Electronic Supplementary Information

for

Molecular Binding Behaviors of Triazole-Bridged Bis(*β*-cyclodextrin)s towards Cinchona Alkaloids

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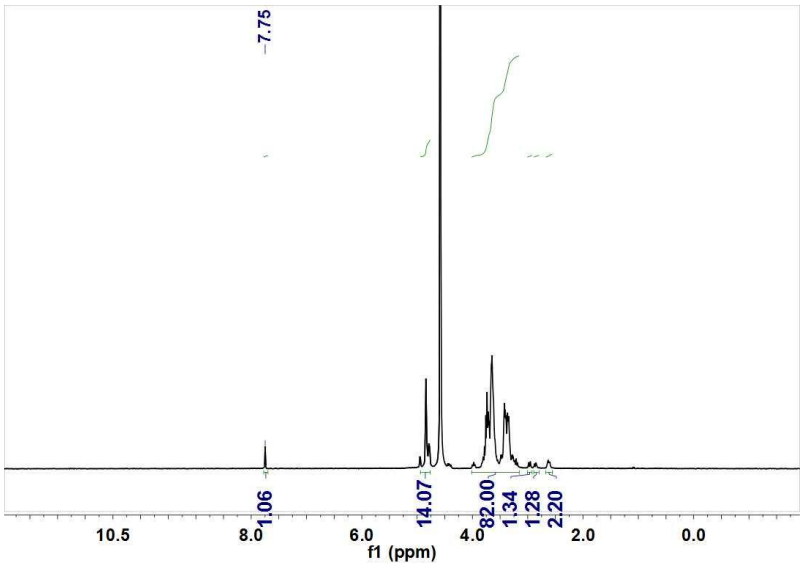

Fig. S1 ^{1}H NMR spectrum of compound **3** in D_2O (400 MHz, 25 °C)

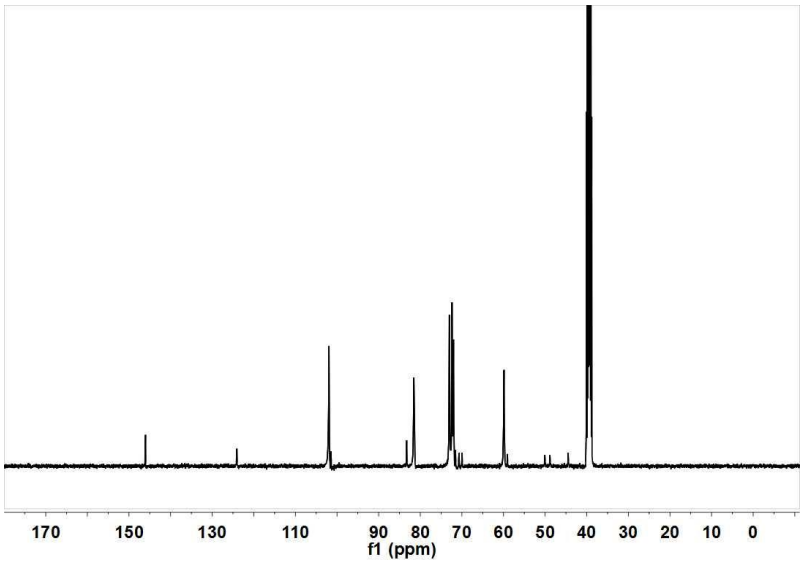

Fig. S2 ^{13}C NMR spectrum of compound **3** in DMSO-d_6 (100 MHz, 25 °C)

