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β and γ-Cyclodextrin dimers: design, characterization and in silico studies to explore the cooperative effect of the cavities

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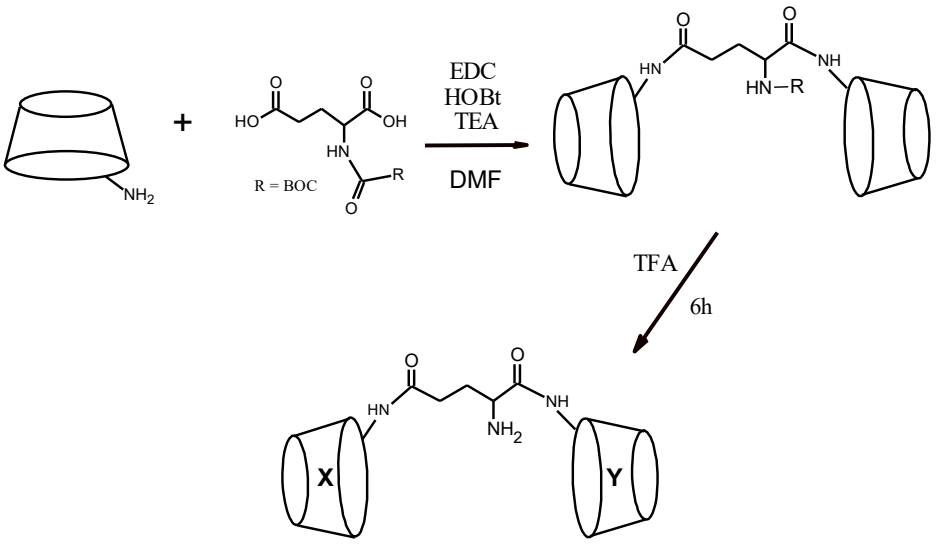

Figure 1S. Synthesis scheme of CyD2Glu systems. R is BOC group

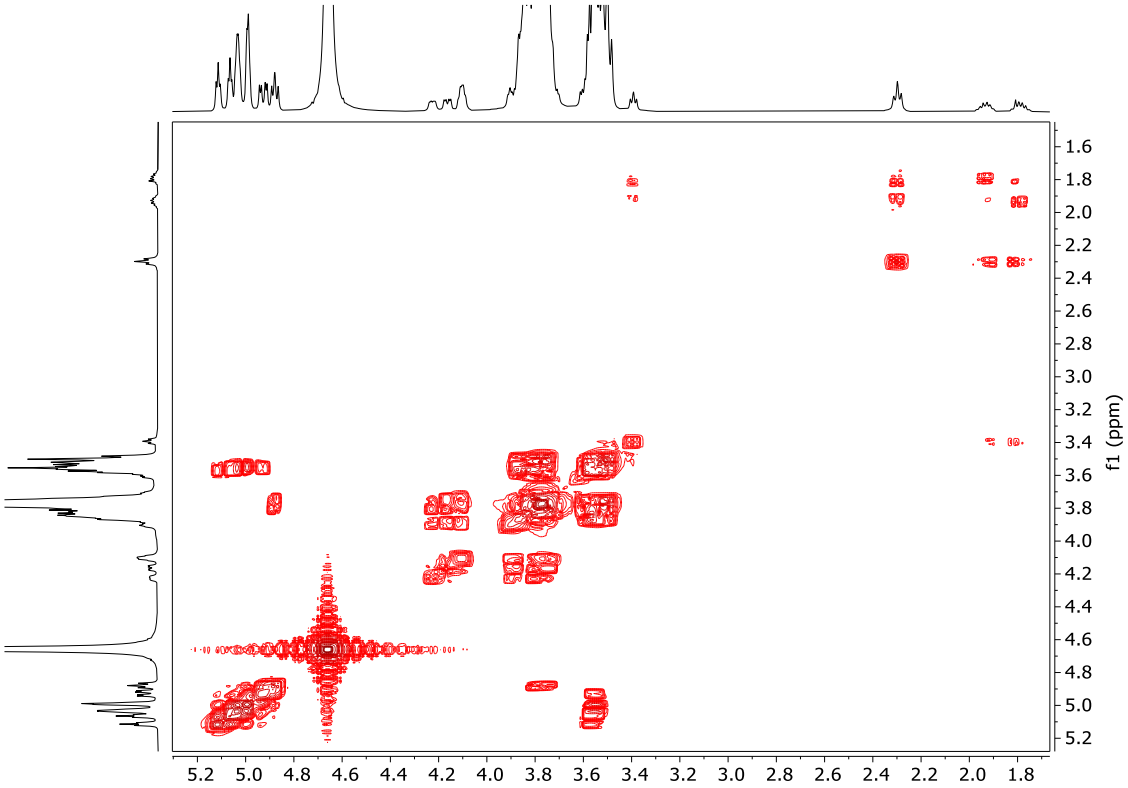

Figure 2S. COSY spectrum of γCyD2Glu (D_2O, 500 MHz)

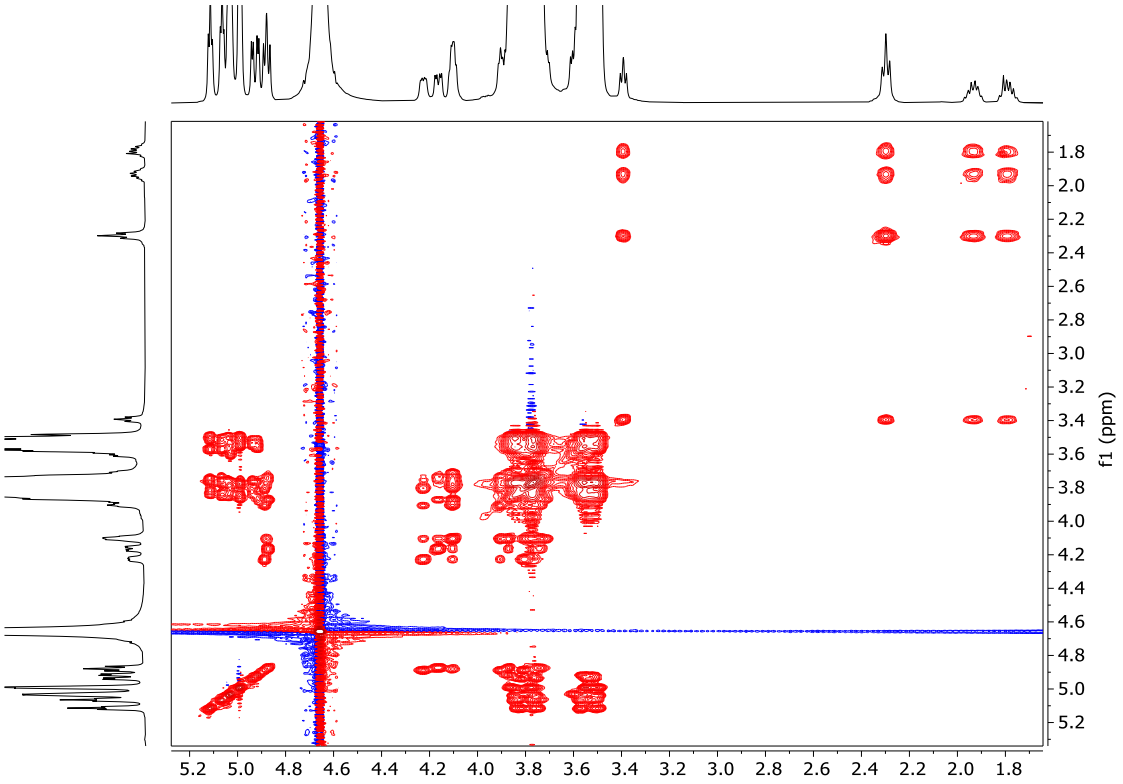

Figure 3S. TOCSY spectrum of γCyD2Glu (D_2O, 500 MHz)

