

Supplementary Table S3 Docking Energies, Free Binding Energies, and Release Behaviors of Inclusion Complexes (ICs) Compared with Published Data.

	Host:guest	Docking energy (kcal/mol)	Binding energy (kcal/mol)	Release behavior	Ref.
Eugenol/ β -CD ICs	1:1	-4.00	-10.76	-	[48]
LMA/ β -CD ICs	1:1	-3.6	-	diffusion	[21]
TA/ β -CD ICs	1:1	-3.7	-	diffusion	[21]
γ -terpinene/ β -CD ICs	1:1	-3.4	-	-	[47]