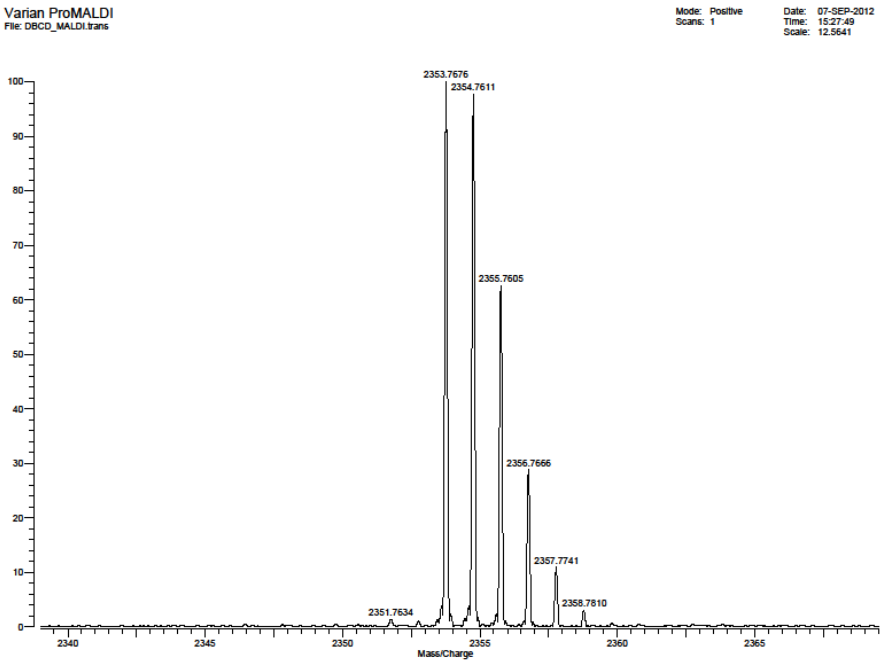

Fig. S3 ESI-MS spectrum of compound **3**

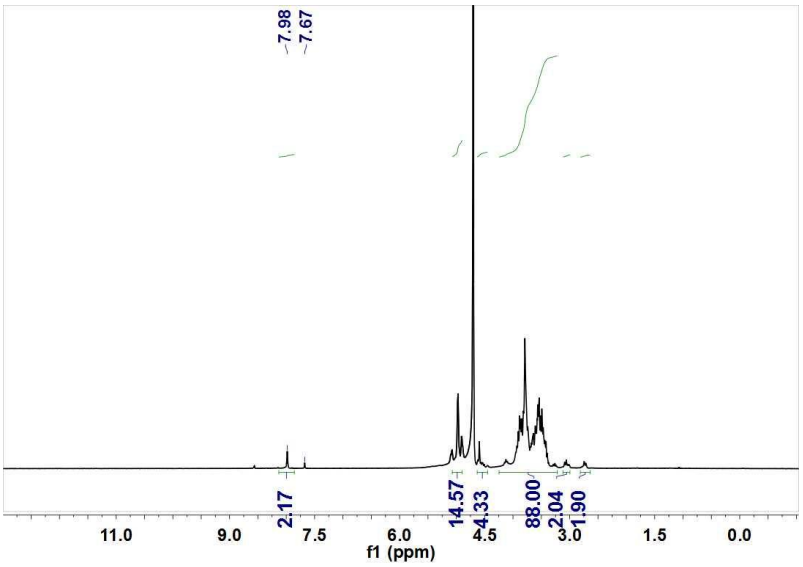

Fig. S4 ^{1}H NMR spectrum of compound **4** in D_2O (400 MHz, 25 °C)

