Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information for

Molecular Binding Behaviors of Bispyridinium-containing Bis(*β*-cyclodextrin)s and [2]Rotaxane toward Bile Salts

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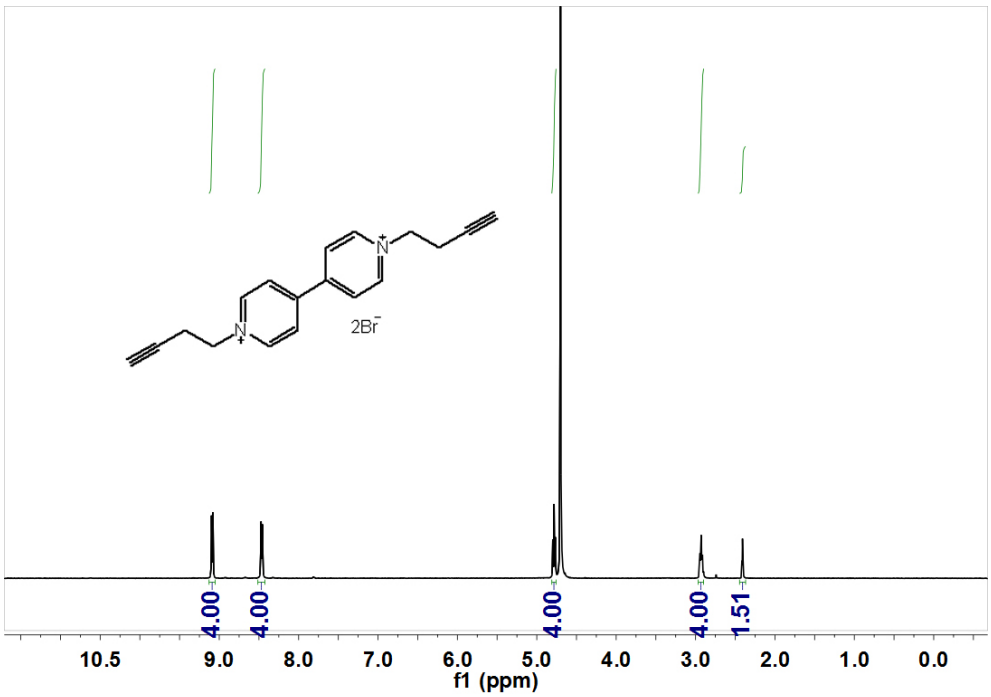

Figure S1. ^{1}H NMR spectrum of compound **3** in D_2O (400 MHz, 25 °C)

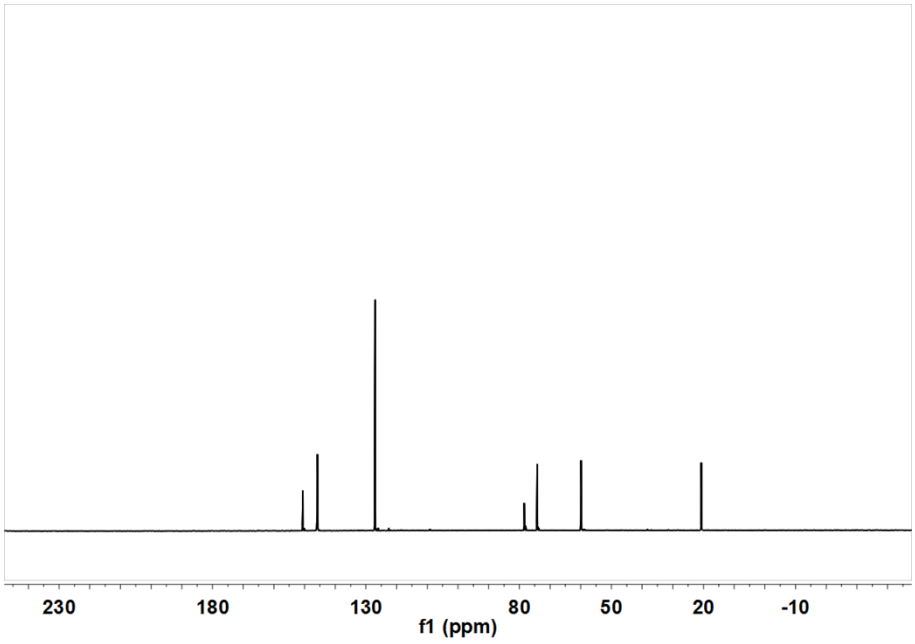

Figure S2. ^{13}C NMR spectrum of compound **3** in D_2O (100 MHz, 25 °C)

