**Supporting Information**

Supramolecular complexation of homocysteine and cysteine with cucurbit[7]uril

Min Jung Leea, Nirmal K. Sheea, Jung-In Sona, Subramanian Karthikeyanb, Kwang-Hwan Jheea, Jin Yong Leec\* and Hee-Joon Kima\*

*aDepartment of Applied Chemistry, Kumoh National Institute of Technology, Gumi 39177, Republic of Korea. bDepartment of Chemistry, Kalaslingam University, Tamil Nadu 626126, India. cDepartment of Chemistry, Sungkyunkwan University, Suwon 16419, Republic of Korea.*

\*To whom correspondence should be addressed: E-mail: hjk@kumoh.ac.kr; jinylee@skku.edu

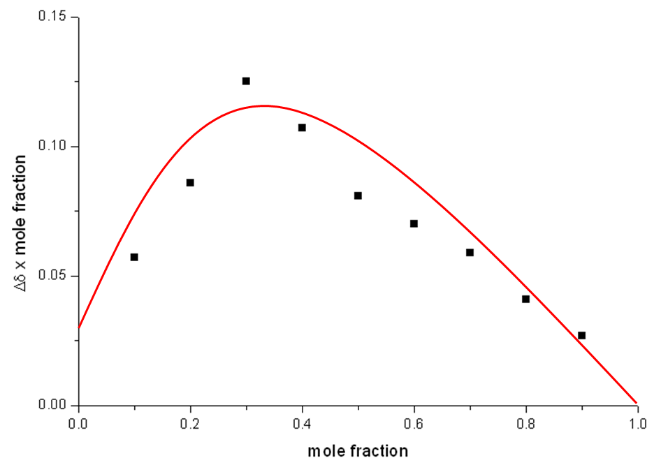
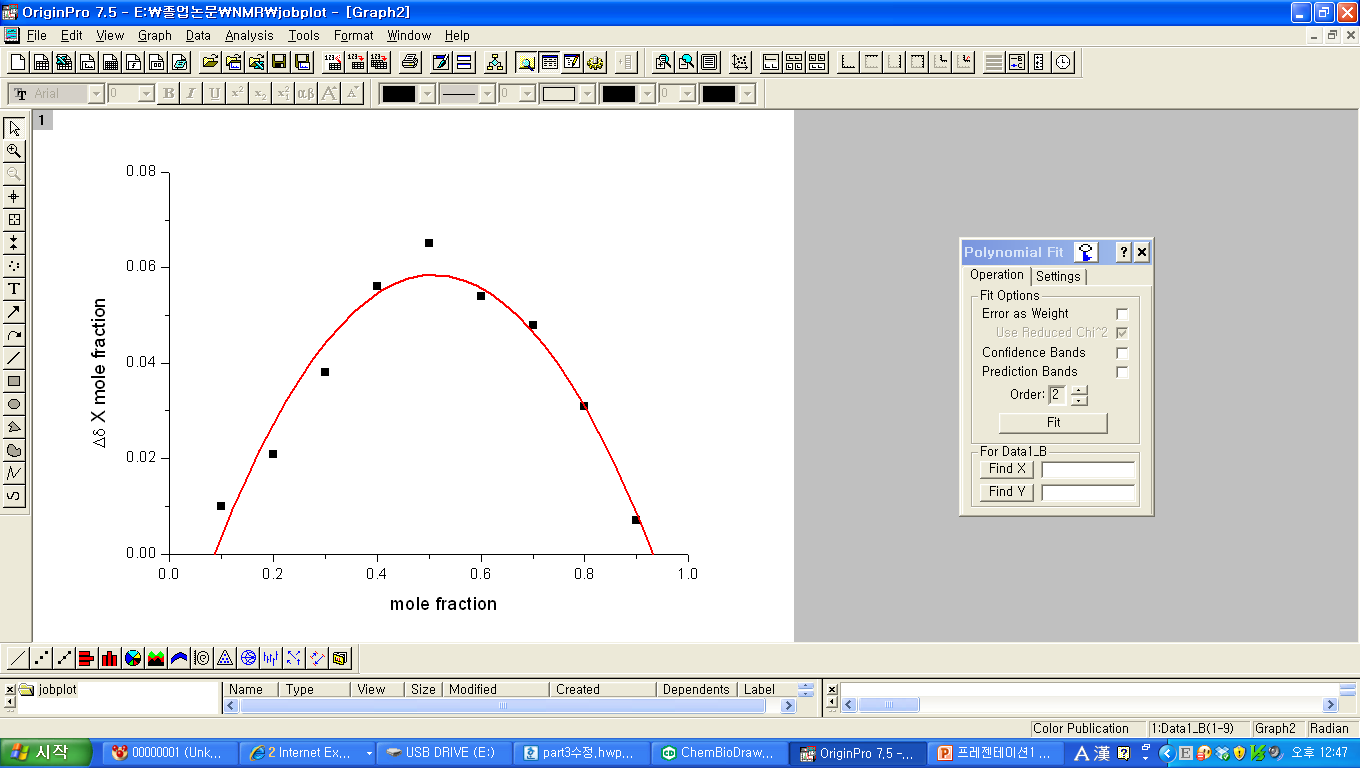
# Experimental

## Materials and Instruments

CB[7], cysteine and homocysteine were purchased from Aldrich. All other reagents were of analytical grade and were used as received. Double-distilled water was used for all experiments. All 1H NMR spectra, including those for titration experiments, were obtained on a Bruker BIOSPIN/AVANCE III 400 spectrometer at 25 °C. The concentrations of the amino acids were 1-2 mM in the NMR experiments. D2O was adjusted to pD = 7.0 with sodium phosphate or pD = 2.45 with 1 M DCl. All pD values were verified on a pH meter calibrated with two standard buffer solutions. ESI mass spectra were recorded on a **Thermo Finnigan Linear Ion Trap Quadrupole Mass Spectrometer**.

