Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A journey from calix[4]arene to calix[6] and calix[8]arene reveals more than a matter of size. Receptor concentration affects stability and stoichiometric nature of the complexes.

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Supporting Information

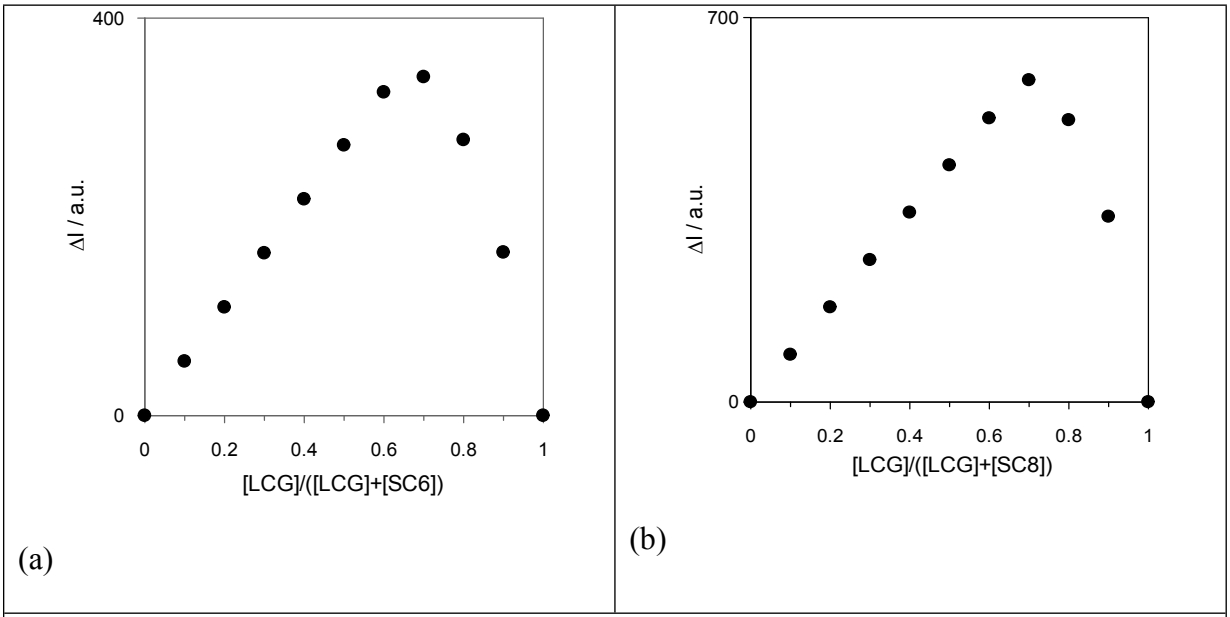


Figure S1 – Job plot analysis at 503 nm for lucigenin (LCG) with (a) SC6 or (b) SC8. The total concentration was 3.0 μM in both cases. Excitation was performed at 368 nm.

