Supporting information

for

Configuration independent AIE-active supramolecular polymers of cyanostilbene through photo stable host-guest interaction of pillar[5]arene

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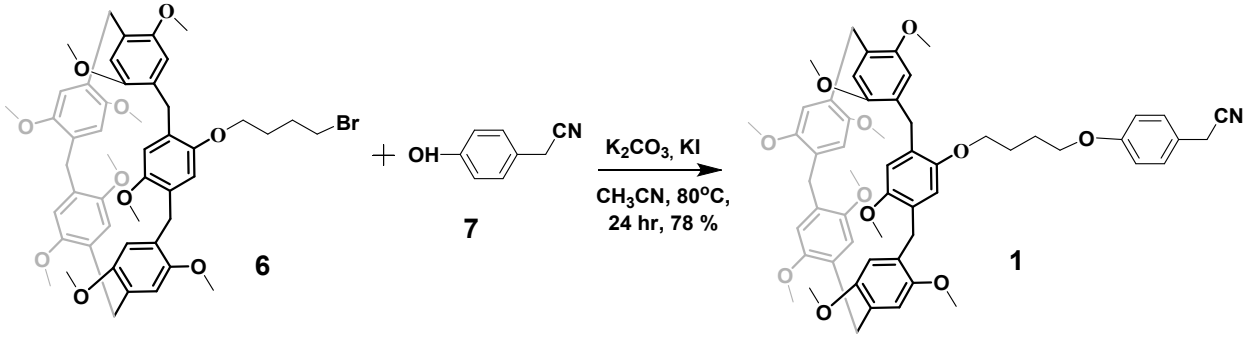
S.I. 1: Synthesis and characterization.

S.I. 1.1: Synthesis and characterization of pillar[5]arene linked phenyl acetonitrile 1.[1]

To the stirred solution of 4-hydroxyphenylacetonitrile, **7** (2.65 mmol., 0.352 g) and K_2CO_3 (3.98 mmol., 0.549 g) in 20 ml acetonitrile under argon, copillar[5]arene, **6** (3.45 mmol, 3 g) and KI (0.4 X 10^{-3} mol., 0.066 g) were added . The reaction mixture was refluxed under argon for 24 hours. After confirming the completion of the reaction by TLC, acetonitrile was removed under vaccum, then reaction mixture was further diluted with DCM and washed with water thrice, The DCM layer was dried with anhydrous $MgSO_4$ and evaporated under vaccum to obtain the crude product, which was further purified by column chromatography to give **1** as white solid, Yeild = 77% (1.883 g).

^{1}H NMR (400 MHz, $CDCl_3$, 298K): 7.18(d, *J* = 8 Hz, 2H, Ar-H), 6.88(d, *J* = 8 Hz, 1H, Ar-H), 6.85(d, *J* = 8 Hz, 2H, Ar-H), 6.78(m, 6.78-6.72, 9H, Ar-H), 4.00(t, *J* = 4 Hz, 2H, OCH_2), 3.90(t, *J* = 4 Hz, 2H, OCH_2), 3.79(m, 3.79-3.77, 10H, CH_2), 3.66(m, 3.66-3.62, 29H, OCH_3 &CH_2CN), 2.01(m, 2.01-1.94, 4H, CH_2).



Scheme S.I.1: Synthesis of Pillar[5]arene linked phenylacetonitrile (**1**).

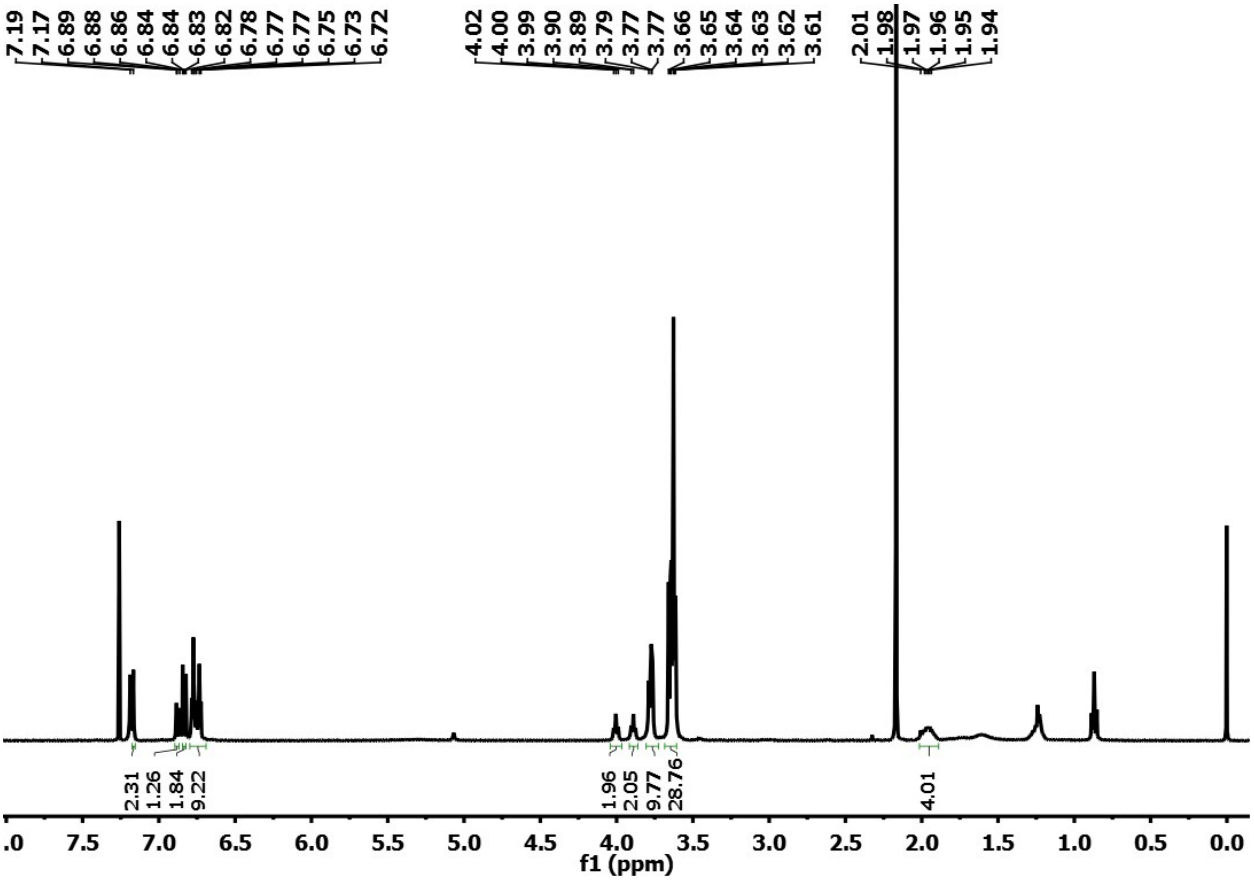
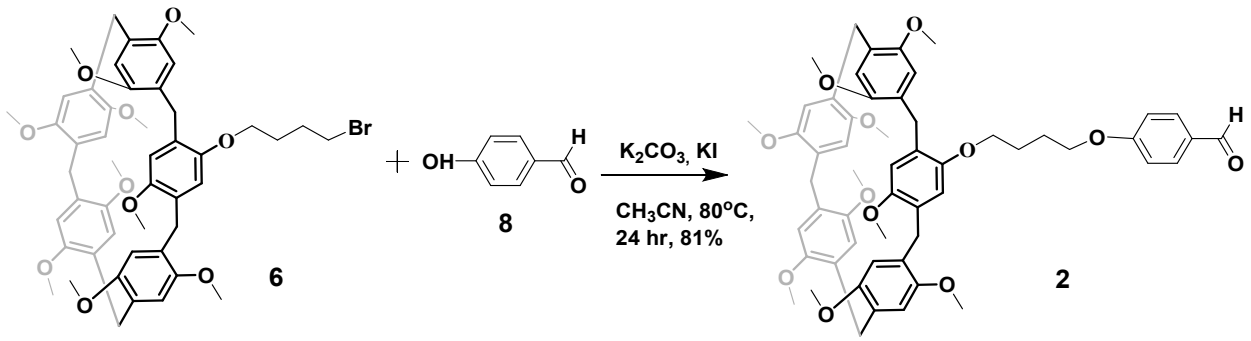


Fig.S.I.1: ^{1}H NMR spectrum of Pillar[5]arene linked phenylacetonitrile (**1**).

