

# Perturbing the AIEE activity of Pyridine Functionalized Cyanostilbenes with Donor Substitutions: An Experimental and DFT study

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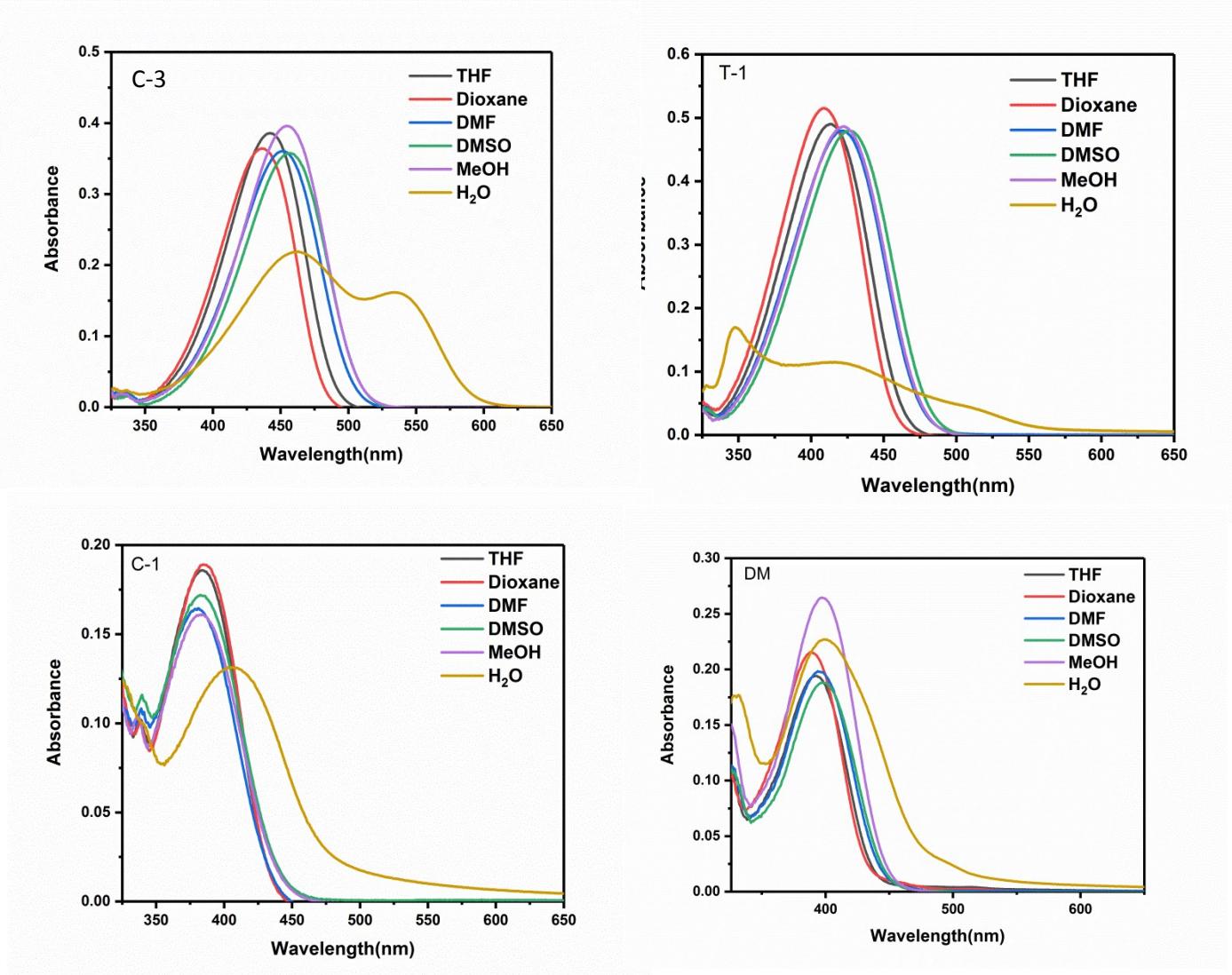


Fig S1: Absorption spectra of pyridylacrylonitriles (C-1, C-3, J-1 and DM) investigated in different solvents.

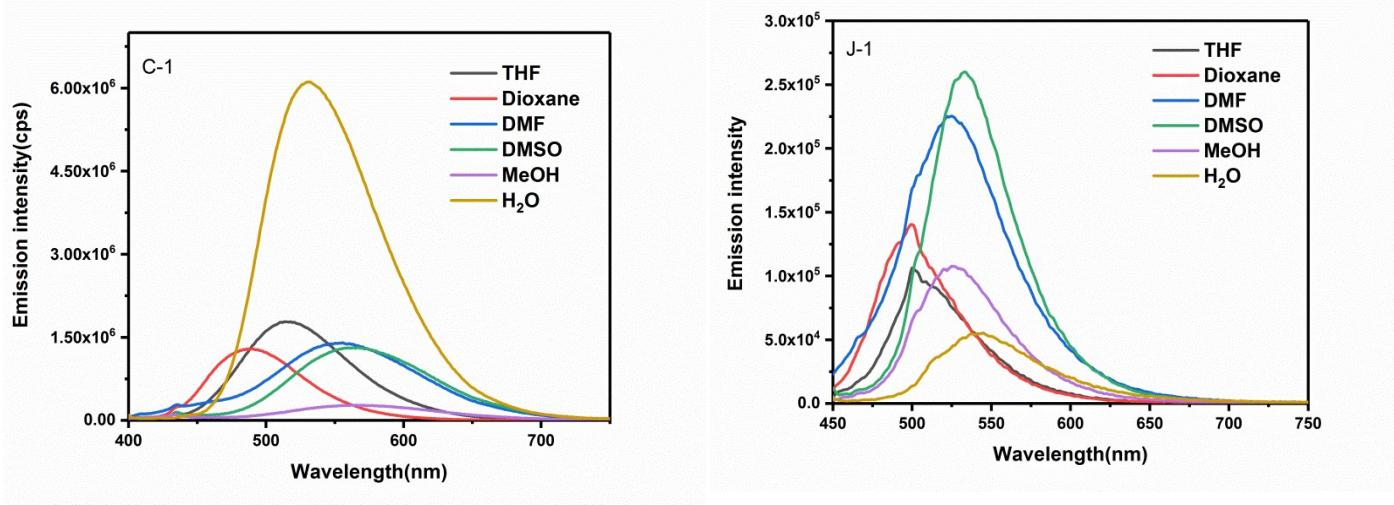


Fig S2: Emission of C-1 and J-1 in various solvents.