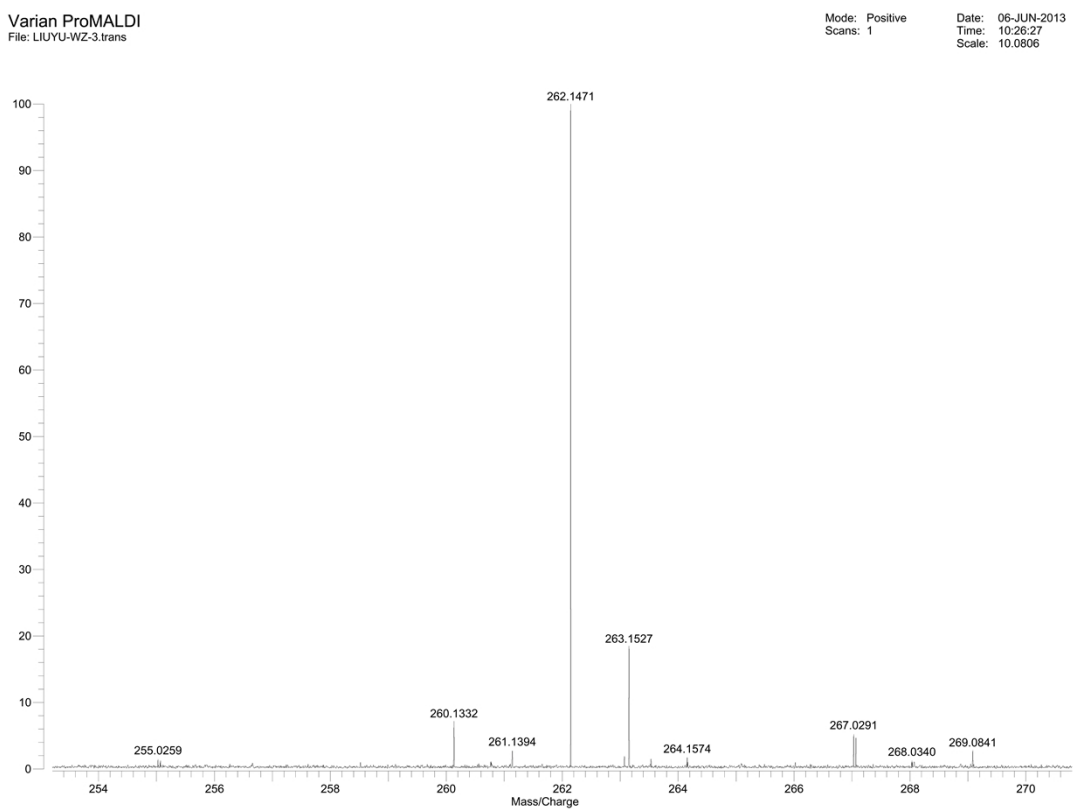

Figure S3. MALDI-MS spectra of compound **3**

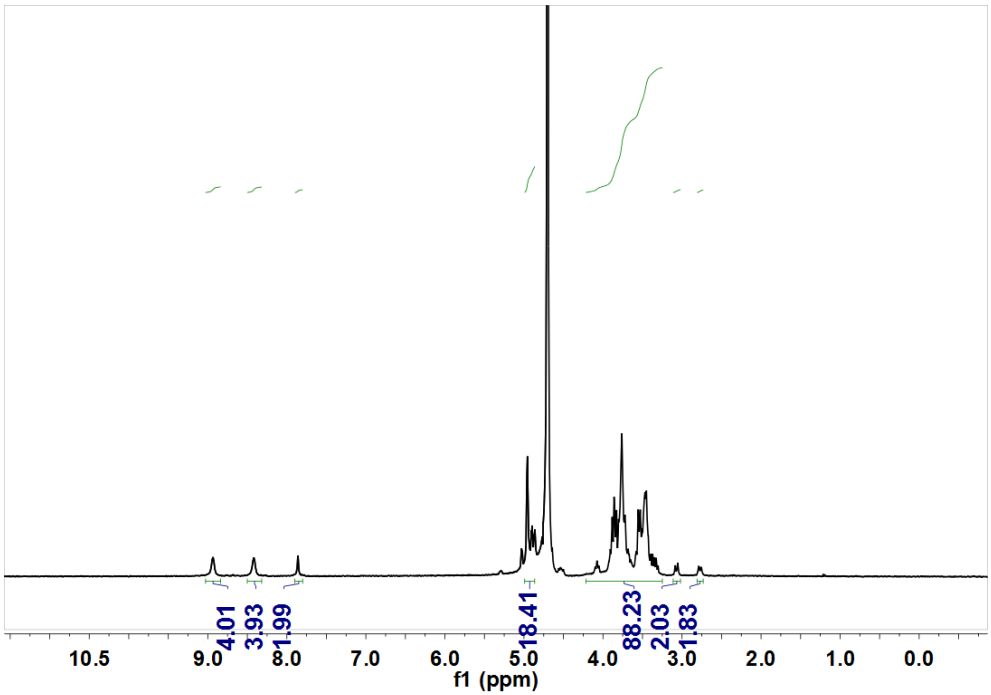

Figure S4. ^{1}H NMR spectrum of compound **1** in D_2O (400 MHz, 25 °C)

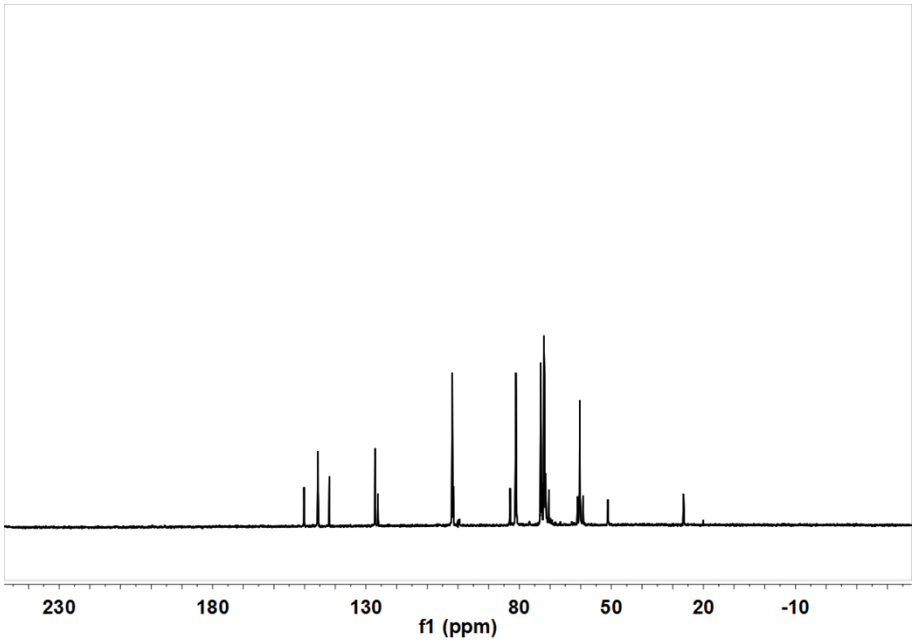

Figure S5. ^{13}C NMR spectrum of compound **1** in D_2O (100 MHz, 25 °C)