S.I. 1.2 : Synthesis and characterization of pillar[5]arene linked benzaldeyde 2.[1]

To the stirred solution of 4-hydroxybenzaldeye, **8** (2.65 mmol, 0.323 g) and K_2CO_3 (3.98 mmol. 0.549 g) in 20 ml acetonitrile under argon copillar[5]arene, **6** (3.45 mmol, 3 g) and KI (0.4 mmol, 0.066 g) was added . The reaction mixture was refluxed under argon for 24 hours. After confirming the completion of the reaction by TLC, acetonitrile was removed under vaccum , the reaction mixture was further diluted with DCM and washed with water thrice, The DCM layer was dried with anhydrous $MgSO_4$ and evaporated under vaccum to obtain the crude product, which was further purified by column chromatography to give **2** as white solid. Yield = 81%(1.957 g). **^{1}H NMR** (400 MHz, $CDCl_3$, 298K): 9.89(1H, s), 7.82(d, *J* = 8 Hz, 2H, Ar-H), 6.95(d, *J* = 8 Hz, 2H, Ar-H), 6.80(m, 6.80-6.73, 10H, Ar-H), 3.99(t, *J* = 4 Hz, 2H, OCH_2), 3.90(t, *J* = 4 Hz, 2H, OCH_2), 3.79(m, 3.79-3.77, 10H, CH_2), 3.66(m, 3.66-3.62, 27H, OCH_3), 1.96(m, 1.96-1.90, 4H, CH_2).



Scheme S.I.2: Synthesis of pillar[5]arene linked benzaldehyde (**2**).

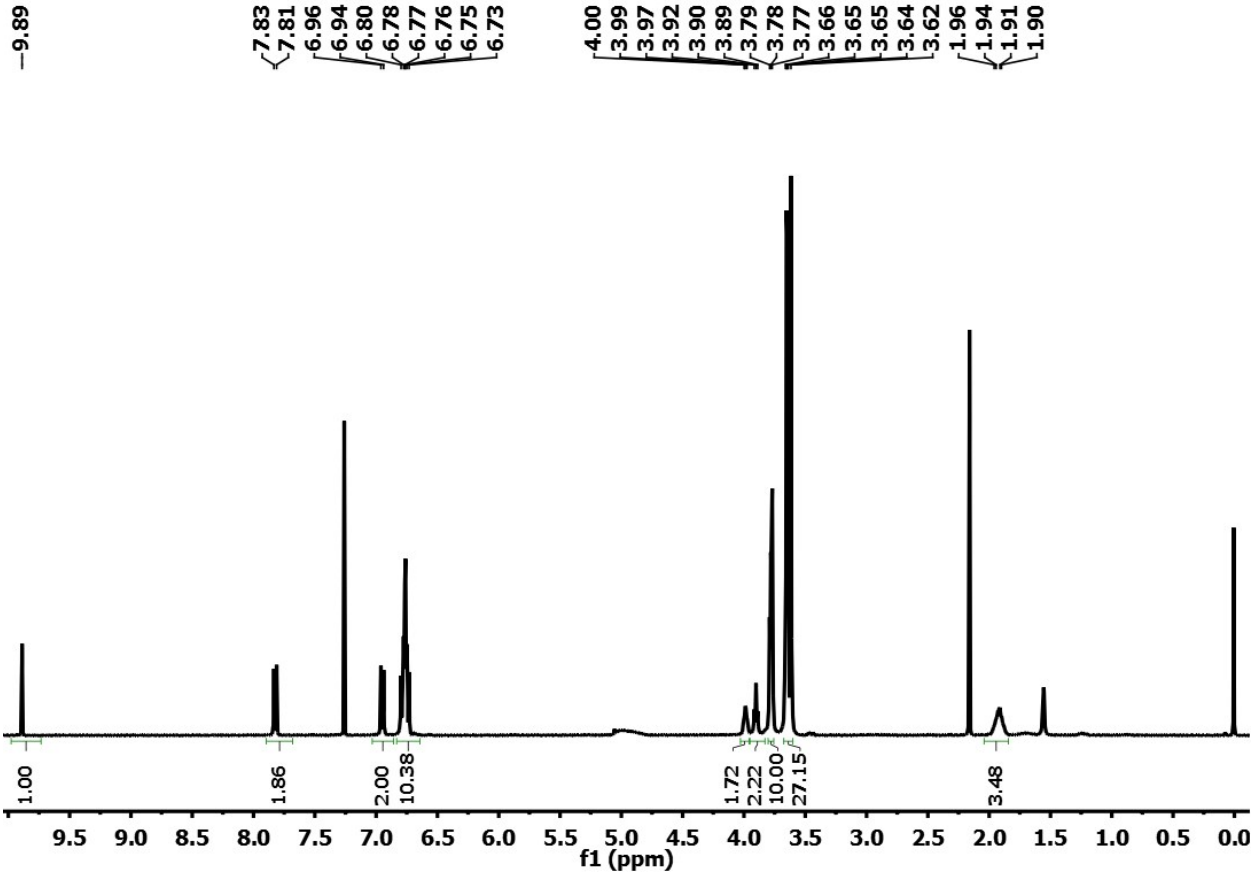


Fig.S.I.2: ^{1}H NMR spectrum of Pillar[5]arene linked benzaldehyde (**2**).

S.I.1.3: Synthesis and characterization of cyanostilbene bridged Pillar[5]arene dimer -(*Z*) CNS(P5)$_2$.