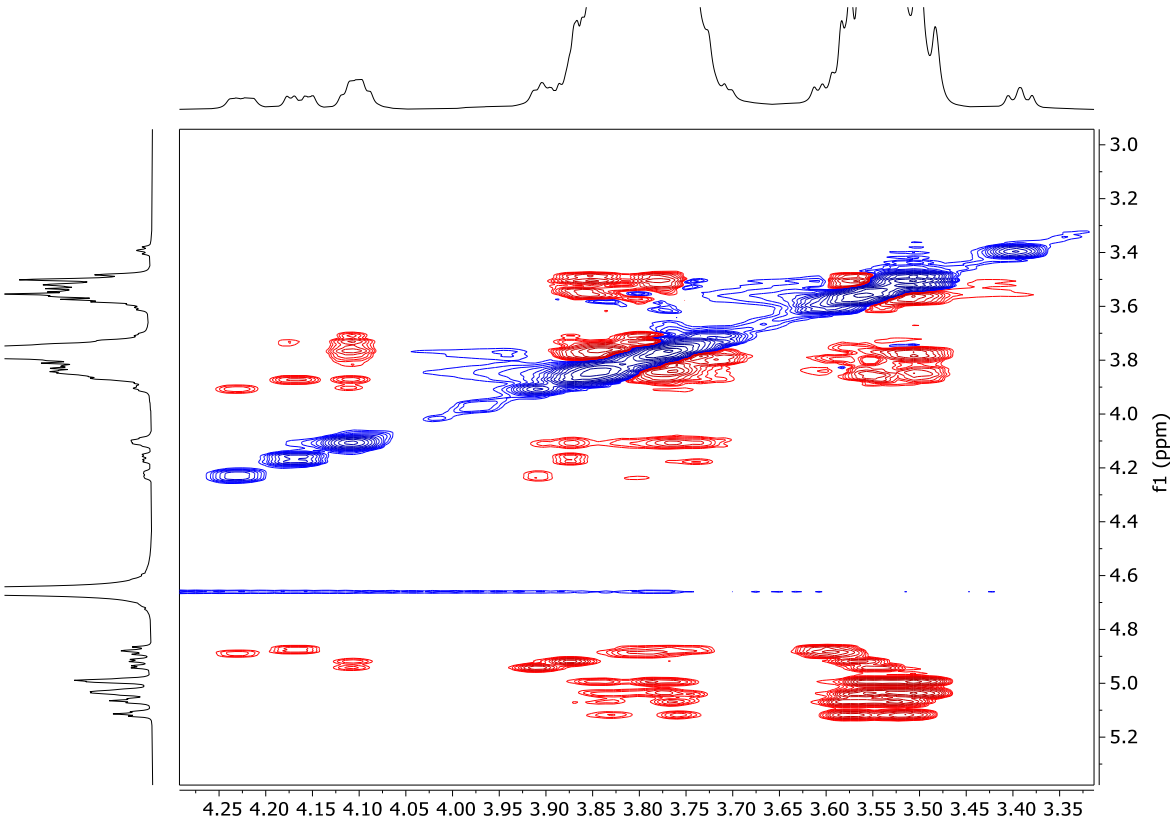

Figure 4S. ROESY of γCyD2Glu (D_2O, 500 MHz)

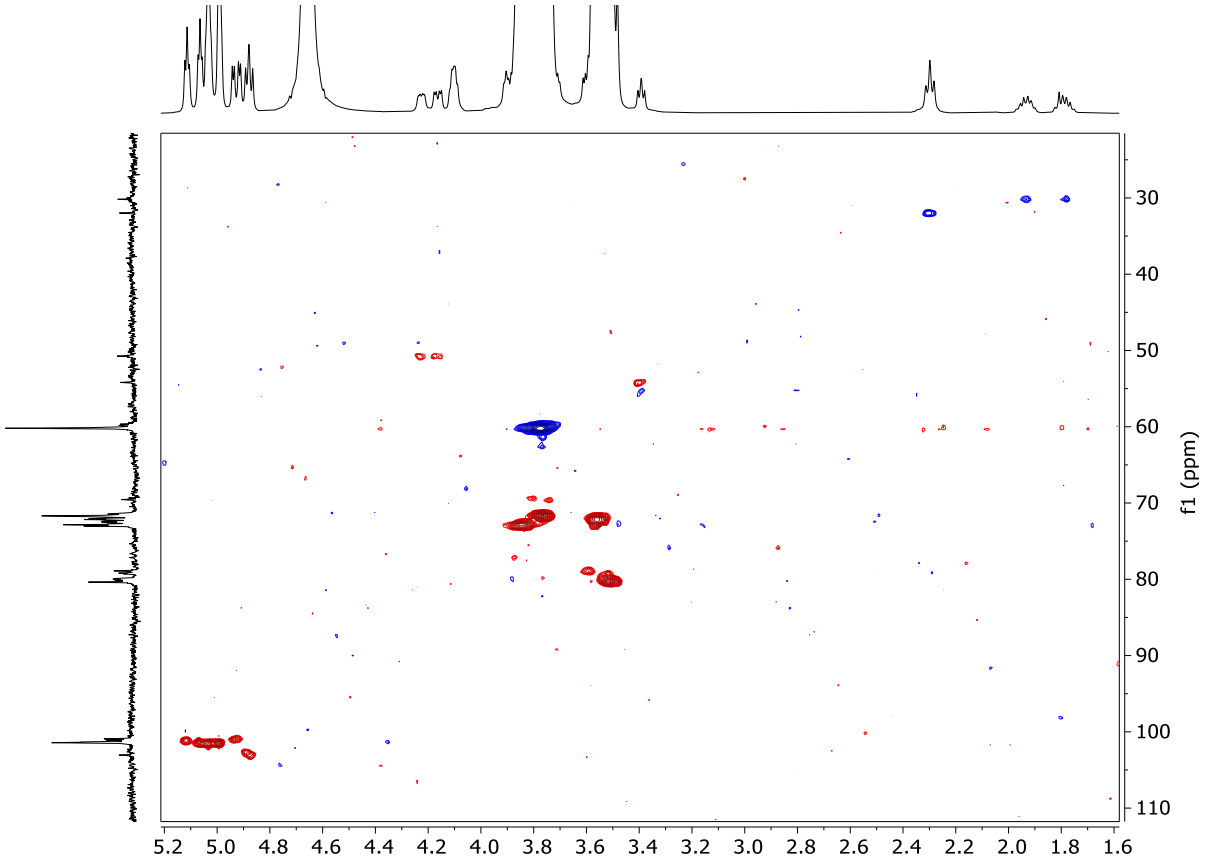

Figure 5S. HSQCAD spectrum of γCyD2Glu (D_2O, 500 MHz)

