Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supplementary Material

Unveiling the Synergy: A Combined Experimental and Theoretical Study of β-Cyclodextrin with Melatonin

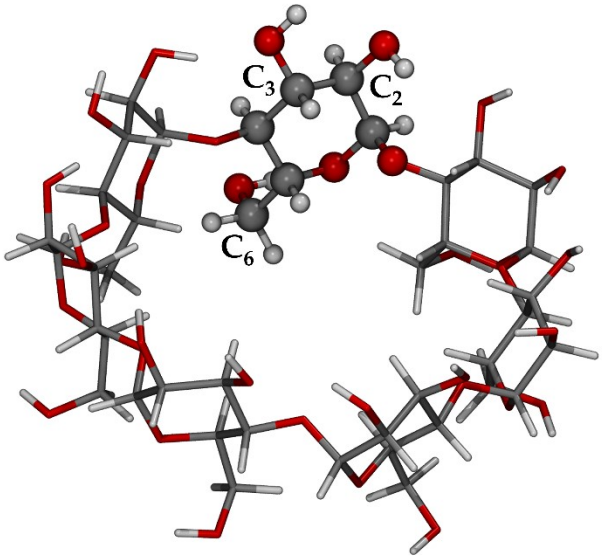
Riccardo Ferrero,[§] Stefano Pantaleone,[§] Cecilia Irene Gho,[‡] Gjylije Hoti, Francesco Trotta, Valentina Brunella,* Marta Corno*

Dipartimento di Chimica and Nanostructured Interfaces and Surfaces (NIS) Centre, Università degli Studi di Torino, Via P. Giuria 7, 10125 Torino, Italy

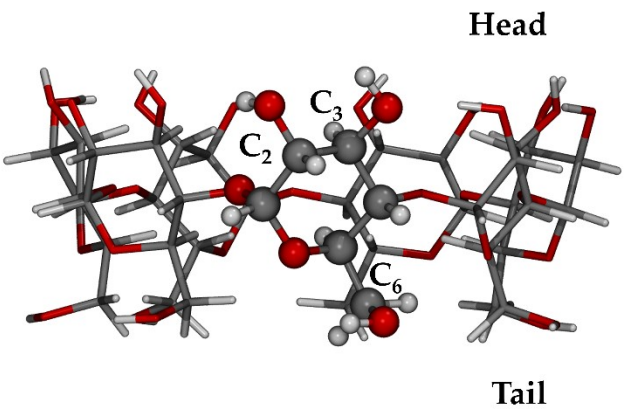
[‡]Present address: Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, C.so Duca degli Abruzzi 24, 10129 Torino, Italy

[§]The authors equally contributed

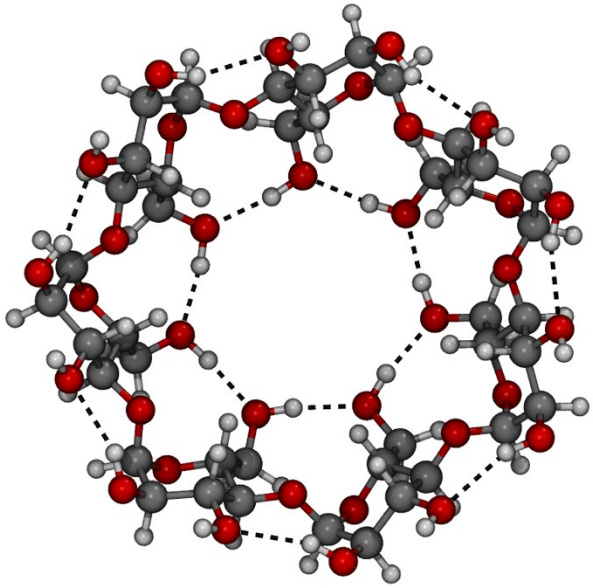
*Correspondence: valentina.brunella@unito.it, marta.corno@unito.it



