Supporting Information 1

for

Association of aescin with β- and γ-cyclodextrins studied by DFT calculations and spectroscopic methods

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Supplement to ^{1}H NMR studies in solution

a) Attemptive Job plot for the H3 proton of γCD in γCD·aescin mixtures

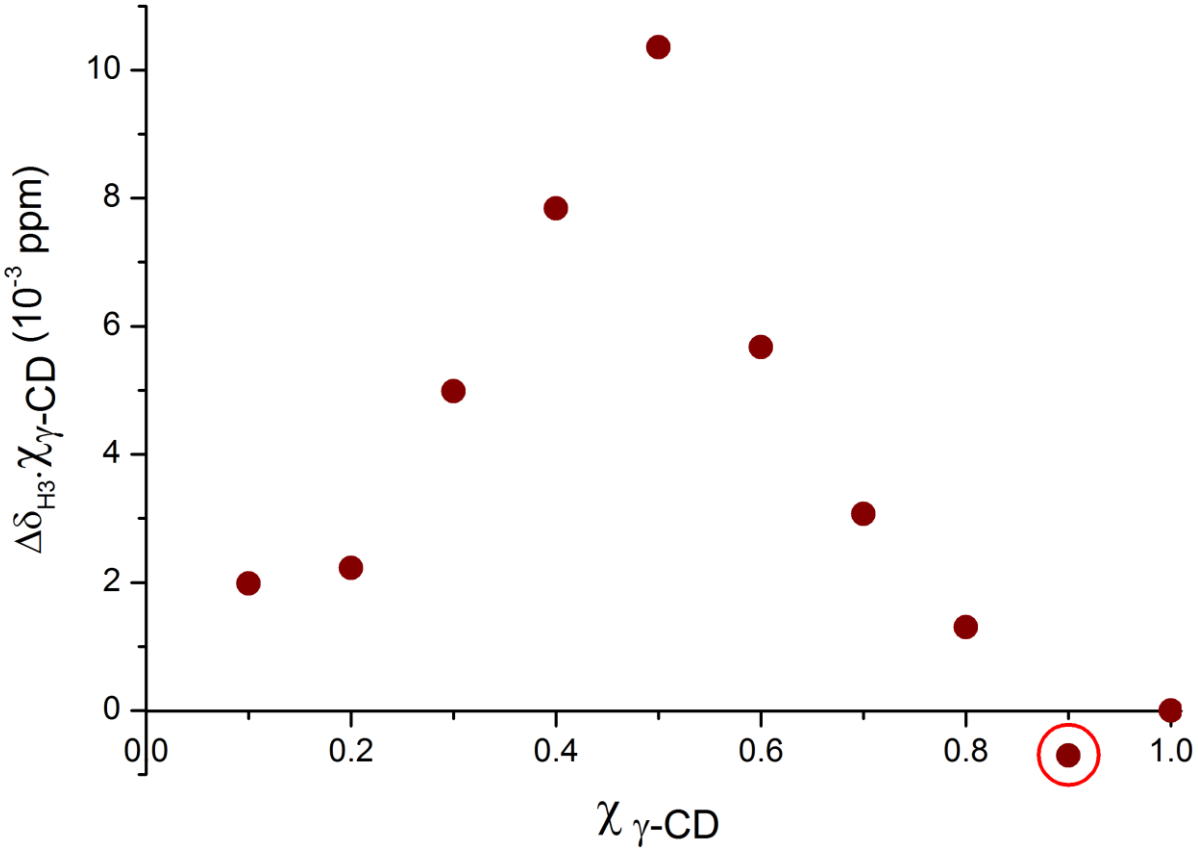

Figure S1.1: Job plot for the H3 proton of γ-CD in aqueous solutions containing γ-CD and aescin in a gradient of molar fraction. Note how the inconsistency in the proton shifts affords a negative value for the data point corresponding to the molar fraction of 0.9 (circled with red).