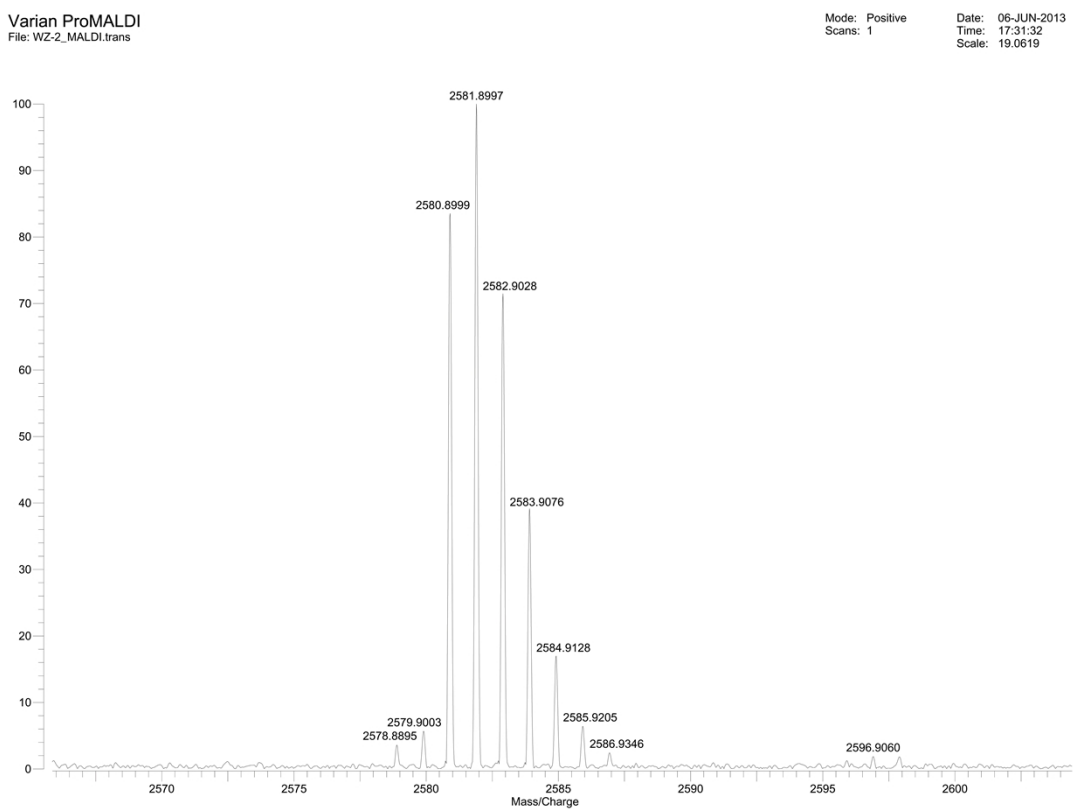

Figure S6. MALDI-MS spectra of compound **1**

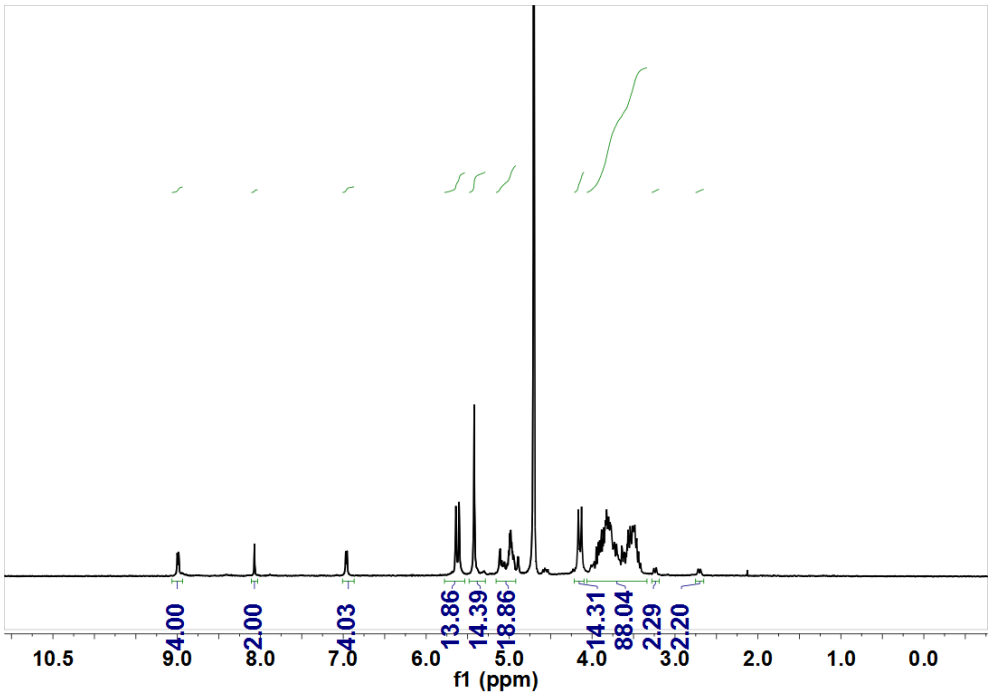

Figure S7. ^{1}H NMR spectrum of compound **2** in D_2O (400 MHz, 25 °C)

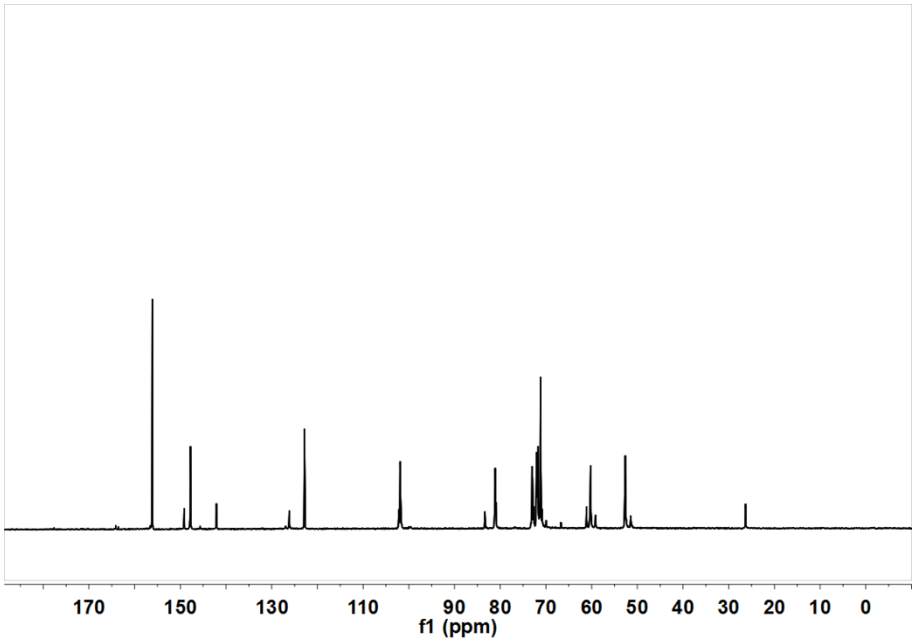

Figure S8. ^{13}C NMR spectrum of compound **2** in D_2O (100 MHz, 25 °C)