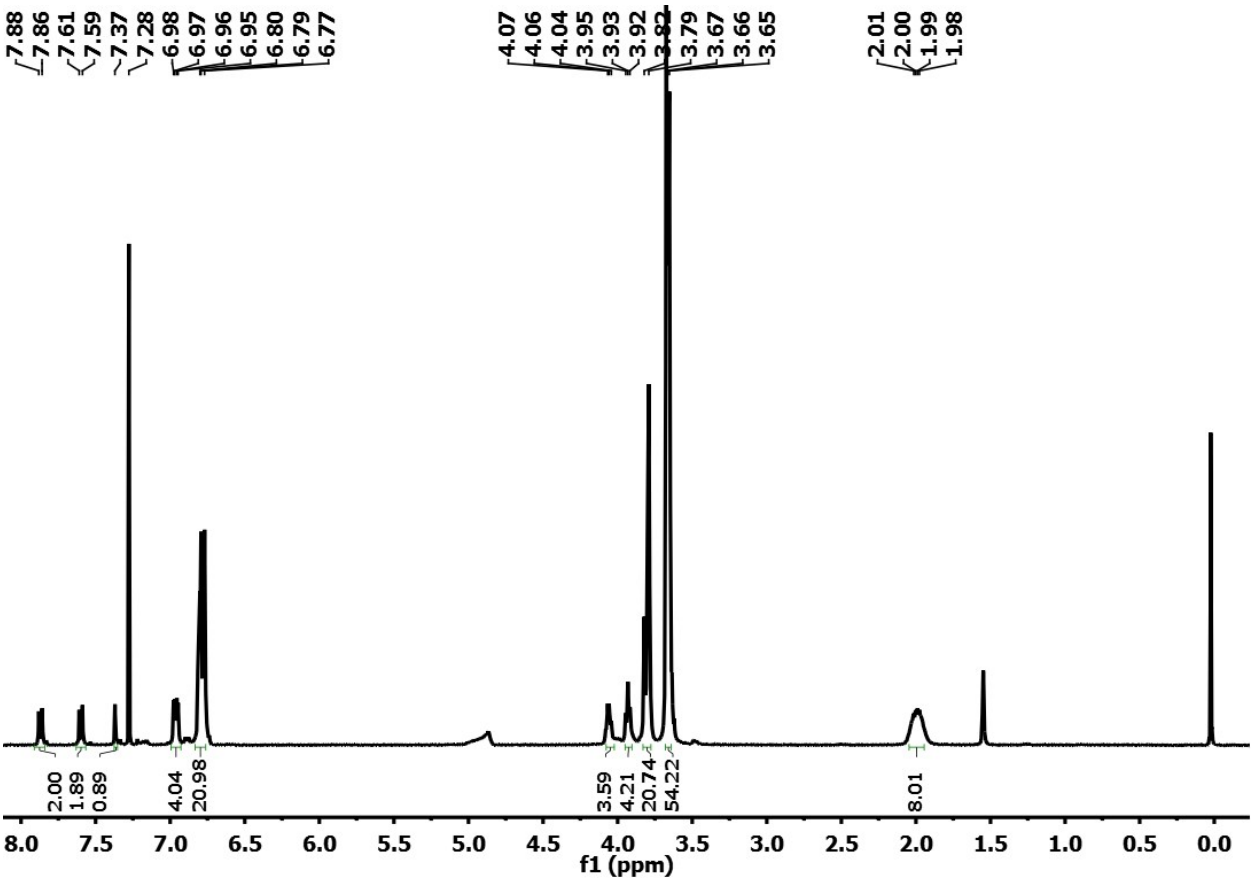


Fig.S.I.3: ^{1}H NMR spectrum of **(*Z*)CNS(P5)$_2$**.

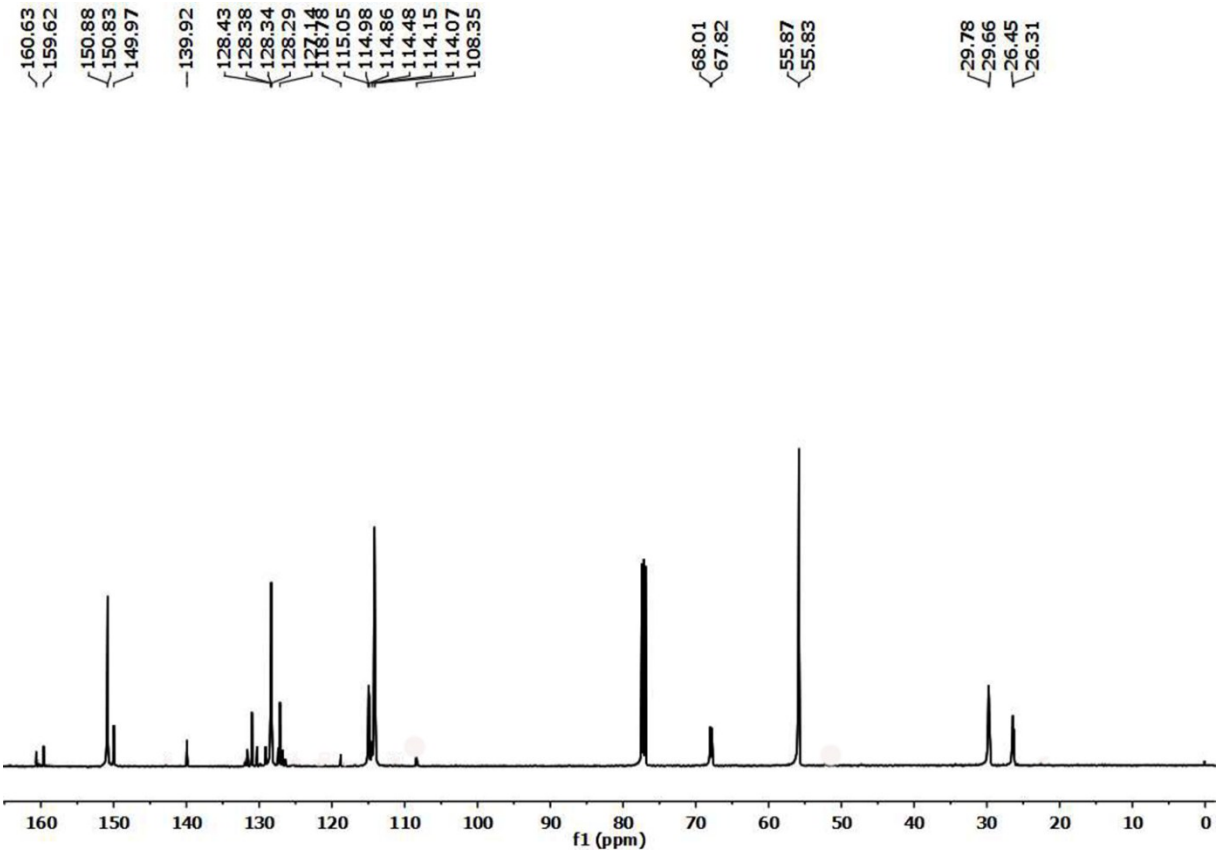


Fig.S.I.4: ^{13}C NMR spectrum of **(*Z*)CNS(P5)$_2$**.

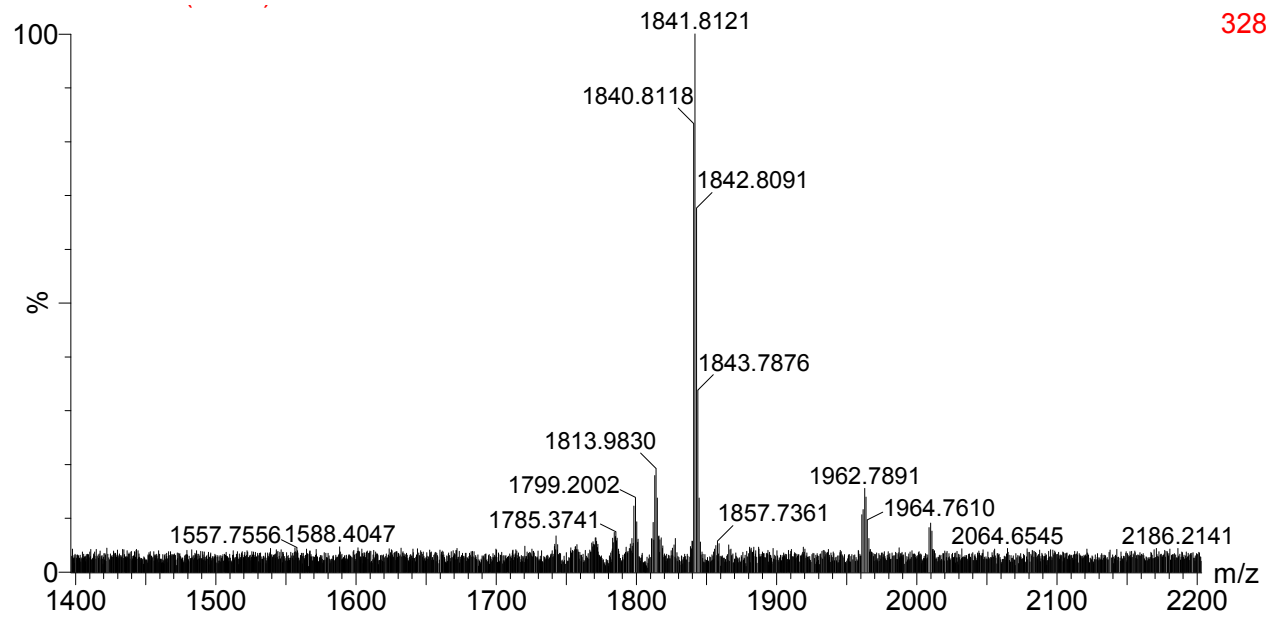


Fig.S.I.5: MALDI-TOF mass spectrum of **(*Z*)CNS(P5)$_2$**.

S.I.1.4: Synthesis and characterization of (*Z*)CNS(MOP)$_2$.