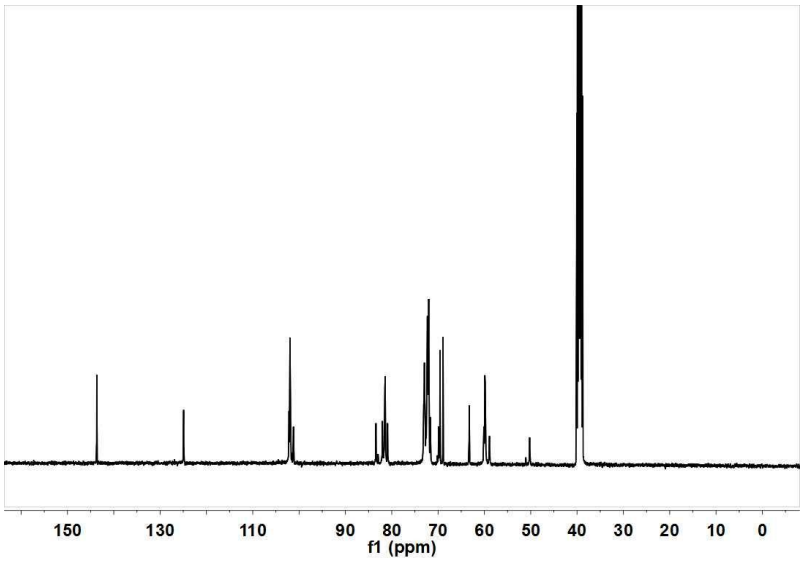

Fig. S5 ^{13}C NMR spectrum of compound **4** in DMSO-d_6 (100 MHz, 25 °C)

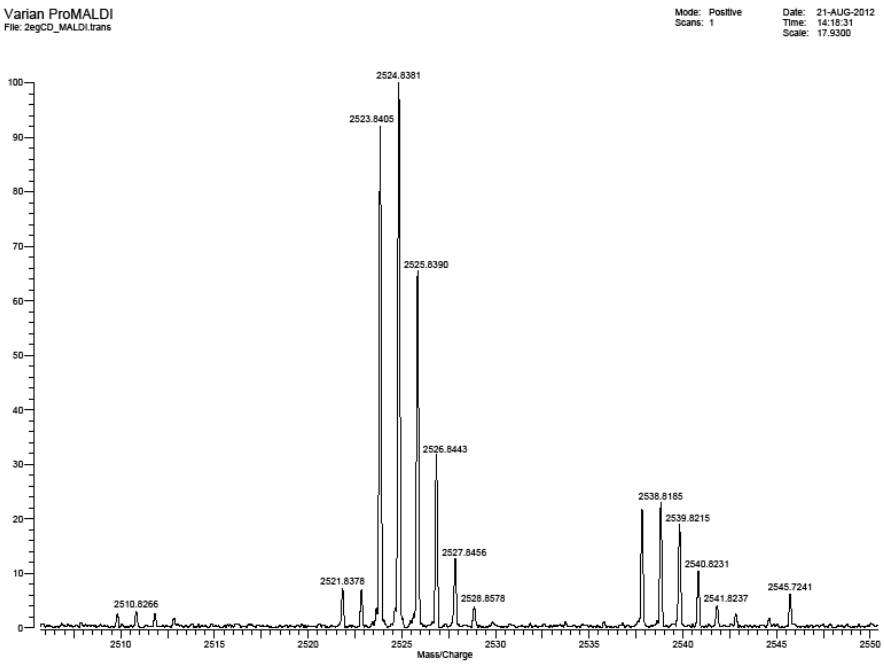

Fig. S6 ESI-MS spectrum of compound **4**

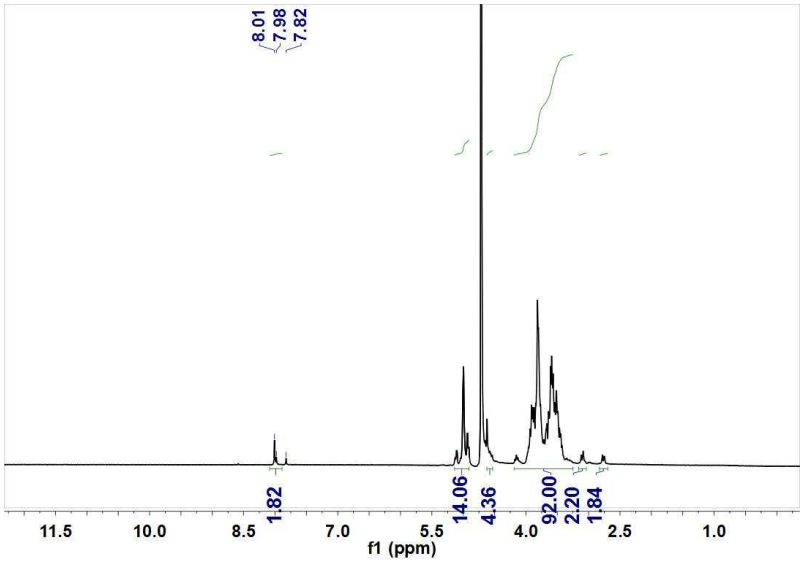

Fig. S7 ^{1}H NMR spectrum of compound **5** in D_2O (400 MHz, 25 °C)

