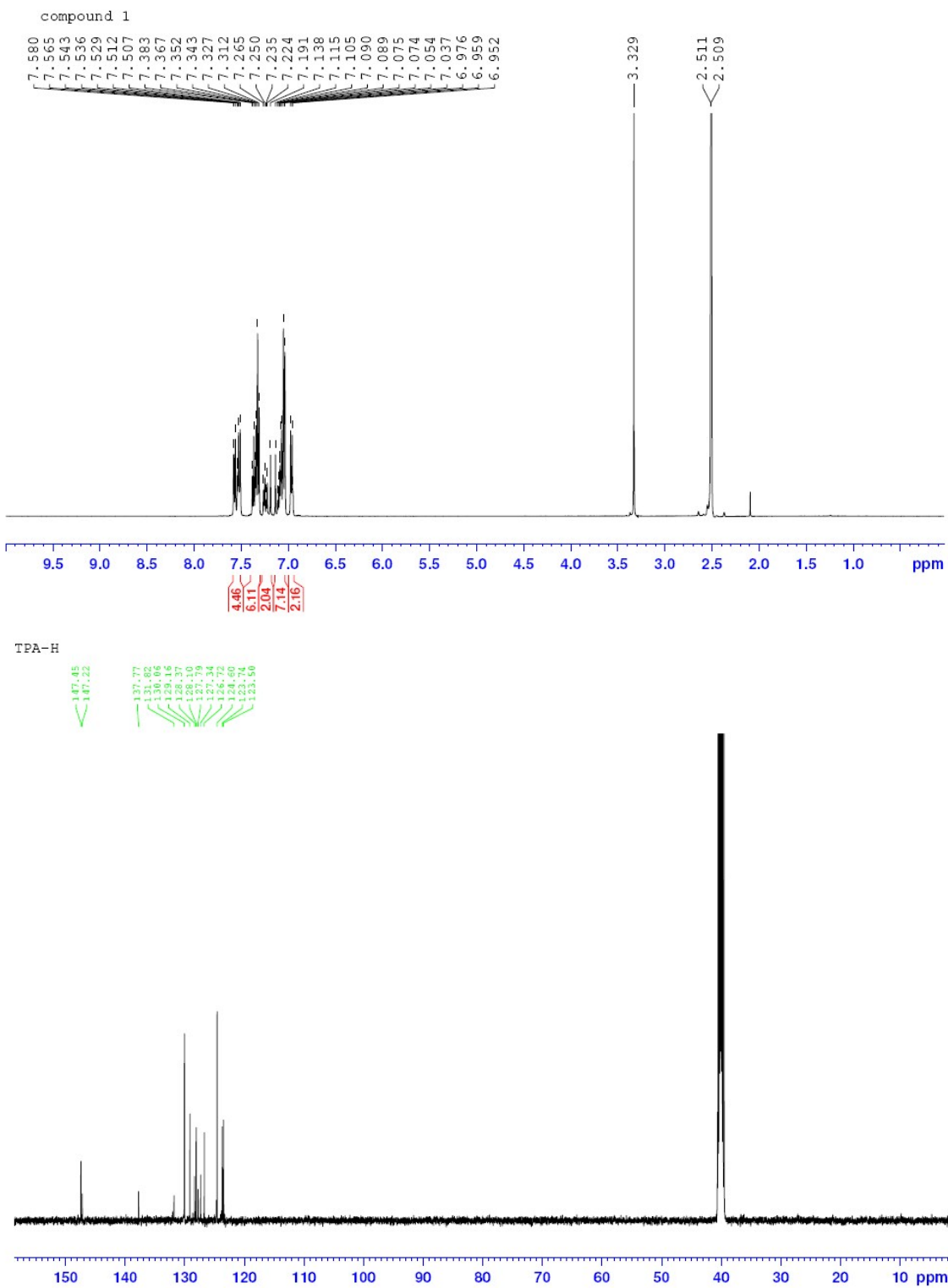
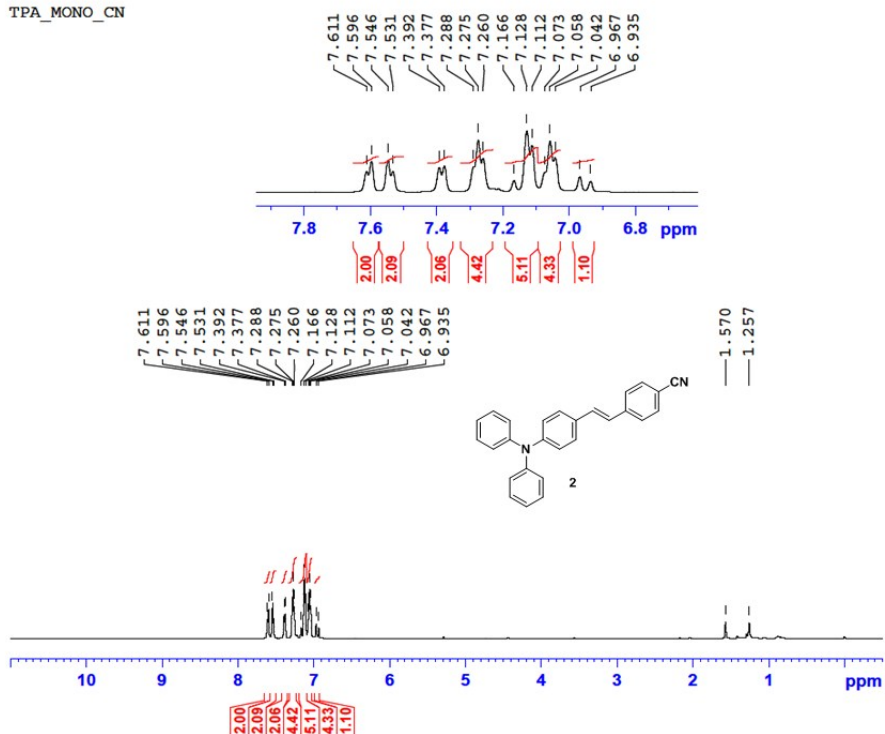