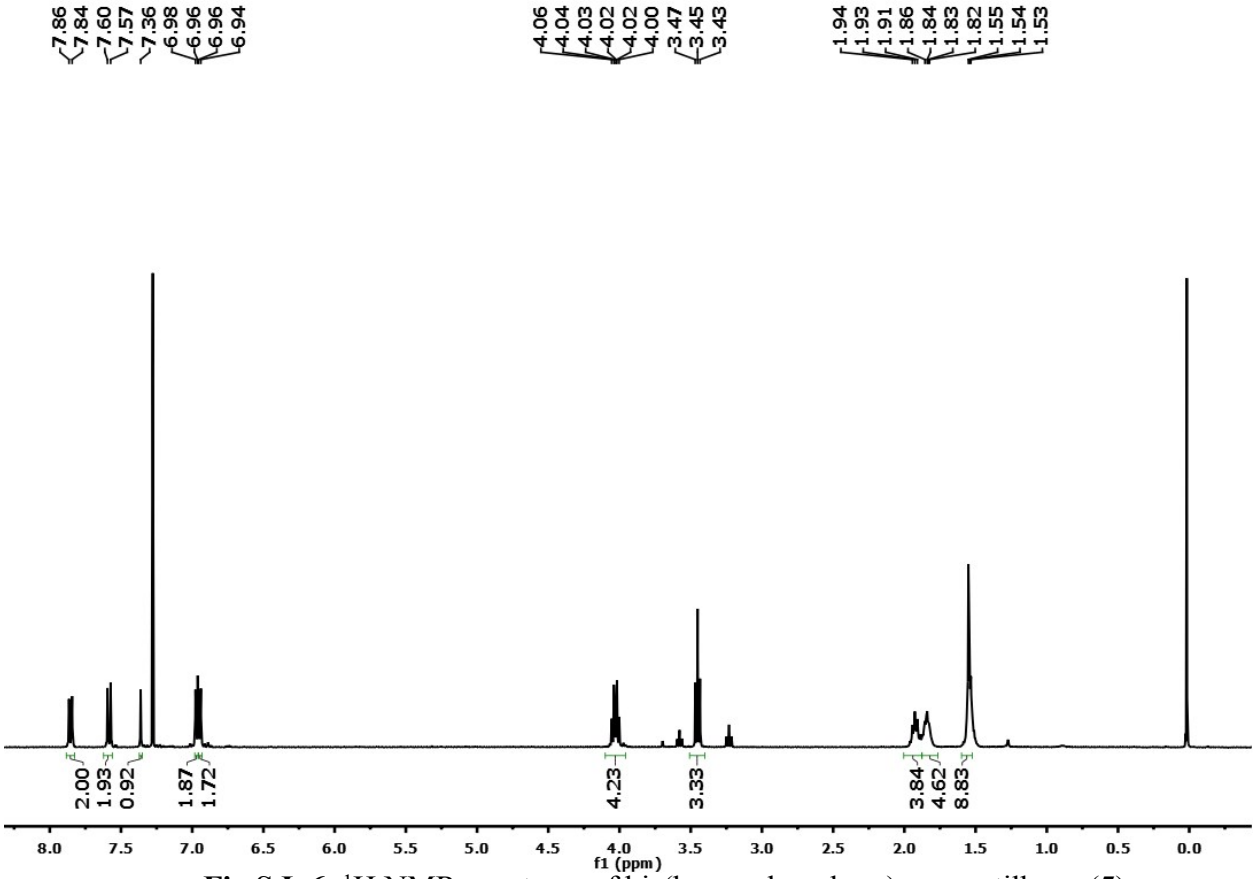


Fig.S.I. 6: ^{1}H NMR spectrum of bis(bromo-hexyloxy) cyanostilbene (**5**).