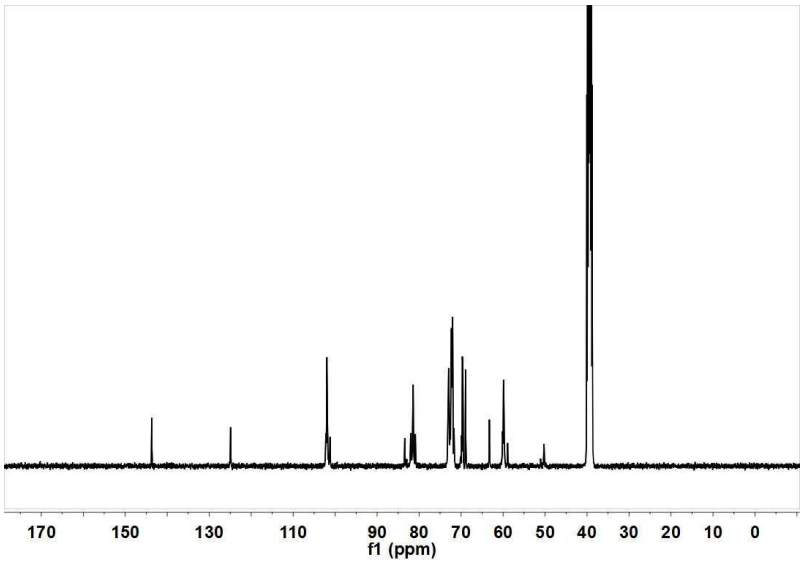

Fig. S8 ^{13}C NMR spectrum of compound **5** in DMSO-d_6 (100 MHz, 25 °C)

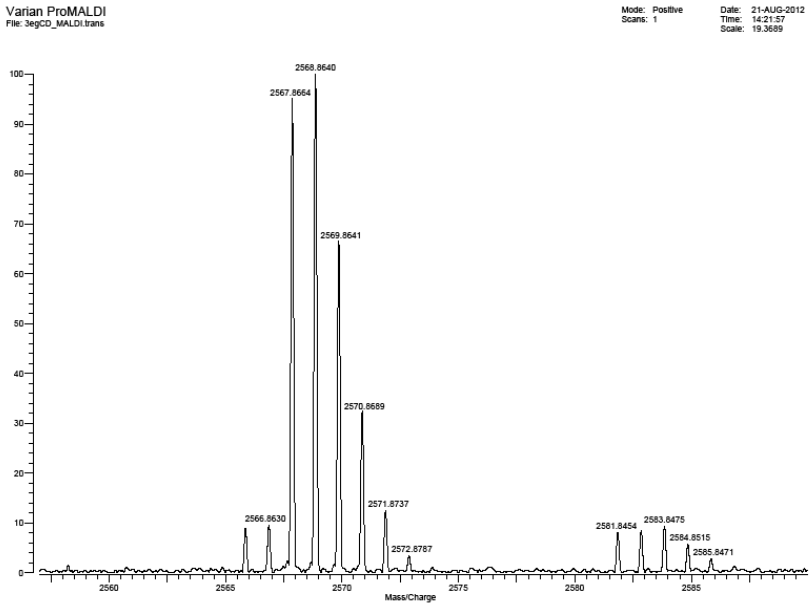

Fig. S9 ESI-MS spectrum of compound **5**

Table S1 Comparative photophysical properties of the 1:1 inclusion complexes between cinchona alkaloids and hosts **3**-**5** in phosphate buffer solution at 25 °C as determined by fluorometric titrations.

