

ESI Supporting Information:

Photophysical Insights on Fullerene-Porphyrazine Supramolecular Interaction In Solution

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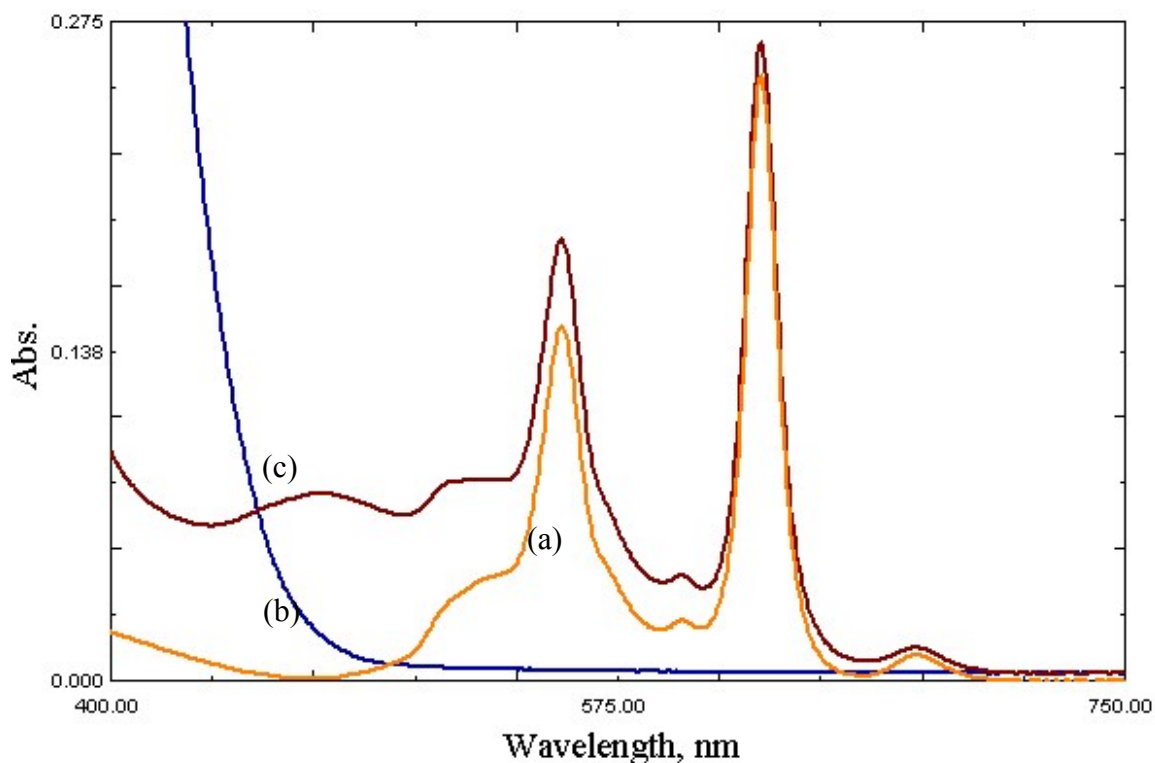


Fig. S1. UV-vis spectral variation of (a) **1** (3.45×10^{-6} M) in DCB recorded against the solvent as reference, (b) *p*-chloranil (1.25×10^{-3} M) in DCB recorded against the solvent as reference and (c) **1** (3.45×10^{-6} M) + *p*-chloranil (1.25×10^{-3} M) in DCB recorded against the pristine acceptor solution in reference; Temp. 298K.

