

Supplementary Materials

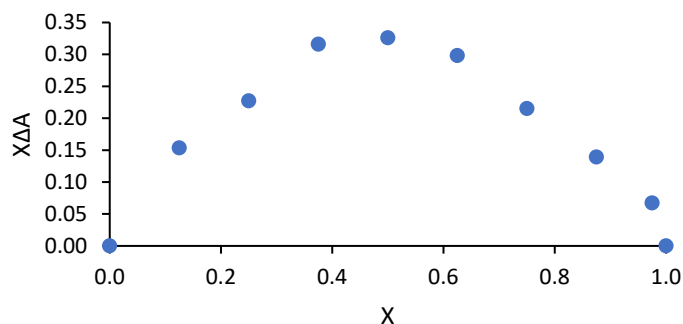


Figure S1. Job plot obtained for the system β -CD-NaSal.

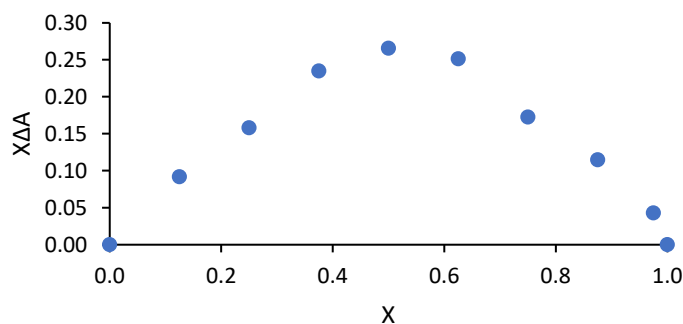


Figure S2. Job plot obtained for the system Na₄EtRA-NaSal.

Table S1. Energy variation of different β -CD-NaSal complexes.

Complex/Property	Hydroxyl end-on	Aromatic end-on	Inclusion outer-side complex	Upper outer-side complex	Bottom outer-side complex
ΔE_c (kcal/mol)	-36.255	-33.487	-30.119	-26.518	-31.984

Table S2. Energy variation of different Na₄EtRA-NaSal complexes.

Complex/Property	Hydroxyl end-on	Aromatic end-on	Upper outer-side complex
ΔE_c (kcal/mol)	-17.5290	-18.0918	-20.362

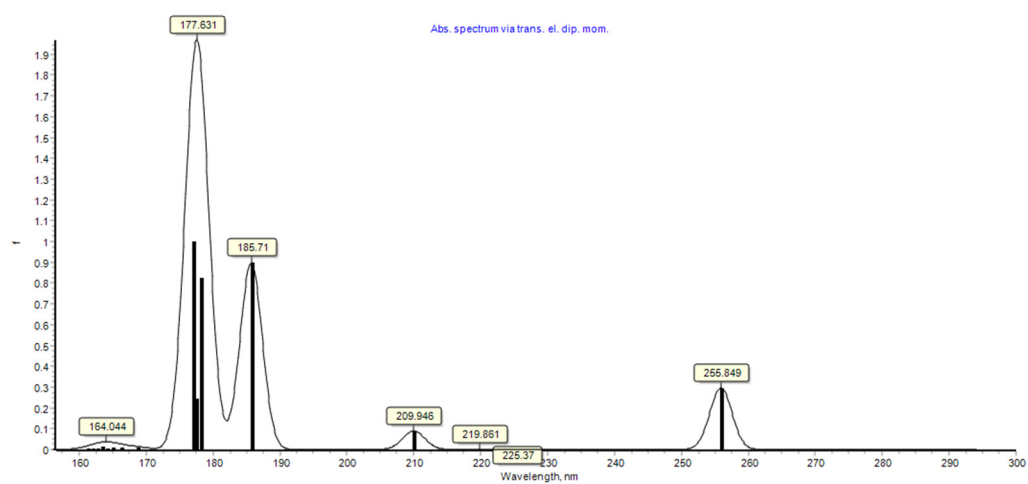
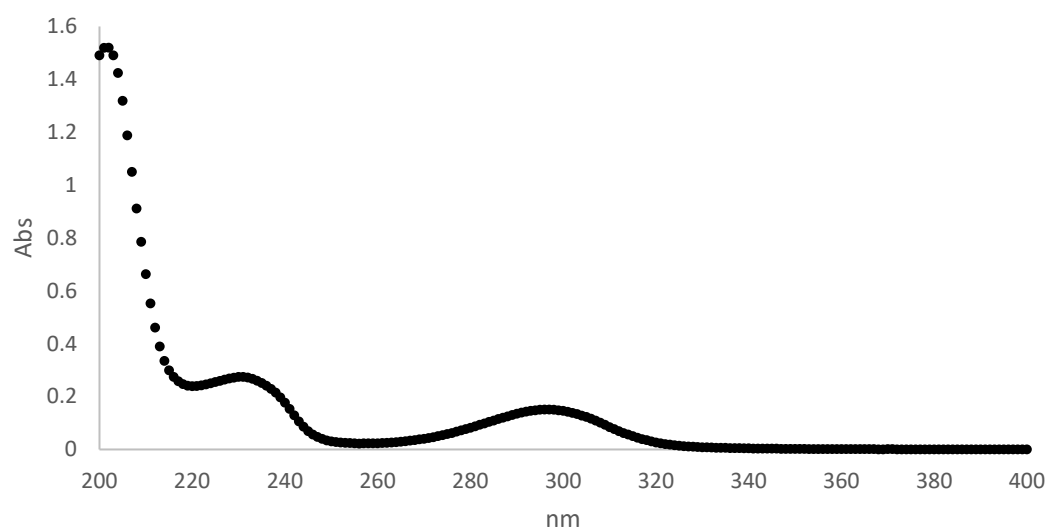