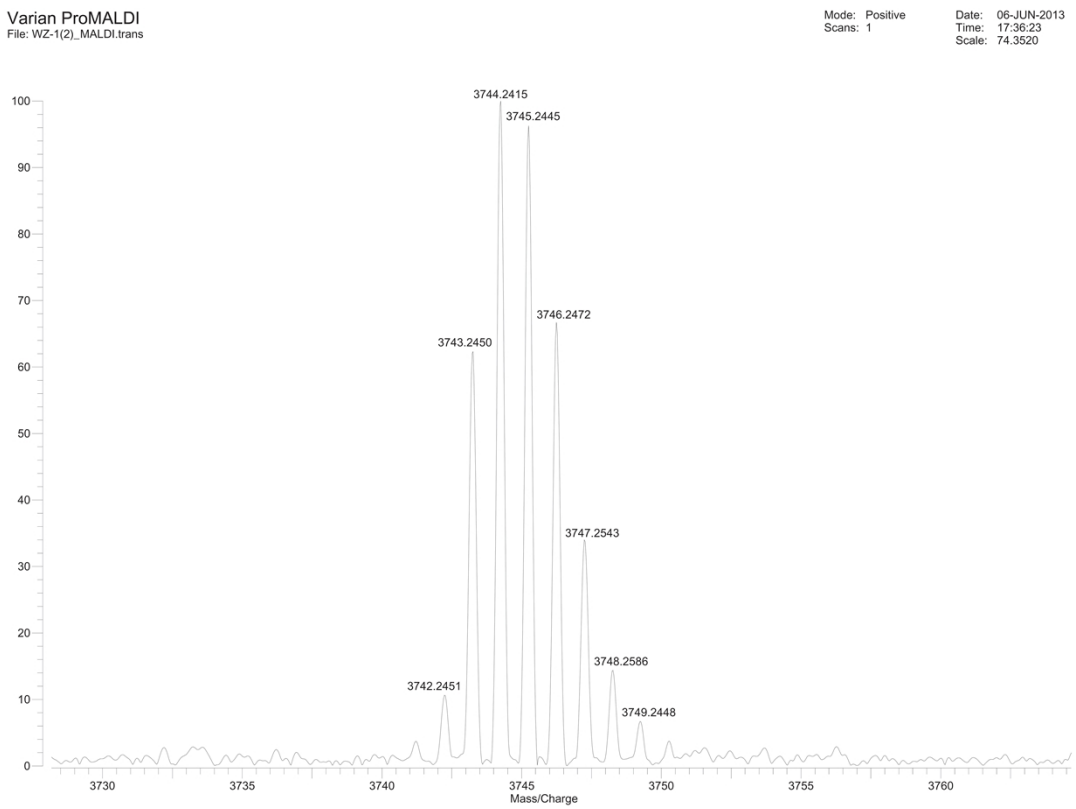

Figure S9. MALDI-MS spectra of compound **2**

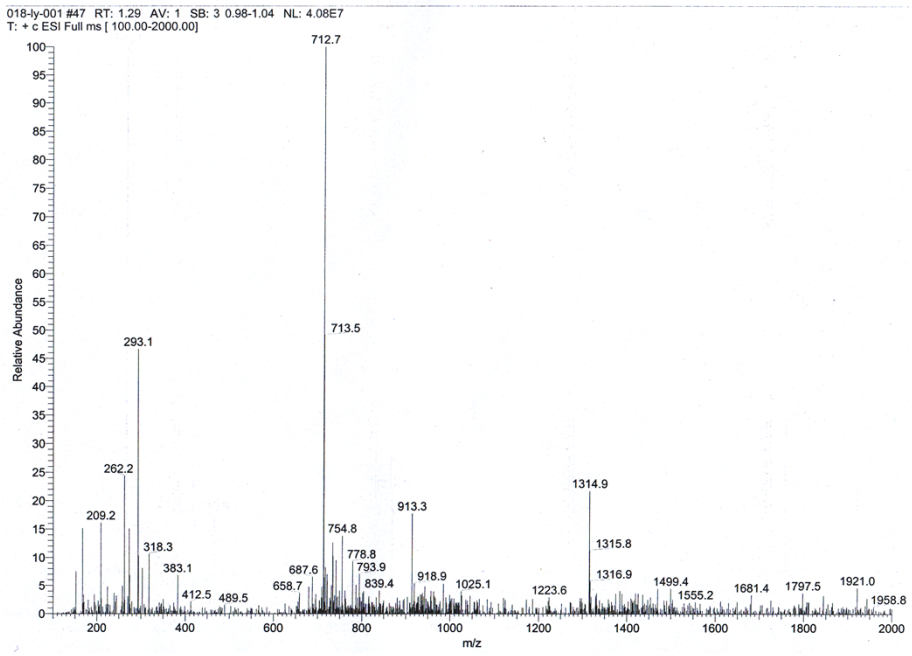

Figure S10. ESI-MS spectra of complex **3**⊂CB[7]