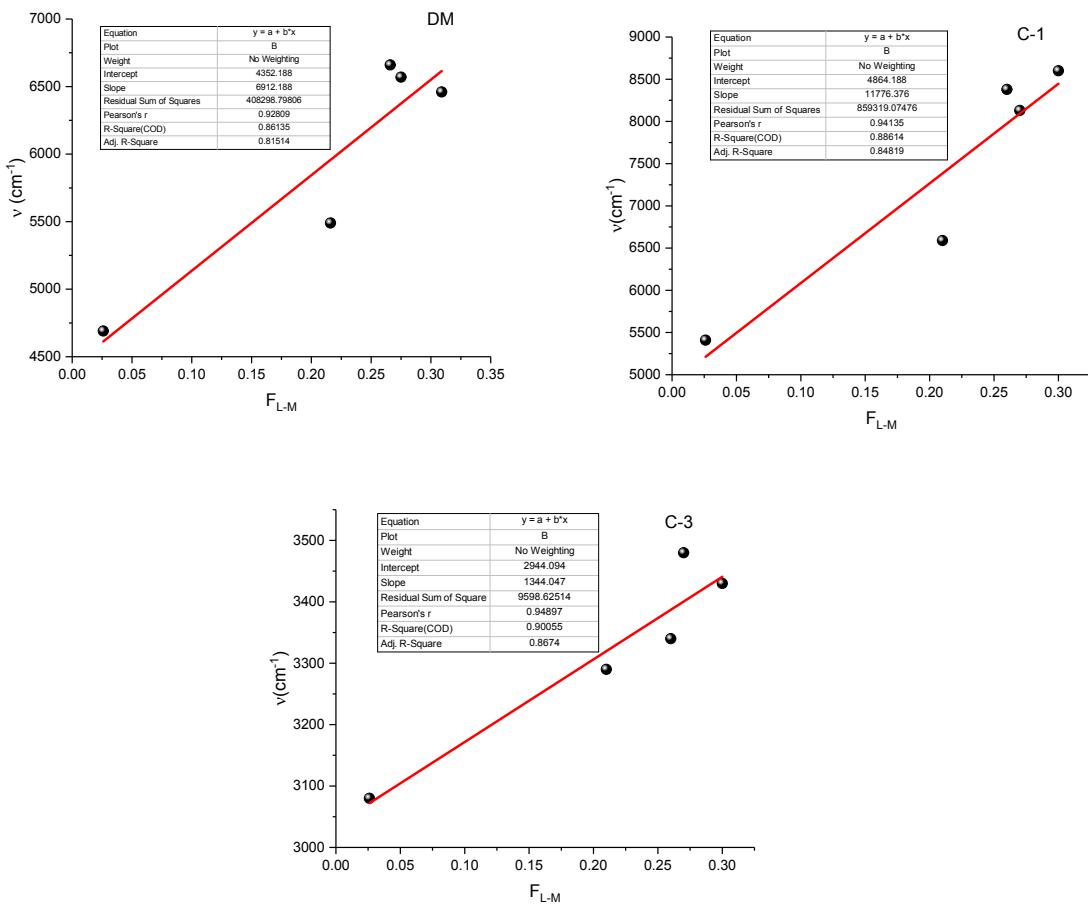


Fig. S2a: Lippert- Mataga plots for C-1, DM and C-3. Poor correlation was obtained for the other compounds.

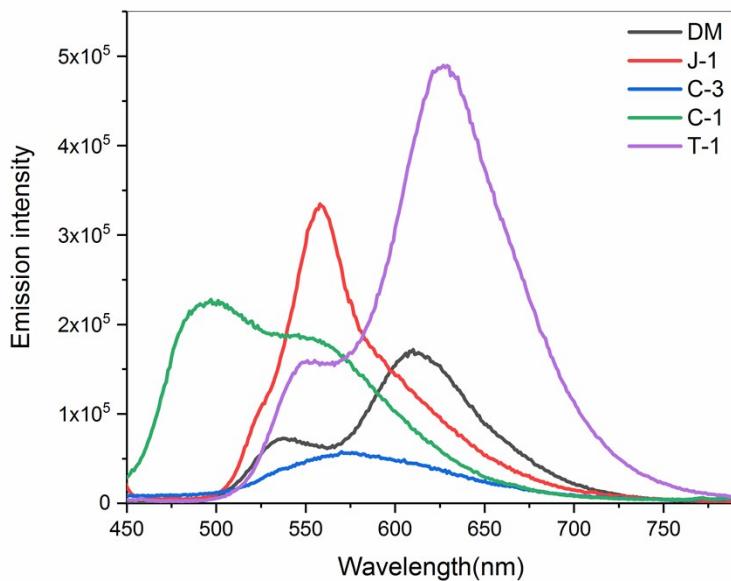


Fig S3: Emission of the compounds in solid state.