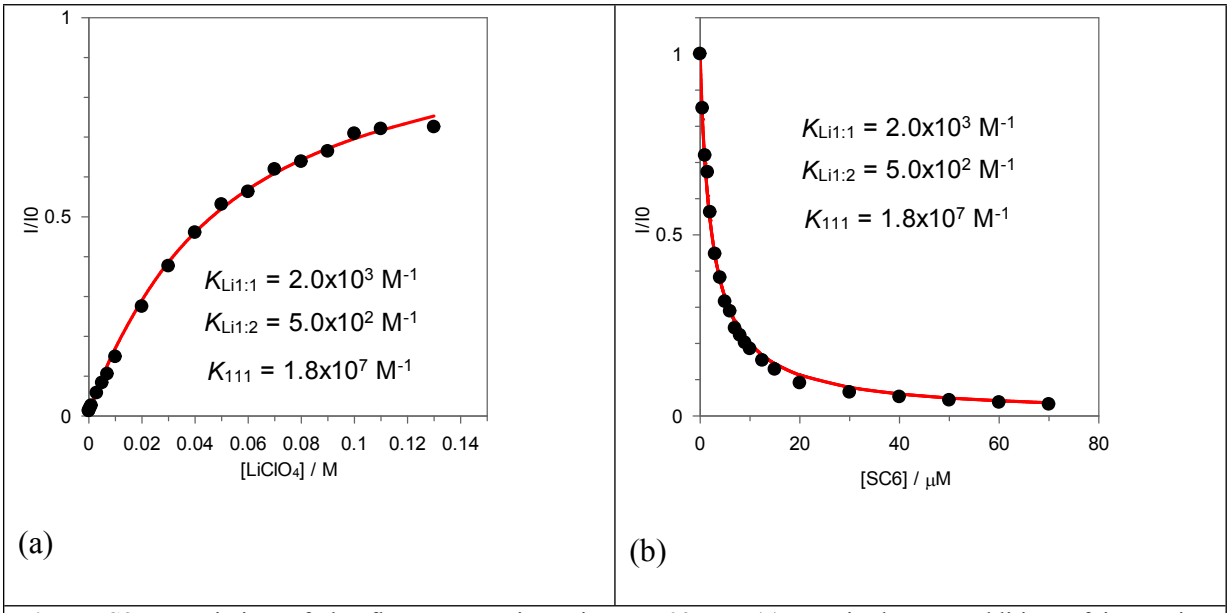
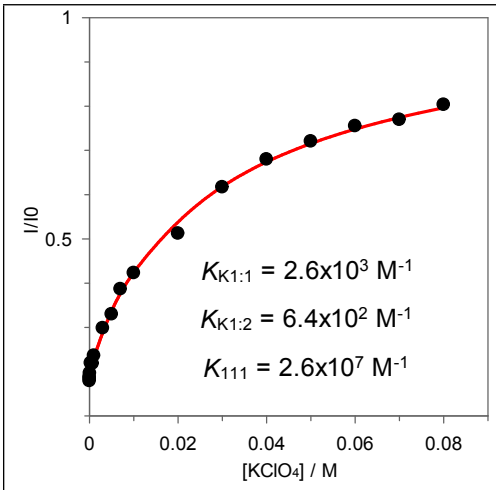
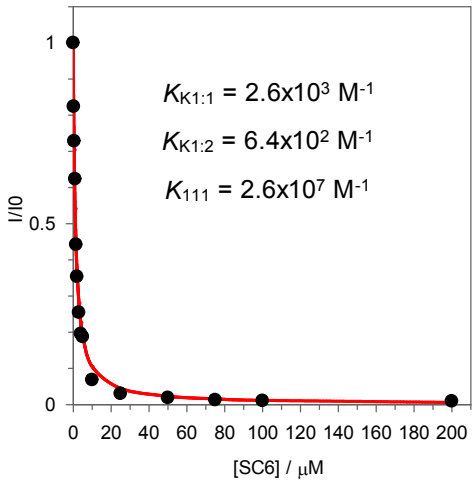


Figure S2 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $LiClO_4$ in a solution containing 1.0 μM of SC6 and 0.5 μM of lucigenin; and (b) upon increasing the concentration of SC6 in solution containing $LiClO_4$ 0.1M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC6 with both lucigenin and Li^+ along with the 1:1:1 heteroternary complex.



(a)



(b)

Figure S3 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $KClO_4$ in a solution containing 0.5 μM of SC6 and 1.0 μM of lucigenin; and (b) upon increasing the concentration of SC6 in solution containing $KClO_4$ 0.05M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC6 with both lucigenin and K^+ along with the 1:1:1 heteroternary complex.

