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White Light Emission in Water through Admixtures of Donor-π-Acceptor Siblings: Experiment and Simulation

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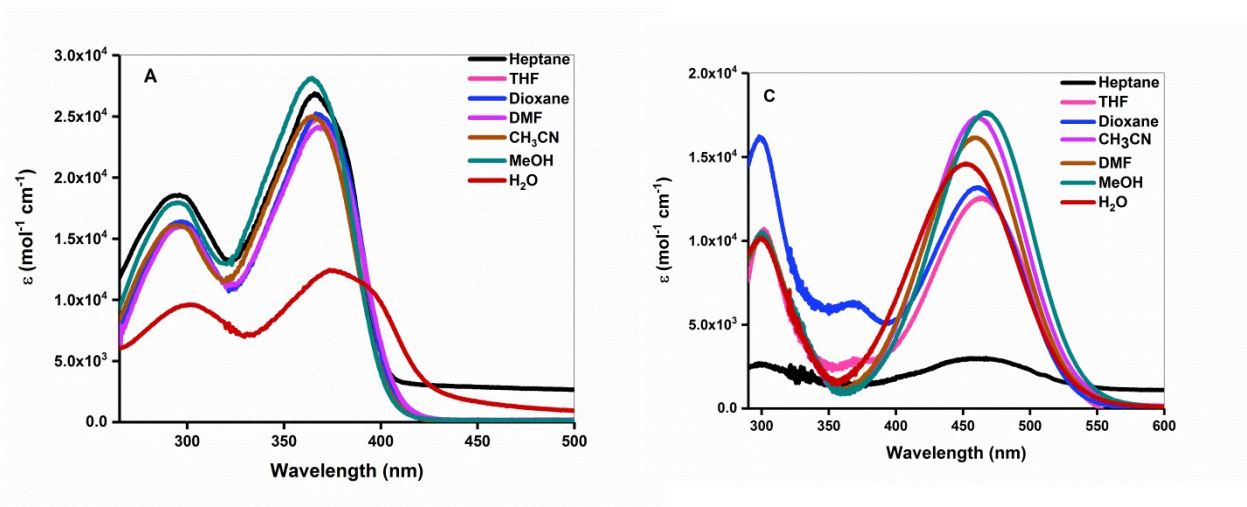