## Isothermal titration calorimetry measurements

The formation constant and thermodynamic parameters for the complexation of Hcys and Cys with CB[7] were measured by the titration calorimetry using a VP-ITC instrument from MicroCal. A stock solution of cysteine and homocysteine solution (50 mM each) were prepared with 10 mM sodium phosphate (pH 7.0) in distilled H2O. CB[7] solution was prepared in distilled water of 0.25 mM. Cysteine and homocysteine solution were injected with 40 μl to host solution 250 μl. The heat evolved was recorded at 25 °C. The heat of dilution was corrected for by injecting the cysteine or homocysteine solution into aqueous solution and subtracting this data from that of the host-guest titration. The data were analyzed and fitted by the Origin software (MicroCal).



(a) (b)

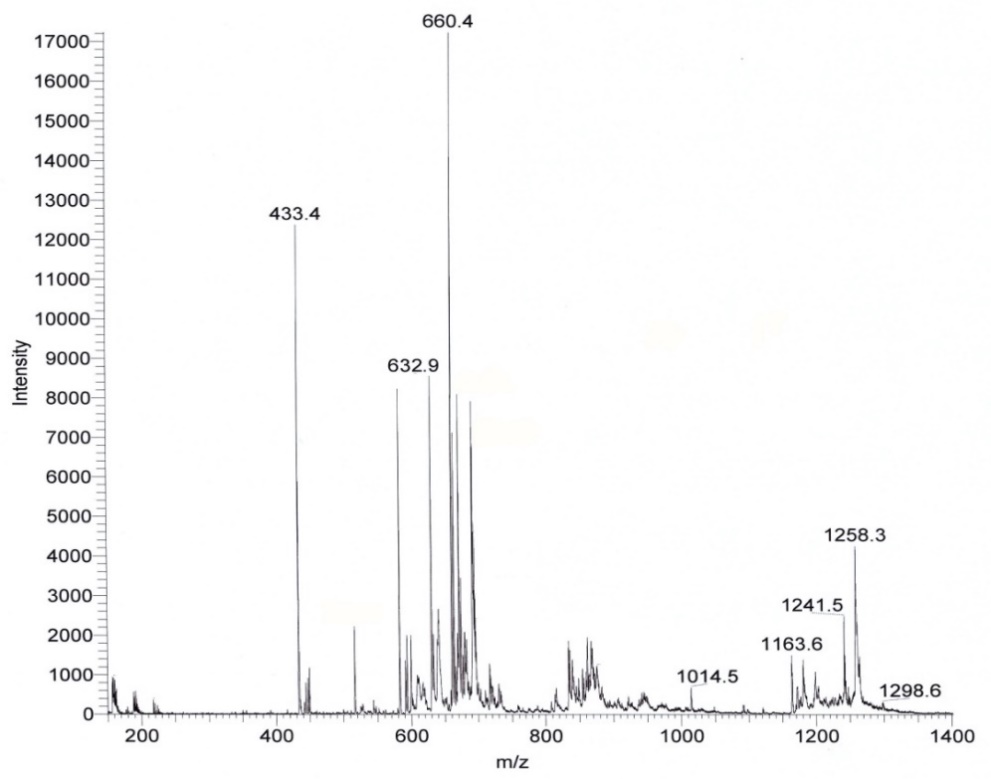
**Figure S1.** Job-plots for the supramolecular complexation of (a) Cys and (b) Hcys with CB[7] (observing the ** proton resonance shift of amino acids).



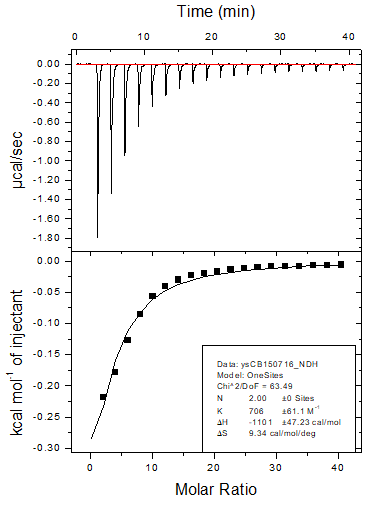
**Figure S2.** 1H NMR spectra (400 MHz, pD =2.45) of Cys (*c* = 1 mM) in the absence and in the presence of CB[7]. The asterisk(\*) denotes the resonances for CB[7]. S due to residual solvent.



**Figure S3.** 1H NMR spectra (400 MHz, pD =2.45) of Hcys (*c* = 1 mM) in the absence and in the presence of CB[7]. The asterisk(\*) denotes the resonances for CB[7]. S due to residual solvent.

****

**Figure S4.** ESI mass spectrum of 1:1 supramolecular complex with Hcys and CB[7] in water.



1. **** (b)

**Figure S5.** ITC titration curves for the supramolecular complexation of CB[7] with (a) Hcys (1:1), (b) Cys (1:2), and (c) Cys (1:1) in aqueous solution.

****

**Figure S6.** 1H NMRtitration profiles obtained upon titration of Cys in D2O with increasing concentration of CB[7] (observing the ** proton shift of Cys).

****

**Figure S7.** DFToptimized geometries of CB[7], cysteine, homocysteine and their complexes.

****

**Figure S8.** Shortest hydrogen bonding interactions in the each optimized geometry for the supramolecular complexes of CB[7] with Cys and Hcys.