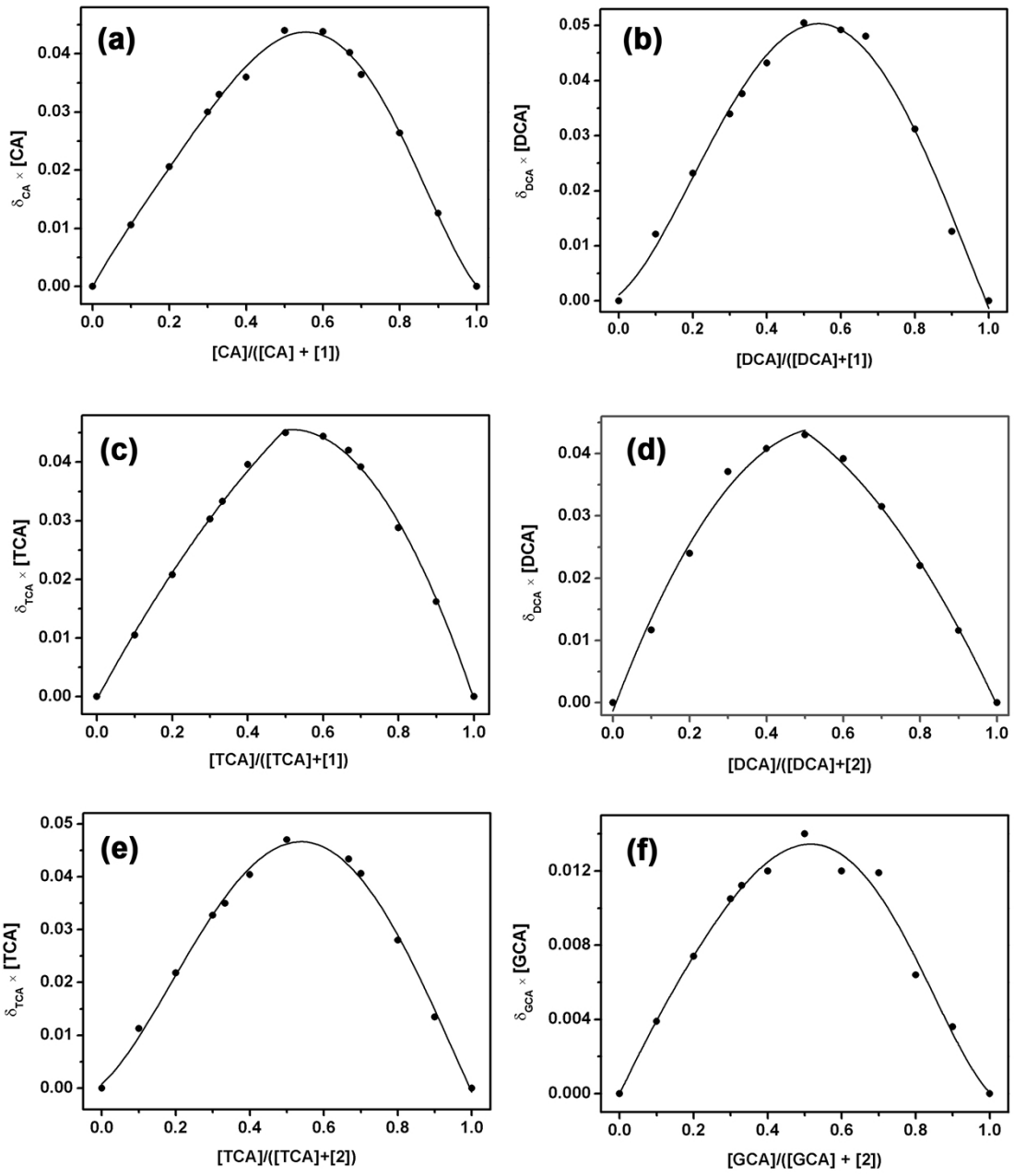

Figure S11. Typical Job's plots of complexes (a) CA⊂**1**, (b) DCA⊂**1**, (c) TCA⊂**1**, (d) DCA⊂**2**, (e) TCA⊂**2**, and (f) GCA⊂**2** in D_2O at 25 °C, respectively ([Host] + [Guest] = 1.0×10^{-3} M).

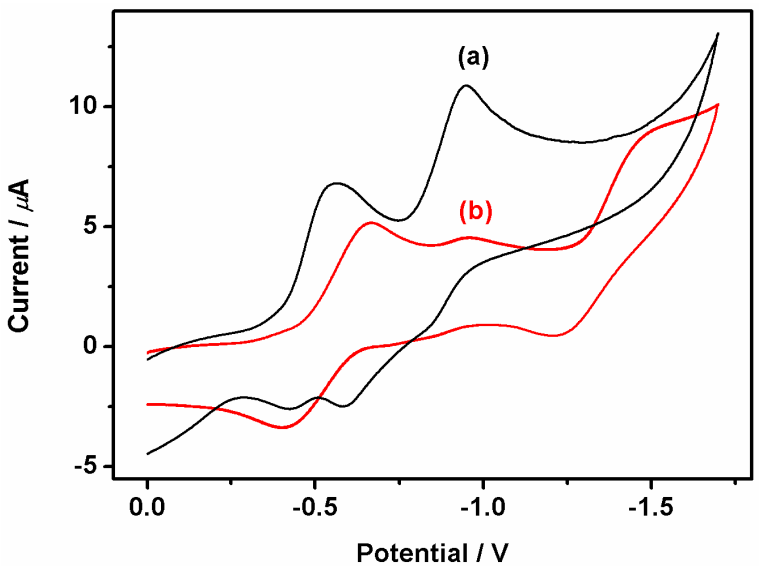

Figure S12. Cyclic voltammograms of (a) **1** and (b) **2** in water containing 0.1 M NaCl as the supporting electrolyte (vs. Ag/AgCl) at 100 mV·s^{-1} ([**1**] = [**2**] = 1.0 × 10^{-3} M).

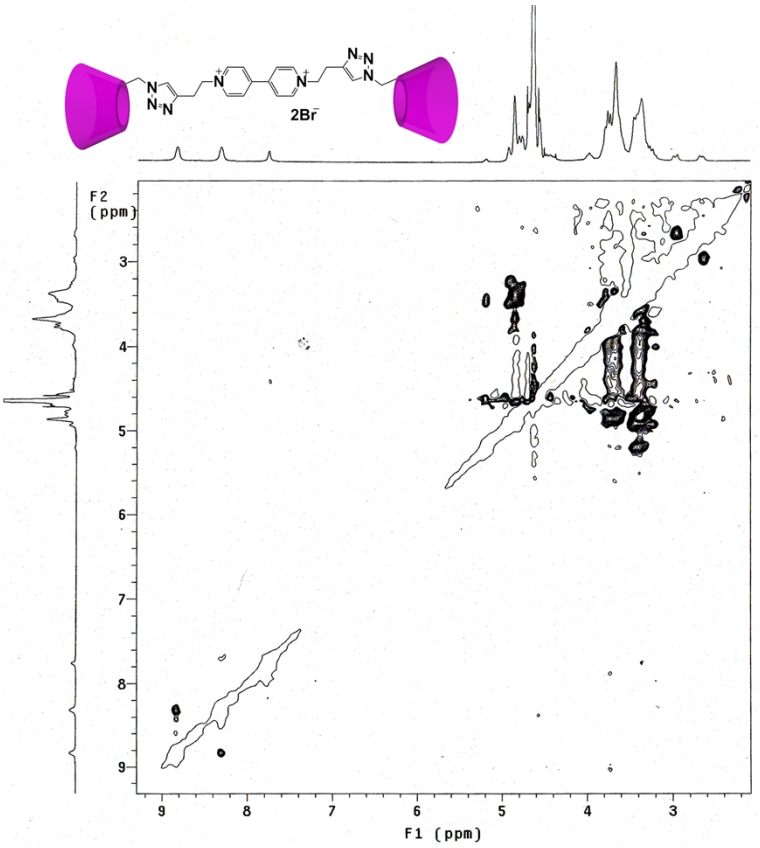

Figure S13. ^{1}H ROESY spectrum of host **1** after a mixing time of 0.220 s ([**1**] = 2.2 ×

10^{-3} M, 300 MHz, D_2O, 25 °C).