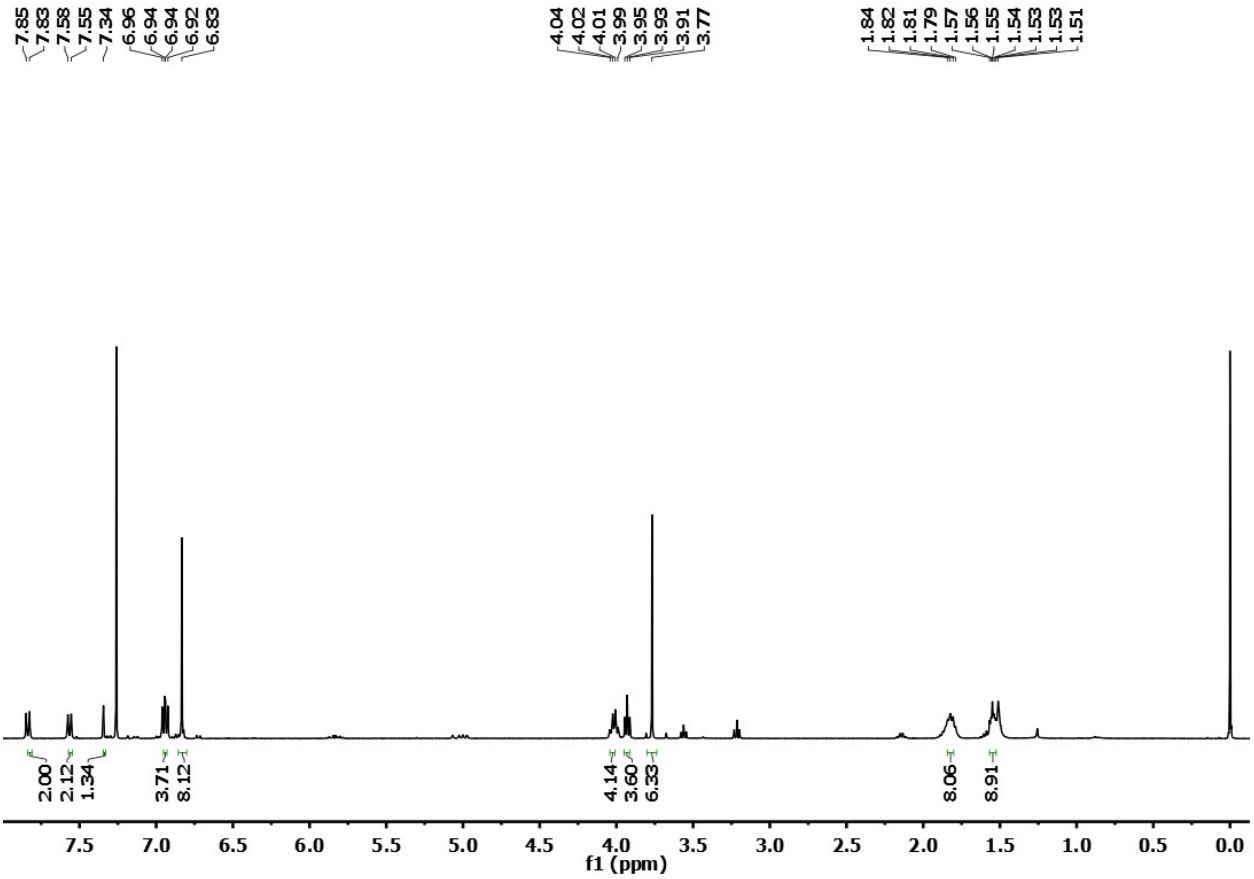


Fig.S.I.7: ^{1}H NMR spectrum of **(*Z*)CNS(MOP)$_2$.**

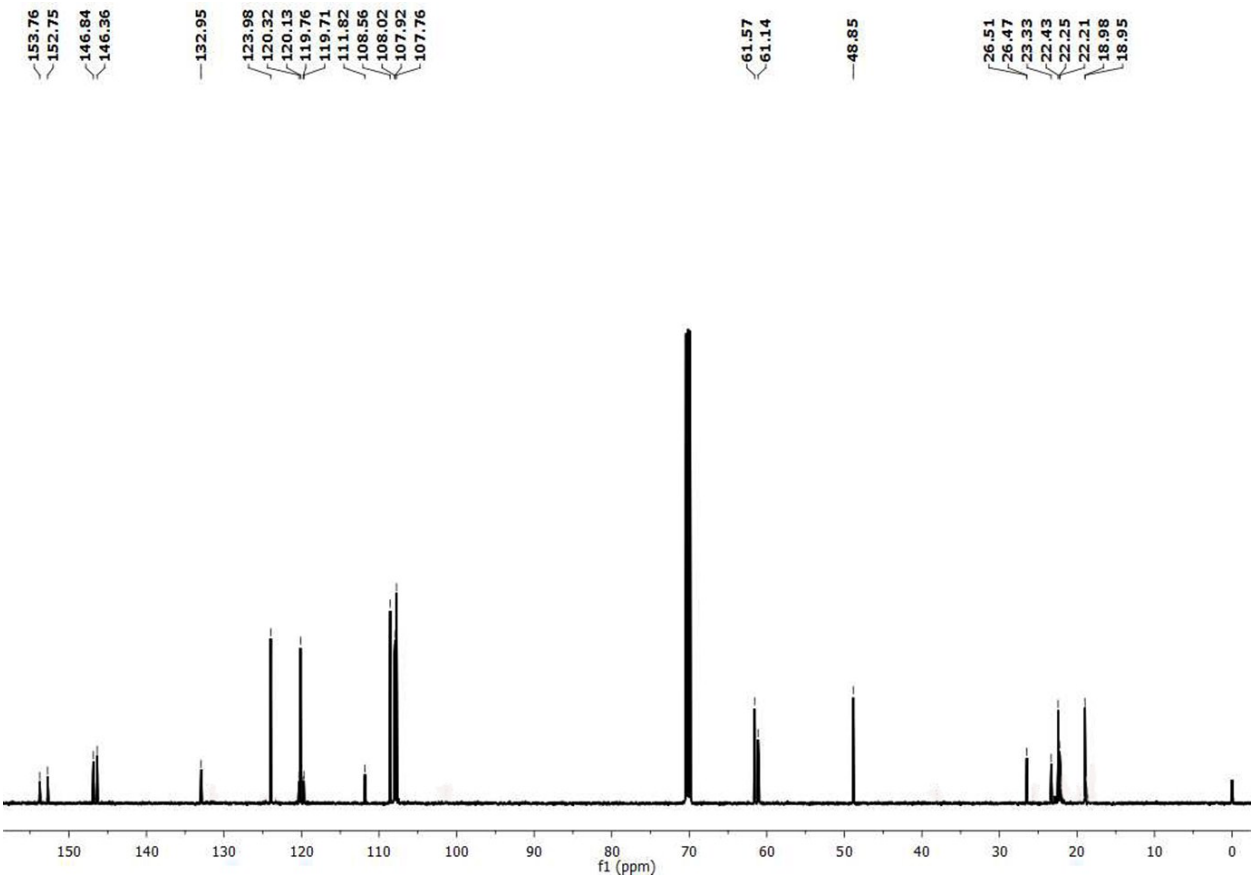
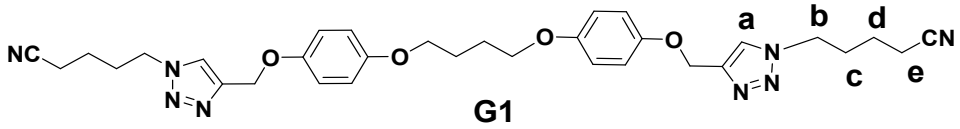


Fig. S.I.8: ^{13}C NMR spectrum of **(*Z*)CNS(MOP)$_2$.**

S.I. 1.5: Synthesis and characterization of guest (G1).

The bis(nitrile triazole) guest G1 was synthesized according to reported literature.[2]



G1

^{1}H NMR (400 MHz, $CDCl_3$, 298K): 7.61(s, 2H, Trz-H), 6.90(d, *J* = 8 Hz, 4H, Ar-H), 6.82(d, *J* = 8 Hz, 4H, Ar-H), 5.16(s, 4H, OCH_2), 4.42(t, J = 8 Hz, 4H, OCH_2), 3.97(t, J = 4 Hz, 4H, OCH_2), 2.39(t, J = 8 Hz, 4H, CH_2), 2.12(m, 2.12-2.05, 4H, CH_2), 1.94(m, 1.94-1.92, 4H, CH_2), 1.71(m, 1.71-1.66, 4H, CH_2).

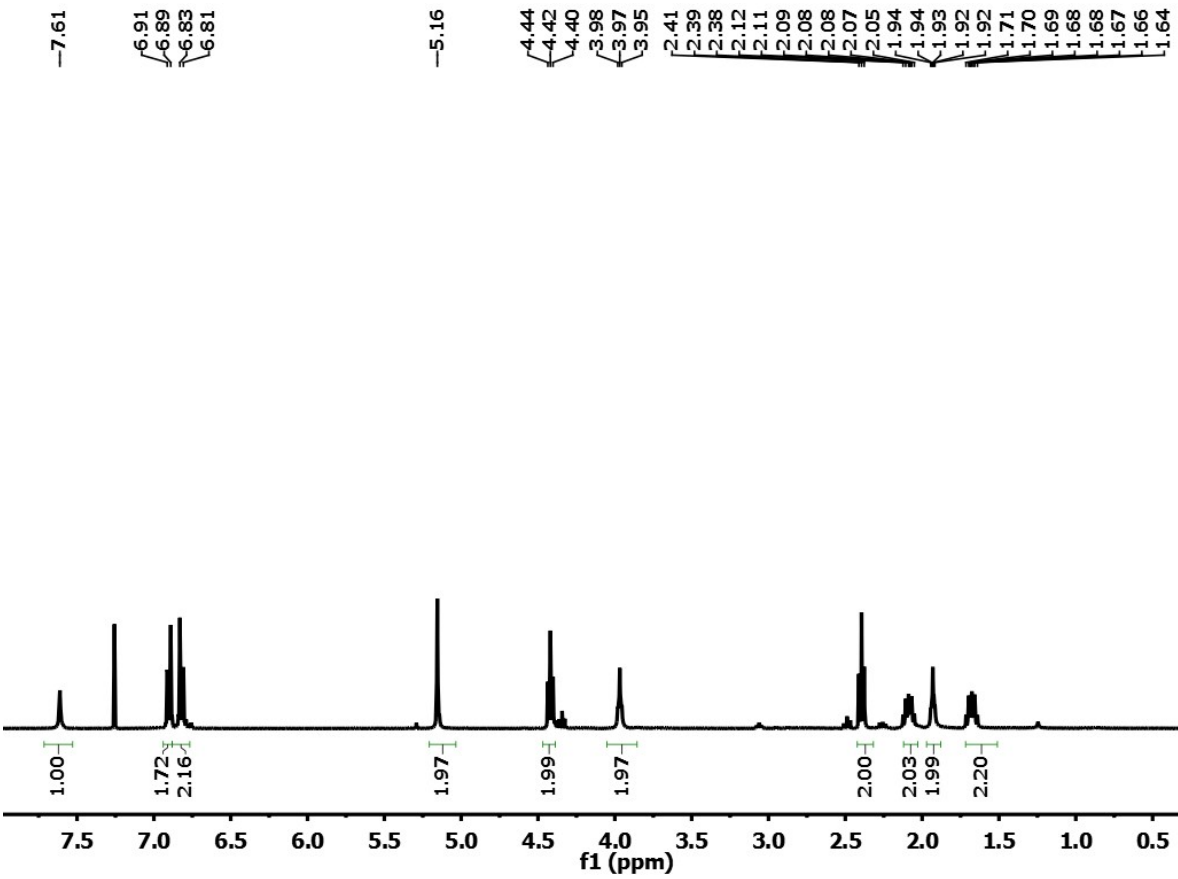


Fig. S.I.9: ^{1}H NMR spectrum of **G1**.

S.I.2: Supramolecular polymerization.

S.I.2.1: Fluorescence studies.

