

Supplementary Table S1 Energy contributions data.

	form	-TΔS (kcal/mol)	ΔE _{vdw} (kcal/mol)	ΔE _{ele} (kcal/mol)	ΔG _{sol} ^{GB} (kcal/mol)	ΔG _{sol} ^{PB} (kcal/mol)
Chavibetol/ β-CD	B1	2.23	-19.86	-4.03	8.73	10.97
	B2	1.67	-20.26	-2.47	7.40	9.80
	B3	2.20	-20.22	-3.24	7.92	10.66
	M1	3.01	-19.71	-3.12	8.44	10.89
	M2	4.49	-19.79	-4.09	9.86	13.11
	M3	3.19	-19.72	-2.75	7.41	10.13
Eugenol/ β-CD	B1	3.20	-19.64	-2.68	8.21	10.67
	B2	2.83	-18.80	-3.13	8.32	10.20
	B3	1.59	-19.75	-3.81	7.80	10.71
	M1	1.17	-19.99	-3.63	7.55	10.37
	M2	3.31	-19.31	-4.71	9.51	12.81
	M3	1.89	-20.28	-5.02	8.87	12.37
Alpha-pinene/ β-CD	E1	3.75	-20.58	-0.22	3.90	2.91
	E2	3.81	-20.67	-0.20	4.26	3.67
	E3	3.39	-20.62	-0.21	4.15	3.20
	P1	4.12	-20.65	-0.30	4.18	3.14
	P2	3.21	-20.63	-0.26	4.09	3.22
	P3	4.34	-20.74	-0.25	4.27	3.29

The computed $\Delta G^{\text{MM/GBSA}}$ and $\Delta G^{\text{MM/PBSA}}$ values ranked the complexes as alpha-pinene/ β -CD > chavibetol/ β -CD > eugenol/ β -CD. Specifically, $\Delta G^{\text{MM/GBSA}}$ ranged from -3.22 ± 0.15 to -4.00 ± 0.32 kcal/mol for alpha-pinene/ β -CD, -1.58 ± 0.32 to -4.17 ± 0.12 for chavibetol/ β -CD, and -1.65 ± 0.29 to -3.58 ± 0.43 for eugenol/ β -CD. Similarly, $\Delta G^{\text{MM/PBSA}}$ ranged from -1.94 ± 0.15 to -2.42 ± 0.24 , -0.94 ± 0.23 to -1.46 ± 0.15 , and -0.94 ± 0.17 to -1.40 ± 0.19 kcal/mol, respectively.