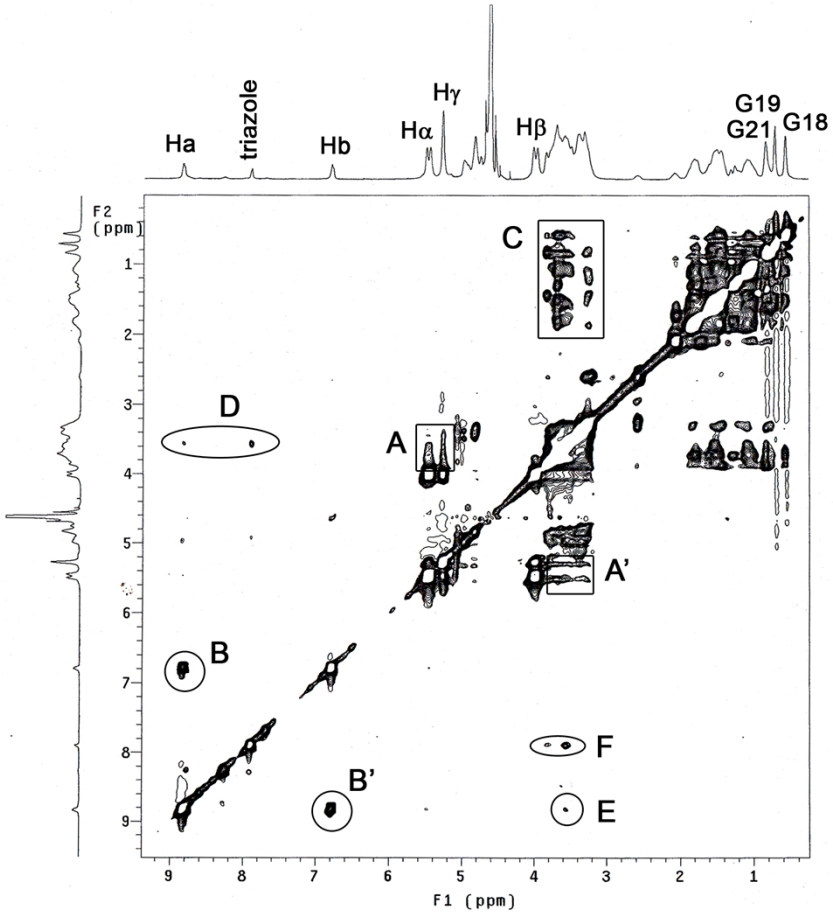

Figure S14. ^{1}H NOESY spectrum of host CA⊂**2** after a mixing time of 0.190 s ([**2**] = 2.2×10^{-3} M and [CA] = 5.0×10^{-3} M, 300 MHz, D_2O, 25 °C).

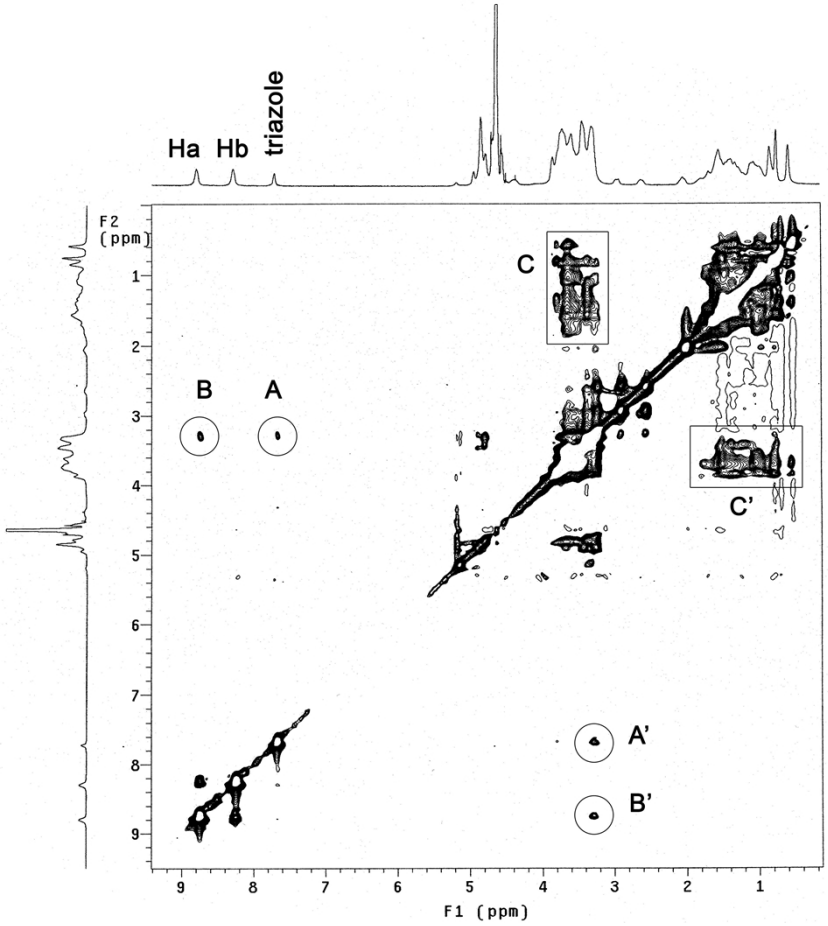

Figure S15. ^{1}H NOESY spectrum of complex DCA⊂**1** after a mixing time of 0.200 s ([**1**] = 2.2 × 10^{-3} M and [DCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)