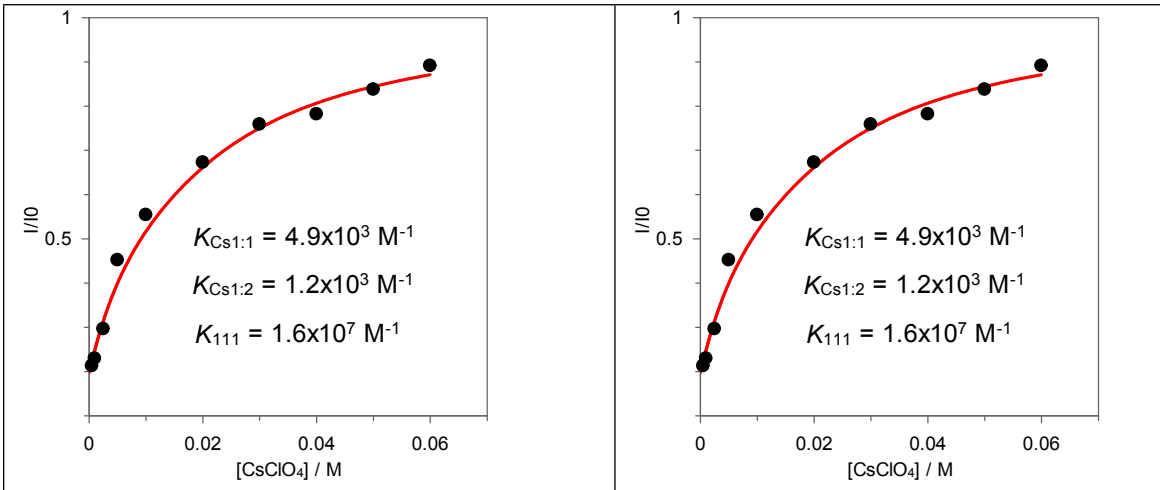
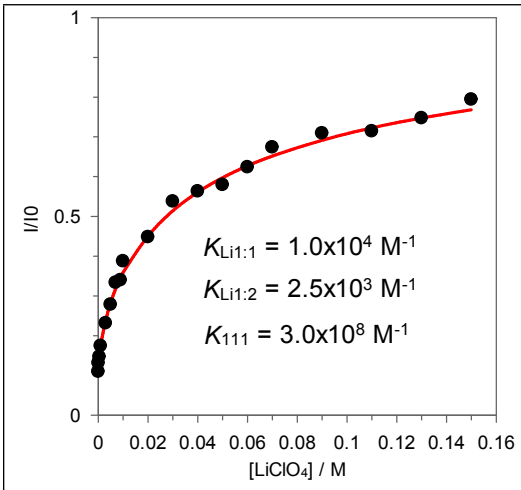
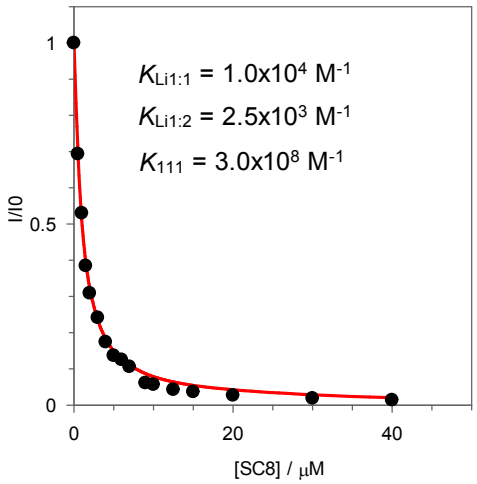


Figure S4 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $CsClO_4$ in a solution containing 0.5 μM of SC6 and 1.0 μM of lucigenin; and (b) upon increasing the concentration of SC6 in solution containing $CsClO_4$ 0.05M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC6 with both lucigenin and Cs^+ along with the 1:1:1 heteroternary complex.

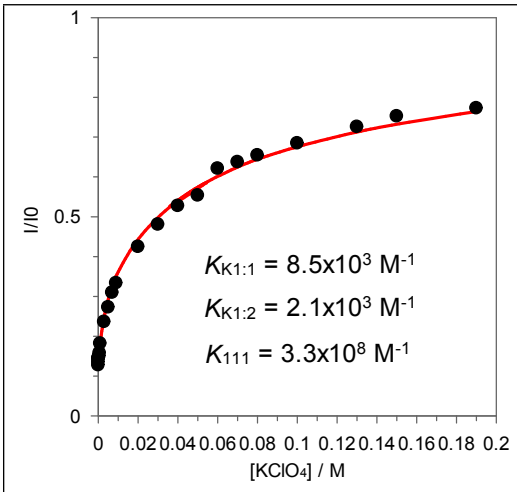


(a)

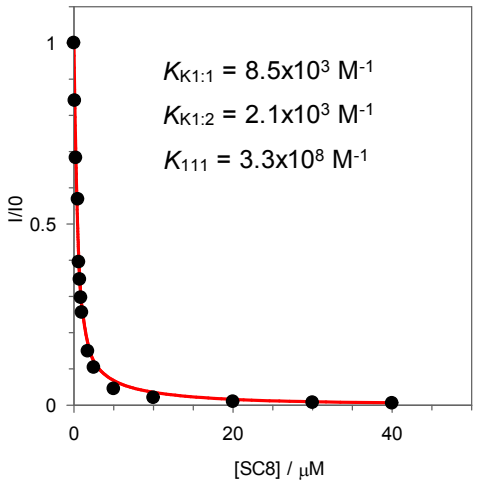


(b)

Figure S5 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $LiClO_4$ in a solution containing 0.5 μM of SC8 and 1.0 μM of lucigenin; and (b) upon increasing the concentration of SC8 in solution containing $LiClO_4$ 0.1M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC8 with both lucigenin and Li^+ along with the 1:1:1 heteroternary complex.