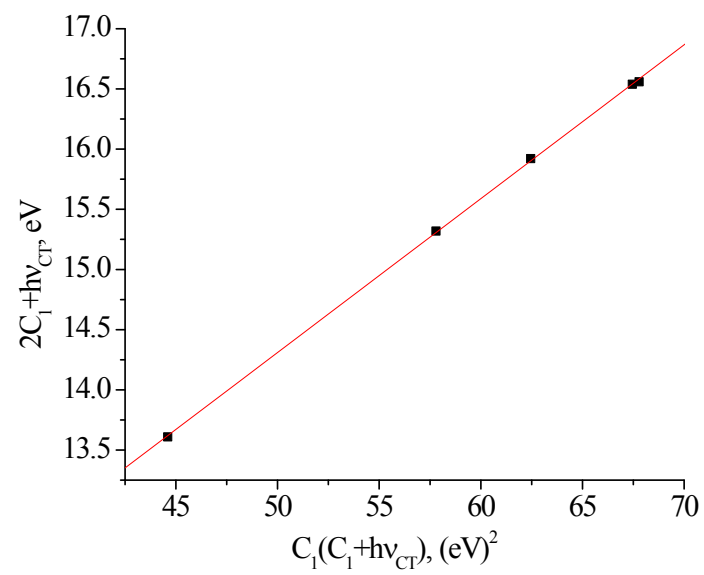
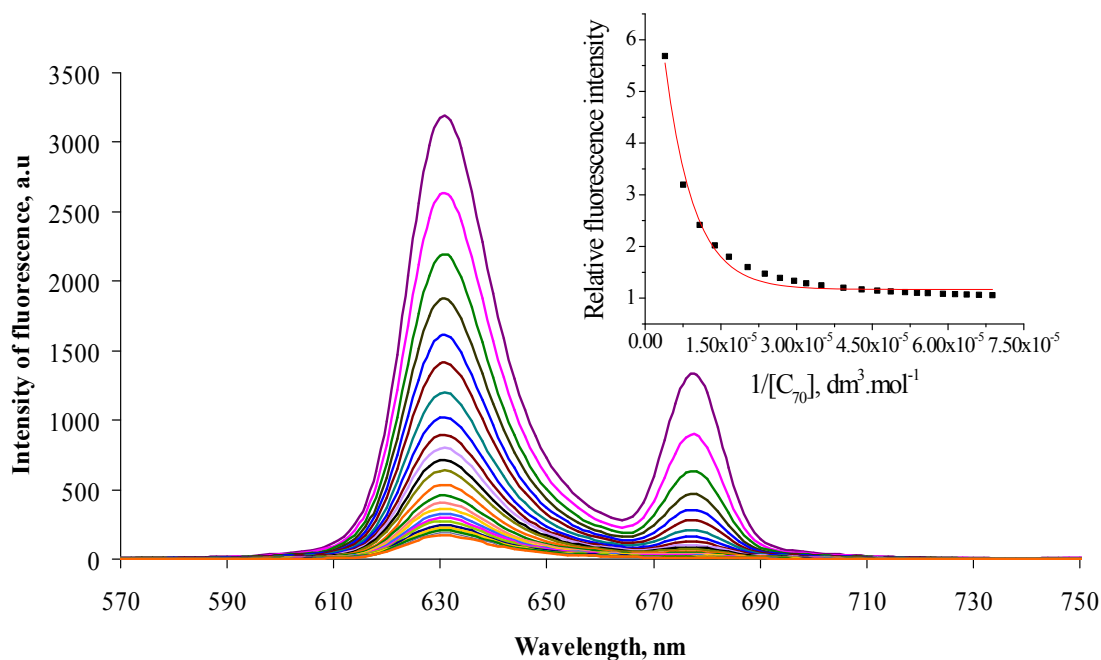
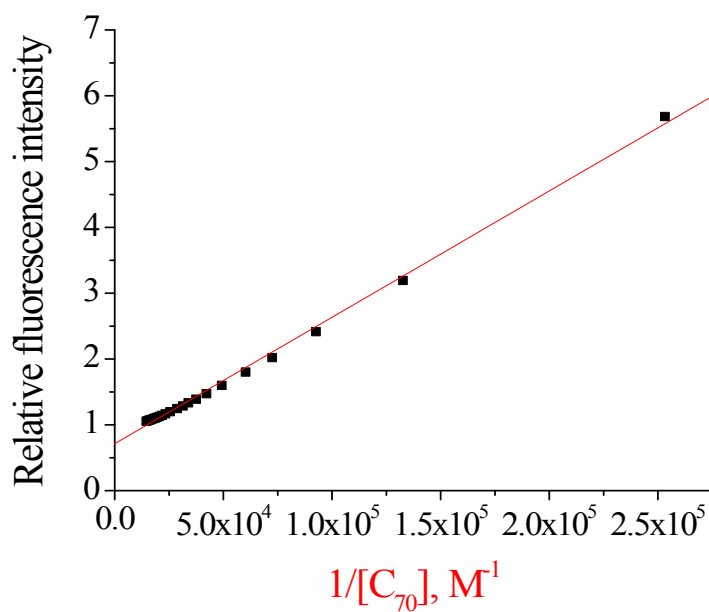


Fig. S2. Determination of I_D^v of **1**.