Host	Guest	Intensity	Emission peak (nm)
3	CID	enhanced	413
	CIN	enhanced	413
	QUD	enhanced	393
	QUN	quenched	383
4	CID	enhanced	432
	CIN	enhanced	431
	QUD	—[a]	390
	QUN	quenched	382
5	CID	enhanced	435
	CIN	enhanced	434
	QUD	—[a]	383
	QUN	quenched	382

[a] The isoluminescence points of **4**/QUD and **5**/QUD systems were 399 and 402 nm, respectively.

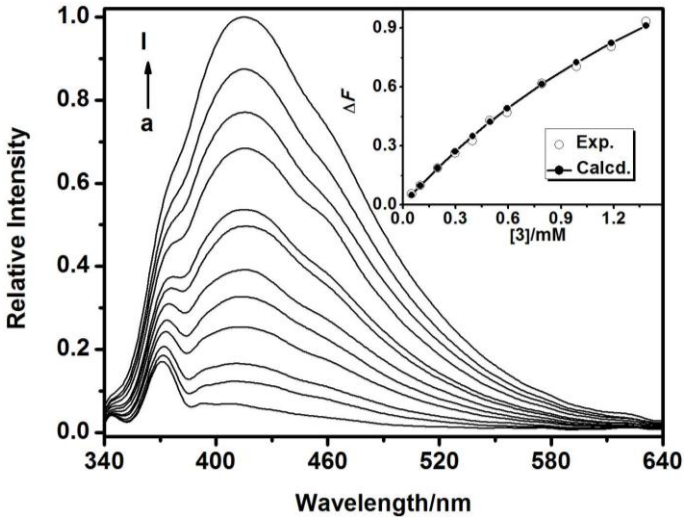

Fig. S10 Emission spectral changes of CIN upon addition of **3** in phosphate buffer solution (0.1 M, pH 7.2) at 25 °C ([CIN] = 1.0×10^{-5} M, [**3**] = 0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0, 1.2, 1.4×10^{-3} M, respectively, from a to l). Inset: The nonlinear least squares analysis of the differential spectral changes (ΔF) at 415 nm to calculate the stability constant (K_S) between **3** and CID (λ_{ex} = 330 nm).

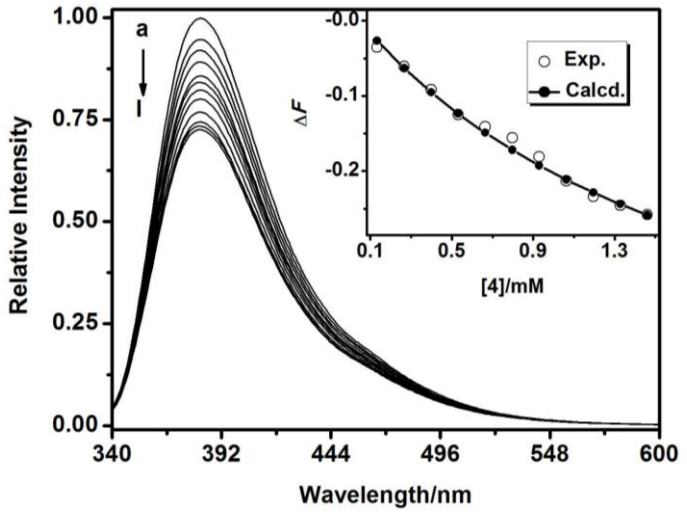

Fig. S11 Emission spectral changes of QUN upon addition of **4** in phosphate buffer solution (0.1 M, pH 7.2) at 25 °C ([QUN] = 1.0×10^{-5} M, [**4**] = 0, 0.1, 0.3, 0.4, 0.5,

0.7, 0.8, 0.9, 1.1, 1.2, 1.3, 1.5 × 10^{-3} M, respectively, from a to l). Inset: The nonlinear least squares analysis of the differential spectral changes (ΔF) at 385 nm to calculate the stability constant (K_S) between **4** and QUN (λ_{ex} = 330 nm).

