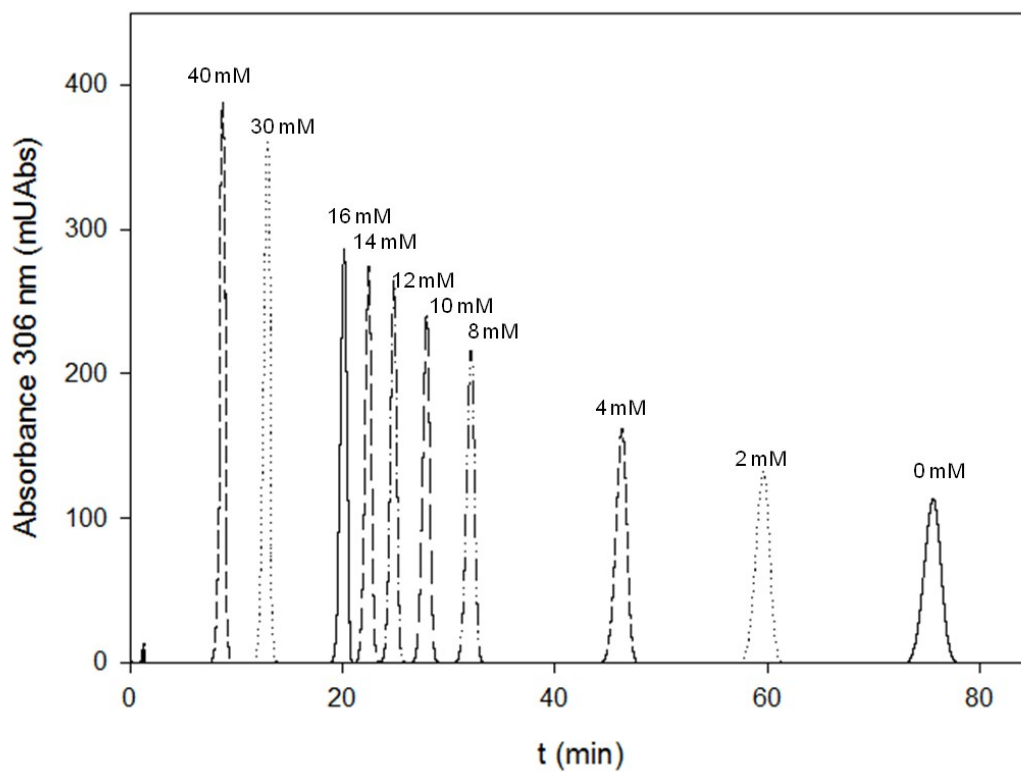
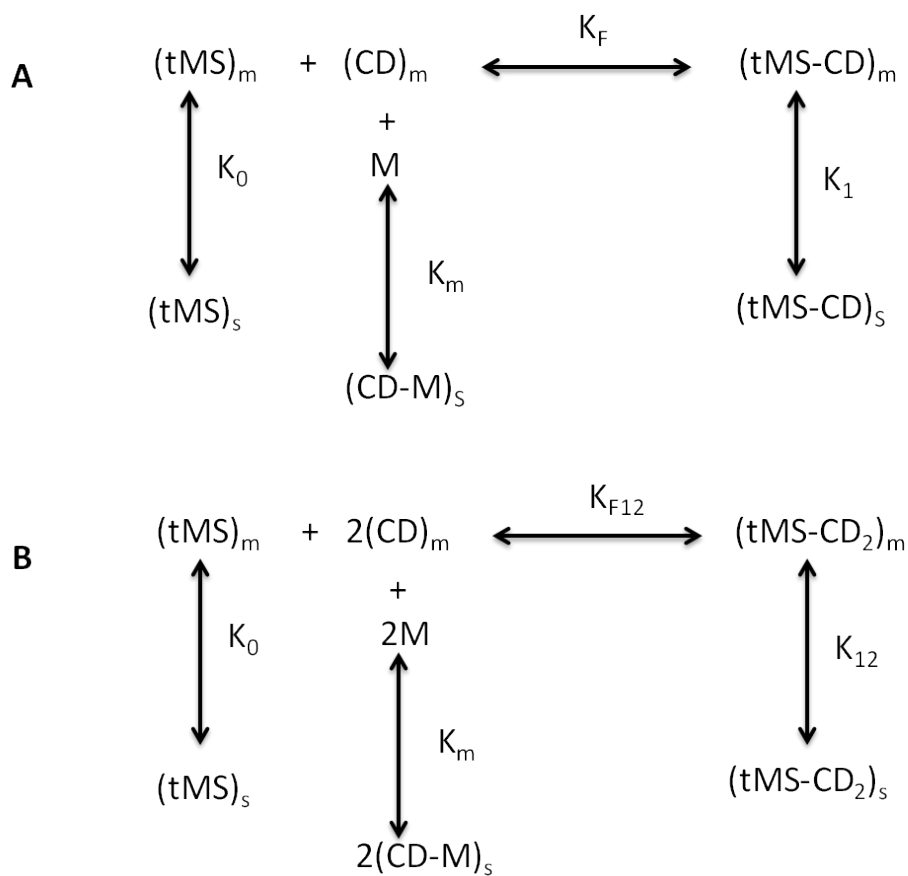


### Supplementary information.

**Supplementary fig 1.** HPLC chromatograms for increasing concentration of M $\beta$ CD (0-40 mM) at 25 °C, 60/40 MeOH/Water and 1.5 mL/min in C18 column.



**Supplementary Fig 2.** (A) Equilibrium proposed for a 1:1 tMS–CD inclusion complex. (B) Equilibrium proposed for a 1:2 tMS–CD inclusion complex <sup>16</sup>. Abbreviations: tMS: trans- $\alpha$ -Methylstilbene; CD:-cyclodextrin; tMS–CD: trans- $\alpha$ -Methylstilbene–CD complex; tMS–CD<sub>2</sub>: trans- $\alpha$ -Methylstilbene–CD<sub>2</sub> complex; m: mobile phase; s: stationary phases; M: organic modifier; K<sub>m</sub>: affinity constant of the modifier for the-CD cavity; K<sub>F</sub>: formation constant for the tMS–CD complex in a 1:1 model; K<sub>F12</sub>: formation constant for the tMS–CD complex in a 1:2 model; K<sub>0</sub>: equilibrium constant of tMS between mobile and stationary phase; K<sub>1</sub>: equilibrium constant of tMS–CD complex between mobile and stationary phase; K<sub>12</sub>: equilibrium constant of tMS–(CD)<sub>2</sub> complex between mobile and stationary phase.



***Supplementary fig 3.*** Animated .gifs for each docking simulation.

(See attach file)