Fig S1. Absorption spectra of stilbenes **1** and **3** in various solvents

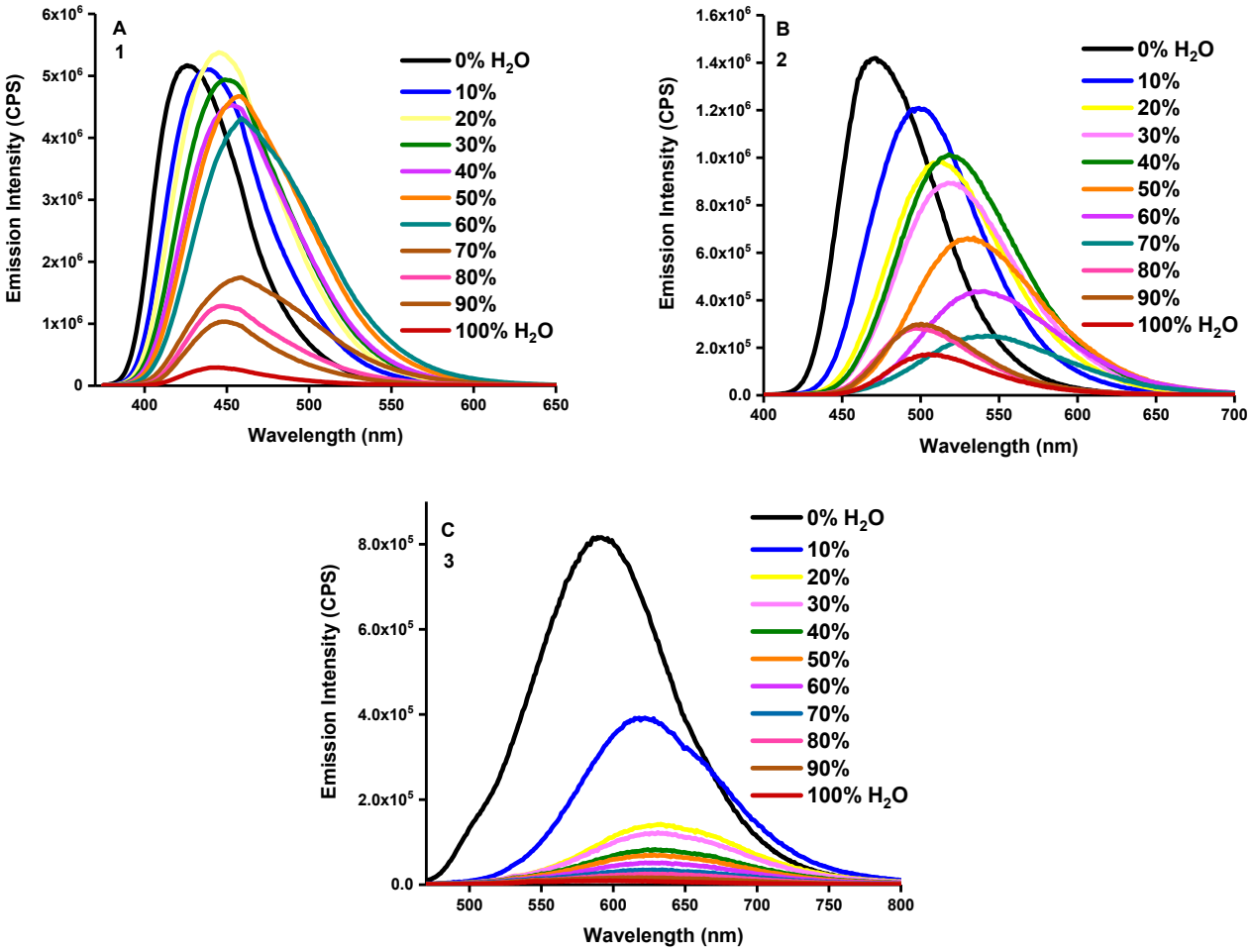

Fig S2. Emission spectra of Stilbenes **1-3** in dioxane-water binary mixture: Water fraction is gradually increased.