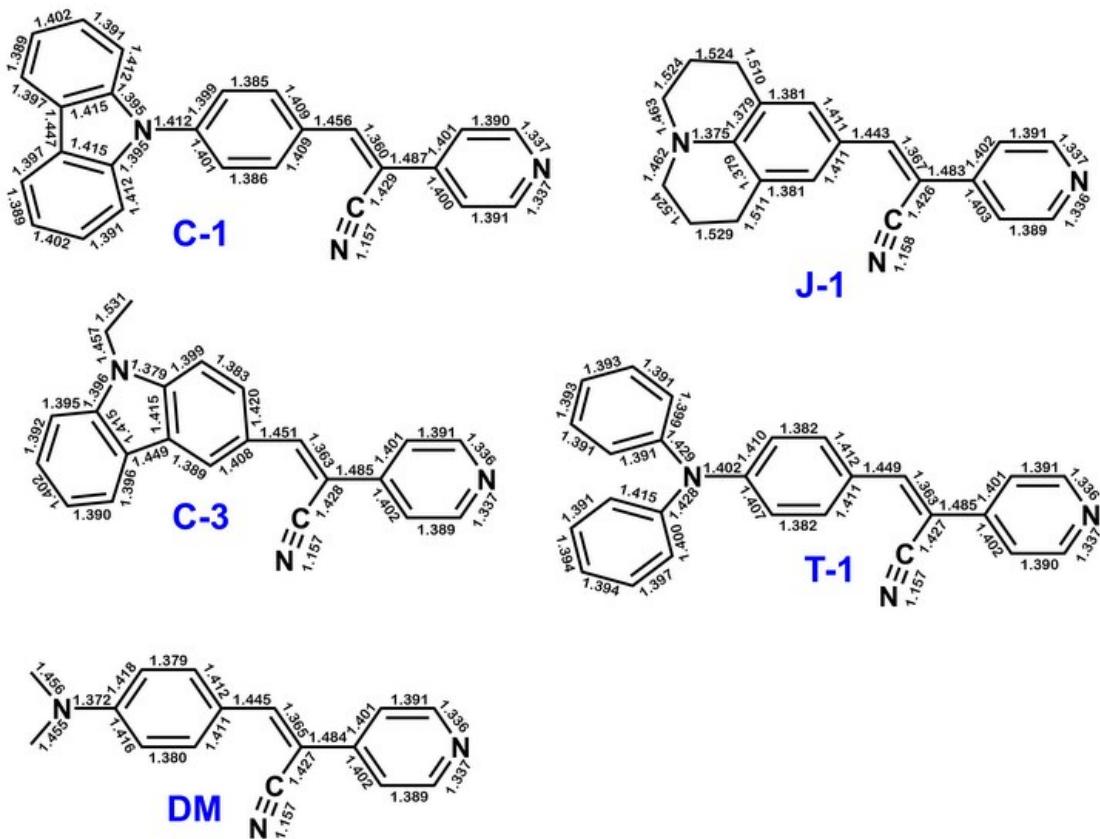
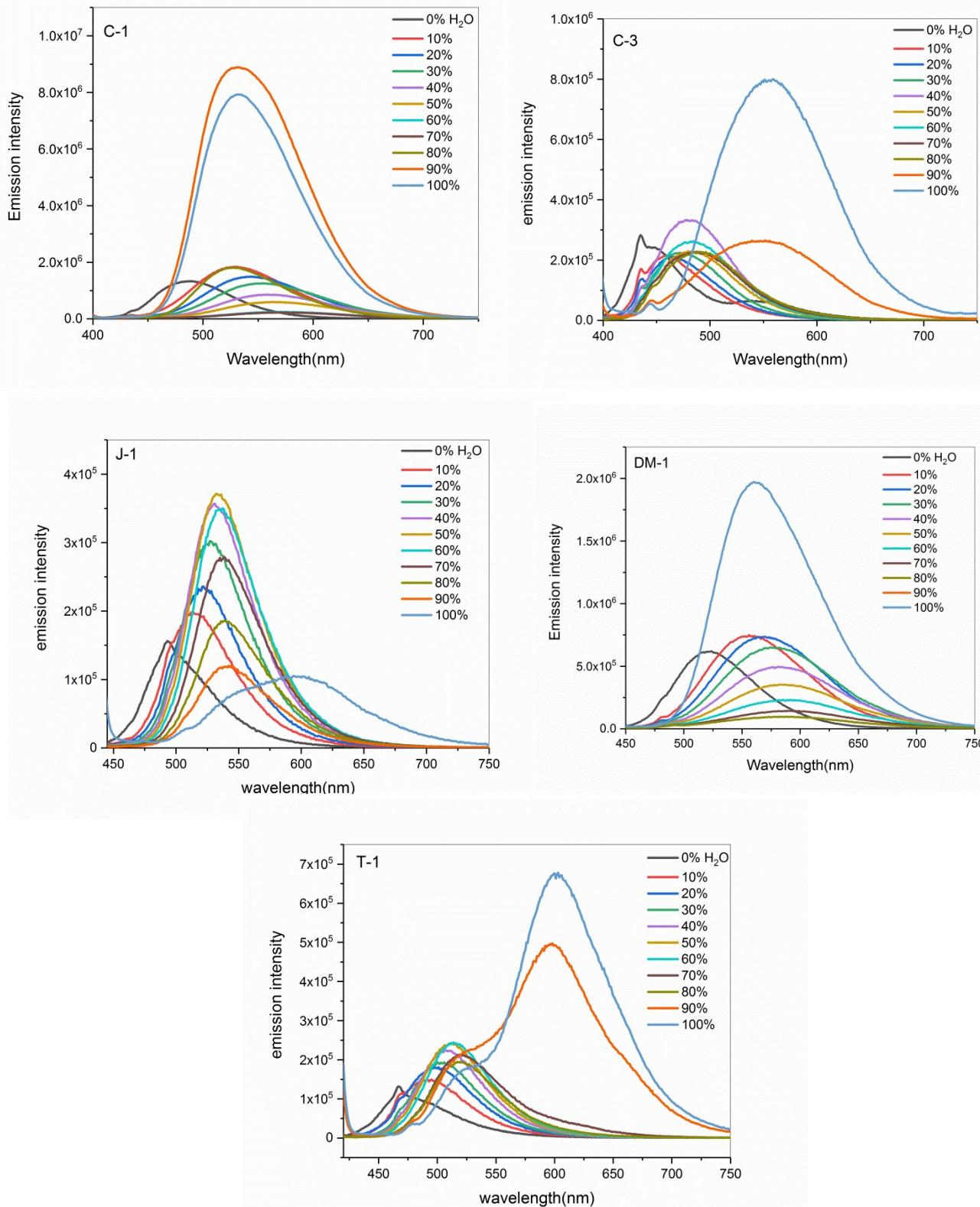
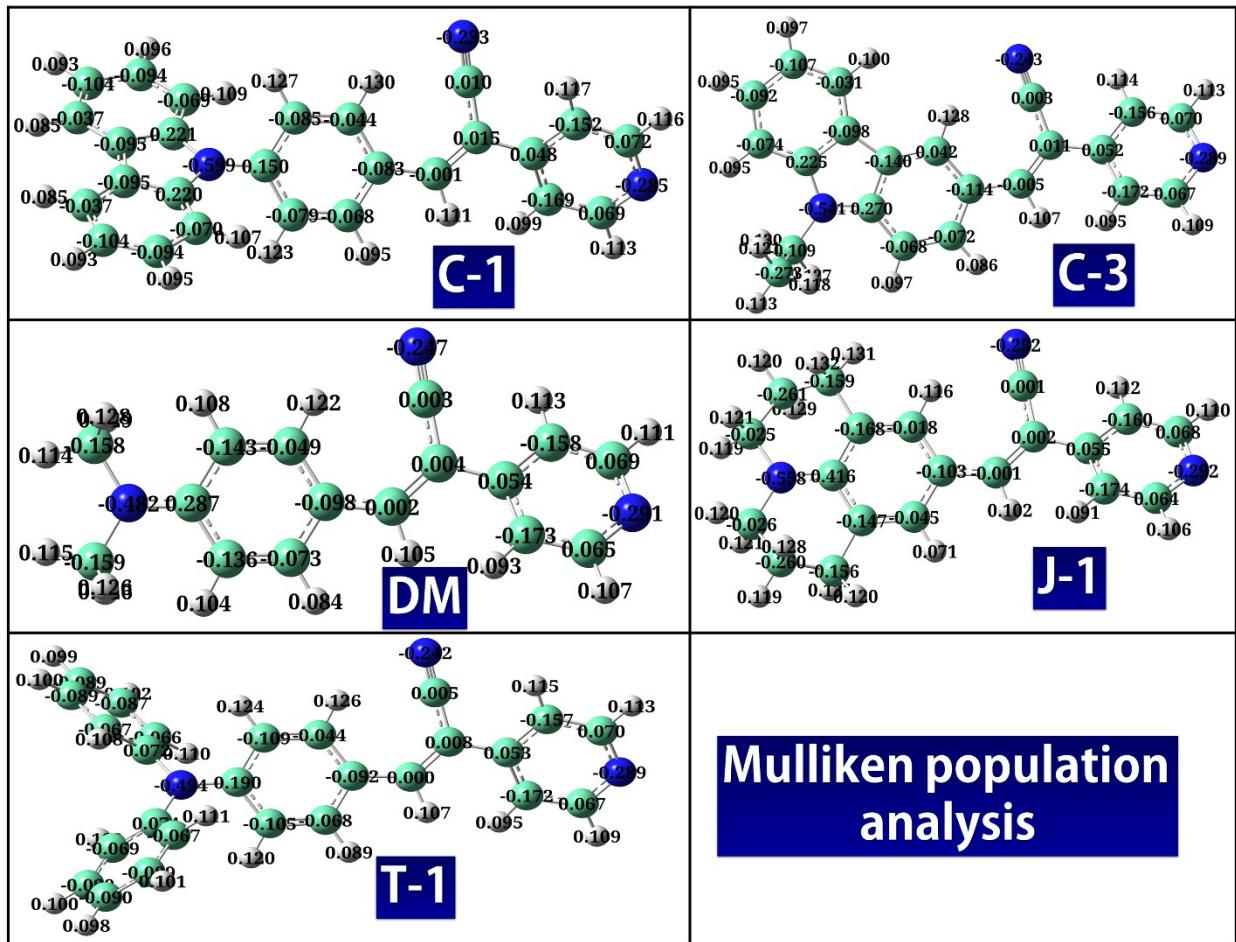