Fig S8.  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and mass data of stilbene 1

TPA\_MONO\_CN

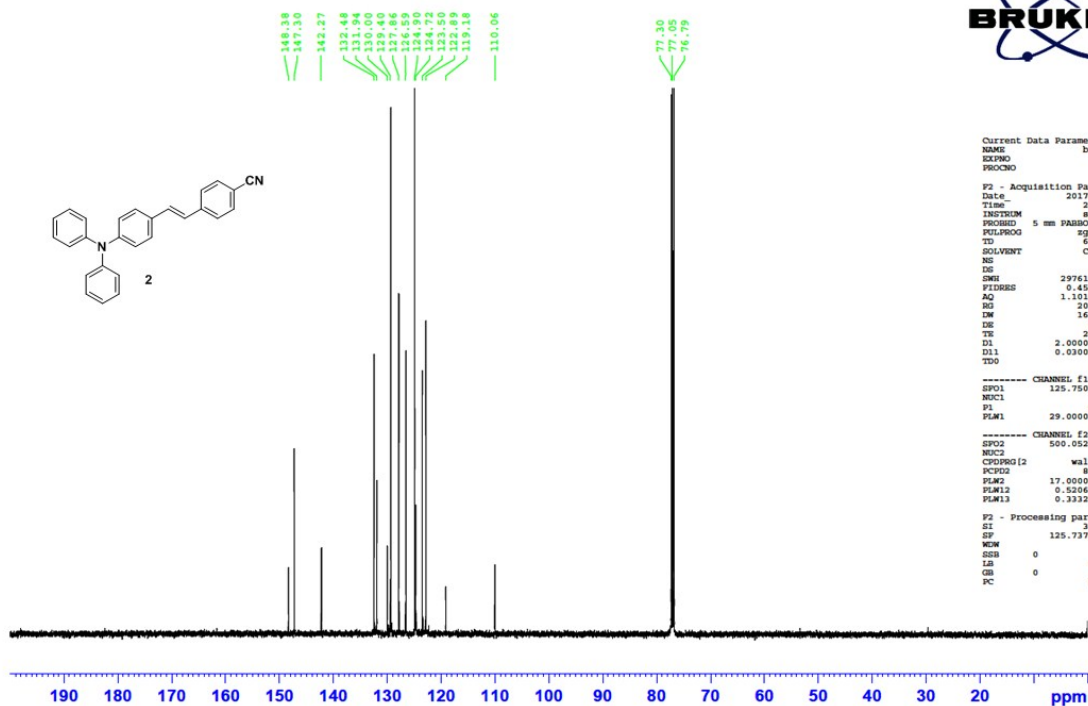


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Fig S9. <sup>1</sup>H, <sup>13</sup>C NMR spectra of Stilbene 2