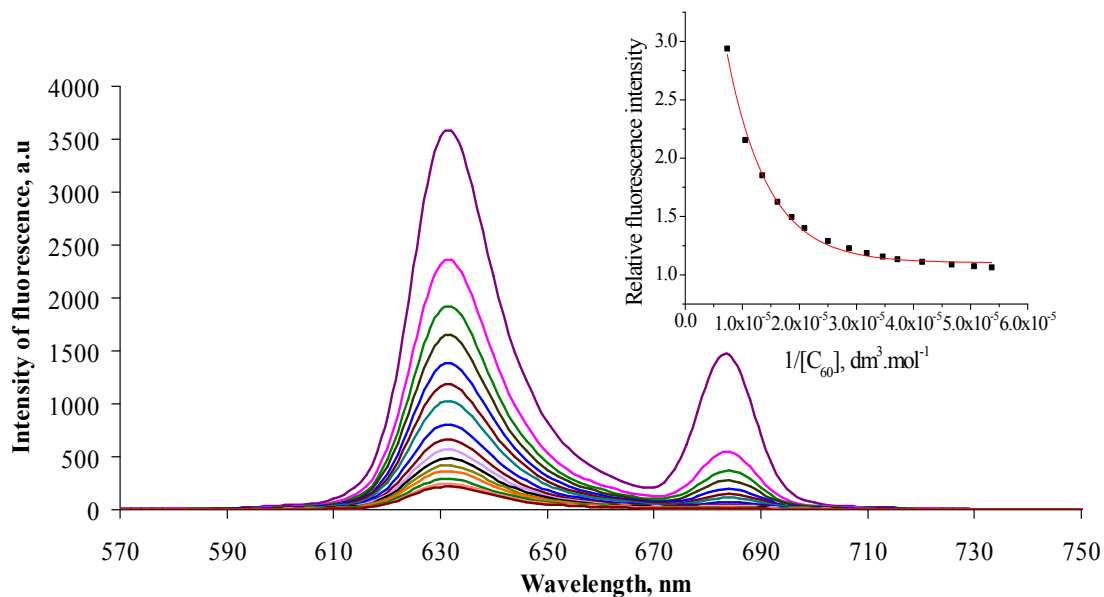


(a)

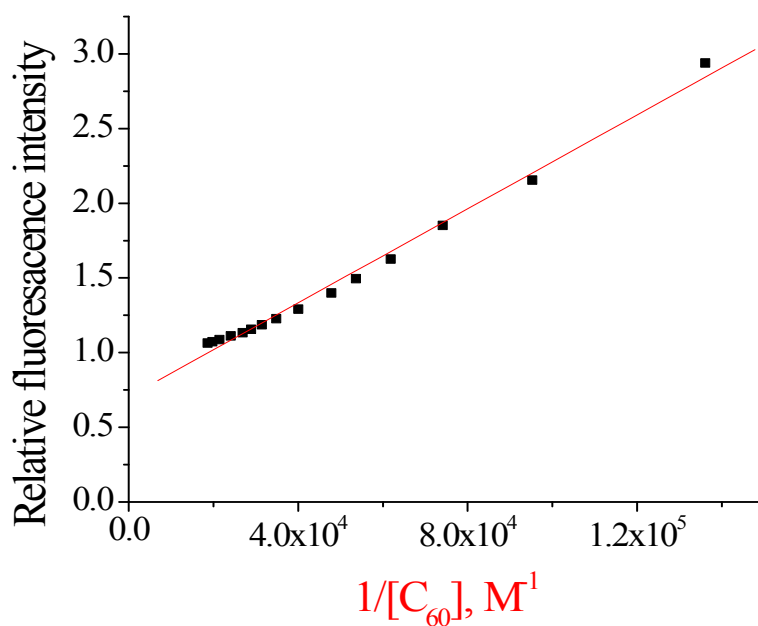


(b)

Fig. S3. (a) Steady state fluorescence spectral variation of **1** (2.60×10^{-6} M) in presence of C_{70} (3.95×10^{-6} to 6.90×10^{-5} M) recorded in toluene at 298K; the inset of **Fig. S3** indicates fluorescence induced curve for the same system. (b) Fluorescence BH plot for C_{70} -**1** system in toluene. $\lambda_{ex} = 337$ nm; $\lambda_{em} = 630$ nm.

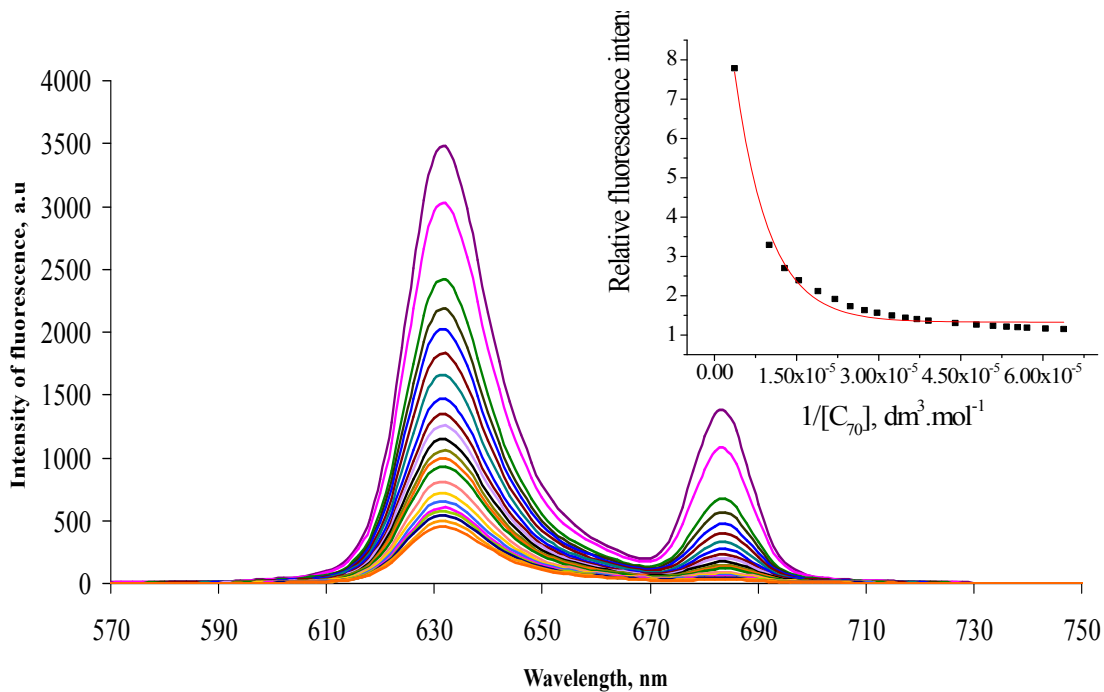


(a)