Figure S3. Upper: Experimental absorption spectrum of B-CD-NaSal complex. Bottom: Simulated absorption spectrum of B-CD-NaSal complex.

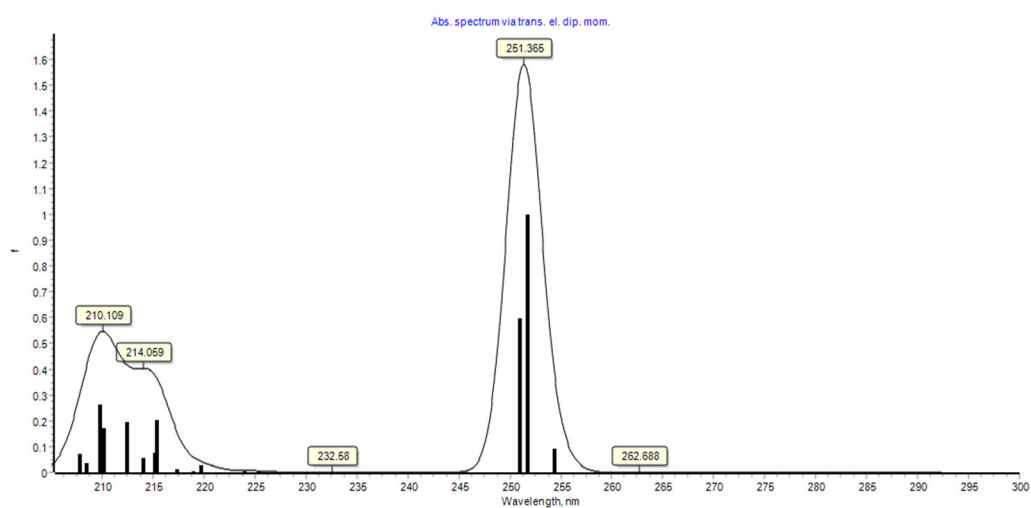
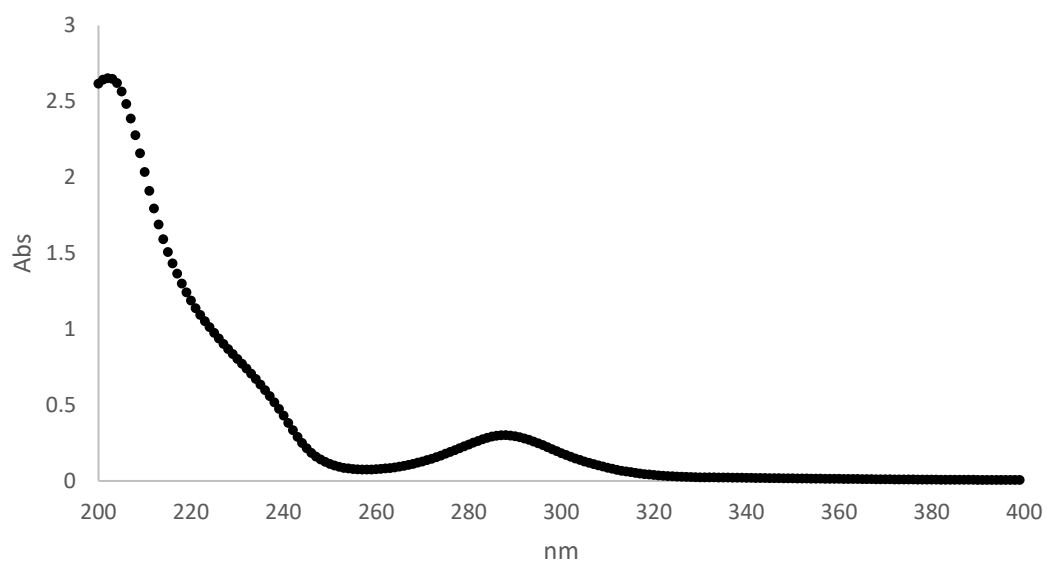


Figure S4. Upper: Experimental absorption spectrum of Na₄EtSN-NaSal complex. Bottom: Simulated absorption spectrum of Na₄EtSN-NaSal complex.