Supplementary Information

Encapsulation of L-Valine, D-Leucine and D-Methionine by Cucurbit[8]uril

Zeng-Hui Zhang,[a] Rui-Lian Lin,[b] Xiang-Yun Yu,[a] Li-Xia Chen,[a] Zhu Tao,[a] Xin Xiao,*[a] Gang Wei,*[c] Carl Redshaw,[d] and Jing-Xin Liu *[b]

[a.] Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, P. R. China. E-mail: gyhxxiaoxin@163.com

[b.] College of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan 243002, P. R. China. E-mail: jxliu411@163.com

[c.] CSIRO Mineral Resources, PO Box 218, Lindfield, NSW 2070, Australia. E-mail: gang.wei@csiro.au

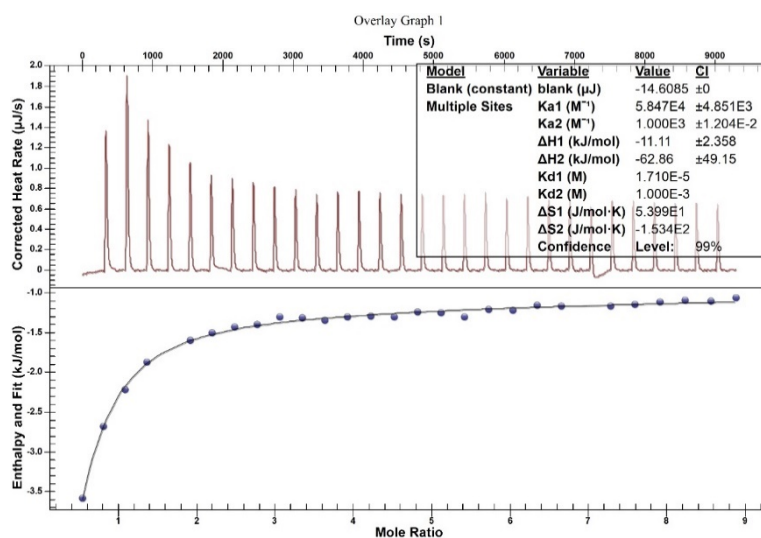[d.] Department of Chemistry, University of Hull, Hull HU6 7RX, U.K
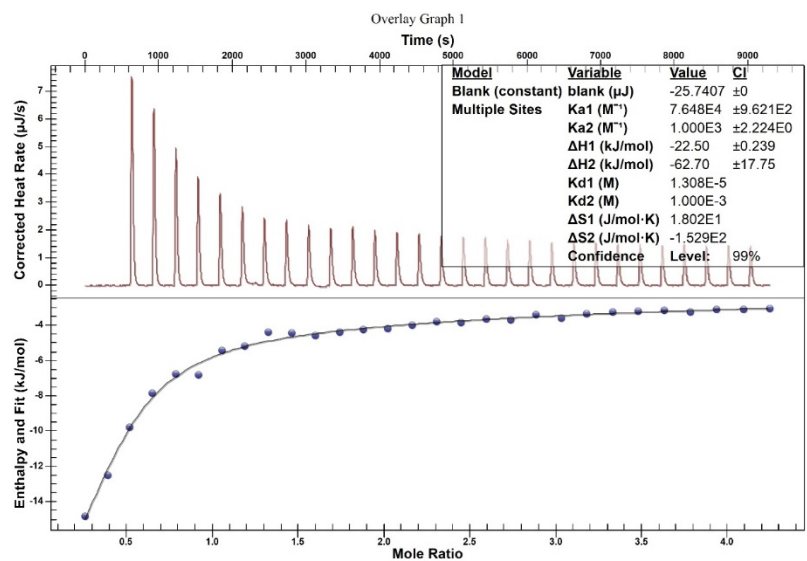
Figure S1. ITC profile of Q[8] with L-Val at 298.15 K

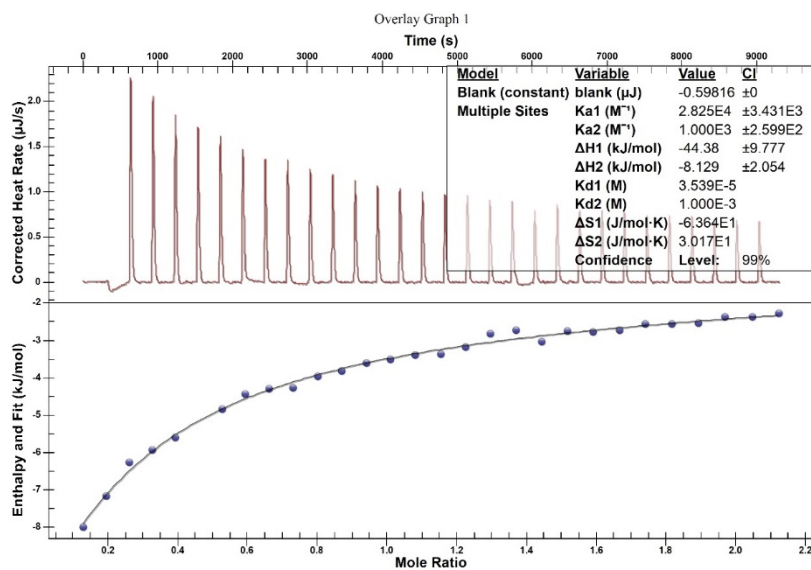**Figure S2**. ITC profile of Q[8] with D-Leu at 298.15 K.

Figure S3. ITC profile of Q[8] with D-Met at 298.15 K.

Table S1. ITC measurements of the thermodynamics for the interactions between amino acids and

Q[8] at 298.15 K

Date	L-Val$_2$@Q[8]	D-Leu$_2$@Q[8]	D-Met$_2$@Q[8]
Ka (M^{-2})	5.847×10^7	7.648×10^7	2.825××10^7
K$_{a1}$ (M^{-1})	(5.847±0.4851) ×10^4	（7.648±0.09621）×10^4	（2.825±0.3431）×10^4
K$_{a2}$ (M^{-1})	1.000×10^3 ±1.204×10^{-2}	1.000×10^3 ± 2.224	（1.000±0.2599）×10^3
ΔH$_1$ (kJ·mol^{-1})	-11.11±2.358	-22.50±0.239	-44.38±9.777
ΔH$_2$ (kJ·mol^{-1})	-62.86±49.15	-62.70±17.75	-8.129±2.054
TΔS_1 (kJ·mol^{-1})	16.0971185	5.372663	-18.974266
TΔS_2 (kJ·mol^{-1})	-45.73621	-45.587135	8.9951855