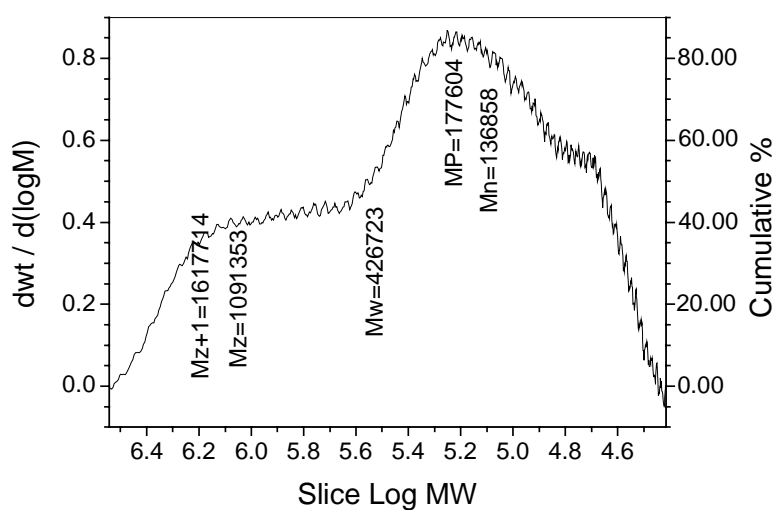# Supporting Information

for

Inter-locked Bis(polyrotaxane) of Cyclodextrin-Porphyrin Systems

Mediated by Fullerenes

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Dist Name	Mn	Mw	MP	Mz	Mz+1	Polydispersity
1	136858	428723	177604	1091353	1617714	3.132614

Figure S1 GPC trace of assembly **3** in DMF elution *vs.* polystyrene standards.

The apparent association constant of the supramolecular complex between cyclodextrin-porphyrin conjugate **3** and fullerene was determined by investigating the fluorescence spectrum of **3** by adding fullerene.[1]

$$(\mathbf{3} + C60)_m \xrightleftharpoons{K_{app}} (\mathbf{3} + C60)_{m-n} + n[\mathbf{3} + C60] \qquad (1)$$
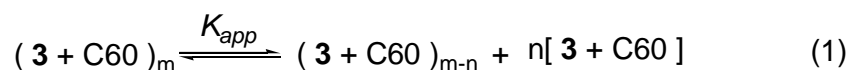
The observed fluorescence quantum yield ($\phi_f(obsd)$) of porphyrin units in **3** was related to the fluorescence quantum yields of uncomplexed (ϕ_f^0) and complexed (ϕ_f') porphyrin units by the equation (2).

$$\phi_f(obsd) = (1-\alpha)\phi_f^0 + \alpha\phi_f' \qquad (2)$$

α was the degree of association between porphyrin and fullerene.

Simplifying the equation (2), we get the following equation (3).

$$\phi_f^0 - \phi_f(obsd) = \alpha(\phi_f - \phi_f') \qquad (3)$$

For high concentration of C60 cluster and [C60] » porphyrin, α was given as the following form.

$$\alpha = \frac{K_{app}[C60]}{1 - K_{app}[C60]} \qquad (4)$$

From equation (3) and (4), the following relation was obtained.

$$\frac{1}{\phi_f^0 - \phi_f(obsd)} = \frac{1}{\phi_f^0 - \phi_f'} + \frac{1}{K_{app}(\phi_f^0 - \phi_f')[C60]} \qquad (5)$$

