

## Supporting Information

### **Psoralidin-Cucurbit[7]uril Complex with Improved Solubility to Tackle Human Colorectal Cancer: an Experimental and Computational Study**

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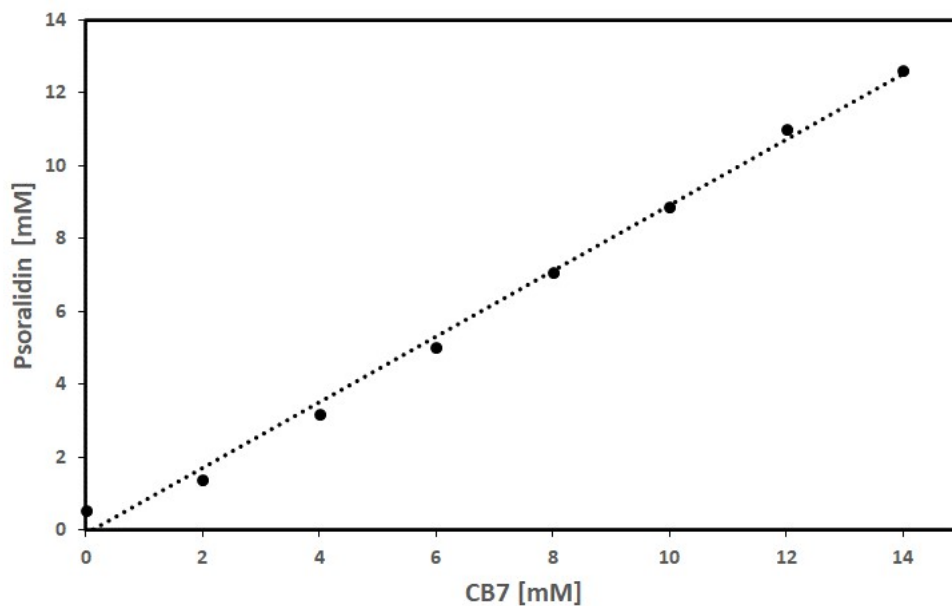
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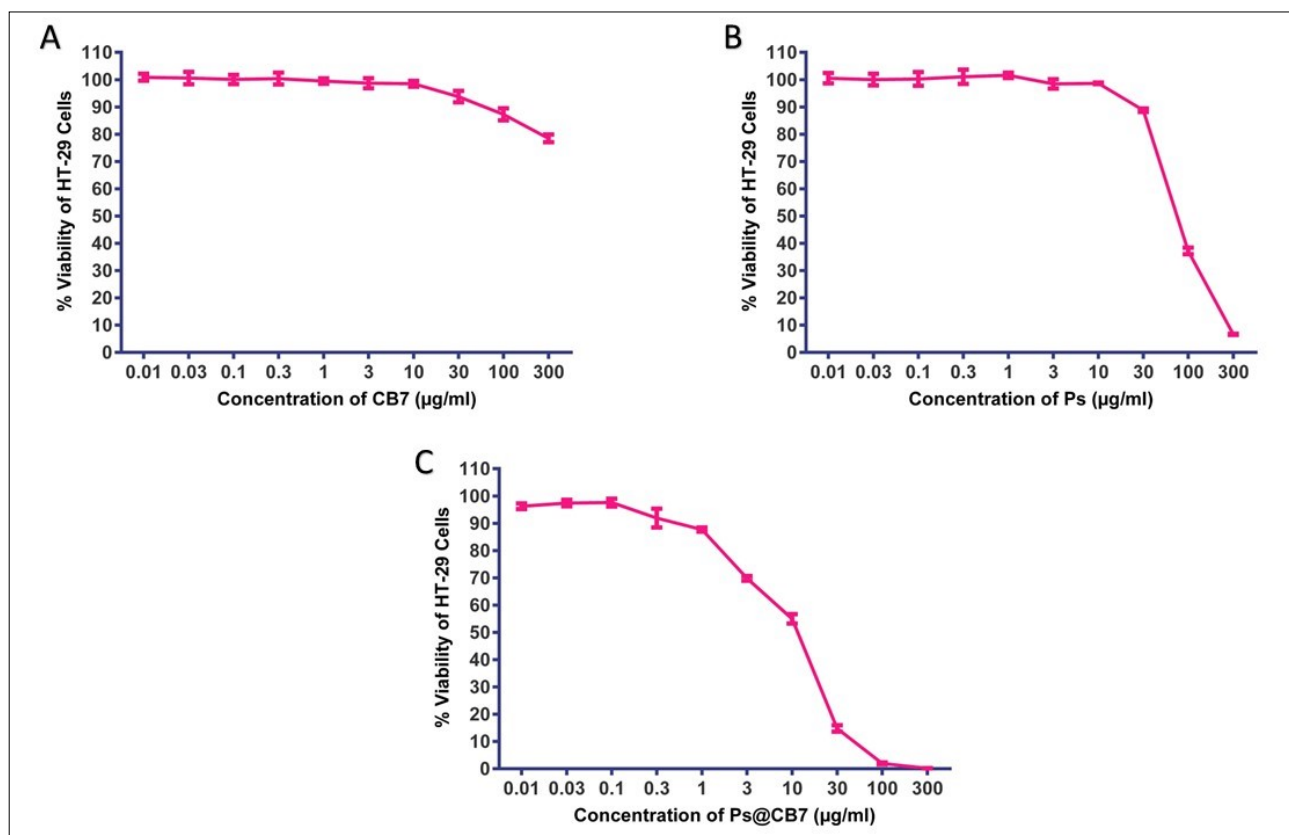
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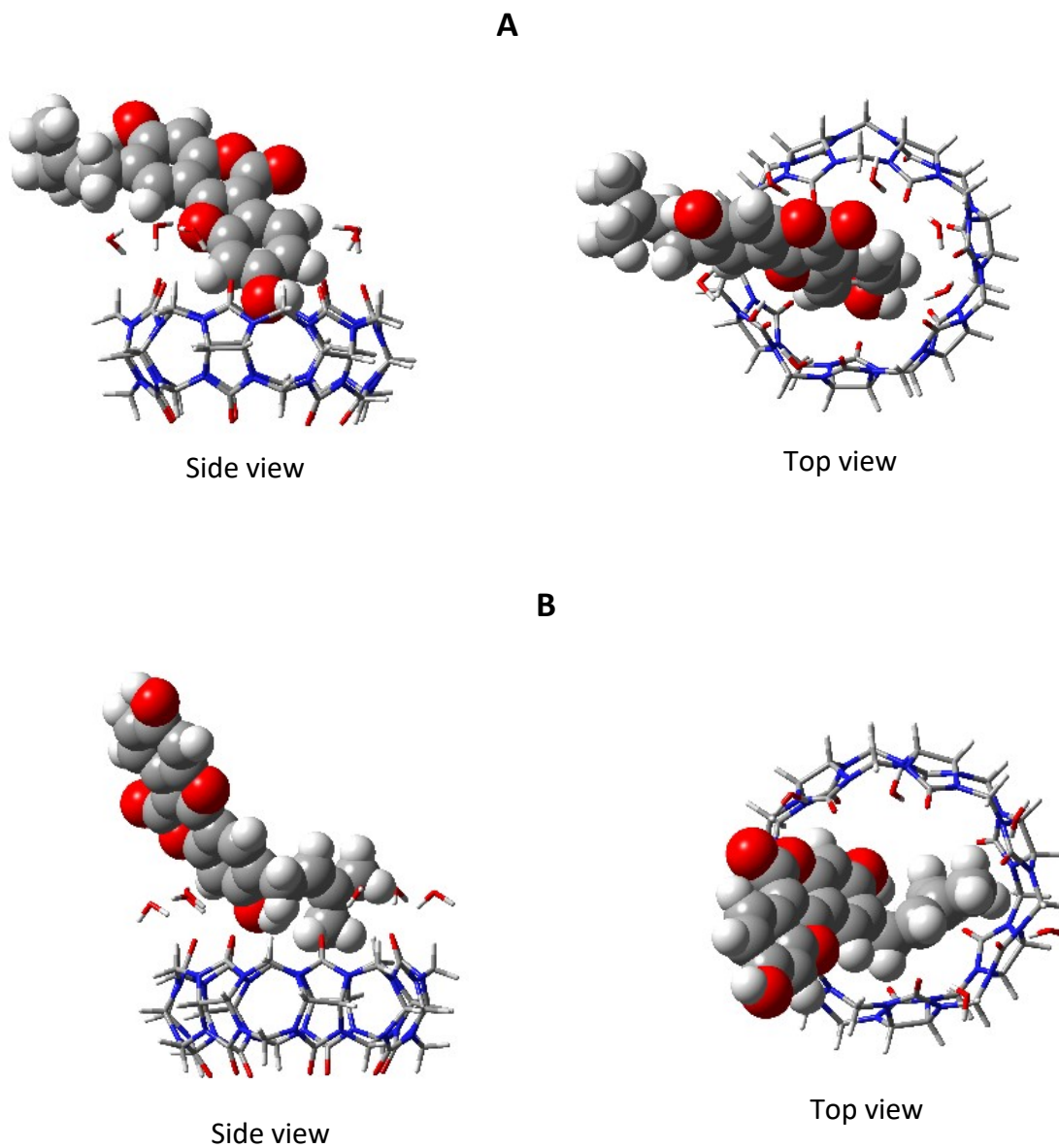
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**Figure S1.** Phase solubility diagram of Ps in aqueous solutions containing increasing concentrations of CB7 at 24 °C.



**Figure S2.** Cellular viability Percent of HT-29 cells following exposure to CB7 only (A), Ps only (B) and Ps@CB7 (C) for 48 h. Data are displayed as triplicates  $\pm$  SD.



**Figure S3.** Side and top views of the representation of the Ps-CB7 A and B arrangements, in which a model of interpenetrating spheres of van der Waals radii has been used for the guest.