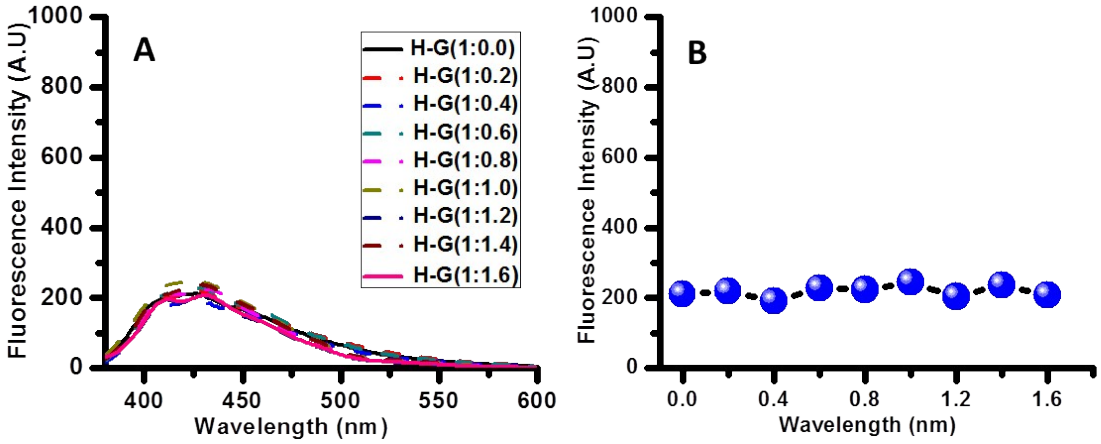


Fig. S.I.10: Fluorescence spectra of A) **(*Z*)G1cCNS(P5)$_2$**, [**(*Z*)CNS(P5)$_2$** = 0.1 mM fixed], Profiles of fluorescence emission intensity changes at λ_{em}=430nm against Guest molar ratio B) **(*Z*)G1cCNS(P5)$_2$**,. Note: λ_{ex}=360 nm, H = **(*Z*)CNS(P5)$_2$**, G= **G1**. Solvent = $CHCl_3$.

S.I.2.2: DLS studies.

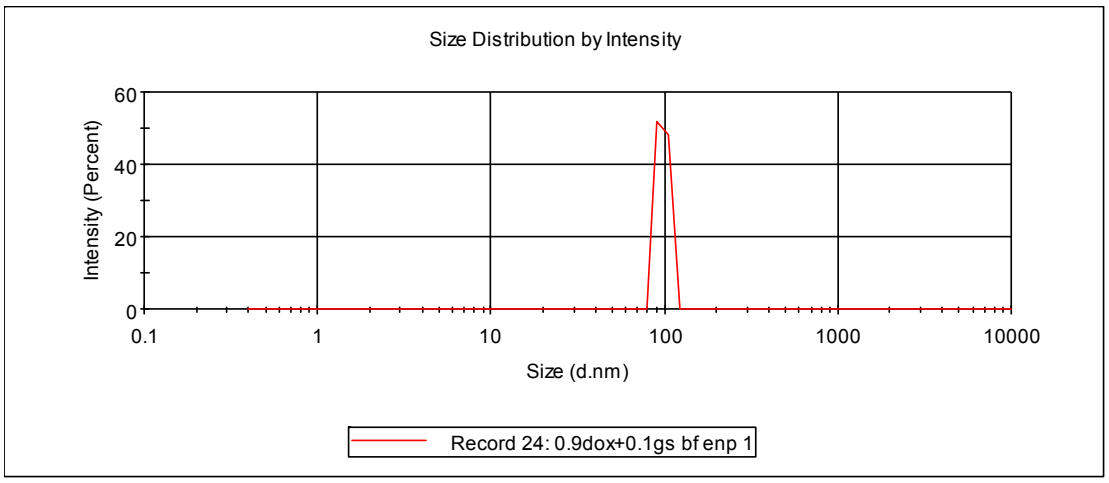


Fig.S.I.11: DLS data for **(*Z*)G1cCNS(P5)$_2$** in THF (25 mM).

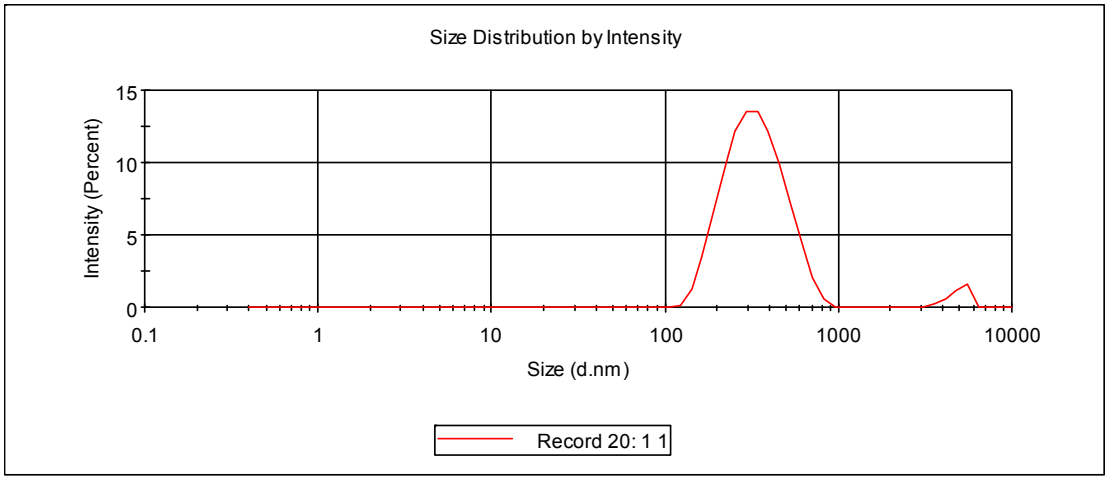


Fig.S.I.12: DLS data for **(*Z*)G1cCNS(P5)$_2$** in $CHCl_3$ (25 m).

S.I.2.1: NMR studies.

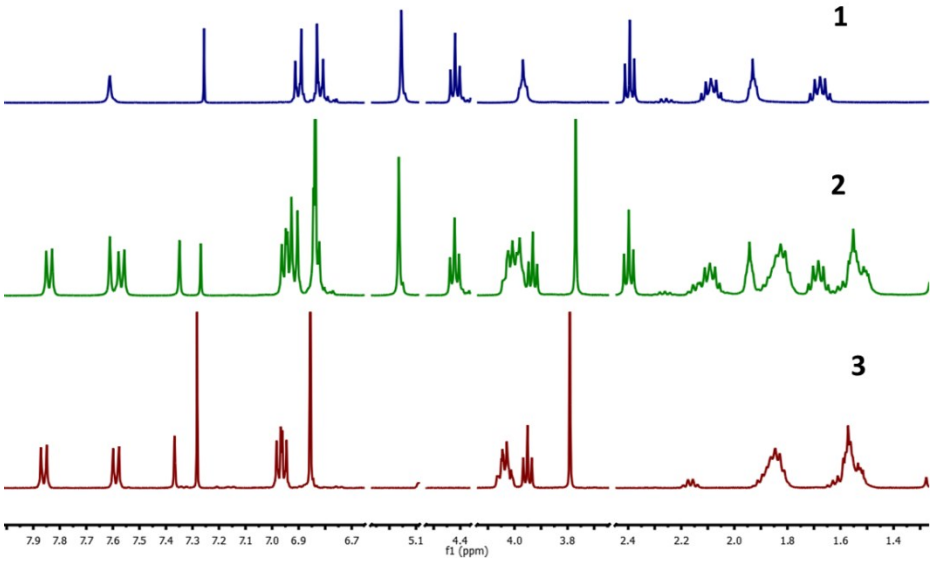


Fig. S.I.13 : Partial ^{1}H NMR(400MHz, $CDCl_3$, 298 K) of of 1) 20 mMole **G1**, 2) 27 mMole **G1** + 30 mmol **(*Z*)CNS(MOP)$_2$**, 3)15 mMole **(*Z*)CNS(MOP)$_2$**.

S.I. 3: AIE studies.

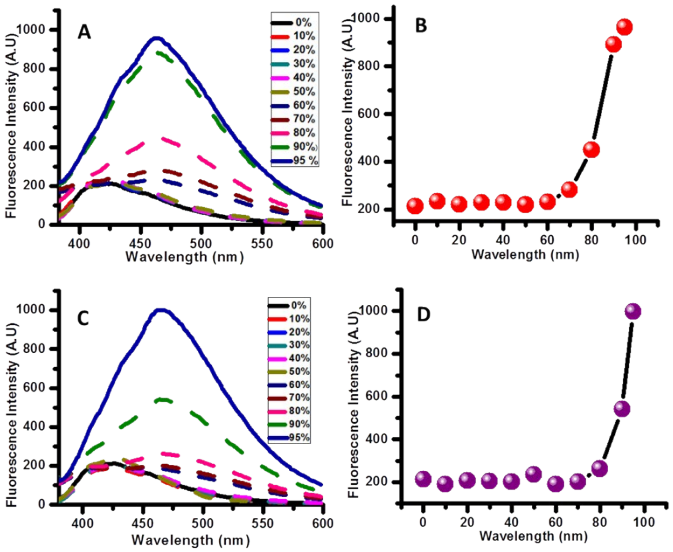


Fig.S.I.14: Fluorescence spectra of A) **(*Z*)CNS(P5)$_2$, B) (*Z*)G1cCNS(P5)$_2$,** in THF-water mixture with increasing the proportion of water from 0-95%. Profiles of fluorescence emission intensity changes at λ_{em} = 430 nm against water proportion C) **(*Z*)CNS(MOP)$_2$,** D) **(*Z*)G1cCNS(MOP)$_2$.** Note: λ_{ex}= 360 nm.