Using the equation (5), we obtained a linear dependence of $1/(\phi_f^0 - \phi_f(obsd))$ on the concentration of C60 clusters. Therefore, we calculated the K_{app} to be 7800 M^{-1}.
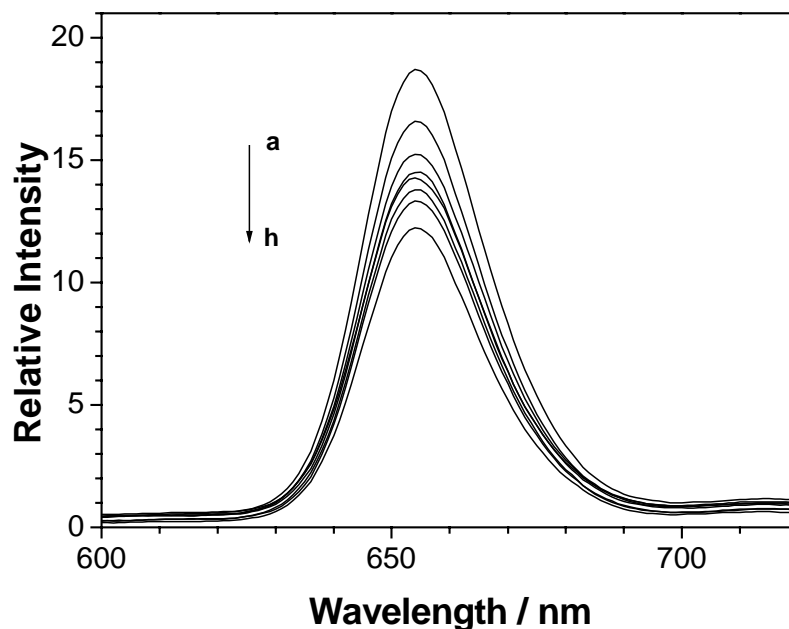
Figure S2. Fluorescence emission spectra of **3** (0.02 mM based on the number of the porphyrins) in DMF/toluene (v/v 3:1) at various concentrations of C60 at 298 K. ([C60]=0, 0.05, 0.1 0.15, 0.2, 0.25, 0.3, 0.4 mM, excition wavelength 410 nm, excitation and emission slit 5 nm)
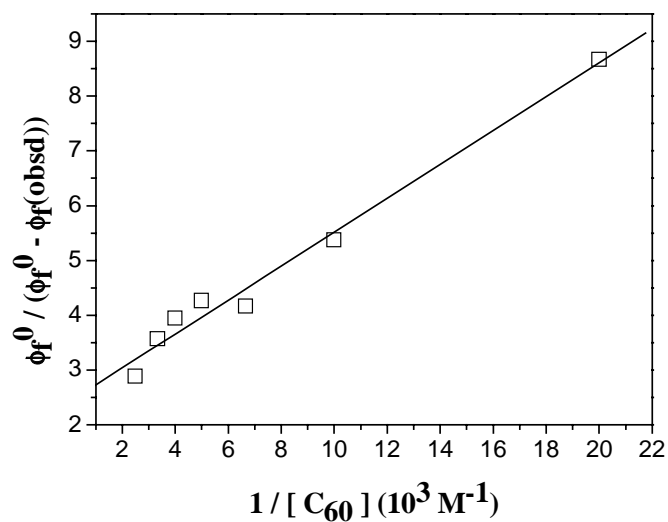

Figure S3. Dependence of $\phi_f^0/(\phi_f^0-\phi_f(obsd))$ on the reciprocal of C60 in DMF/toluene (v/v 3:1). (ϕ_f^0 is the initial fluorescence yield of **3**; $\phi_f(obsd)$ is the observed

fluorescence quantum yield of **3** in the presence of C60 with various concentration.)
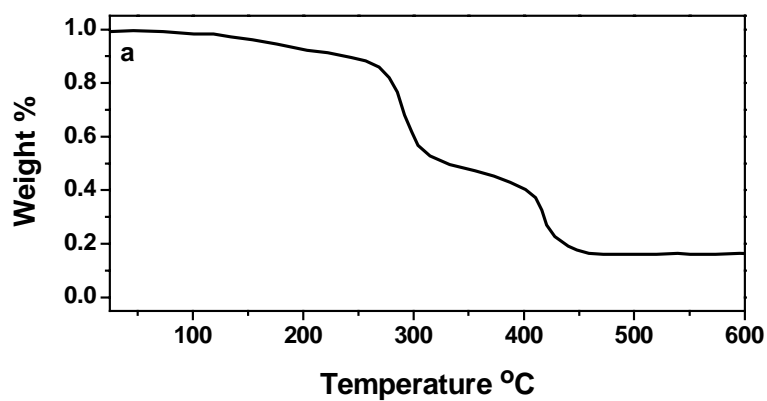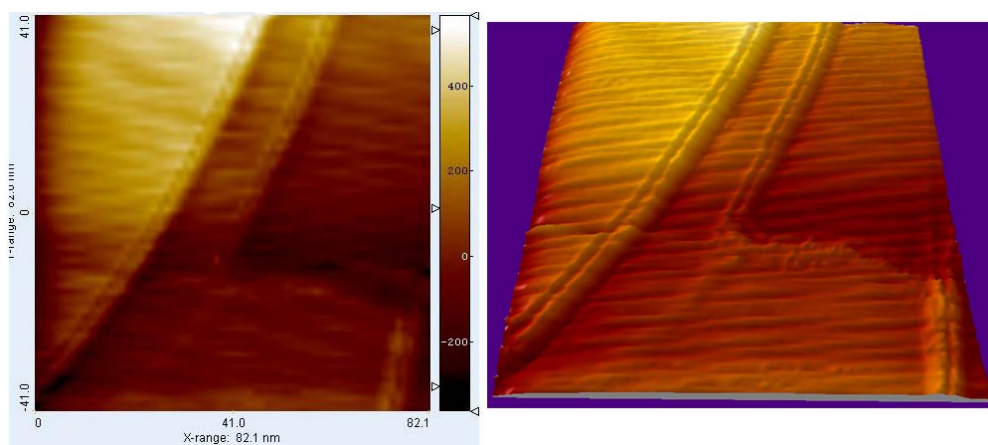

Figure S4. The thermogravimetric curve of **4**.

Figure S5 STM image of the end of **4** on HOPG surface (tunneling current 1.0 nA)

[1] Hasobe, T.; Imahori, H.; Kamat, P. V.; Ahn, T. K.; Kim, S. K.; Kim, D.; Fujimoto, A.; Hirakawa T.; Fukuzumi, S. *J. Am. Chem. Soc.* **2005**, *127*, 1216-1228.