b) Apparent Inclusion Constants for βCD·aescin and γCD·aescin

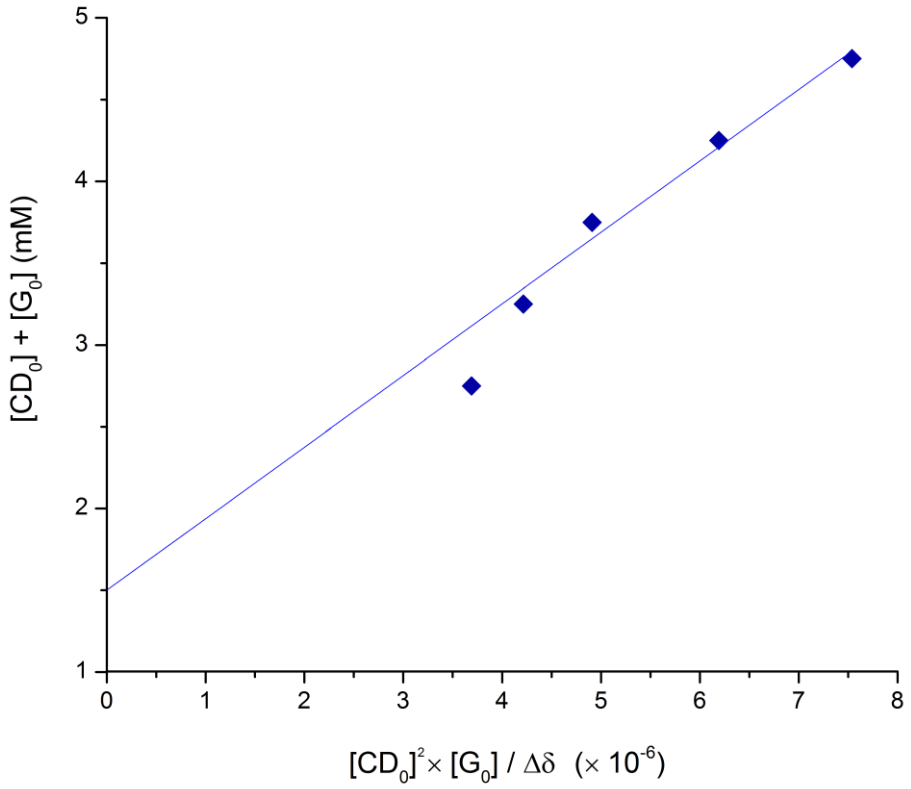

Figure S1.2: Graphical analysis of ^{1}H NMR shifts of the H5 proton of β-CD of one assay comprising a series of aqueous solutions containing 0.25 mM of β-CD and 2.5, 3.0, 3.5, 4.0 and 4.5 mM of aescin. Data is fitted to a line with r^2 value of 0.972 and x_0 (yy-intercept) of 0.00151, which allows estimating, for this data set, $K_{app} = 1/x_0 = 662$ M^{-1} (the values presented in the manuscript are the average (± RSD) of different calculated K_{app} values). The first data point was not used in the data fitting.

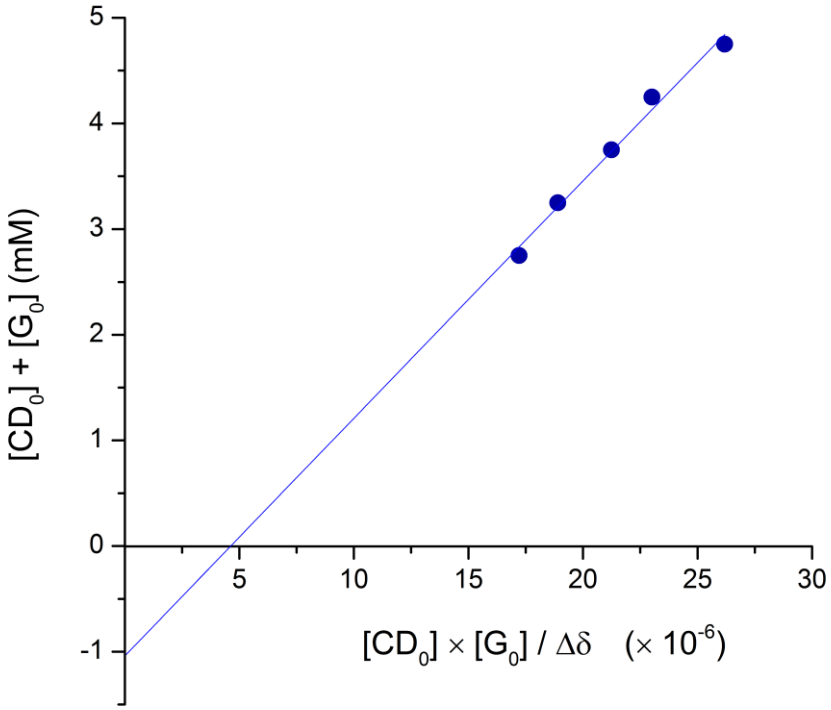

Figure S1.3: Graphical analysis of ^{1}H NMR shifts of the H5 proton of γ-CD of one assay comprising a series of aqueous solutions containing 0.25 mM of γ-CD and 2.5, 3.0, 3.5, 4.0 and 4.5 mM of aescin. Data is fitted to a line with r^2 value of 0.9834 and x_0 (yy-intercept) of -0.00102, which allows estimating $K_{app} = 1/x_0 = 980\ M^{-1}$.