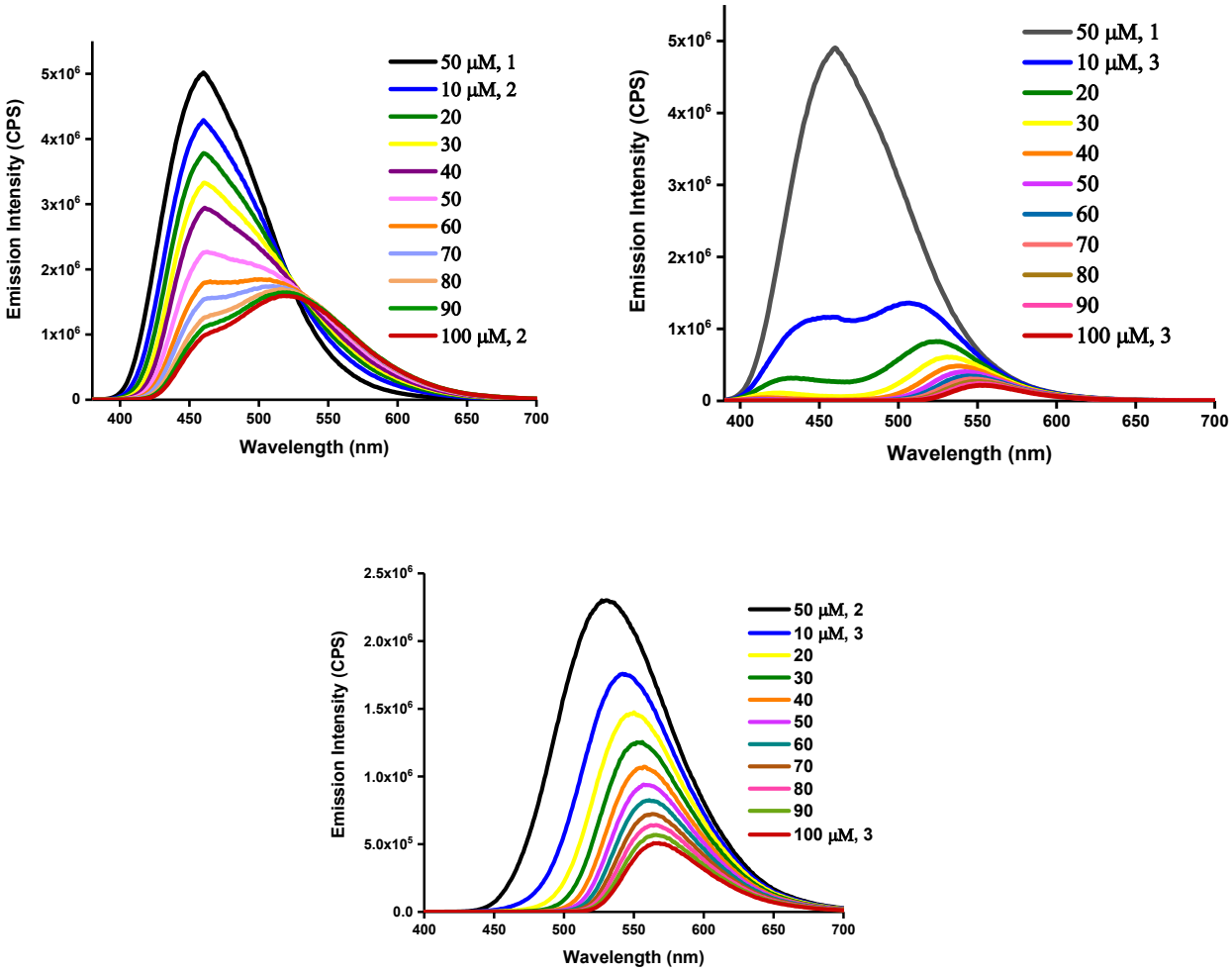

Fig S3. Emission spectra of binary mixtures of stilbenes (**1-2**, **1-3** and **2-3**) in acetonitrile.

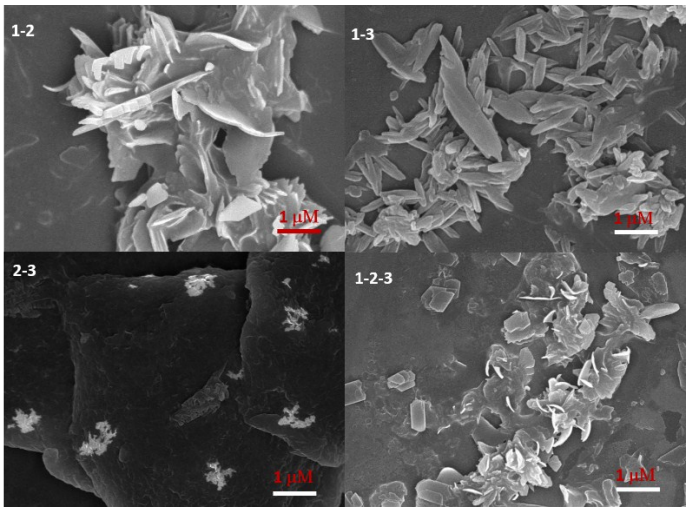

Fig S4. SEM images of mixtures of stilbenes (**1-2**, **1-3**, **2-3 and 1-2-3**) in water.

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

	Water: 1+3 (μM)	**CIE Coordinates**	**CH_3CN: 1+2** (μM)	**CIE Coordinates**
1	50 μM & 10 μM	0.40,0.42	50 μM & 10 μM	0.18,0.22
2	50 & 20	0.38,0.37	50 μM & 20 μM	0.19, 0.28
3	50 & 30	0.37,0.35	50 μM & 30 μM	0.20,0.36
4	50 & 40	0.35,0.33	50 μM & 40 μM	0.22,0.40
5	50 & 50	0.34,0.33	50 μM & 50 μM	0.49, 0.32
6	50 & 60	0.31, 0.32	50 μM & 60 μM	0.60, 0.41
7	50 & 70	0.28,0.30	-	-