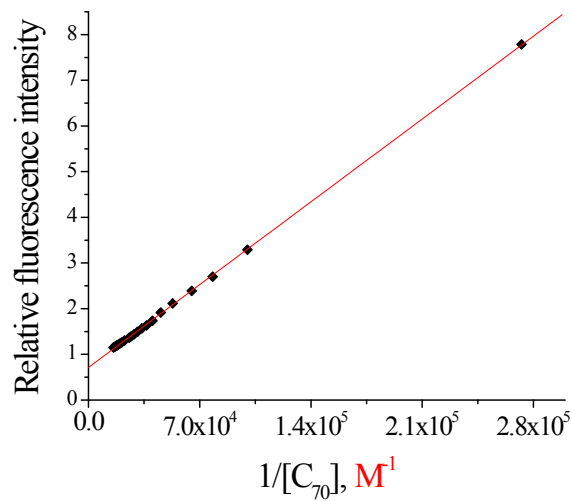


(b)

Fig. S4. (a) Steady state fluorescence spectral variation of **1** (2.70×10^{-6} M) in presence of C_{60} (7.35×10^{-6} to 5.40×10^{-5} M) recorded in DCB at 298K; the inset of **Fig. S4** indicates fluorescence induced curve for $C_{60}/\mathbf{1}$ system. (b) Fluorescence BH plot for C_{60} -**1** system in DCB. $\lambda_{\text{ex}} = 340$ nm; $\lambda_{\text{em}} = 632$ nm.



(a)



(b)

Fig. S5. (a) Steady state fluorescence spectral variation of **1** (2.70×10^{-6} M) in presence of C_{70} (3.65×10^{-6} to 6.40×10^{-5} M) recorded in DCB at 298K; the inset of **Fig. S5** indicates fluorescence induced curve for C_{70} -**1** system. (b) Fluorescence BH plot for C_{70} -**1** system in DCB. $\lambda_{\text{ex}} = 340$ nm; $\lambda_{\text{em}} = 632$ nm.