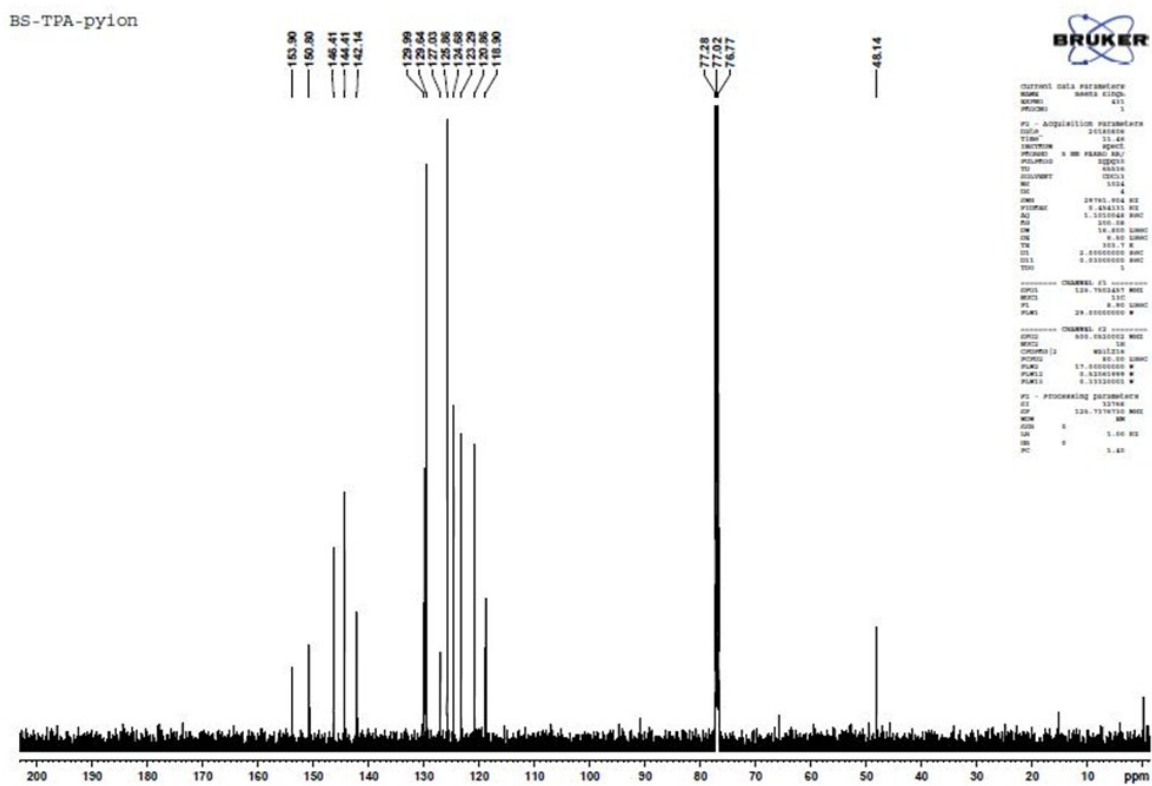
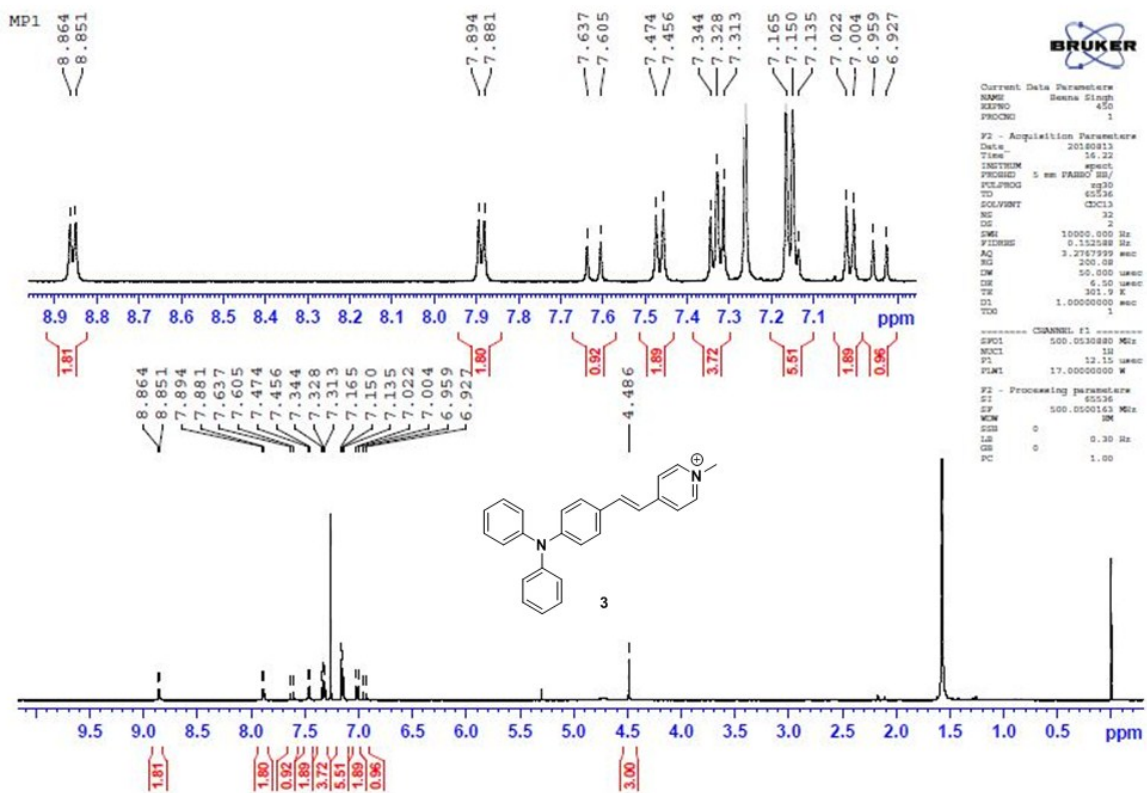


Fig S10. <sup>1</sup>H, <sup>13</sup>C NMR and LC-MS spectra of stilbene 3