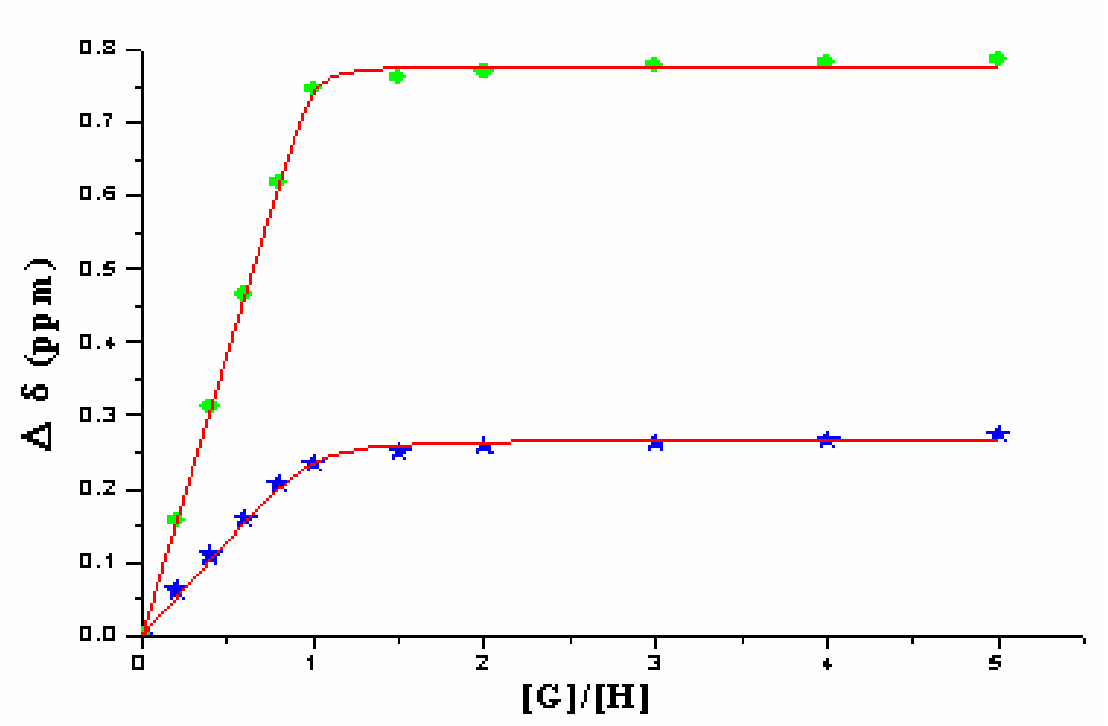
Supporting Information for

Cholic acid-based fluorescent probe for enantioselective recognition of trifunctional aminoacids

Hao Wang, Wing-Hong Chan* and Albert W. M. Lee

Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Hong Kong SAR, China

1. Binding saturation curves based on ^{1}H NMR titrations of sensor **1a** with antipodal forms of serine



S-Figure 1. Binding saturation curves based on ^{1}H NMR titrations of sensor **1a** with L-serine (★) and D-serine (●) in CD_3CN, [**1a**] = 2mM. $\triangle\delta$ is the complexation induce shift (CIS) difference of the anthracenylmethylene protons of **1a** after an aliquot of guest has been added compared to before any guest addition

S-Table 1. Association constants $\mathbf{K_{ass}}$ (M^{-1}) and relative coefficients (R) of sensor **1a** with L-serine and D-serine in CD_3CN at 25°C as determined by ^1H NMR titration

guests	K_{ass} (M^{-1})[a]	R[a]	δ_{max}[b] (ppm)
L-serine	$(3.18\pm0.21)\times10^4$	0.9942	0.29
D-serine	$(2.44\pm0.06)\times10^5$	0.9963	0.79