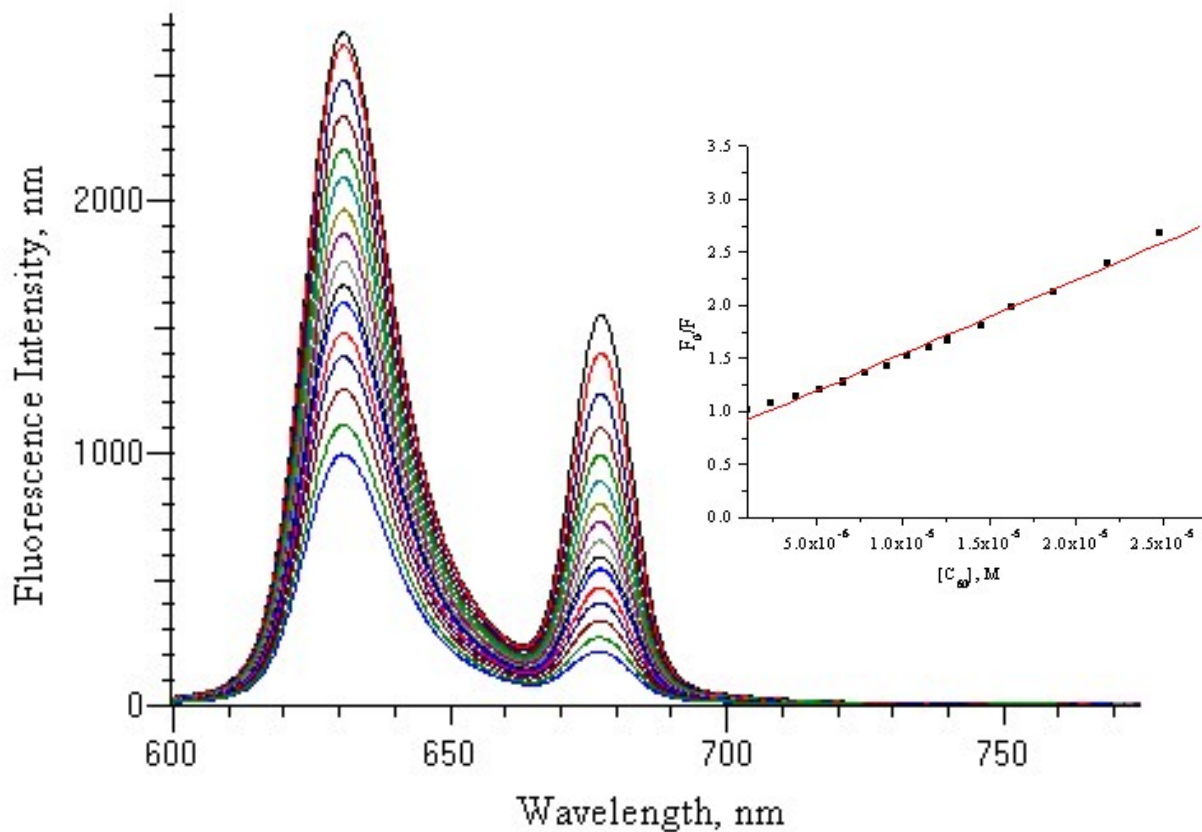


Fig. S6. Steady state fluorescence spectral variation of **1** (2.6×10^{-6} M) in presence of C₆₀ (1.0×10^{-6} to 2.5×10^{-5} M) recorded in toluene at 298K; the inset of **Fig. S6** shows SV plot. $\lambda_{\text{ex}} = 337$ nm; $\lambda_{\text{em}} = 630$ nm.

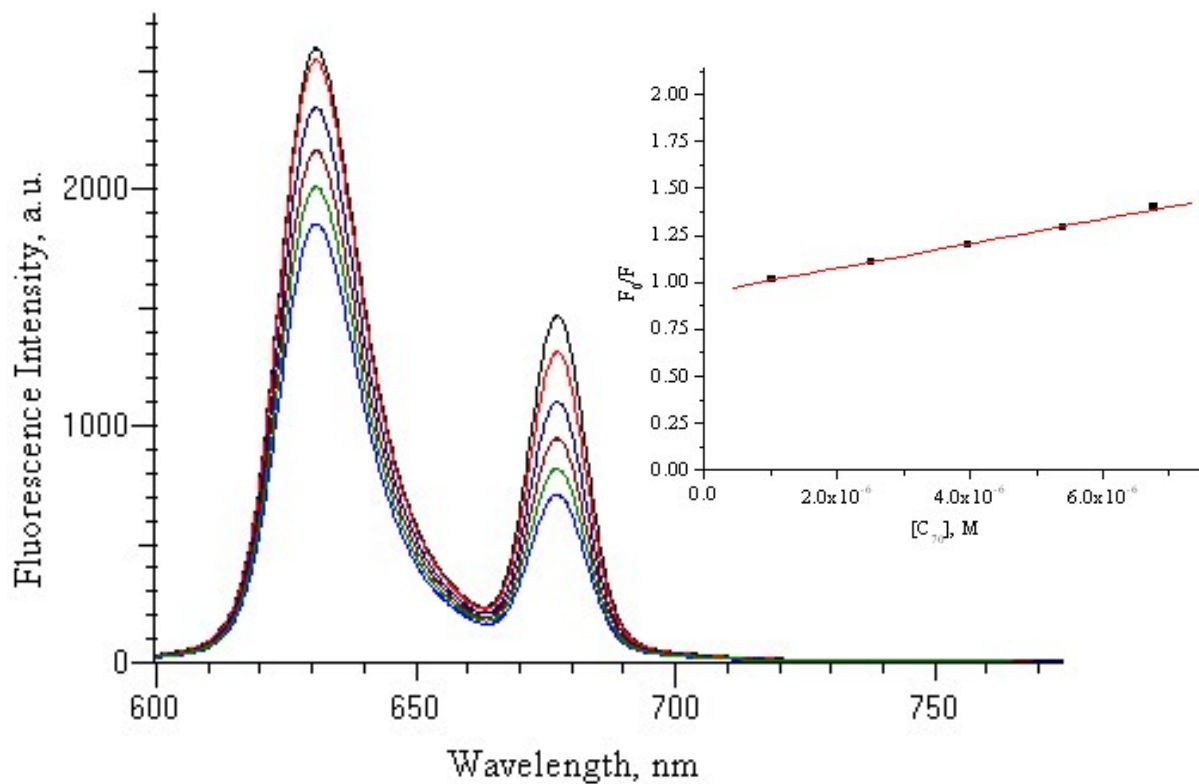


Fig. S7. Steady state fluorescence spectral variation of **1** (2.6×10^{-6} M) in presence of C_{70} (1.0×10^{-6} to 6.80×10^{-6} M) recorded in toluene at 298K; the inset of **Fig. S7** shows SV plot. $\lambda_{\text{ex}} = 337$ nm; $\lambda_{\text{em}} = 630$ nm.