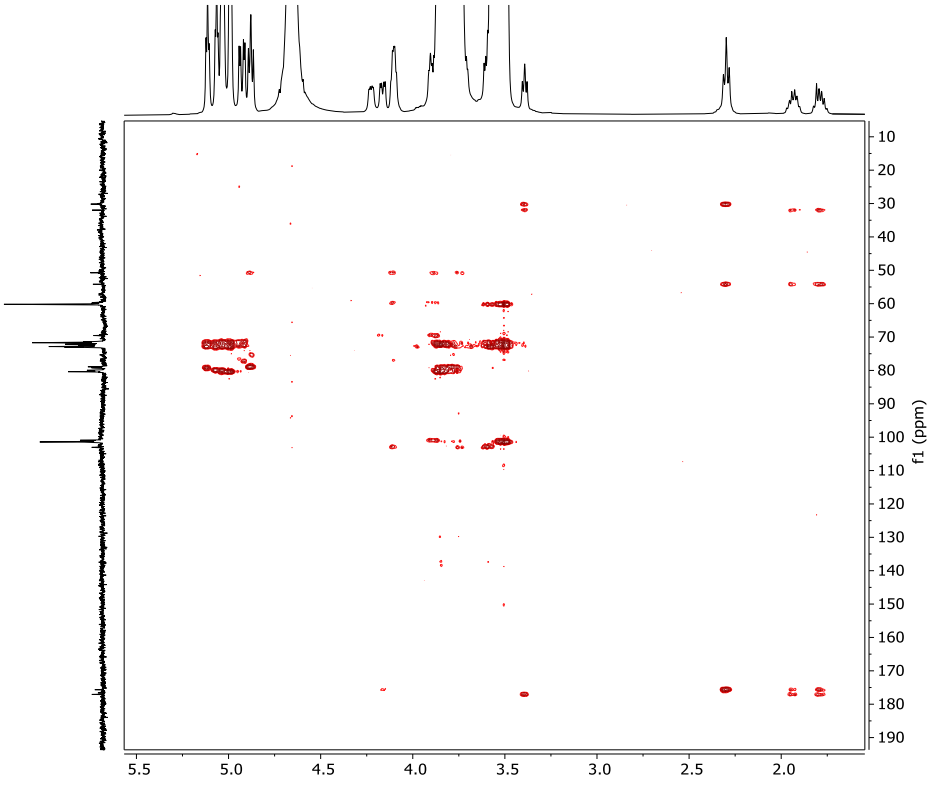

Figure 6S. HMQC spectrum of γCyD2Glu (D_2O, 500 MHz)

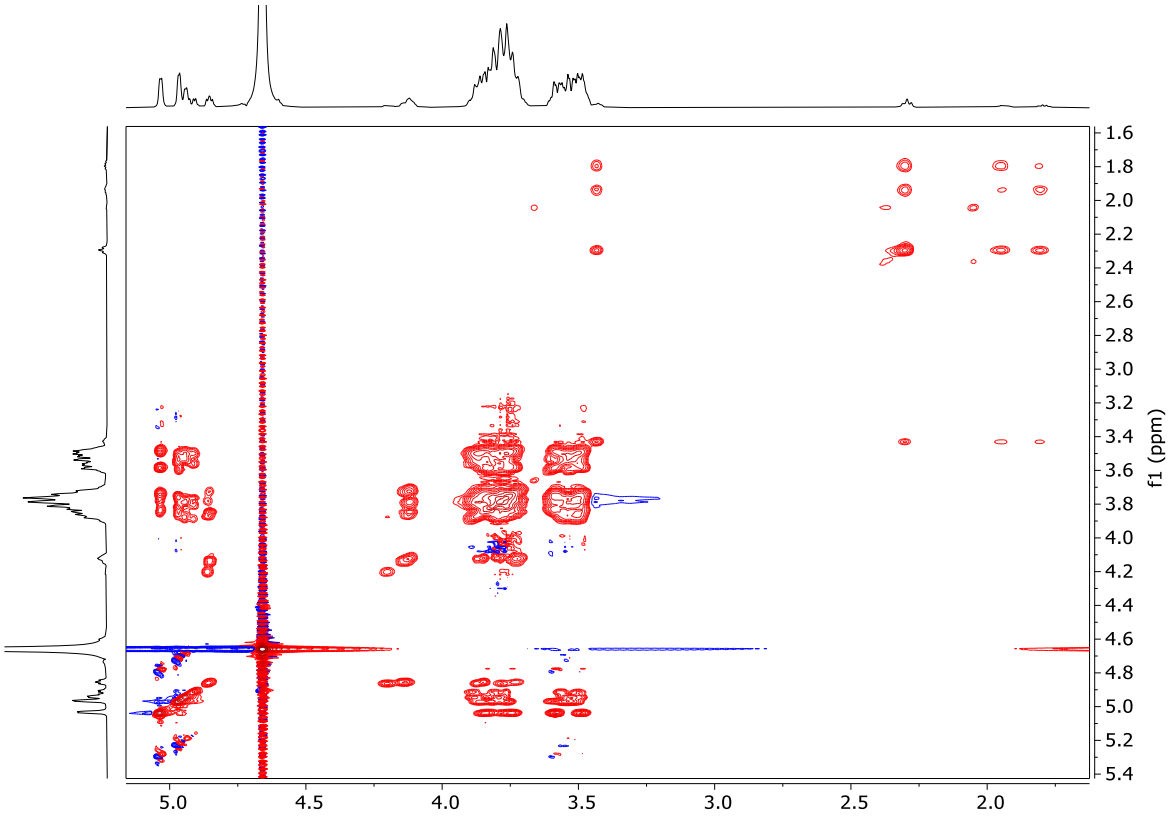

Figure 7S. COSY spectrum of βCyD2Glu (D_2O, 500 MHz)

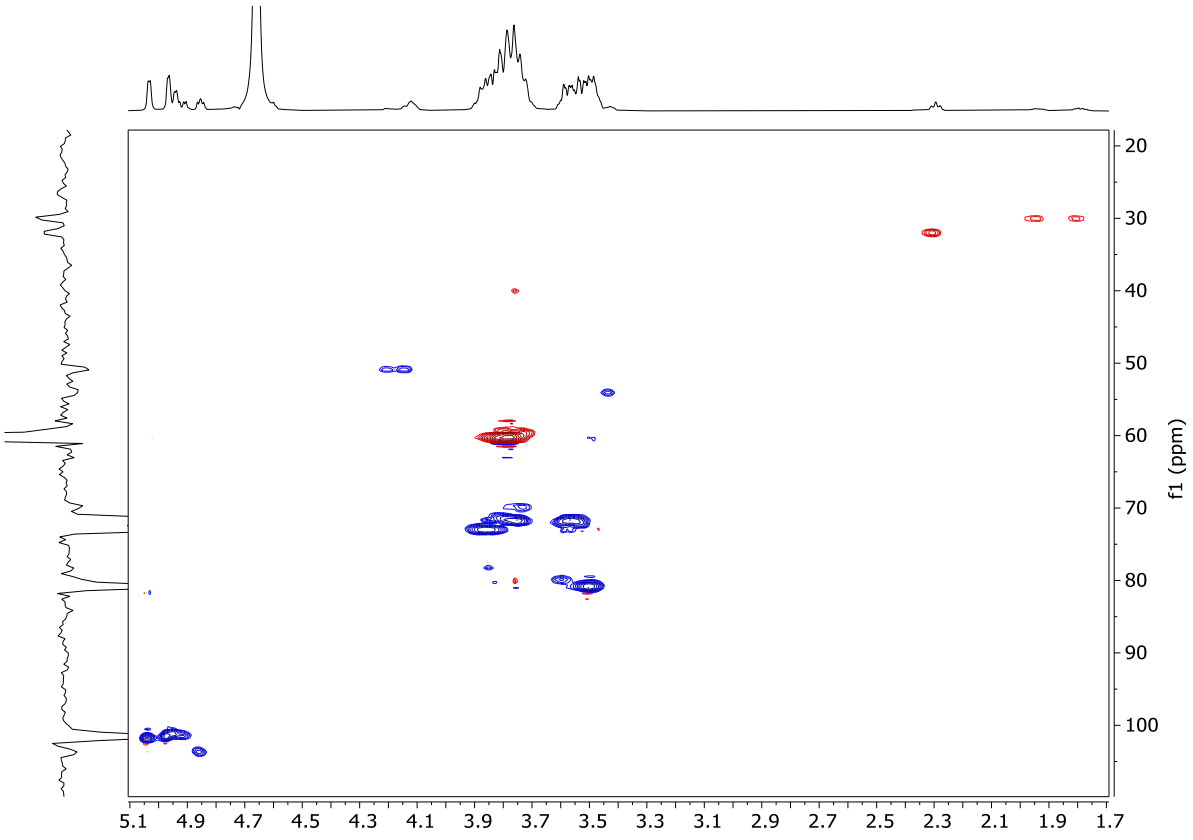

Figure 8S. HSQC spectrum of βCyD2Glu (D_2O, 500 MHz)

