

Structure of genipin in solution: a combined experimental and theoretical study

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SUPPLEMENTARY INFORMATION

Table S1. Activation Gibbs free energies (ΔG^\ddagger , kcal/mol) and products stabilization (ΔG , kcal/mol) calculated for the ring-opening ($1 \rightarrow 2'$) and tautomerization ($2' \rightarrow 2$) reactions of genipin in the gas phase and in ethanol. Explicit solvent molecules have been also considered.

	REACTANTS	ΔG^\ddagger	ΔG
GAS PHASE	1	46.6	13.0
	1 + H₂O	27.7	14.1
	1 + 2H₂O	18.5	4.0
ETHANOL	1 + 2H₂O	17.6	4.5
GAS PHASE	2'	55.8	-5.6
	2' + H₂O	34.6	2.7
	2' + 2H₂O	27.8	-0.9
	2' + 2H₂O (+2H₂O)	20.8	2.0
ETHANOL	2' + 2H₂O (+2H₂O)	18.5	-0.4