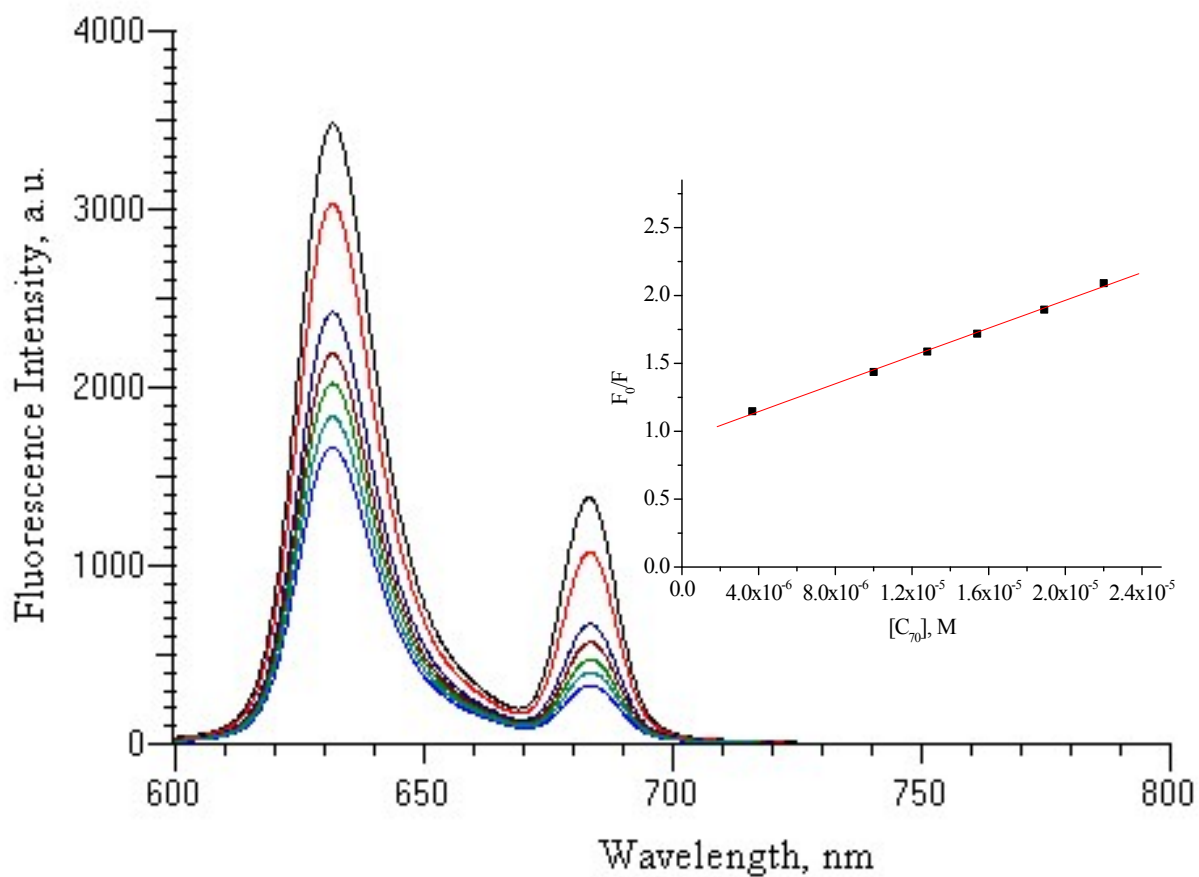


Fig. S8. Steady state fluorescence spectral variation of **1** (2.6×10^{-6} M) in presence of C_{70} (1.0×10^{-6} to 2.2×10^{-5} M) recorded in DCB at 298K; the inset of **Fig. S8** shows SV plot. $\lambda_{ex} = 340$ nm; $\lambda_{em} = 632$ nm.

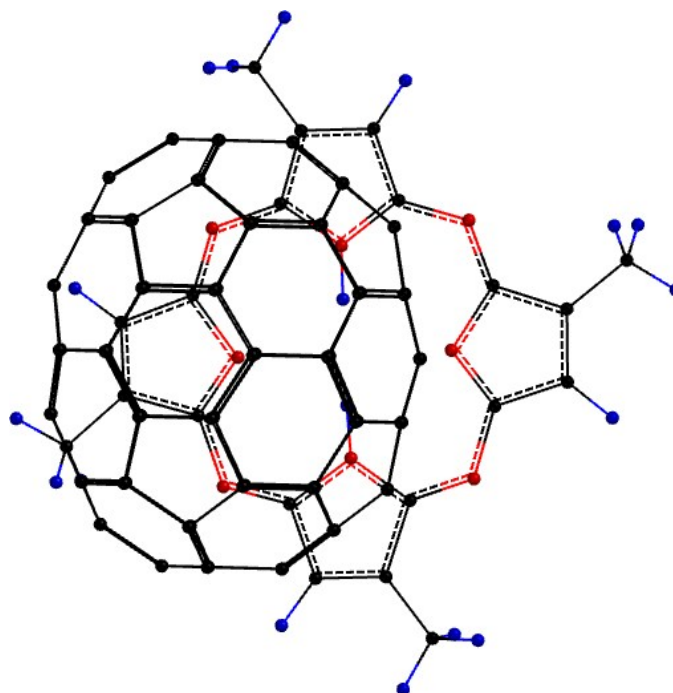


Fig. S9. *Ab initio* optimized geometric structure of C₇₀-1 complex done in *vacuo* at side-on orientation of C₇₀.