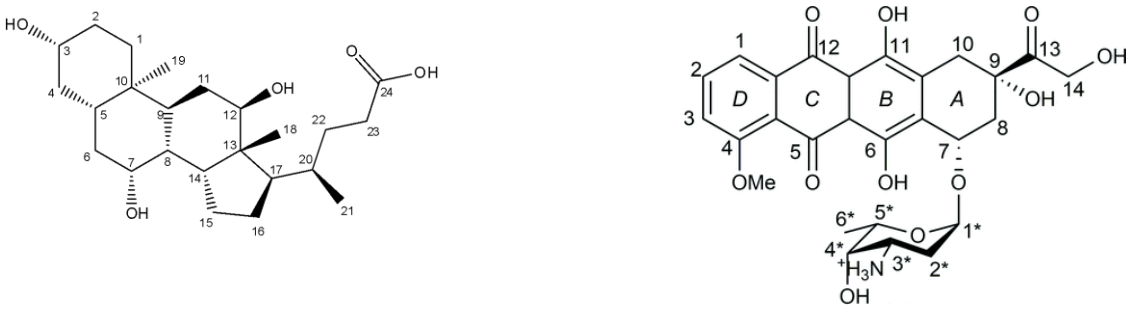

Figure 9S. Cholic acid and DOXO numbering

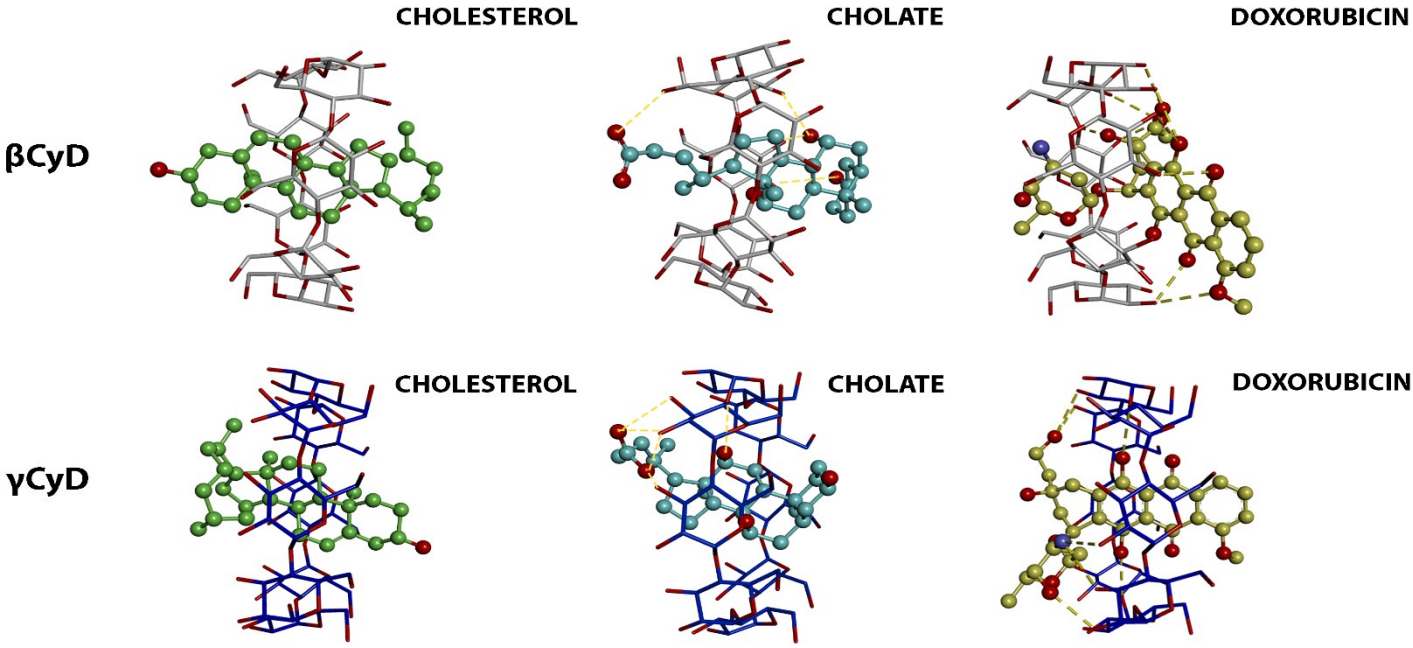

Figure 10S. Docking poses of cholate (blue) cholesterol (green) and doxorubicin (yellow) into the cavity of native β- and γ-cyclodextrins. H bond interactions are depicted as dotted yellow lines

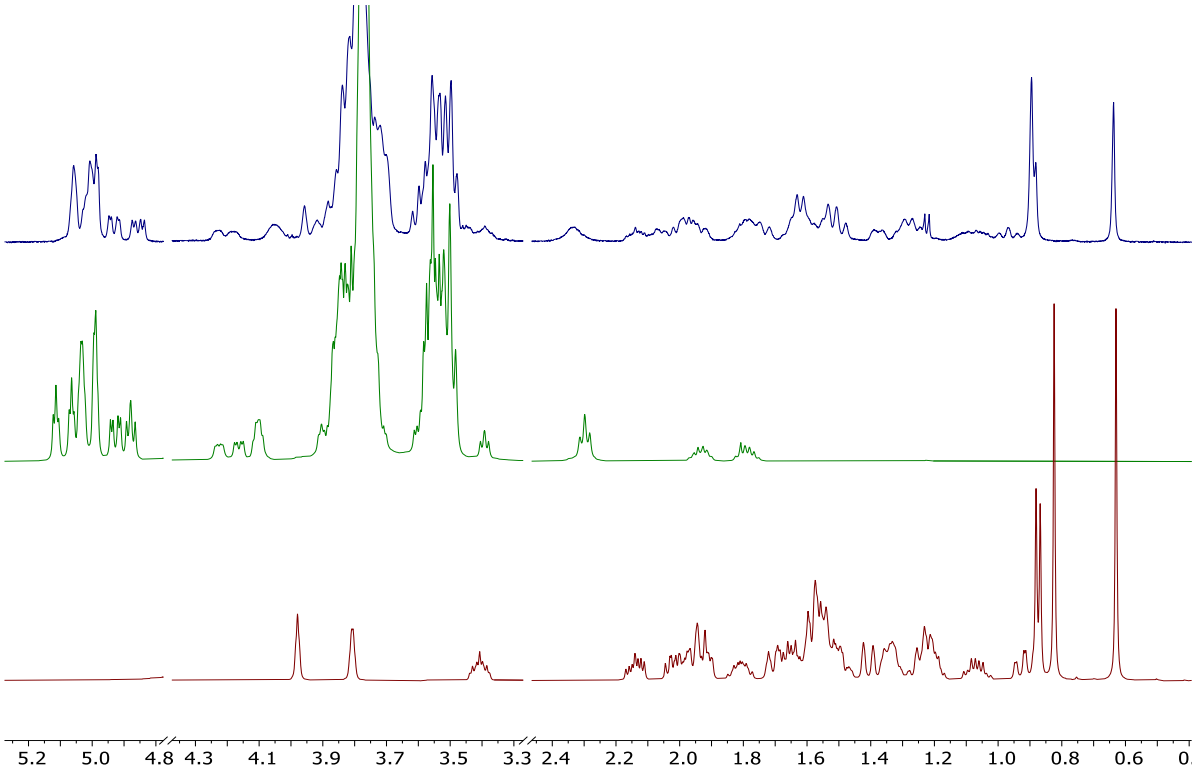

Figure 11S. 1H NMR spectrum of Ch/γCyD2Glu 1:1 molar ratio (500 MHz, D2O): γCh/βCyD2Glu (top), γCyD2Glu (bottom) and Ch alone (middle)

