

# Host-guest interaction of $\beta$ -cyclodextrin toward isomeric ursolic acid and oleanolic acid: physicochemical characterization and molecular modeling study

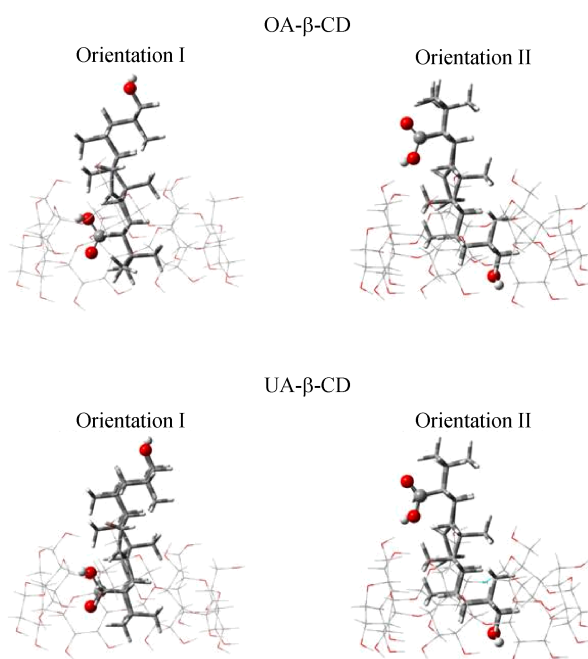
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**Fig. S1** Starting structures employed for the optimization of OA- $\beta$ -CD and UA- $\beta$ -CD complexes with carbonyl (orientation I) and hydroxyl (orientation II) groups being inserted into the cavity of  $\beta$ -CD.

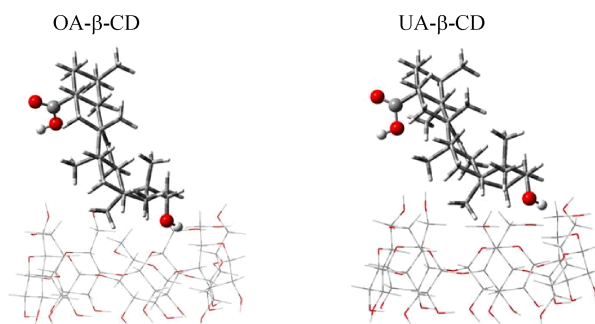
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**Fig. S2** Optimized structures for the OA- $\beta$ -CD and UA- $\beta$ -CD complexes with hydroxyl group being inserted in the cavity of  $\beta$ -CD (orientation II).

Preparative method	Group	
	OA- $\beta$ -CD	UA- $\beta$ -CD
Trituration	9.00	9.67
Ultrasound	0.06	0.06
Ultrasound	3.07	0.26

	$\beta$ -CD	OA	UA	OA- $\beta$ -CD	UA- $\beta$ -CD
Gas phase					
$E$ (a.u.)	-4275.176315	-1397.763329	-1397.752337	-5672.919402	-5672.890688
$\Delta E$ (kcal/mol)	–	–	–	12.70	23.82
Aqueous solution					
$E$ (a.u.)	-4275.354360	-1397.779016	-1397.767660	-5673.097324	-5673.069517
$\Delta E$ (kcal/mol)	–	–	–	22.63	32.95