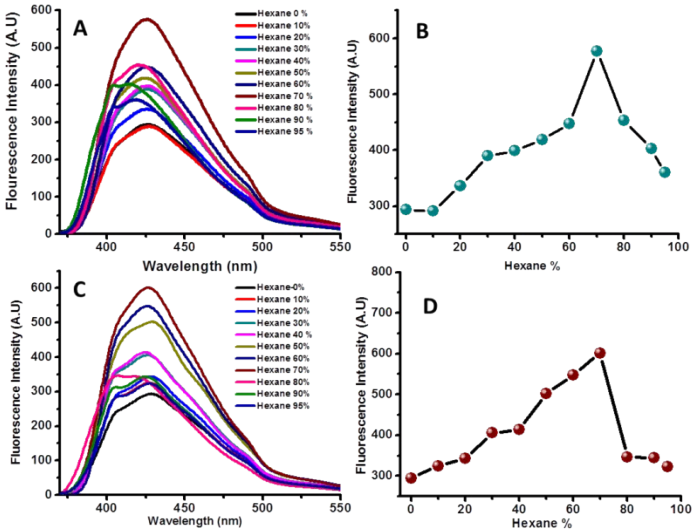


Fig.S.I.15: Fluorescence spectra of A) **(*Z*)CNS(MOP)$_2$, B) (*Z*)G1cCNS(MOP)$_2$,** in $CHCl_3$-Hexane mixture with increasing the proportion of hexane from 0-95%. Profiles of fluorescence emission intensity changes at λ_{em} = 430 nm against hexane propotion, C) **(*Z*)CNS(MOP)$_2$,** D) **(*Z*)G1cCNS(MOP)$_2$.** Note: λ_{ex}= 360 nm.

S.I. 4: Photoresponsive studies.

S.I.4.1. NMR studies.

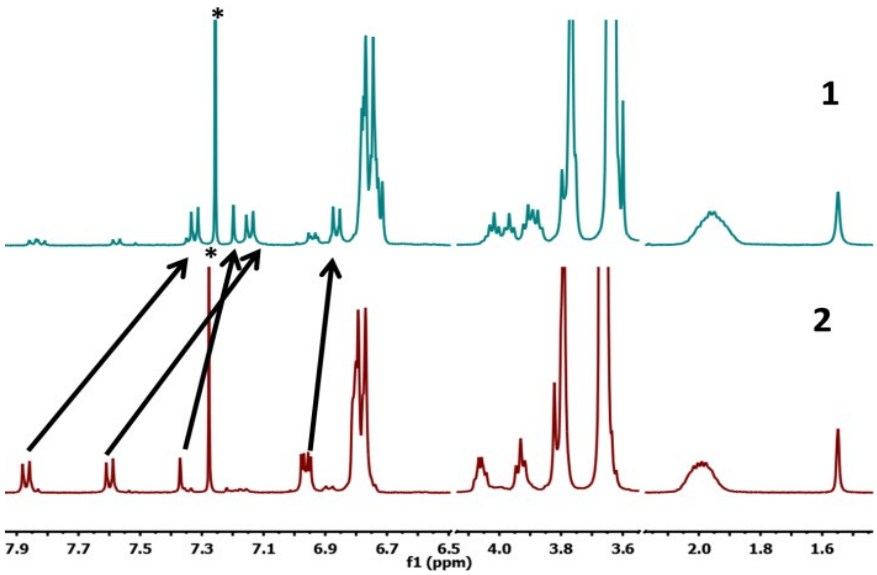


Fig. S.I.16: ^{1}H NMR(400MHz, CDCl3, 298 K) 10 mMol of **(*Z*)CNS(P5)** 1)Before irradiation, 2)After irradiation of UV 365 nm for 2 hrs. *Solvent peak

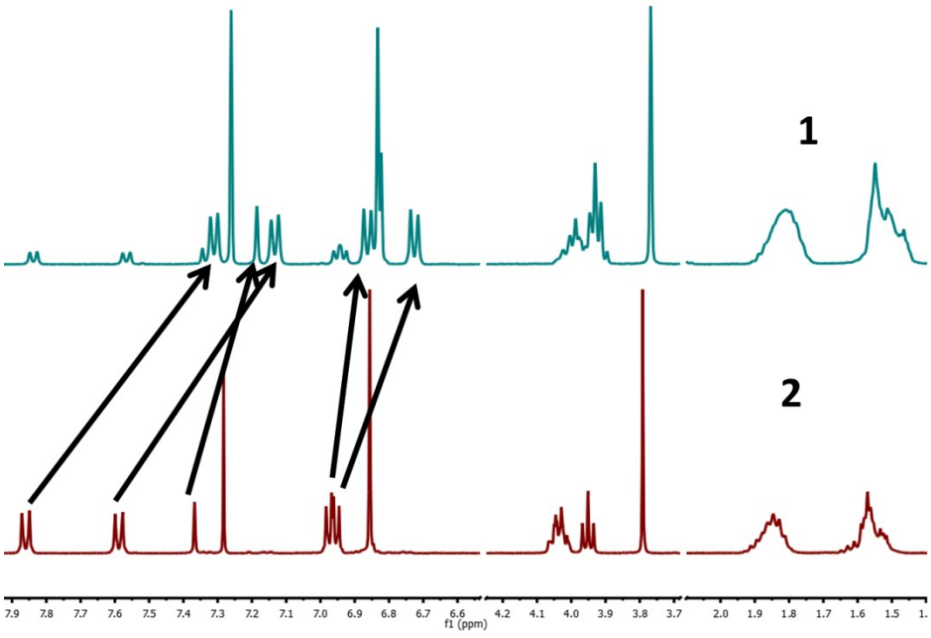


Fig. S.I.17: ^{1}H NMR(400MHz, $CDCl_3$, 298 K) 15 mMol. of **(*Z*)CNS(MOP)$_2$**1)Before irradiation, 2)After irradiation of UV (365 nm) for 2 hrs. ***Solvent peak.**

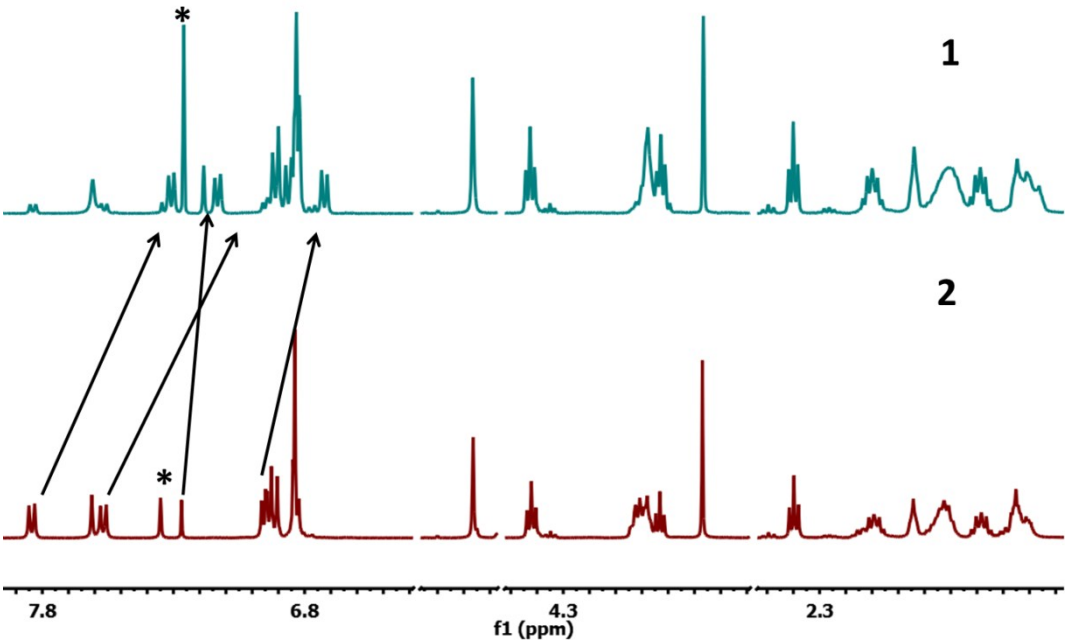


Fig.S.I.18:[1]H NMR(400MHz, $CDCl_3$, 298 K) of **(*Z*)G1cCNS(MOP)$_2$**1) 20 mmol., Before irradiation, 2) 10 mmol., After irradiation of UV (365 nm) for 2 hrs. ***Solvent peak.**

S.I. 4.2: Fluorescence studies.