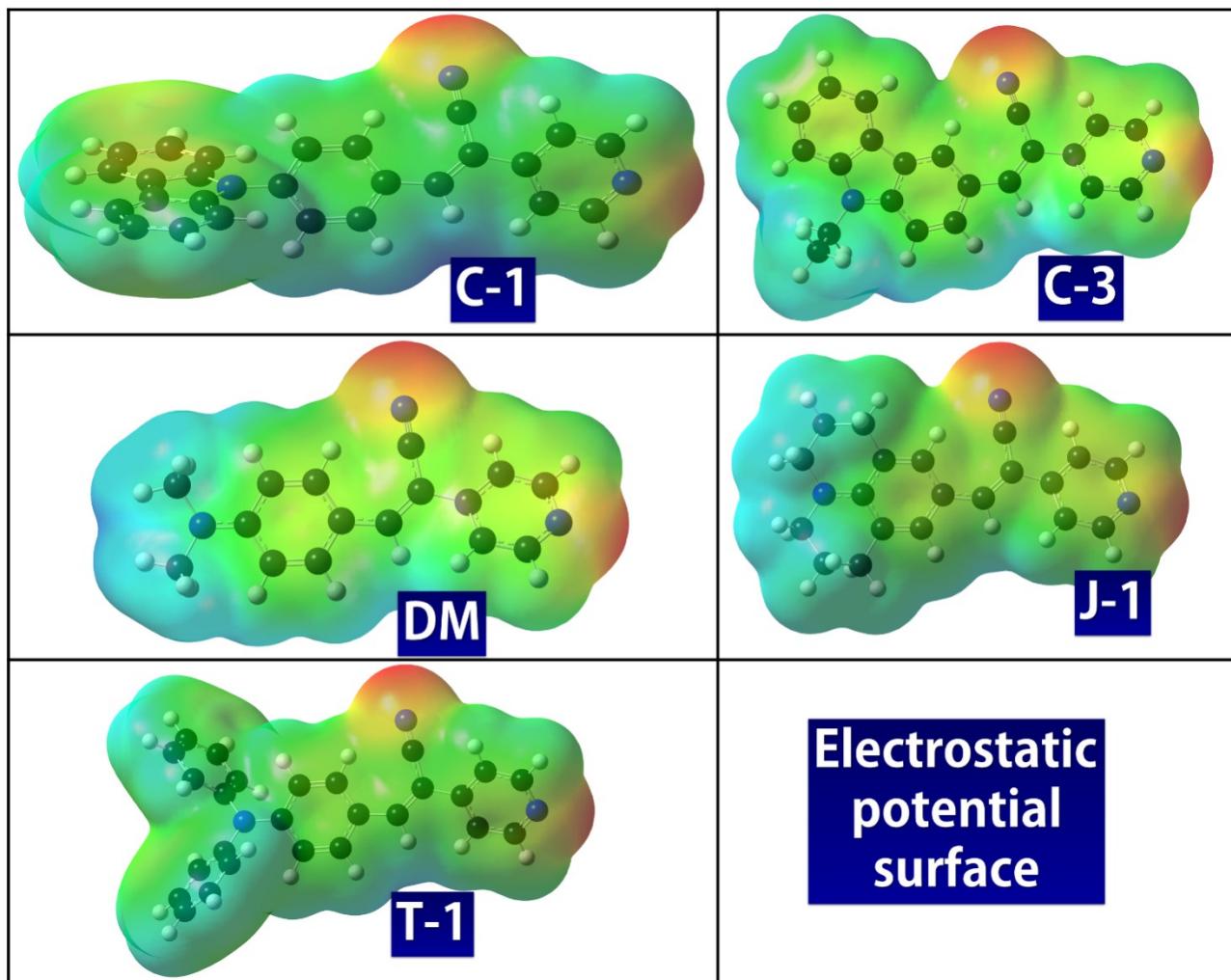
Fig. S4 Geometrical coordinates of the  $\alpha$ -cyanostilbene derivatives.



**Fig S5:** Emission of compounds in dioxane-water binary mixture.



**Fig.S6** Mulliken population analysis on the grouped segments (D,  $\pi$ , and A) of the compounds obtained from DFT/B3LYP/6-311++G (d, p) level of theory.



**Fig.S7** Electrostatic potential map of the compounds obtained from DFT/B3LYP/6-311G++ (d, p) level of theory. The red, green and blue colors are representing negative, neutral and positive charge population on the segments respectively.  $\alpha$ -Cyano moiety and pyridyl group contain negative charge population sites.