(a)



(b)

Figure S6 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $KClO_4$ in a solution containing 0.5 μM of SC8 and 1.0 μM of lucigenin; and (b) upon increasing the concentration of SC8 in solution containing $KClO_4$ 0.1M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC8 with both lucigenin and K^+ along with the 1:1:1 heteroternary complex.

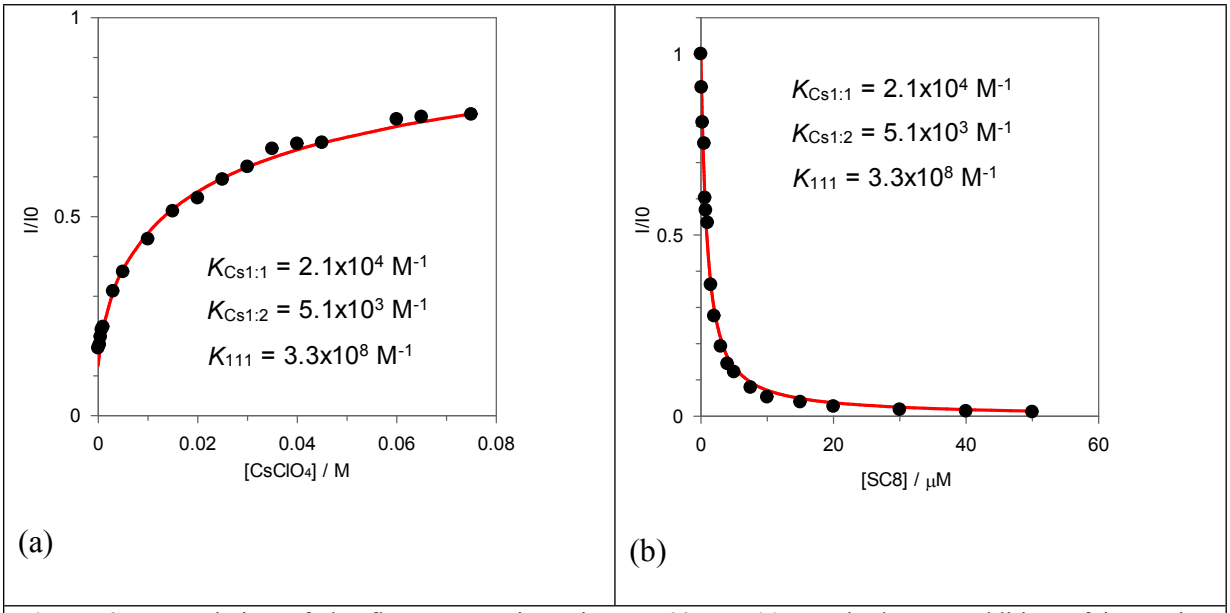


Figure S7 – Variation of the fluorescence intensity at 503 nm (a) acquired upon addition of increasing concentrations of $CsClO_4$ in a solution containing 0.5 μM of SC8 and 1.0 μM of lucigenin; and (b) upon increasing the concentration of SC8 in solution containing $CsClO_4$ 0.05M and lucigenin 0.50 μM. The line represents theoretical curve obtained upon global fitting of the experimental data points to a binding model that considers the formation of 1:1 and 1:2 host:guest complexes of SC8 with both lucigenin and Cs^+ along with the 1:1:1 heteroternary complex.