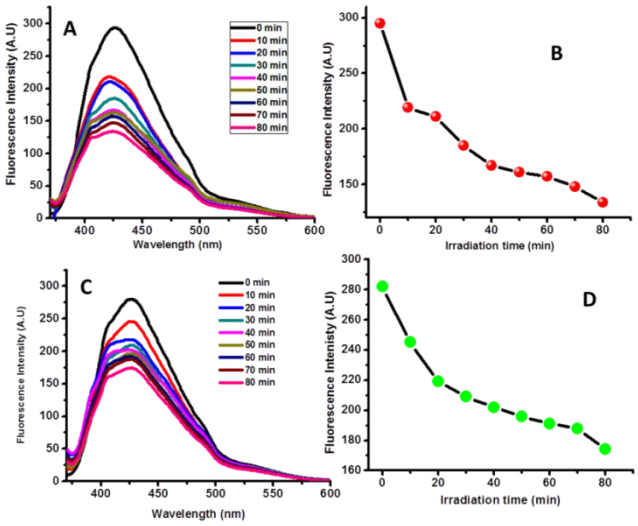


Fig.S.I.19: Fluorescence spectra of A) **(*Z*)CNS(MOP)$_2$, C) (*Z*)G1cCNS(MOP)$_2$,** upon irradiation with UV light (365 nm) in $CHCl_3$. Profiles of fluorescence emission intensity changes at λ_{em} = 430 nm against irradiation time in min B) **(*Z*)CNS(MOP)$_2$** and D) **(*Z*)G1cCNS(MOP)$_2$.** Note: λ_{ex}=360 nm.

S.I. 4.3: AIE studies.

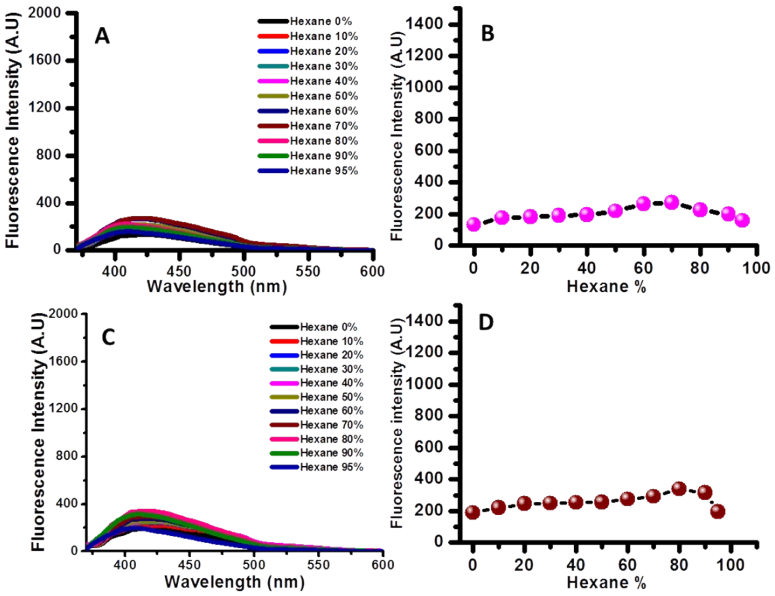


Fig.S.I.20: Fluorescence spectra of UV irradiated **A) (*E*)CNS(MOP)$_2$, C) (*E*)G1cCNS(MOP)$_2$,** in $CHCl_3$-Hexane mixture with increasing the proportion of hexane from 0-95%. Profiles of fluorescence emission intensity changes at λ_{em} = 430 nm against hexane propotion B) **(*E*)CNS(MOP)$_2$** and D) **(*E*)G1cCNS(MOP)$_2$.** Note: λ_{ex}=360 nm.

S.I. 5: Time-resolved fluorescence decay of (*Z*)CNS(P5)$_2$ and (*Z*)G1CCNS(P5)$_2$.

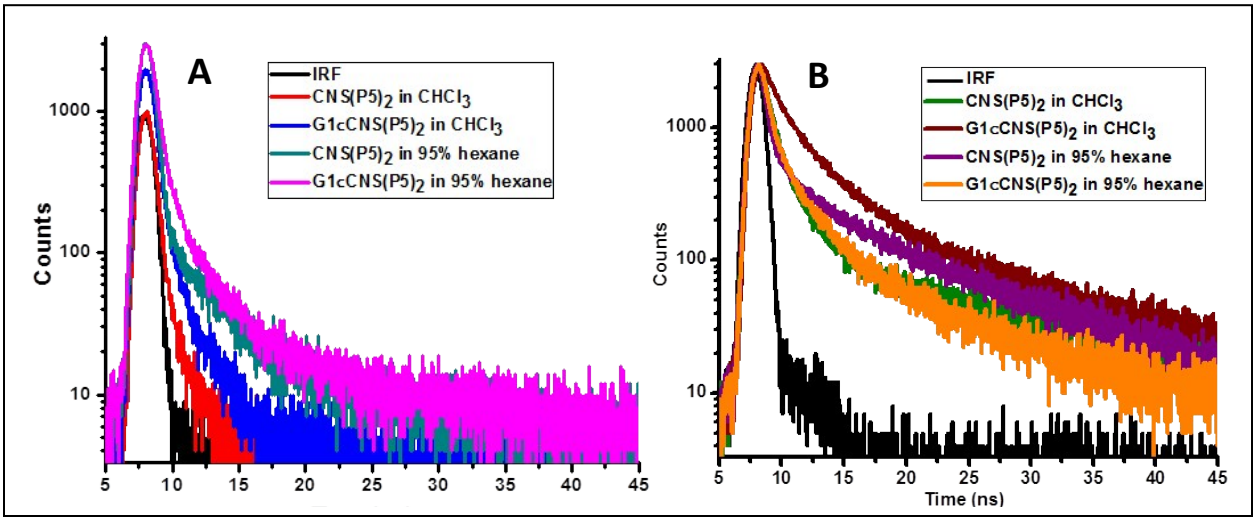


Fig. S.I. 21: Fluorescence decay of **(*Z*)CNS(P5)$_2$** and **(*Z*)G1cCNS(P5)$_2$A**) before irradiation, B) after UV irradiation.

S.No	Sample	Fluorescence Life Time (ns)
1	**Host**	**0.2066**
2	**Host-Guest**	**0.28**
3	**Host in 95% hexane**	**0.8536**
4	**Host-Guest in 95% hexane**	**0.9123**
5	**Host**	**4.7656**
6	**Host-Guest**	**5.8756**
7	**Host in 95% hexane**	**5.22**
9	**Host-Guest in 95% hexane**	**2.744**

S.I. 6: Reference:

1. M. M. Abadía, B. R. Hernández, B. Villacampa, M. R. de la Fuente, R. Giménez and M. B. Ros, *J. Mater. Chem. C*, 2015, **3**, 3038.
2. Y. Zhou, K. Jie, B. Shi and Y. Yao, *Chem. Commun*., 2015, **51**, 11112.