Table S1. DLS data of pyridine acrylonitriles

Compounds	Z-average(d.nm)	PdI
DM	354.1	0.35
J-1	415.4	.502
C-1	172.2	0.243
C-3	653.8	0.342
T-1	3940	1

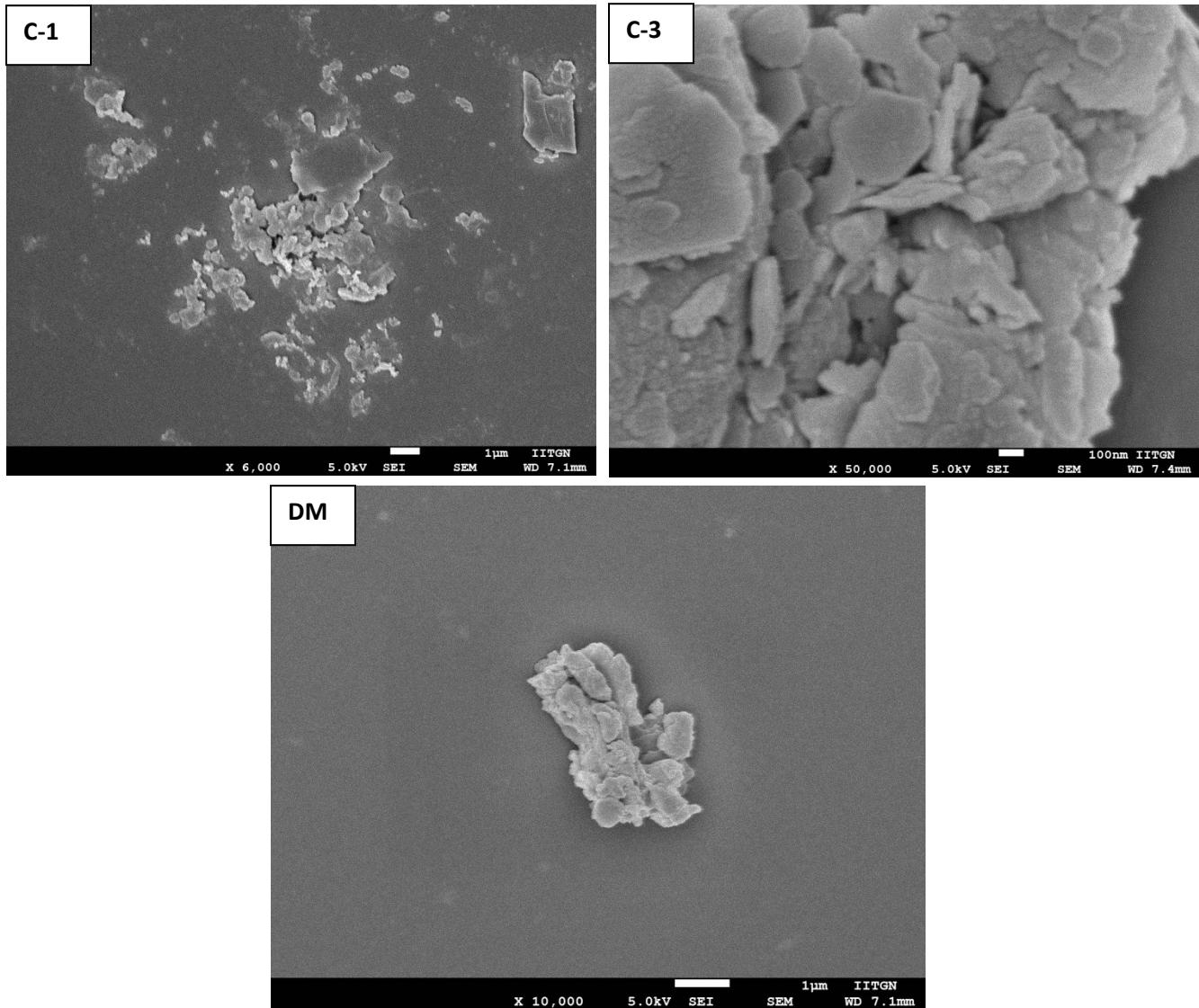


Fig. S8: Drop-cast SEM images of C-1, C-3 and DM in water (concentration 10  $\mu$ M).

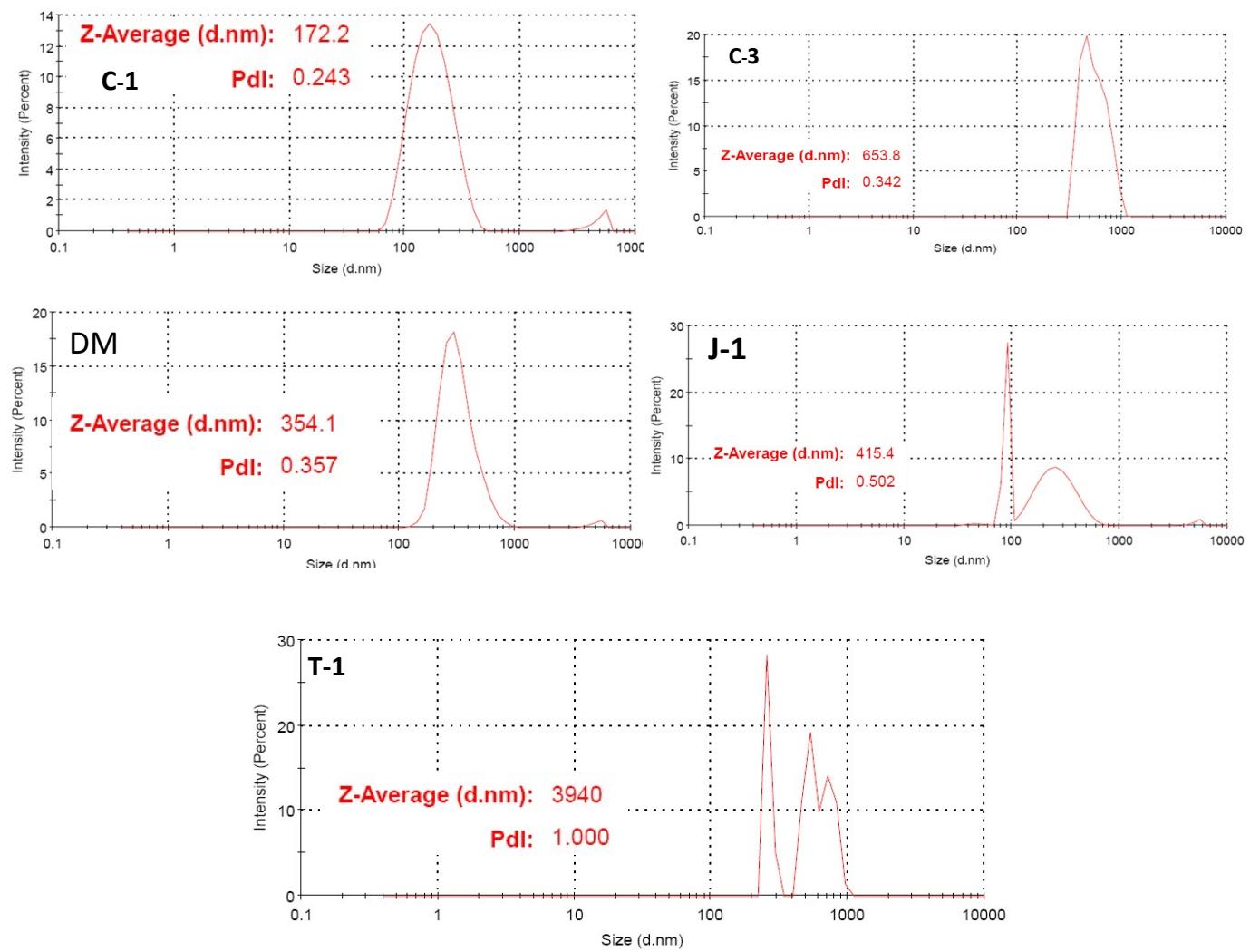


Fig S9: Size distribution of the particles in water as obtained by Dynamic Light Scattering (DLS) measurements