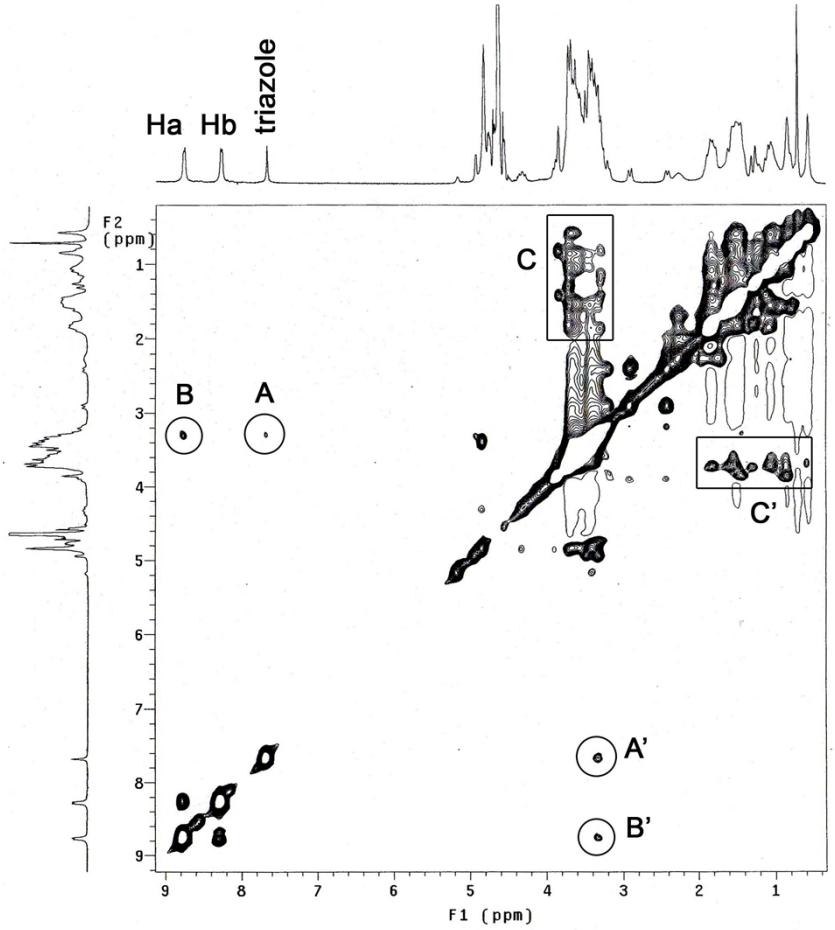

Figure S16. ^{1}H NOESY spectrum of complex GCA⊂**1** after a mixing time of 0.210 s ([**1**] = 2.2 × 10^{-3} M and [GCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)

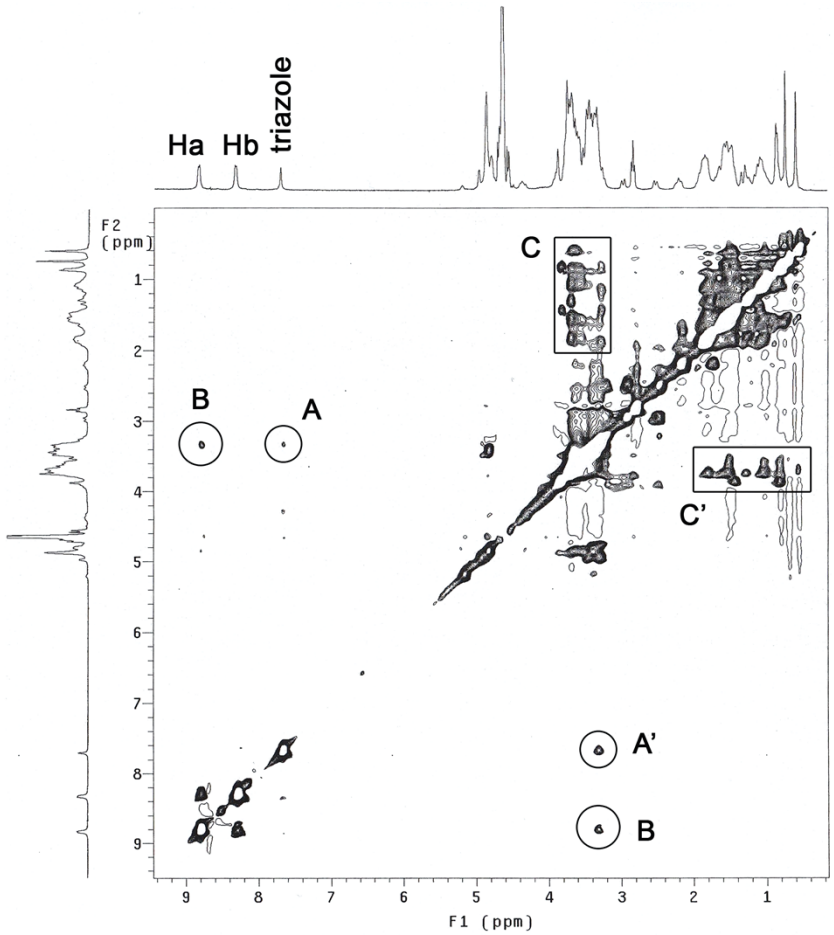

Figure S17. ^{1}H NOESY spectrum of complex TCA⊂**1** after a mixing time of 0.210 s ([**1**] = 2.2 × 10^{-3} M and [TCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)

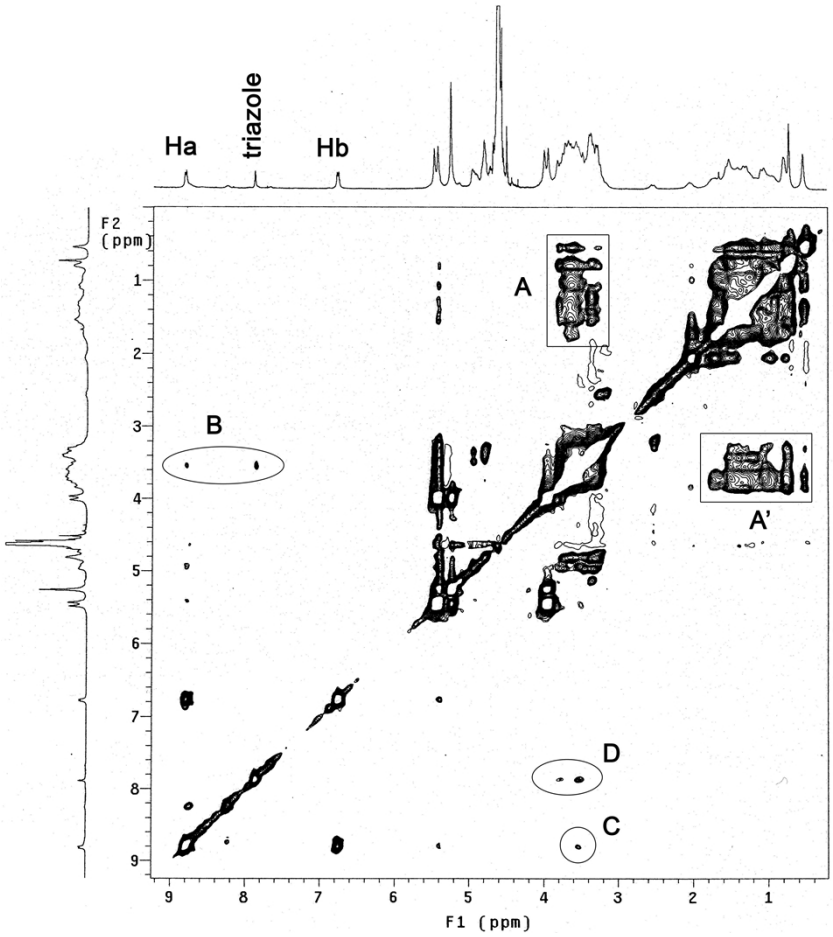

Figure S18. ^{1}H NOESY spectrum of complex DCA⊂**2** after a mixing time of 0.190 s ([**2**] = 2.2 × 10^{-3} M and [DCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)

