

Supporting Information

for

Effect of cyclodextrin complexation on phenylpropanoids' solubility and antioxydant activity

Miriana Kfoury^{1,2,3}, David Landy^{2,3}, Lizette Auezova¹, H el ene Greige-Gerges¹

and Sophie Fourmentin^{2,3} *

Address: ¹Bioactive Molecules Research Group, Doctoral School of Science and Technology, Department of Chemistry and Biochemistry, Faculty of Sciences-2, Lebanese University, Lebanon, ²Univ Lille Nord de France, F-59000 Lille, France and ³ULCO, UCEIV, F-59140 Dunkerque, France

Email : Sophie Fourmentin - lamotte@univ-littoral.fr

* Corresponding author

Phase solubility profiles of CD inclusion complexes and most stable CD/PP inclusion complex conformers

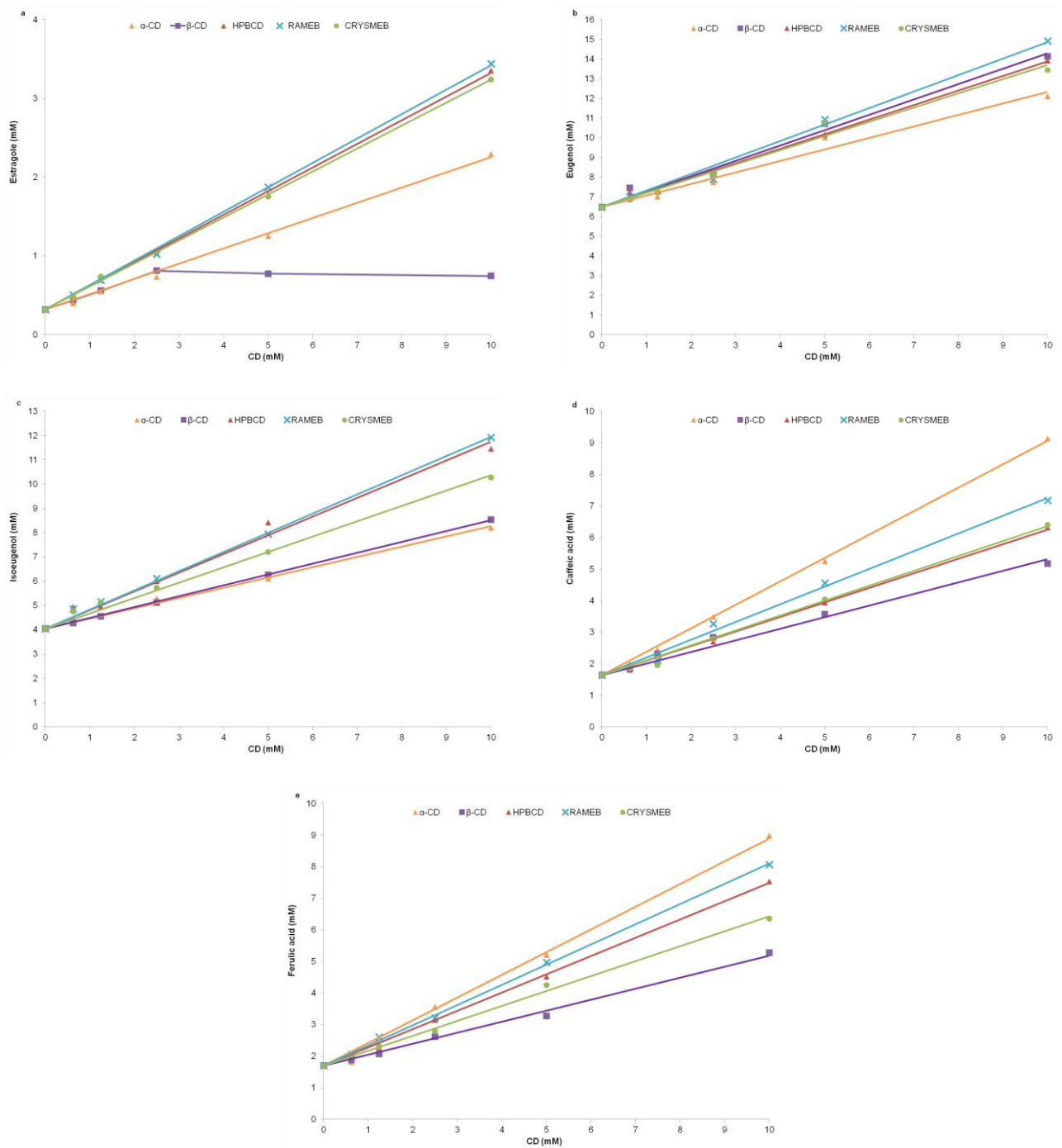
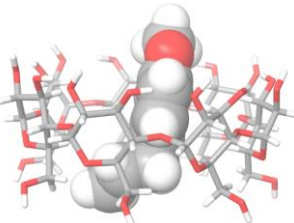
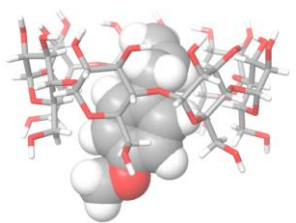
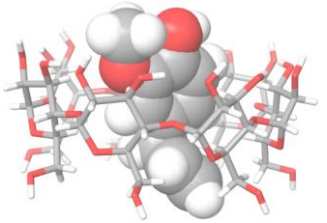
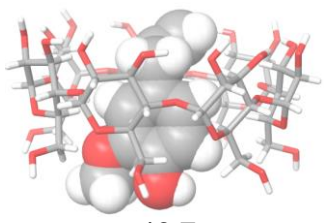