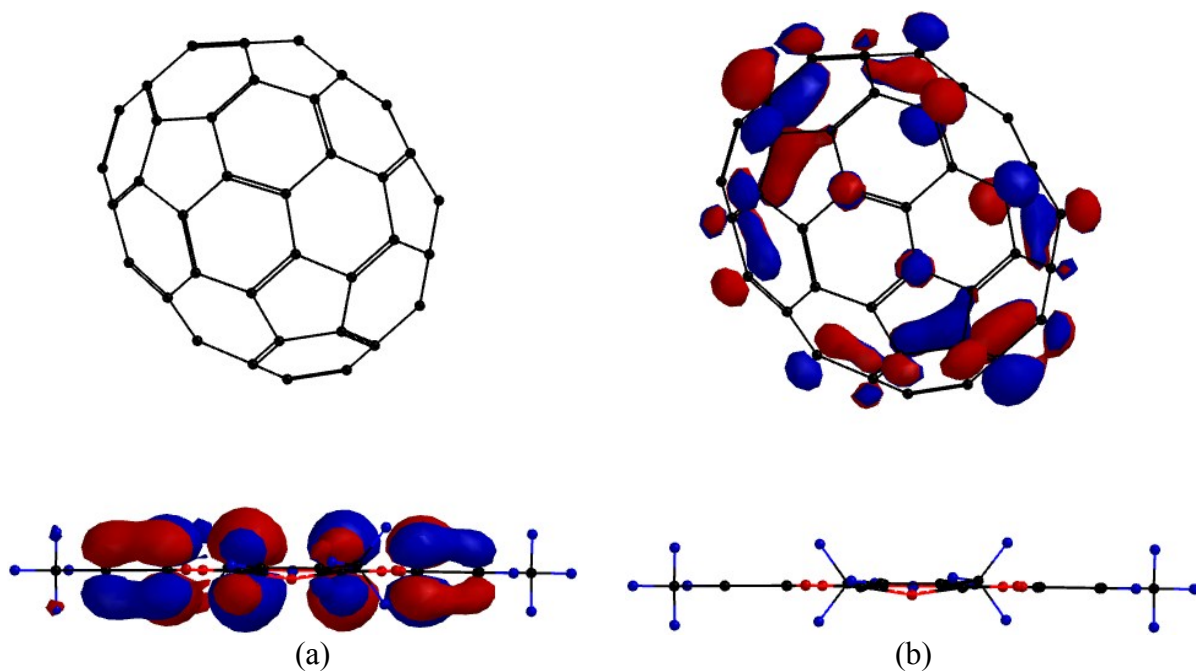


Fig. S10. DFT (B3LYP/6-31G*) calculated frontier (a) HOMO and (b) LUMO for the C₇₀-1 complex done in *vacuo* in end-on orientation of C₇₀. The calculations are done using SPARTAN '14 software.

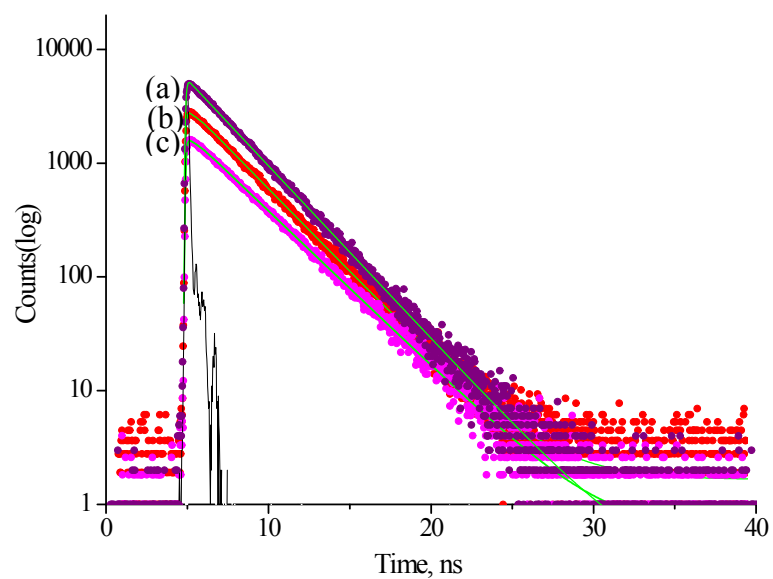
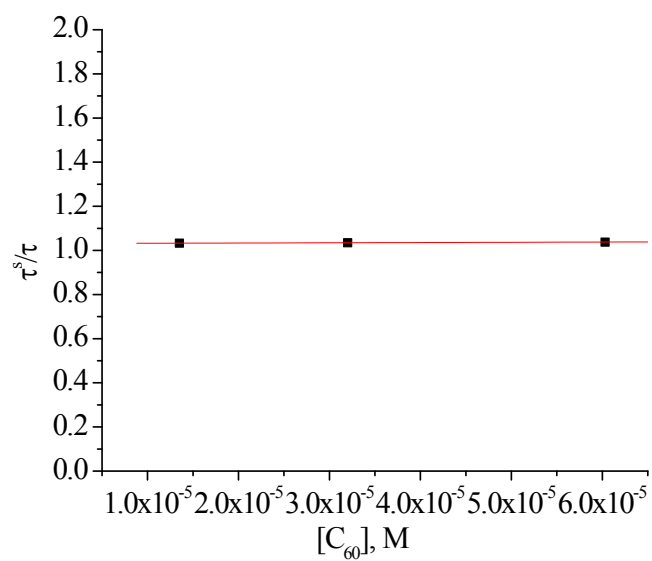
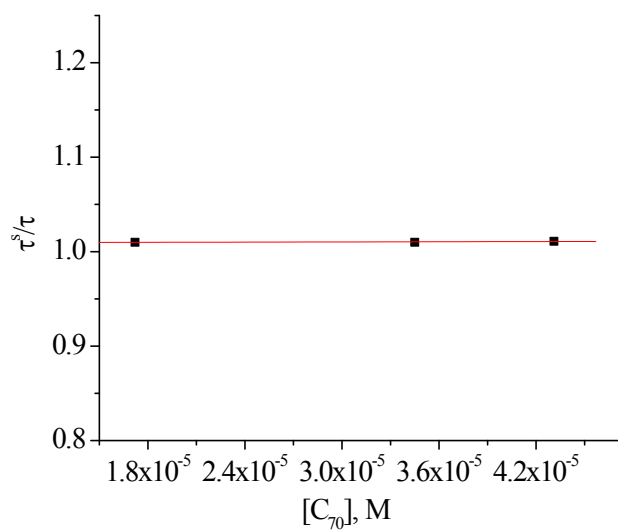