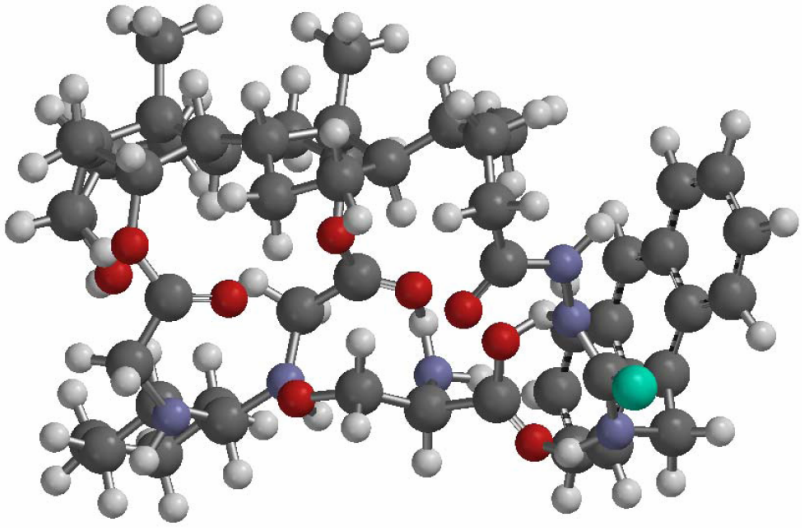
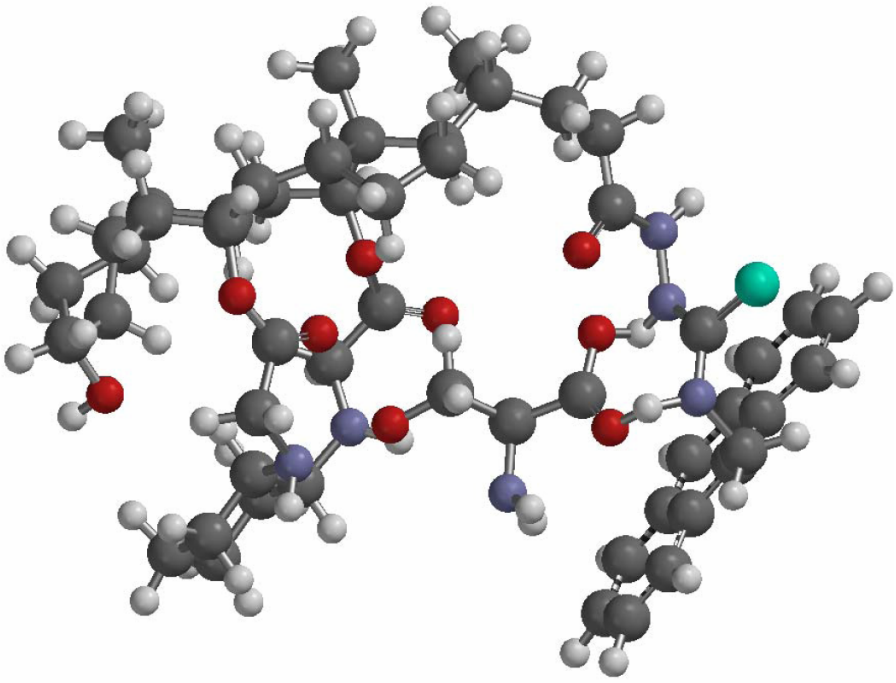
[a] The values were calculated using the 1:1 binding isotherm by iterative curve-fitting methods described elsewhere[ref. 9]. [b] δ_{max} is the saturated CIS calculated by the iterative methods.

2. Free energy difference of the diastereomeric binding of **1a** with antipodal forms of trifunctional aminoacids

S-Table 2. Diastereomeric binding of **1a** with antipodal forms of serine, threonine, lysine and tyrosine

aminoacids	Host **1a**			Host **1c**		
	- △G (Kcal/mol)	△△G	K_D/K_L	- △G (Kcal/mol)	△△G	K_L/K_D
L-serine	6.09			7.12	1.06	6.2
D-serine	7.20	1.11	6.7	6.06		
L-threonine	5.80			6.98	1.23	8.1
D-threonine	7.07	1.27	8.9	5.75		
L-lysine	5.69			6.71	1.17	7.4
D-lysine	6.91	1.22	8.1	5.54		
L-tyrosine	5.93			7.05	1.05	7.2
D-tyrosine	7.11	1.18	7.5	5.90		

3. **S-Figure 2** Molecular modeling studies for the host-guest complex conducted by SPARAN 04

Complex ***1a*** **-** *D-serine* (additional H-bond formed between one of the hydrogen of the α-amino group of D-serine and the C-12 pendant ester oxygen atom)

Complex ***1a*** – *L-serine* with the α-amino group of L-serine pointing away from the core portion of cholic acid derivative


4. Solvent effect on the binding properties of **1a** to D- and L-serine

S-Table 3 Association constants K_{ass} (M^{-1}) of sensor **1a** with serine in different solvent systems

Solvent	D-serine	L-serine	K_D/K_L
CH_3CN	$(2.26\pm0.17)\times10^5$	$(3.36\pm0.23)\times10^4$	6.7
$CH_3CN:H_2O$=8:2	$(9.33\pm0.31)\times10^4$	$(1.73\pm0.11)\times10^4$	5.4
$CH_3CN:H_2O$=6:4	$(4.95\pm0.20)\times10^4$	$(1.05\pm0.06)\times10^4$	4.7
$CH_3CN:H_2O$=5:5	$(3.57\pm0.26)\times10^4$	$(8.71\pm0.42)\times10^3$	4.1