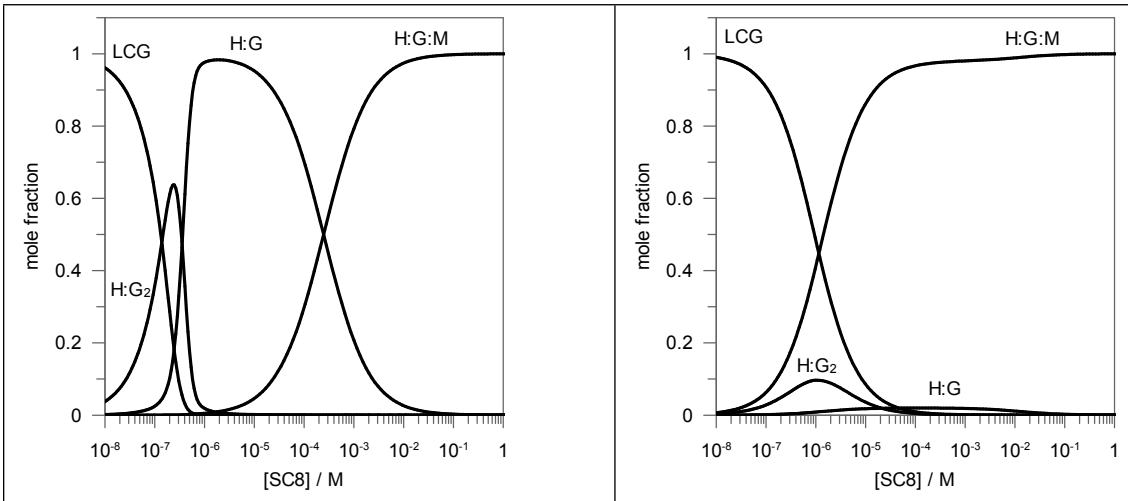


Figure S8 – Mole fraction distribution of SC8:lucigenin complexes (a) in the absence of added $NaClO_4$ and (b) in the presence of 0.1 M of $NaClO_4$. In both cases the sodium counterions are also considered. The simulation was carry out assuming a constant concentration of lucigenin [LCG] = 0.5 μM.

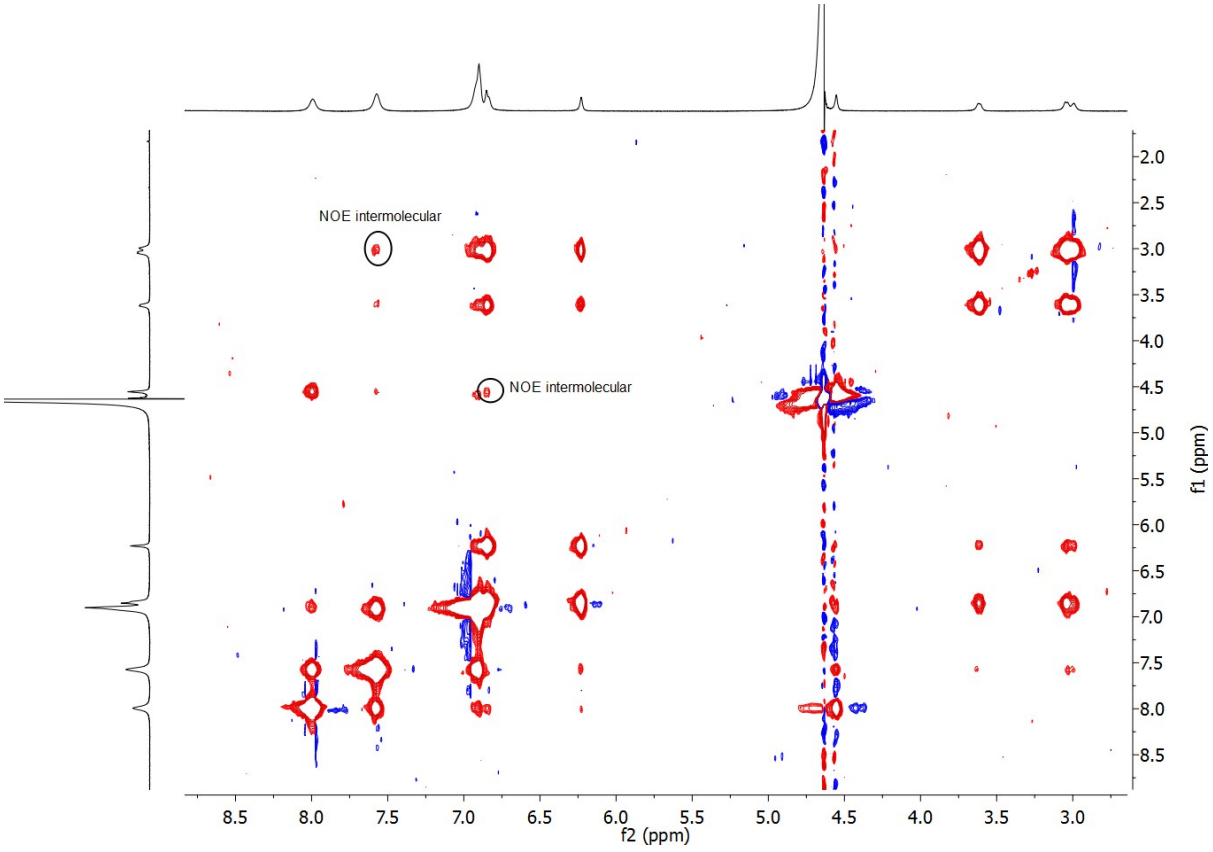


Figure S9 – NOESY spectrum obtained for a solution of lucigenin 1.37 mM with SC6 0.4 mM in D_2O at 5C. Mixing time 400 ms..