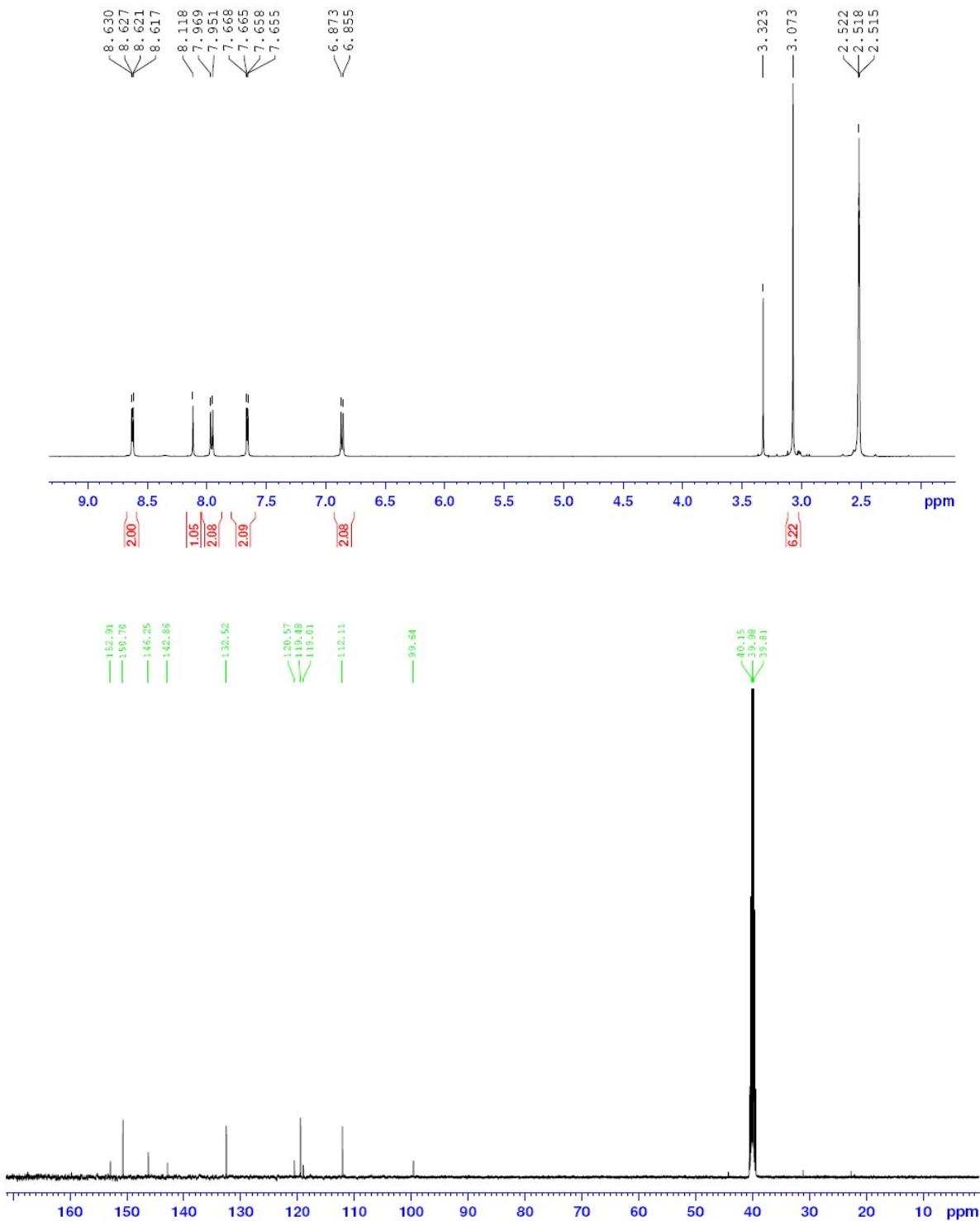


Fig. S10 <sup>1</sup>H-NMR & <sup>13</sup>C spectrum of DM

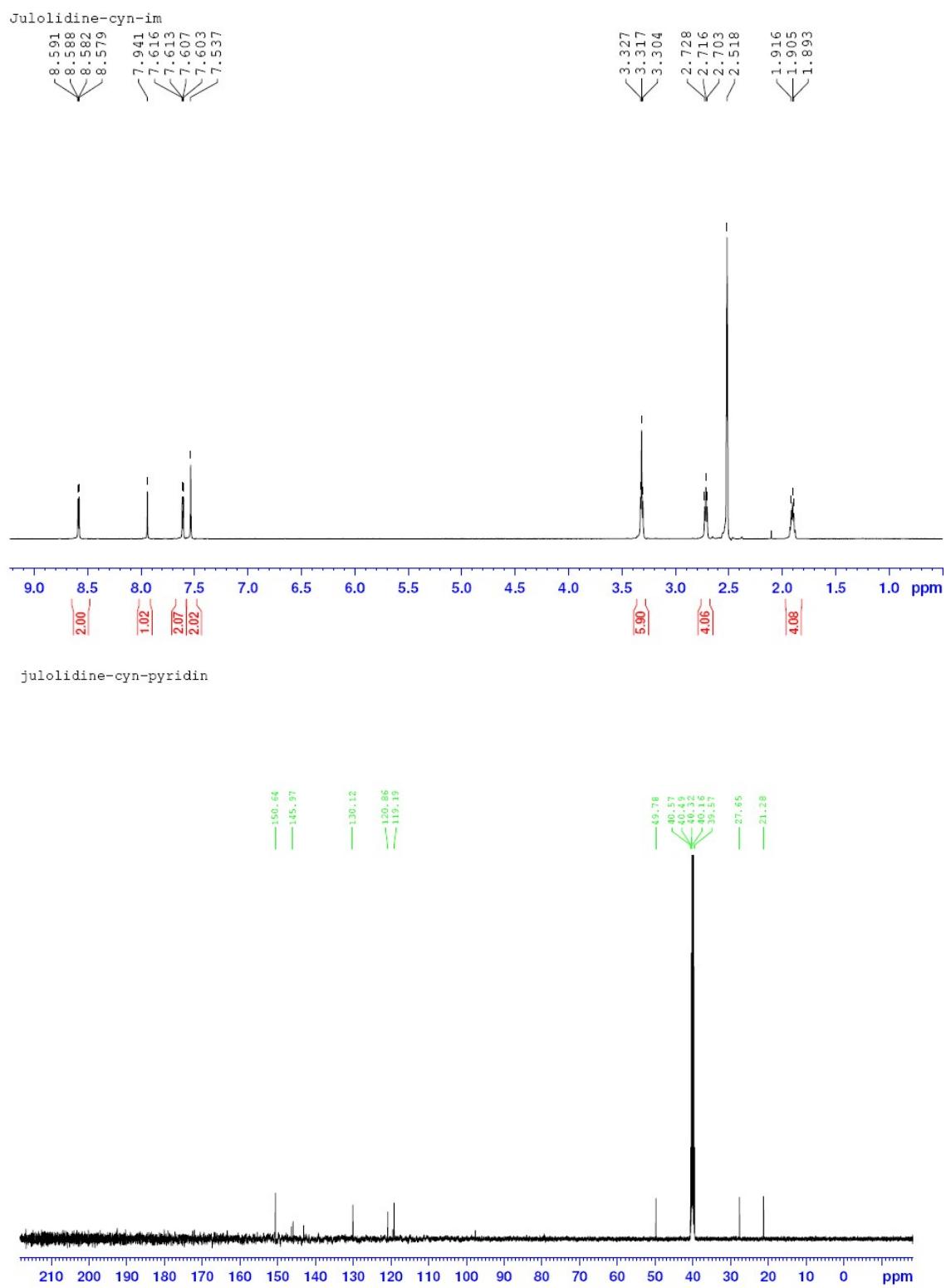


Fig. S11  $^1\text{H}$ -NMR &  $^{13}\text{C}$  spectrum of J-1

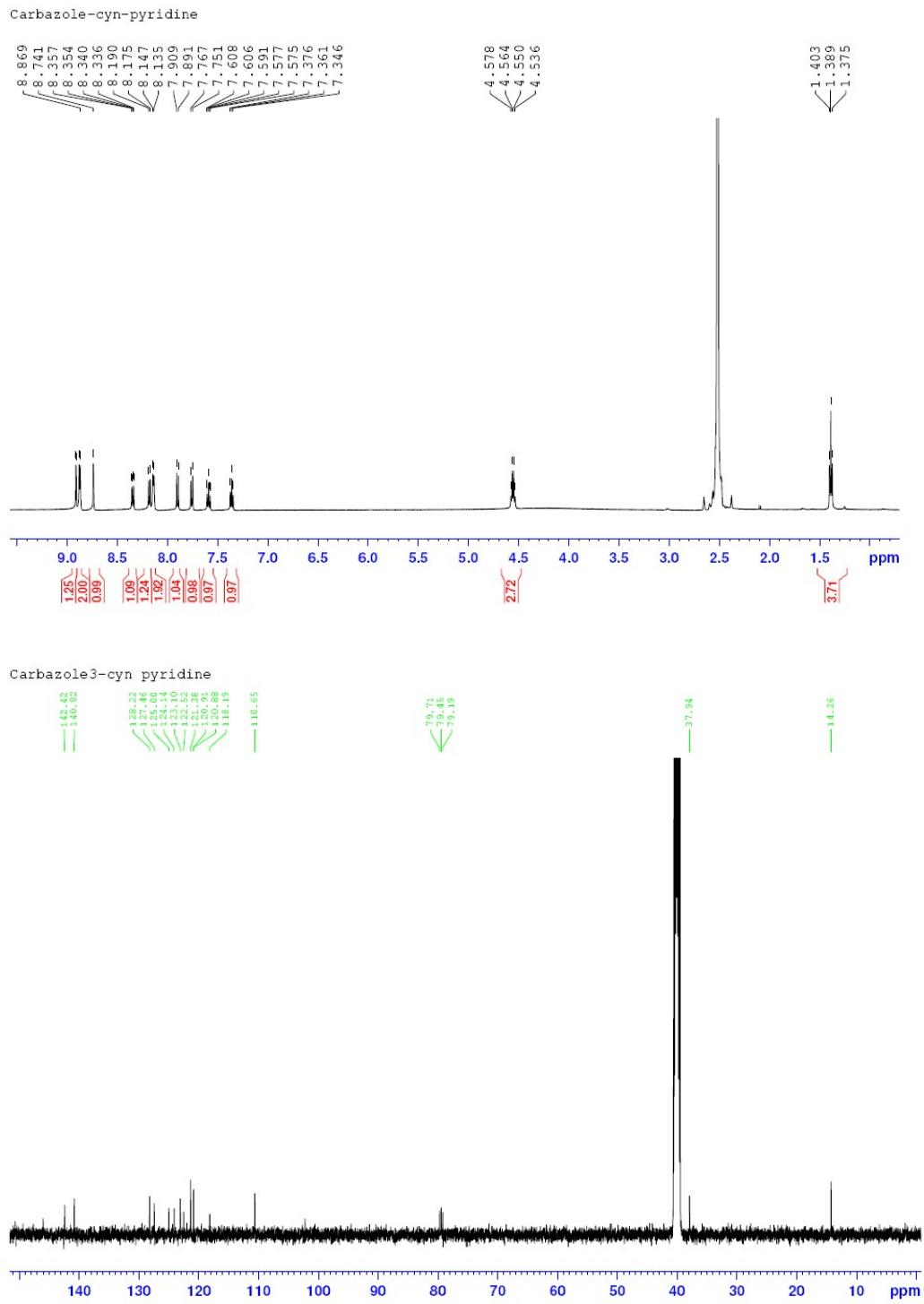


Fig. S12:  $^1\text{H}$ -NMR &  $^{13}\text{C}$  spectrum of C-3

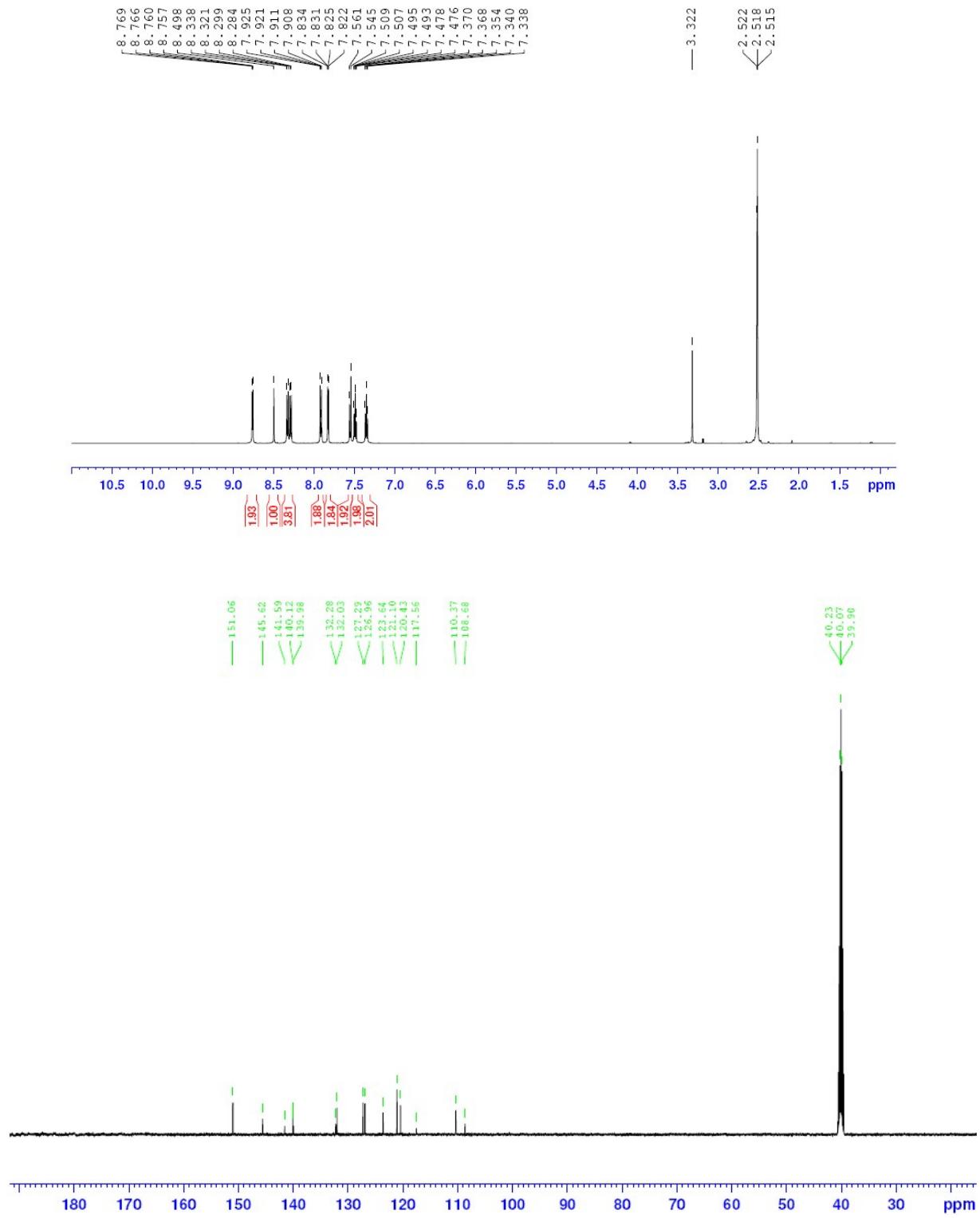