Fig. S11. Time-resolved fluorescence decay profile of (a) **1** (3.0×10^{-6} M) in presence of (b) C₇₀ (5.10×10^{-5} M) and (c) C₆₀ (6.7×10^{-5} M) recorded in toluene at 298K. Black and green colour lines represent instrument response function and fit to decay, respectively.



(a)



(b)

Fig. S12. Plot of τ^s/τ vs. concentration of quencher for (a) C₆₀-1 and (b) C₇₀-1 system recorded in DCB.

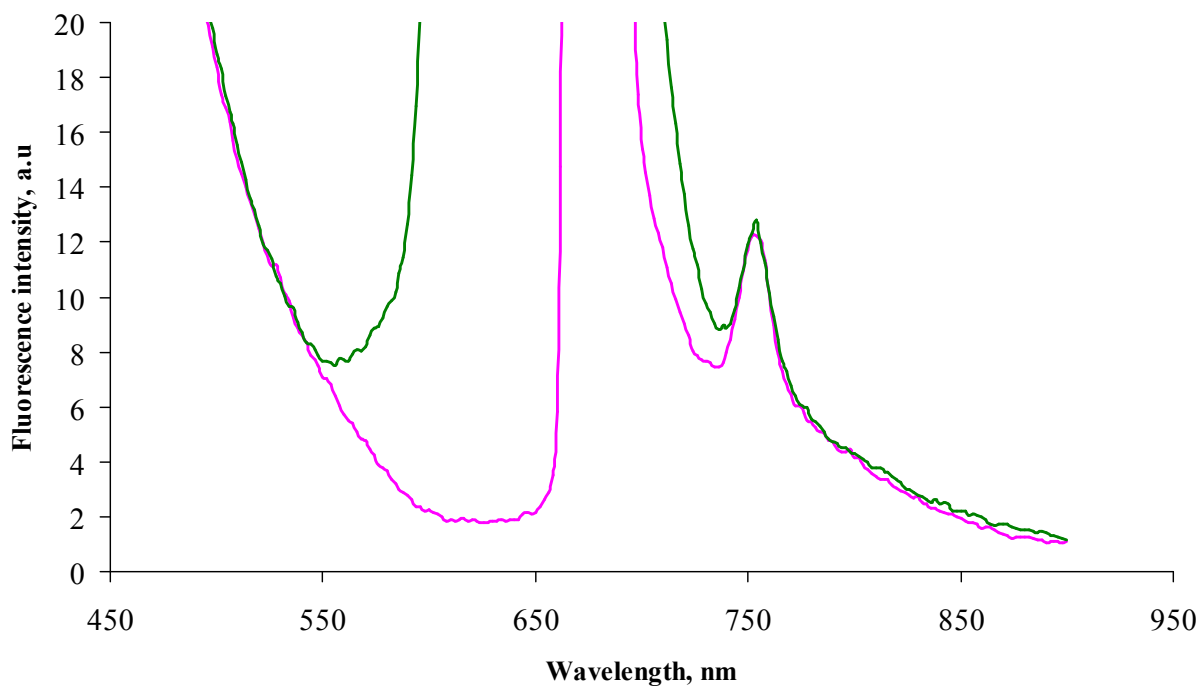


Fig. S13. Steady state fluorescence spectral variation of C₆₀ (3.4×10^{-6} M, magenta colour line) in presence of **1** (2.5×10^{-6} M, green colour line) recorded in toluene at 298K; $\lambda_{\text{ex}} = 337$ nm; $\lambda_{\text{em}} = 753$ nm.