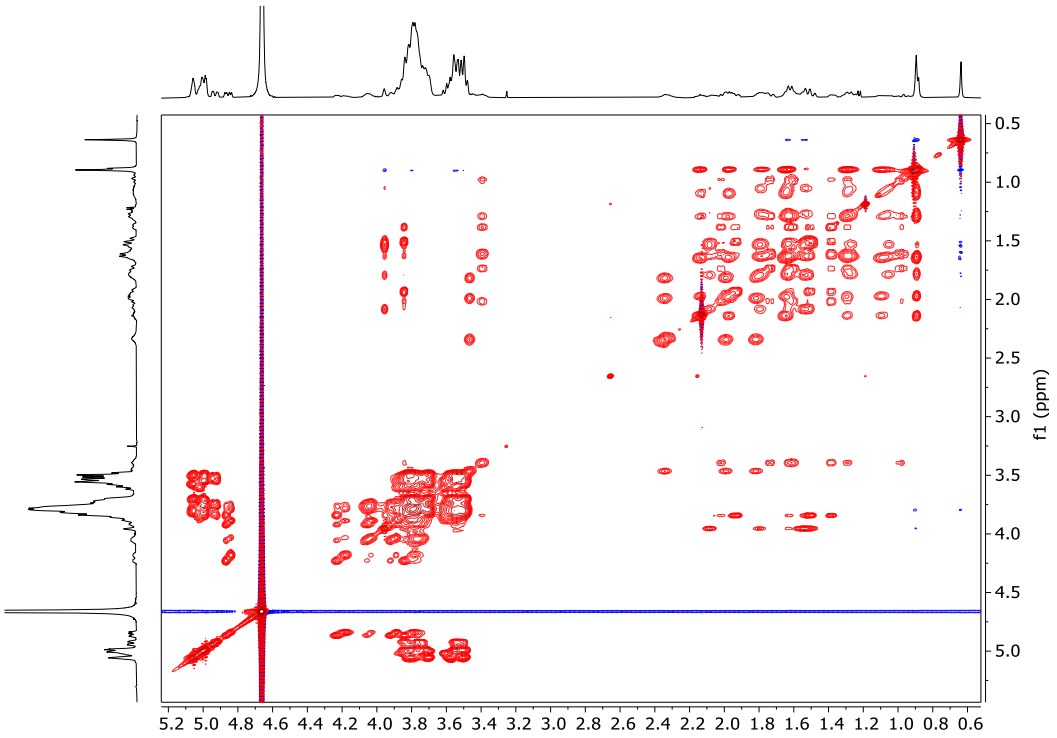

Figure 12S. ^{1}H NMR spectrum of γCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

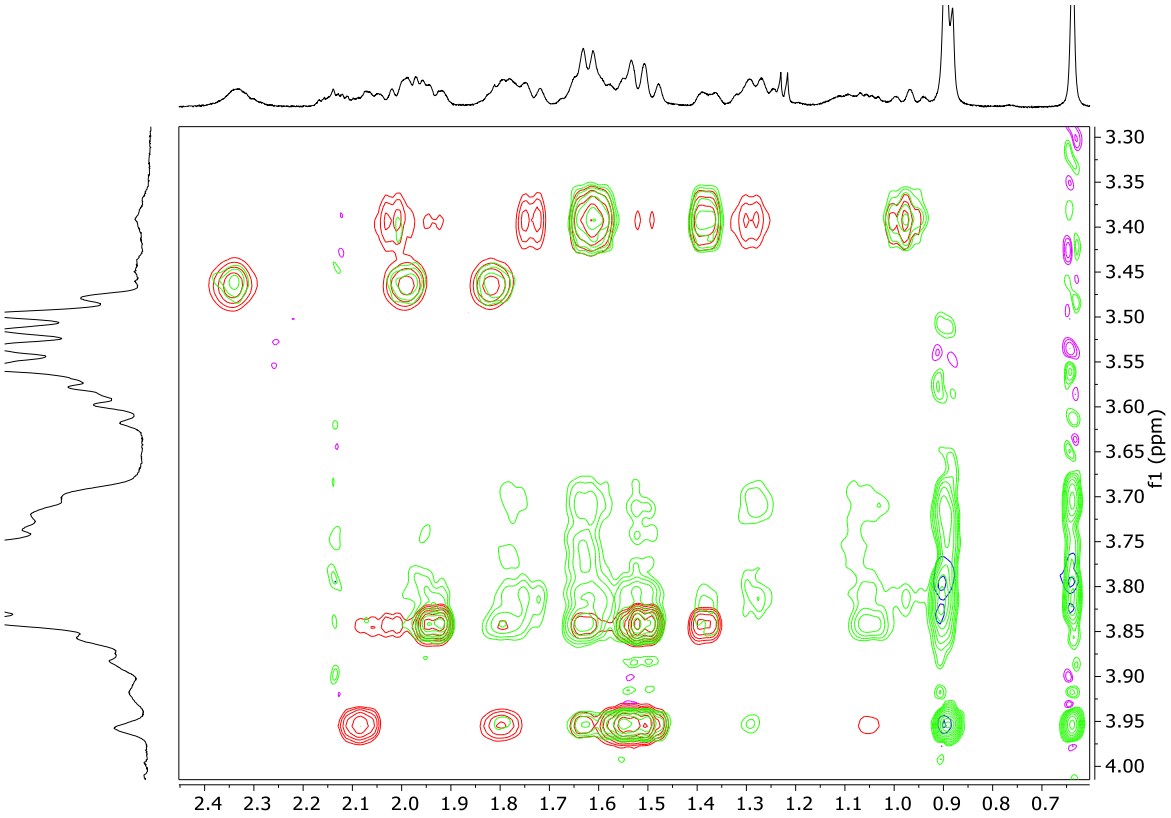

Figure 13S. Overlapped TOCSY (Red) and ROESY (Green) spectra of γCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

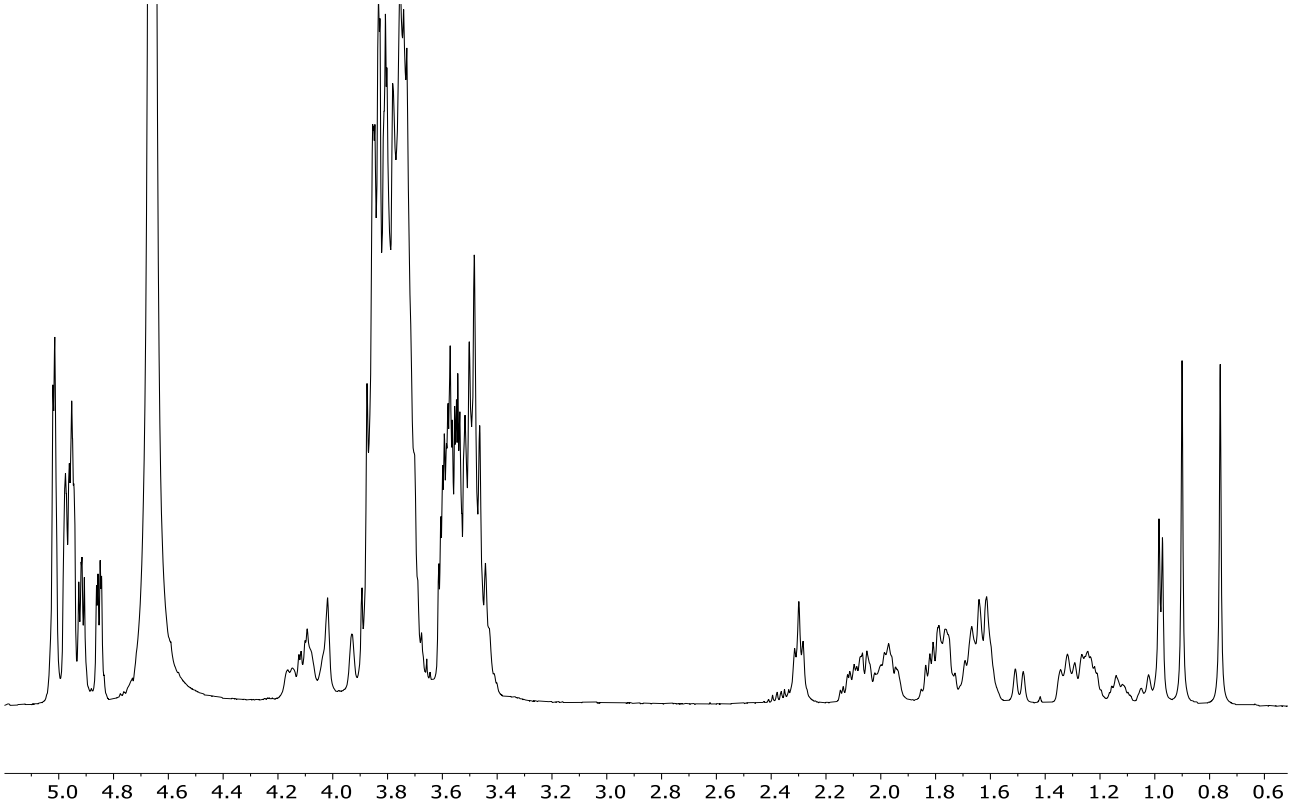

Figure 14S. 1H NMR spectrum of βCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