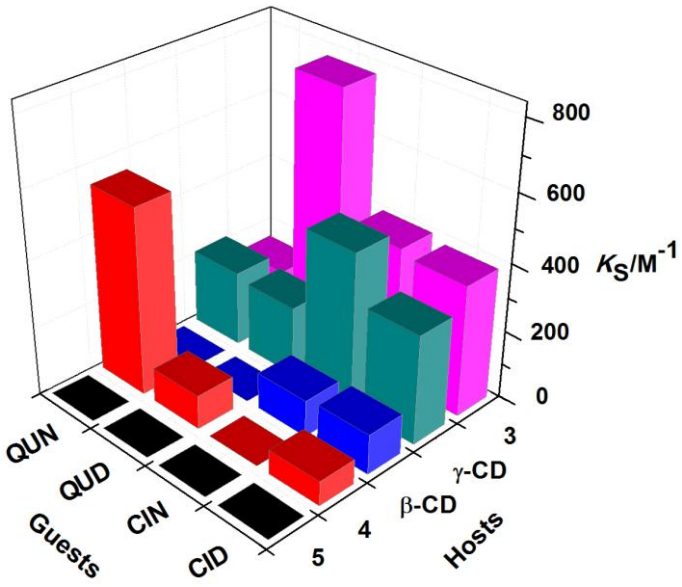

Fig. S12 Complex stability constants (K_S) of cinchona alkaloids with native β-, γ-CD, and hosts **3-5** in phosphate aqueous buffer solution at 25 °C.

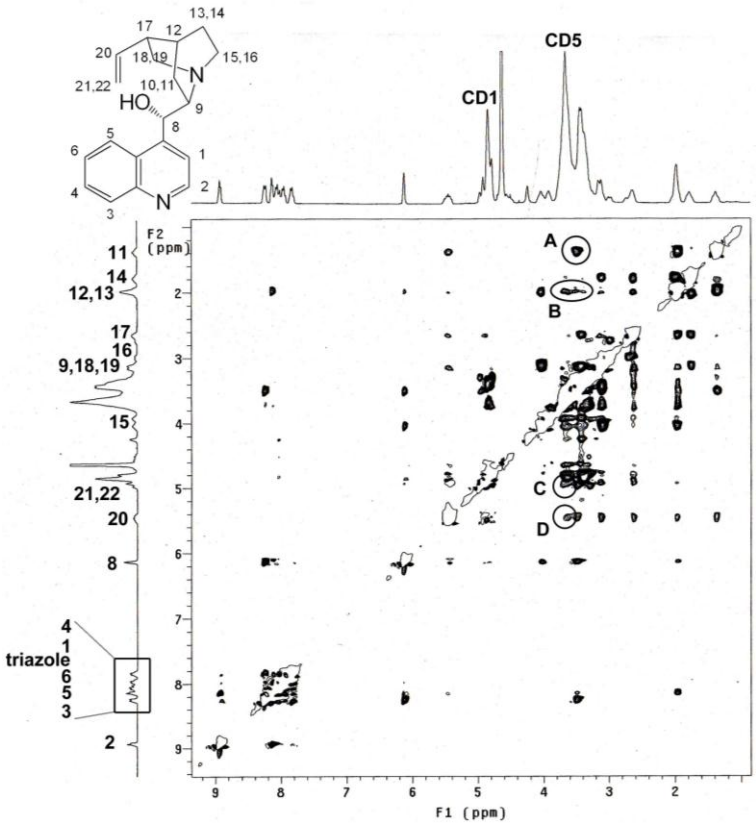

Fig. S13 ^{1}H ROESY spectrum of **3**/CID system with a mixing time of 0.25 s (300 MHz, D_2O, 25 °C).

Table S2 Comparative structural information of the 1:1 inclusion complexes of cinchona alkaloids with *β*-CD and hosts **3** as determined by 2D NMR results.

protons	aliphatic ring	ethenyl group	phenyl ring	pyridyl ring
H5 of **3** [a]	CID	CID	—[c]	—[c]
	CIN	CIN	CIN	—[c]
	QUD	QUD	—[c]	QUD
	QUN	QUN	QUN	QUN
H5 of *β*-CD [b]	CIN	CIN	CIN	—[c]

[a] this work; [b] ref. 13; [c] No correlation can be clearly observed at the corresponding protons of host and the substituent groups of guest.