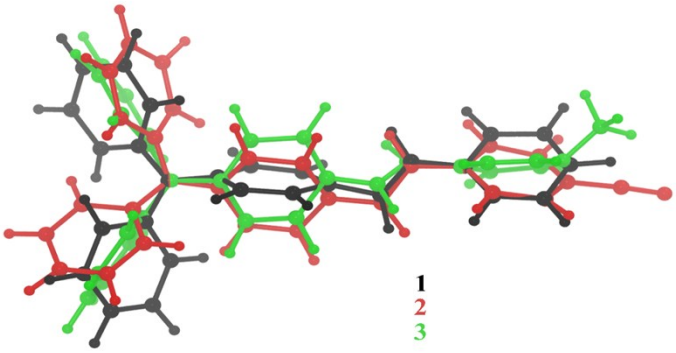

Fig S5. Figure showing superimposition of atomic coordinates of all three molecules obtained after 100 ns equilibrated run from single molecule MD simulation. (**1** in black, **2** in red and **3** in green)

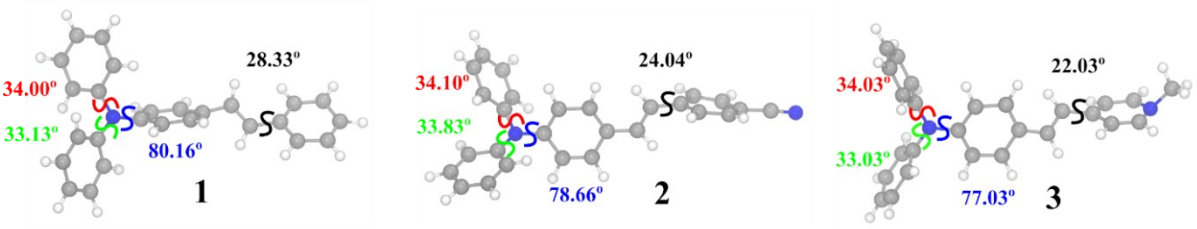

Fig S6. Geometry obtained from 100 ns equilibrated MD simulation with selected dihedral angles.

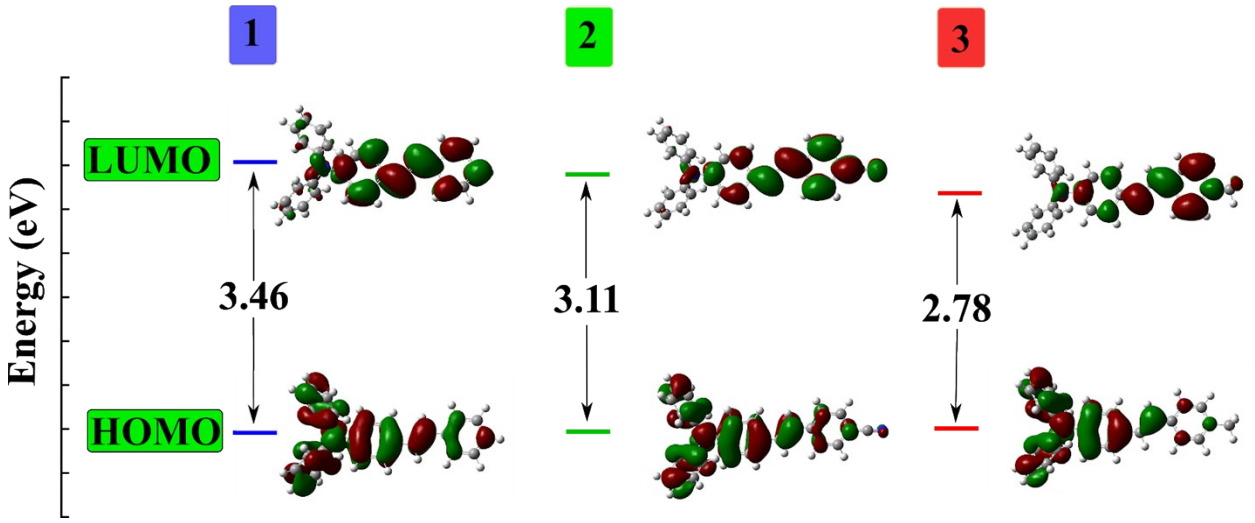

Fig S7. Schematic diagram shows the energy level comparison of the molecules estimated from DFT computation and the isodensity surface plots of the frontier molecular orbitals (FMOs).