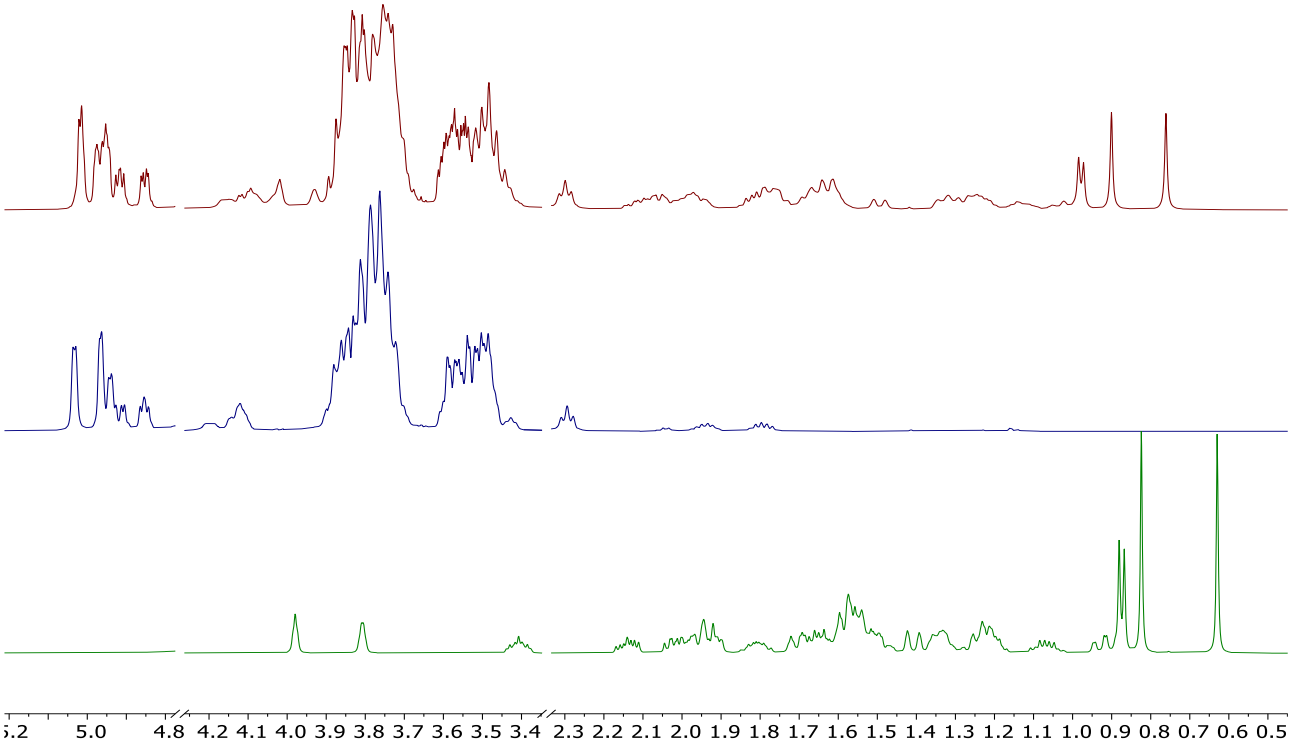

Figure 15S. 1H NMR spectrum of Ch/CyD2Glu 1:1 molar ratio (500 MHz, D2O): Ch/βCyD2Glu (top), βCyD2Glu (bottom) and Ch alone (middle)

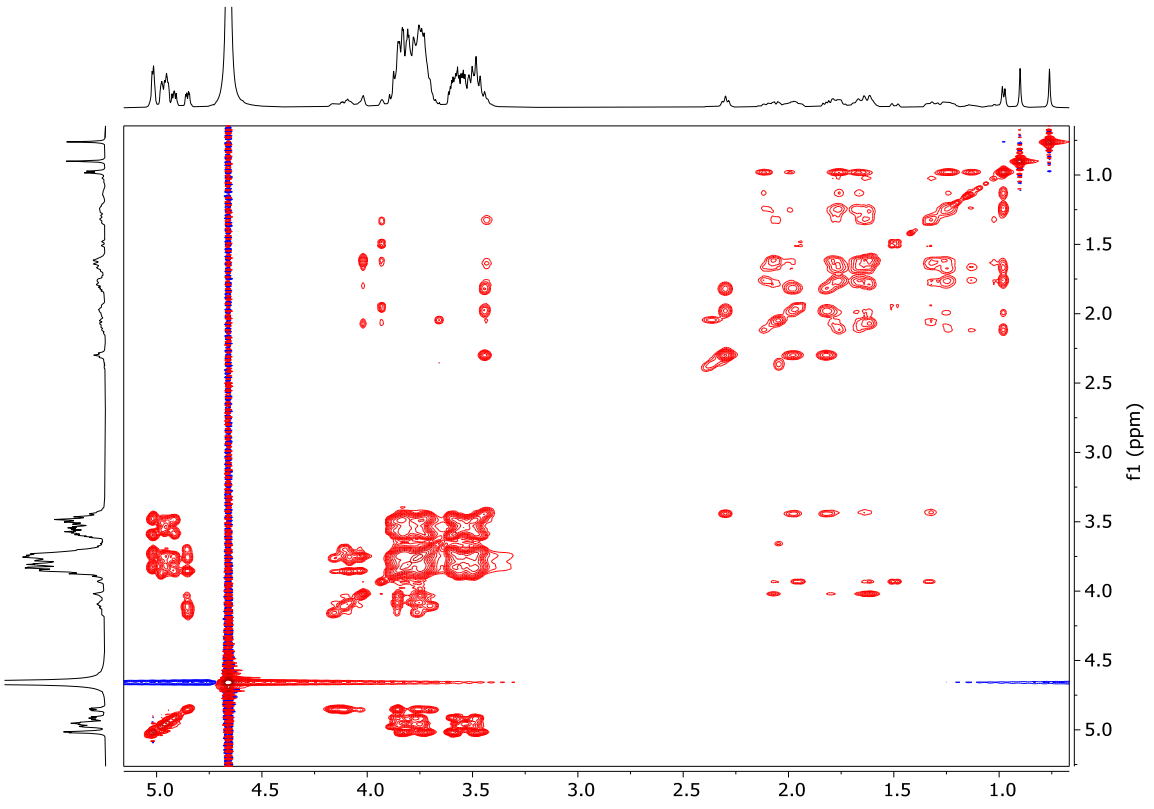

Figure 16S. TOCSY spectrum of βCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