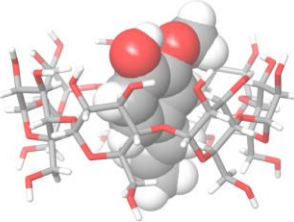
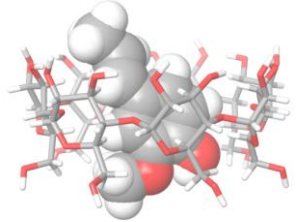
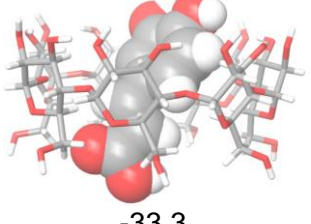
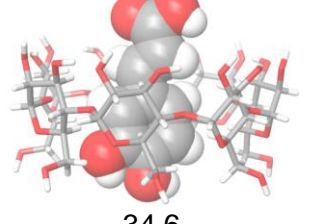
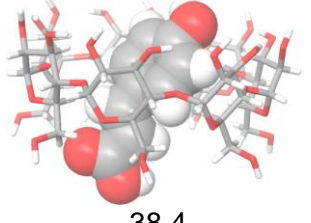
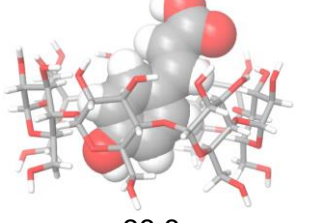
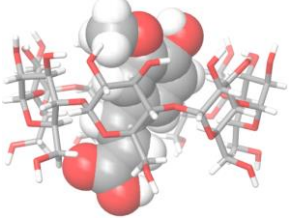
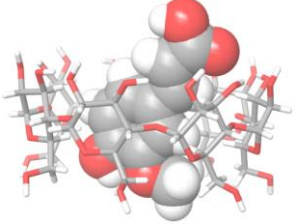


Figure S1: Phase solubility profiles of a) CD/estragole, b) CD/eugenol, c) CD/isoegenol, d) CD/caffeic acid and e) CD/ferulic acid inclusion complexes.

Table S1: Representation of the most stable CD/PP inclusion complex conformers resulting from the two docking strategies.

Host/guest	ΔE (kJ/mol)	
	Inclusion complex E1	Inclusion complex E2
β -CD/ estragole	 -46.0	 -43.6
β -CD/ eugenol	 -45.2	 -46.7
β -CD/ isoeugenol	 -50.9	 -49.9
β -CD/ caffeic acid	 -33.3	 -34.6
β -CD/ <i>p</i> - coumaric acid	 -38.4	 -38.8
β -CD/ ferulic acid	 -32.2	 -28.1