Fig. S13  $^1\text{H}$ -NMR &  $^{13}\text{C}$  spectrum of C-1

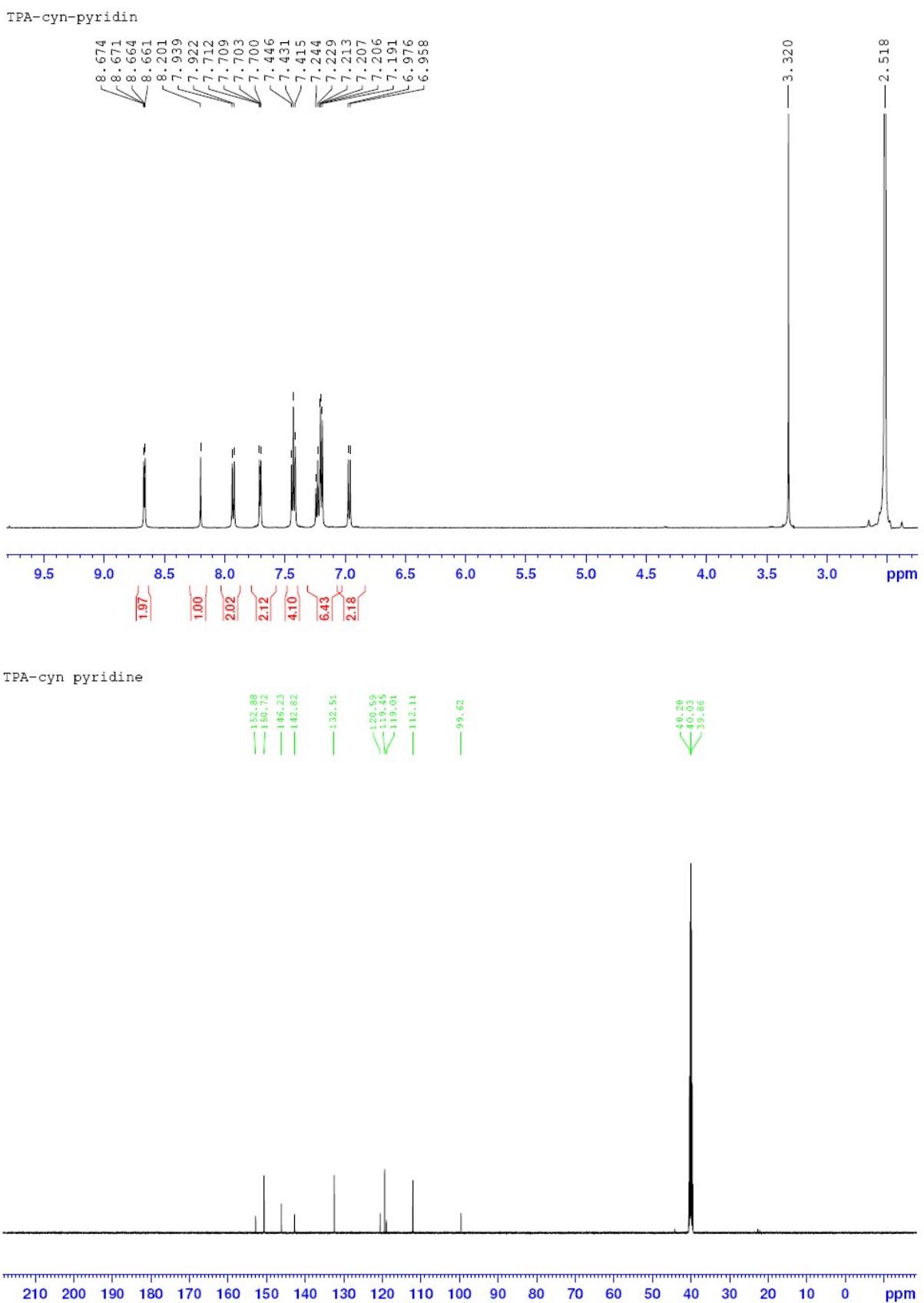


Fig. S14  $^1\text{H}$ -NMR &  $^{13}\text{C}$  spectrum of T-1