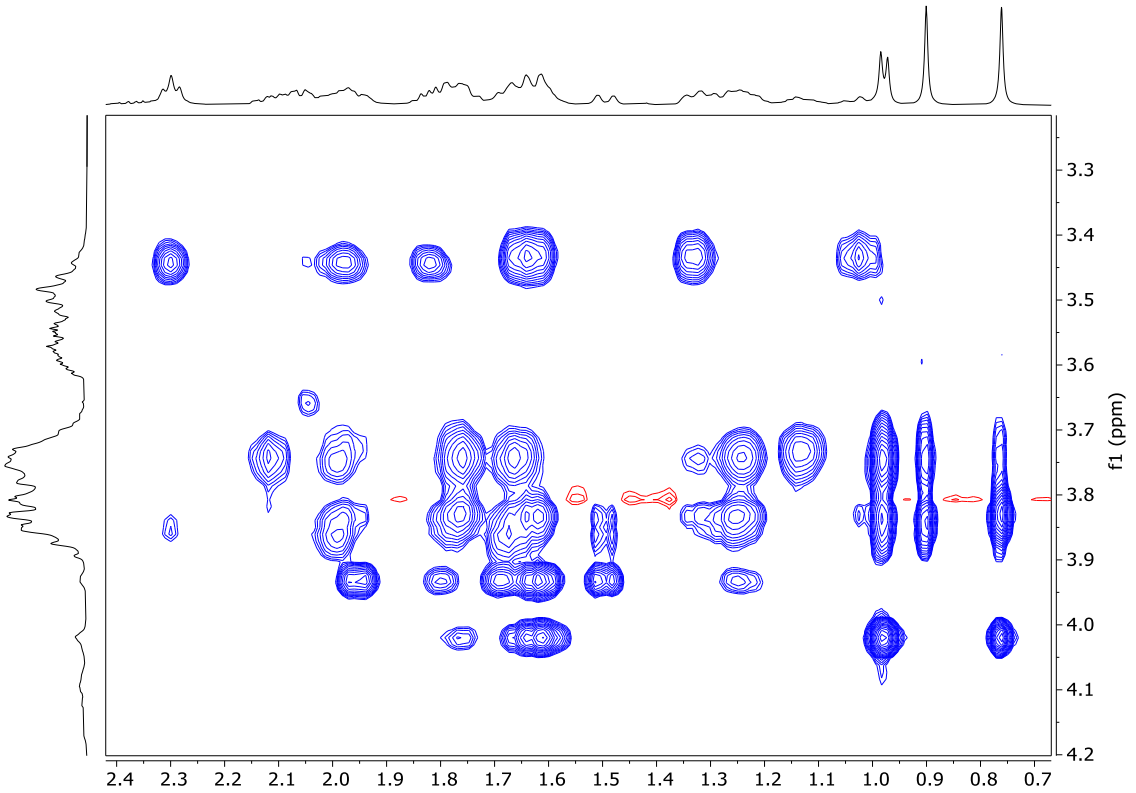

Figure 17S. ROESY of βCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

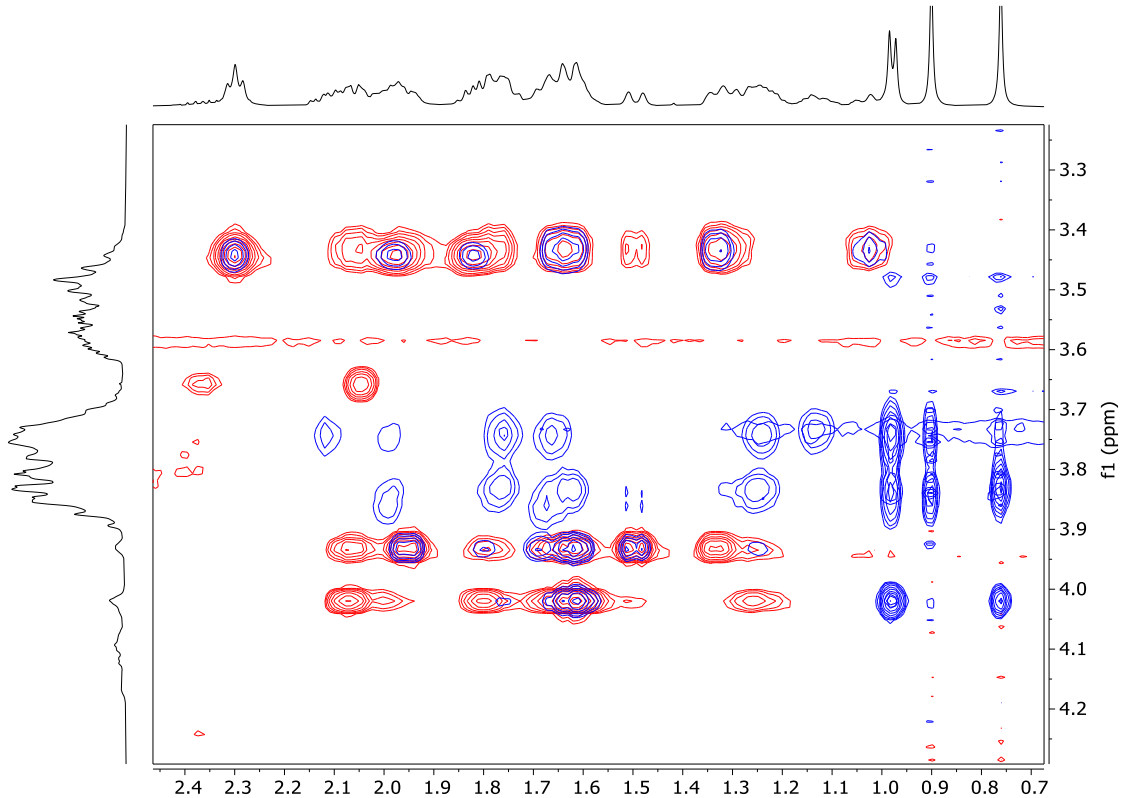

Figure 18S. Overlapped TOCSY (Red) and ROESY (Blue) spectra of βCyD2Glu/Cholate 1:1 (D_2O, 500 MHz)