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

	Energies (Hartrees)				XS_o-GS_o	XS_1-GS_1			Absorption (nm)		Emission (nm)	
Molecule	Ground State (GS_o)	Excited State (XS_o)	Excited State (XS_1)	Ground State (GS_1)	Abs (eV)	Em (eV)	Solvent Contribution (Abs) kcal/mol	Solvent Contribution (Em) kcal/mol	Theor	Expt	Theor	Expt
1	-1058.02664159	-1057.89946191	-1057.91250700	-1058.01162921	3.460737144 35619	2.697 2541 0519 141	-8.12	-0.016776206	358	377	460	451
2	-1150.2736002	-1150.15894980	-1150.171343275	-1150.2585301	3.119797894 55581	2.372 4755 6980 2	-12.95	-16.24	400	400	522.59	504
3	-1574.20239	-1574.10013	-1574.10781505	-1574.191210	2.782637763 99694	2.269 2933 4242 881	-45.29	-48.99	445.67	450	548	670

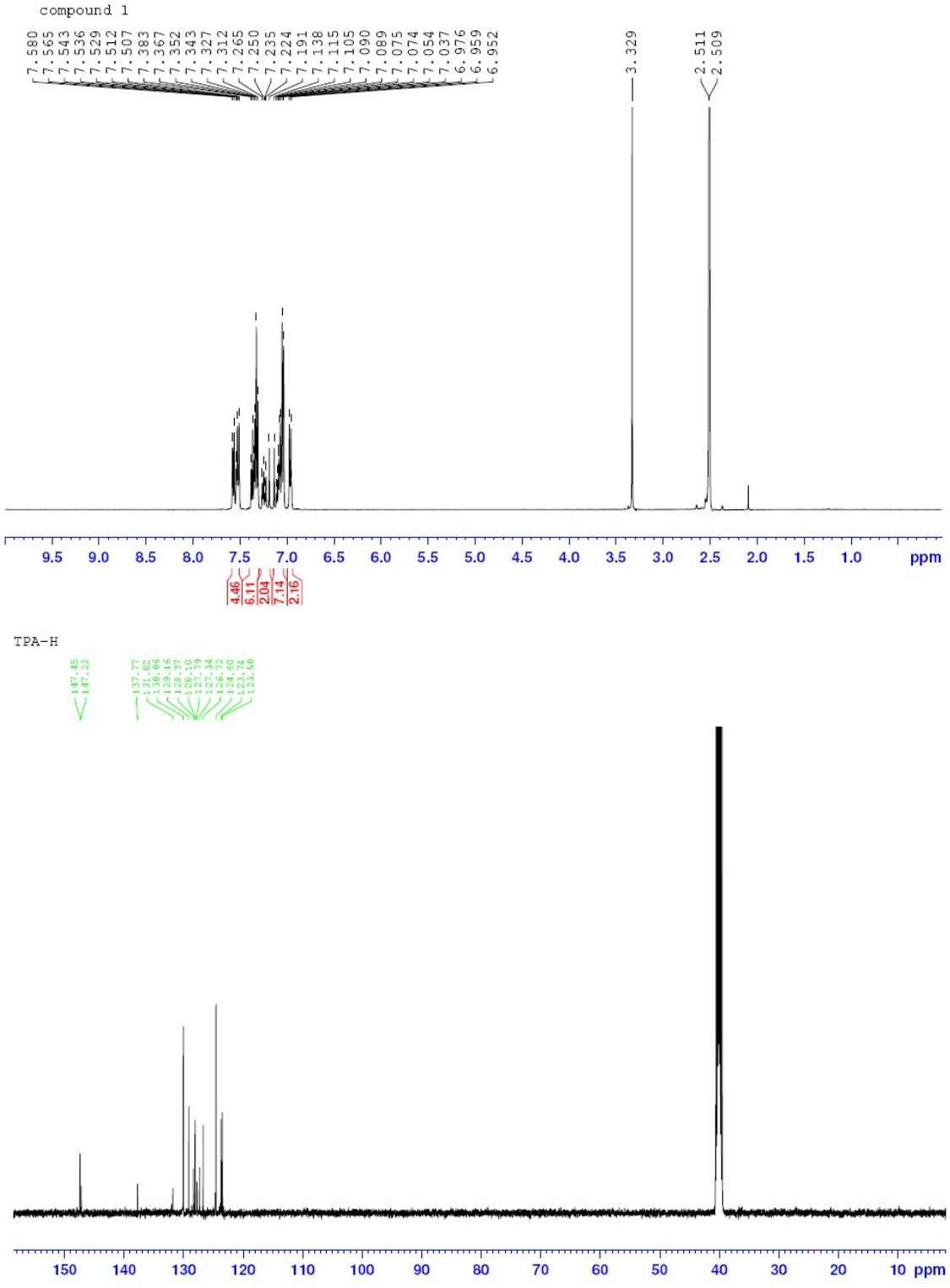

Fig S8. ^{1}H, ^{13}C NMR and mass data of stilbene **1**

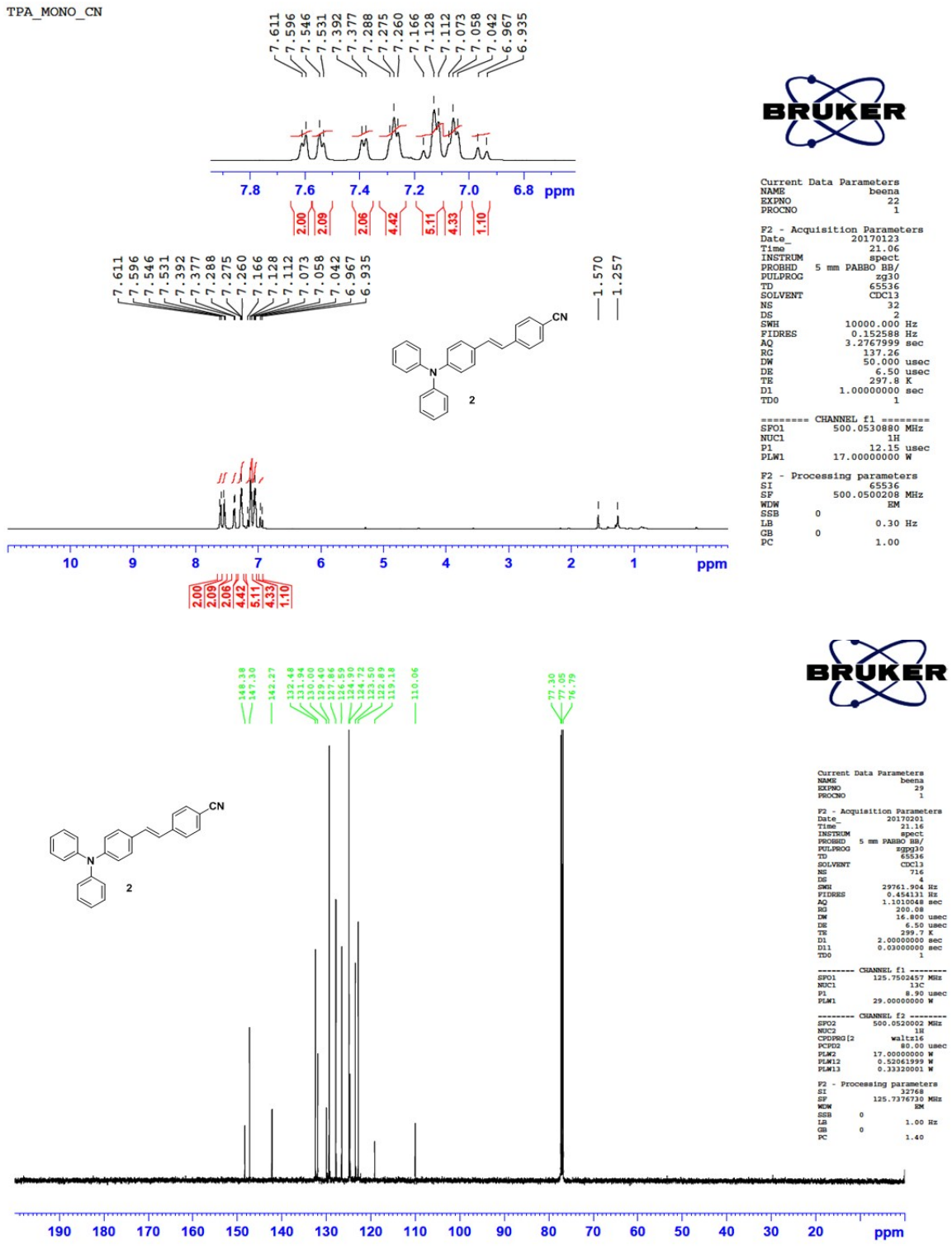

Fig S9. ^{1}H, ^{13}C NMR spectra of Stilbene **2**

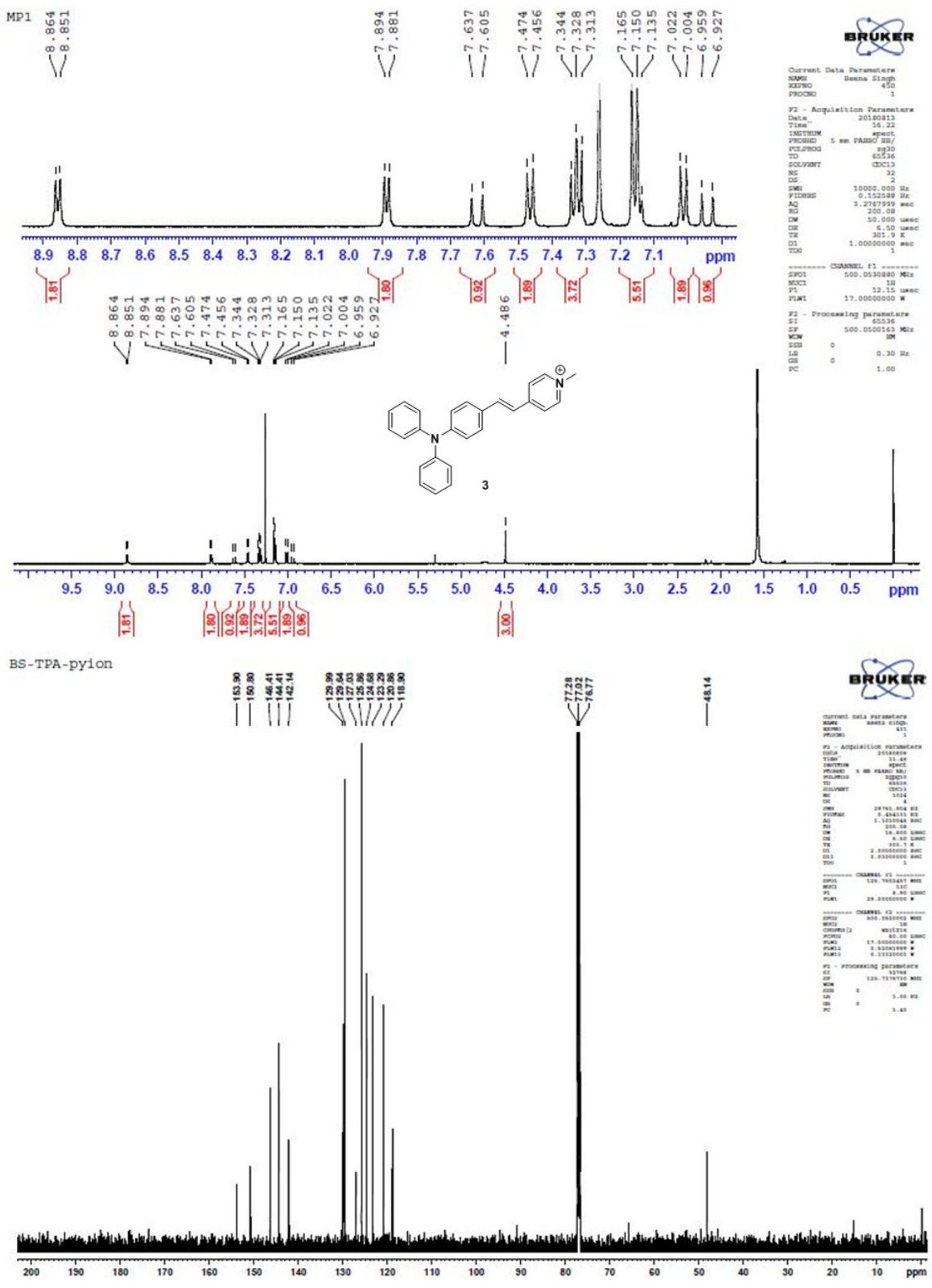

Fig S10. ^{1}H, ^{13}C NMR and LC-MS spectra of stilbene **3**