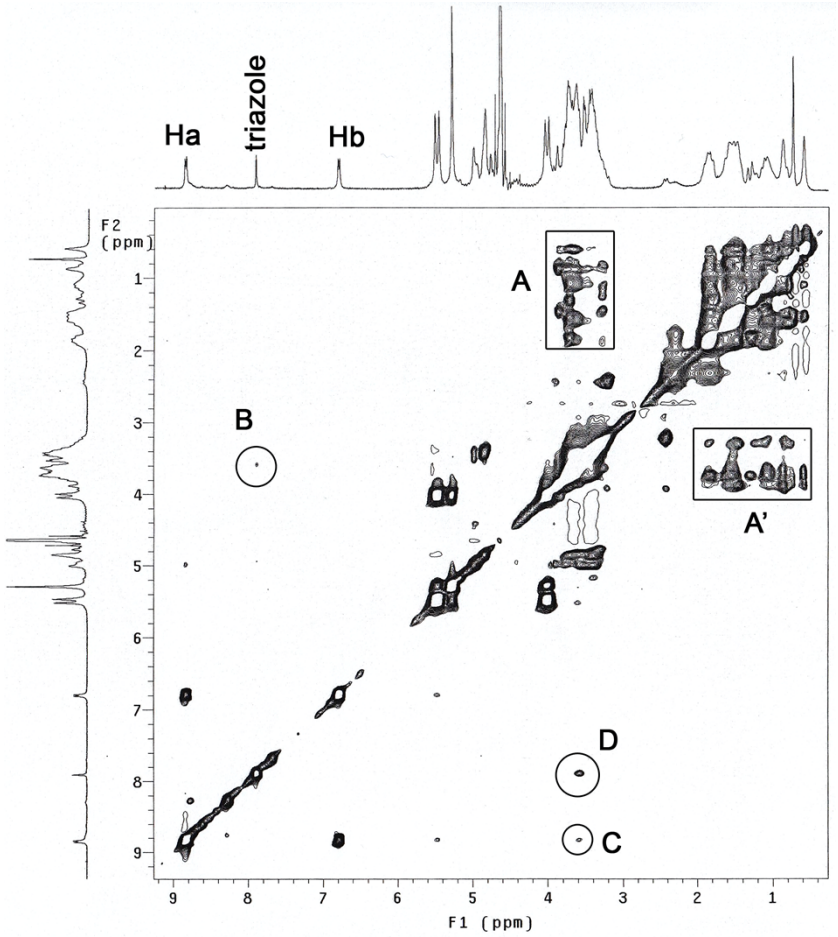

Figure S19. ^{1}H NOESY spectrum of complex GCA⊂**2** after a mixing time of 0.200 s ([**2**] = 2.2 × 10^{-3} M and [GCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)

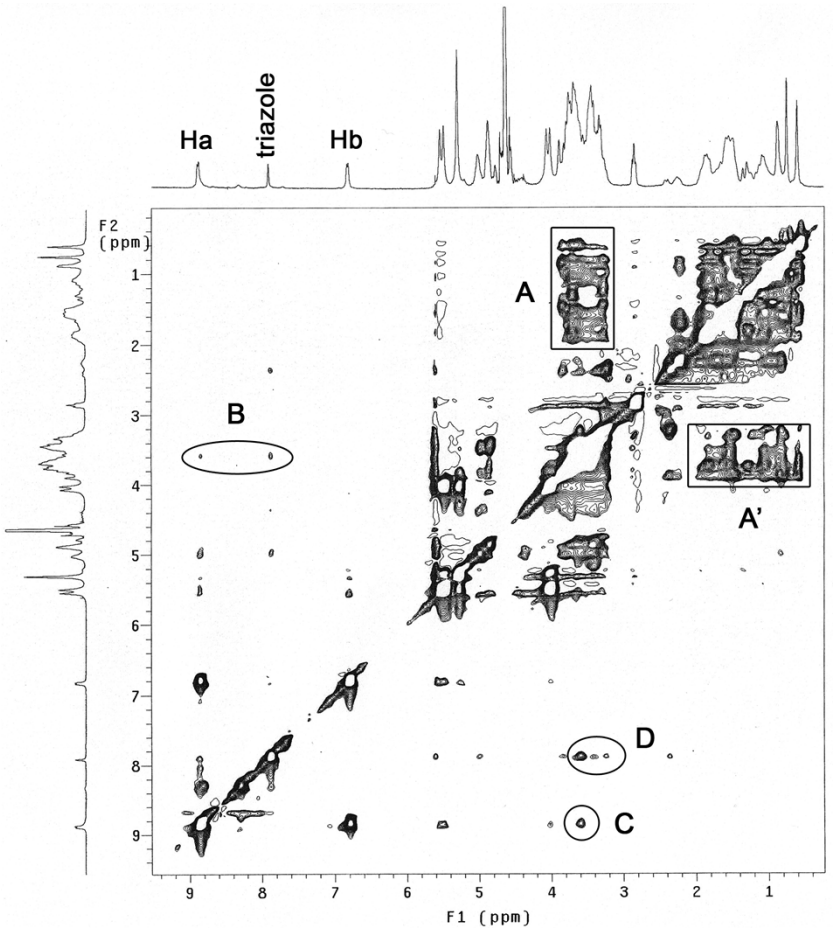

Figure S20. ^{1}H NOESY spectrum of complex TCA⊂**2** after a mixing time of 0.200 s ([**2**] = 2.2 × 10^{-3} M and [TCA] = 5.0 × 10^{-3} M, 300 MHz, D_2O, 25 °C)