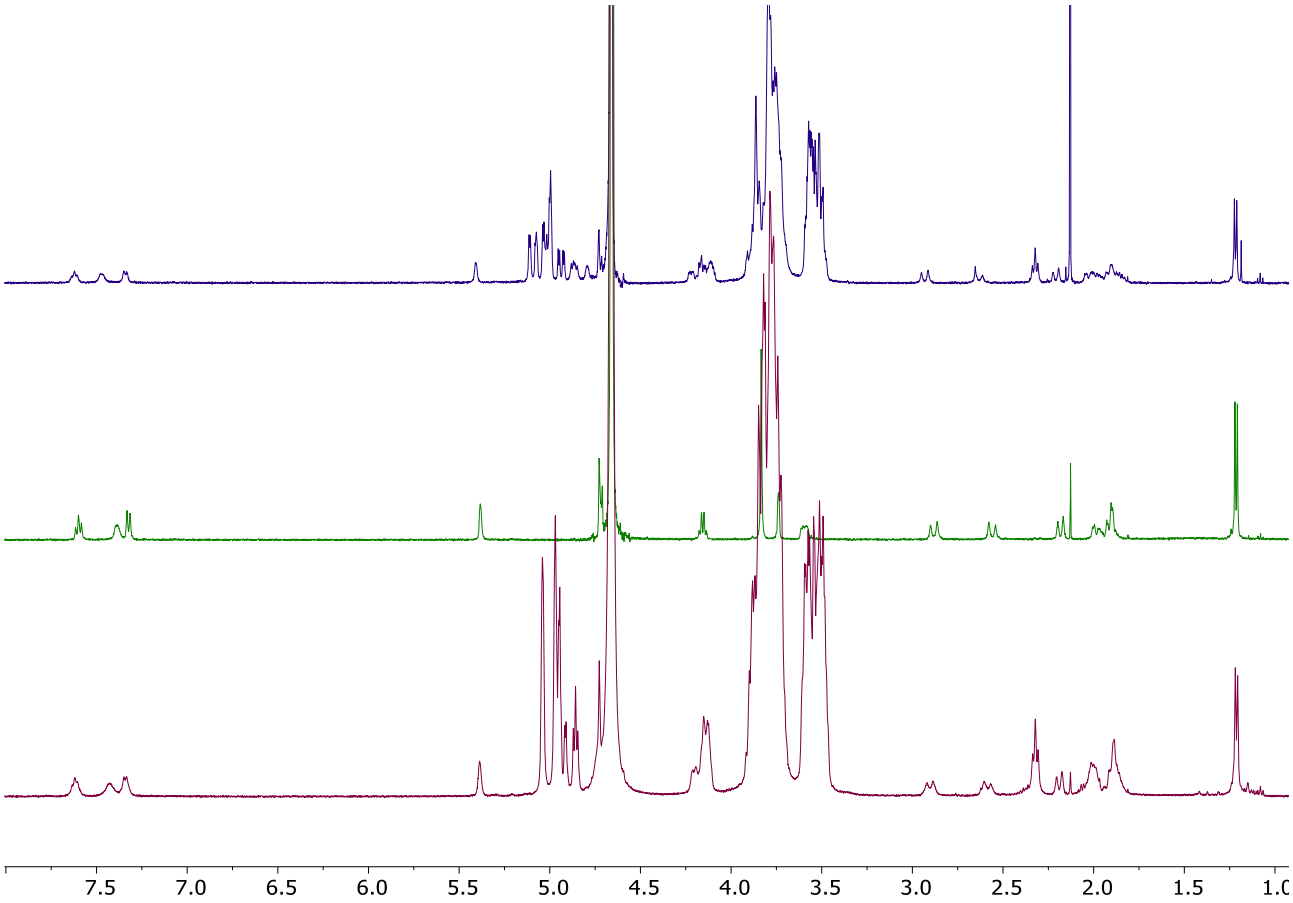

Figure 19S. ^{1}H NMR spectrum (D_2O, 500 MHz) of γCyD2Glu/DOXO (top); doxo (middle); βCyD2Glu/DOXO bottom. Acetone trace are present in γCyD2Glu spectrum at 2.1 ppm

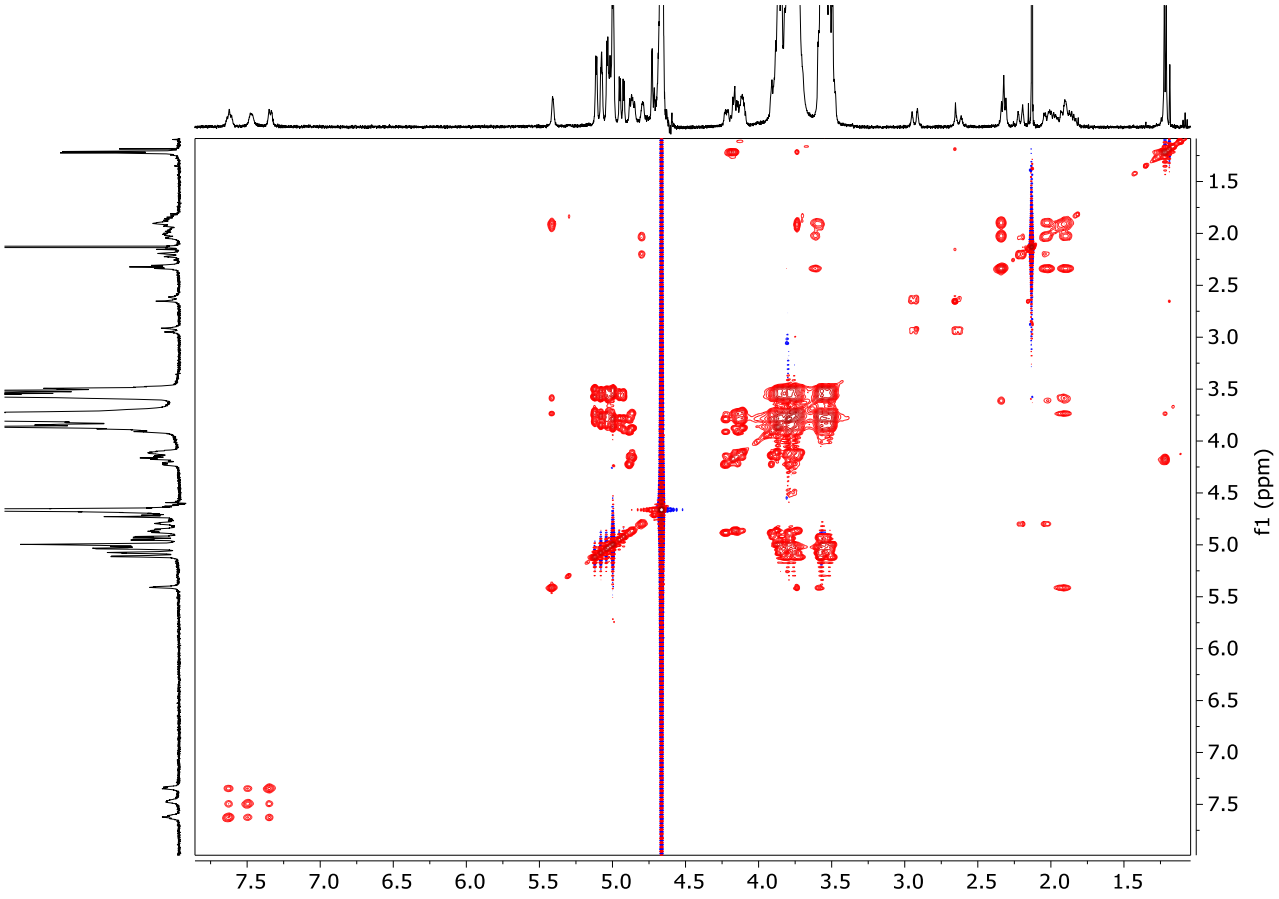

Figure 20S. TOCSY of γCyD2Glu/DOXO 1:1 (D_2O, 500 MHz)

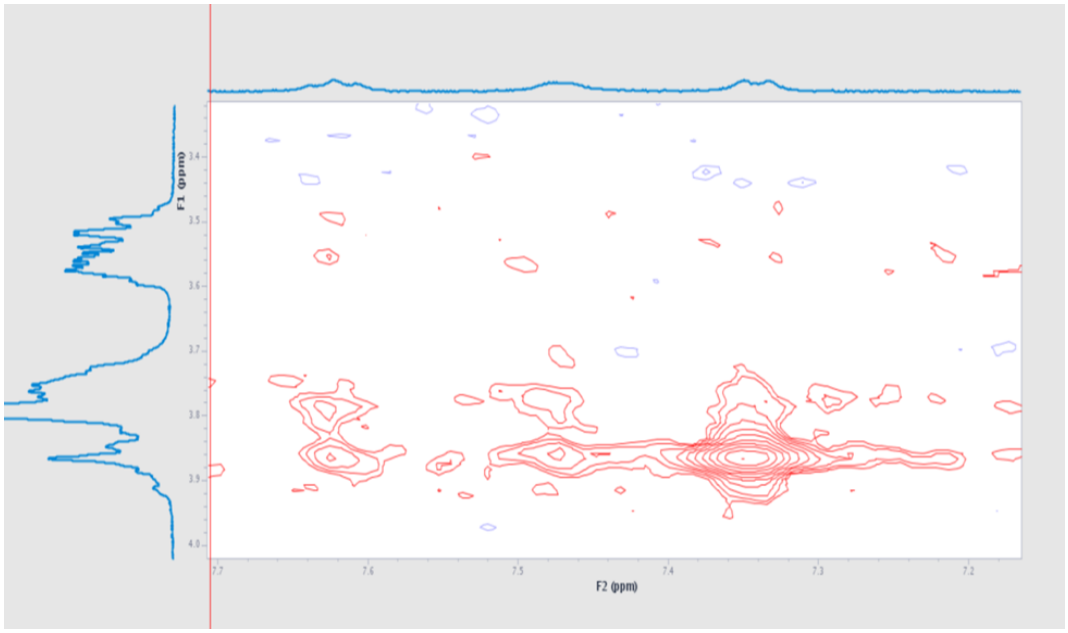

Figure 21S. ROESY of γCyD2Glu/DOXO 1:1 (D_2O, 500 MHz)