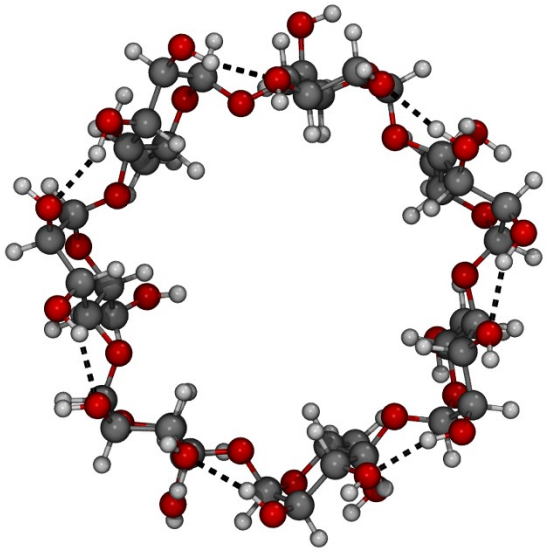
a) β-CD – top view



b) β-CD – side view



c) β-CD1 – top view



d) β-CD2 – top view

Figure S1: Top and side views of β-cyclodextrin (a, b) and open and closed conformations (c, d).

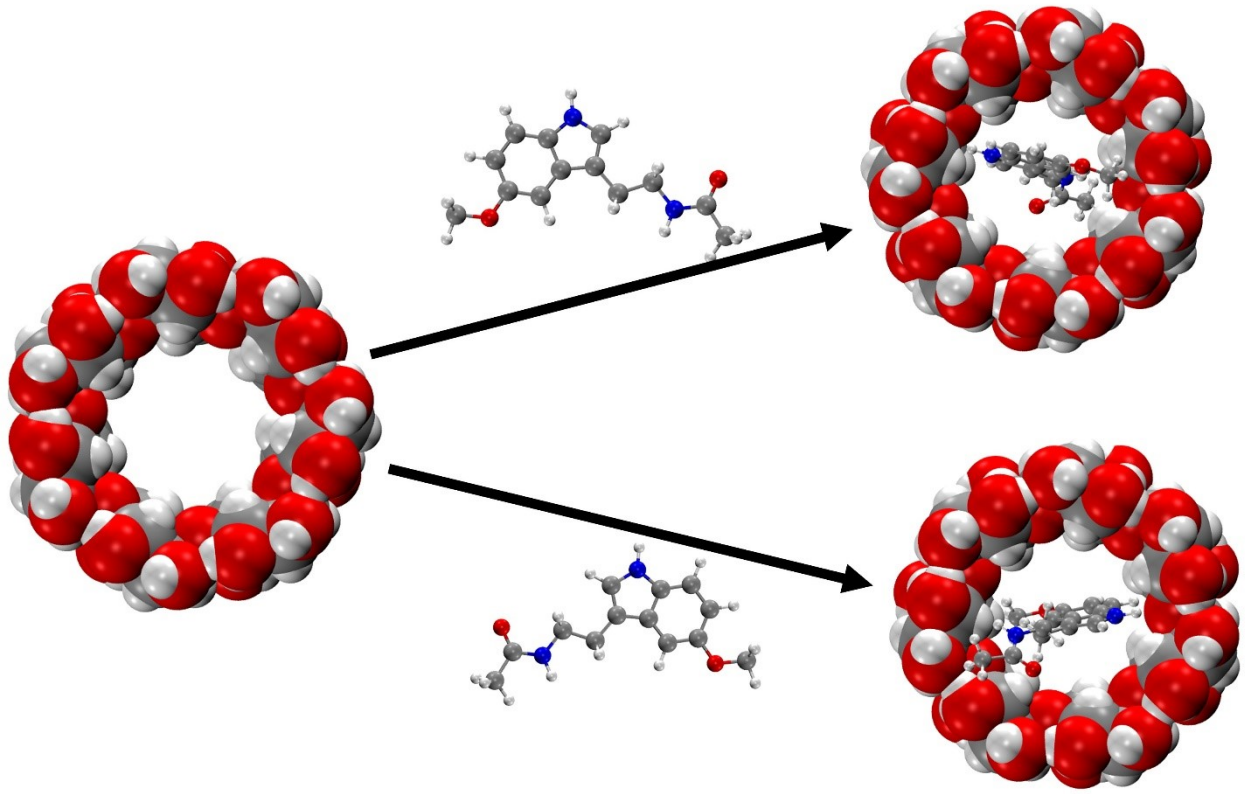


Figure S2: Starting complexes for the conformational search procedure. C in grey, N in blue, O in red, H in white.

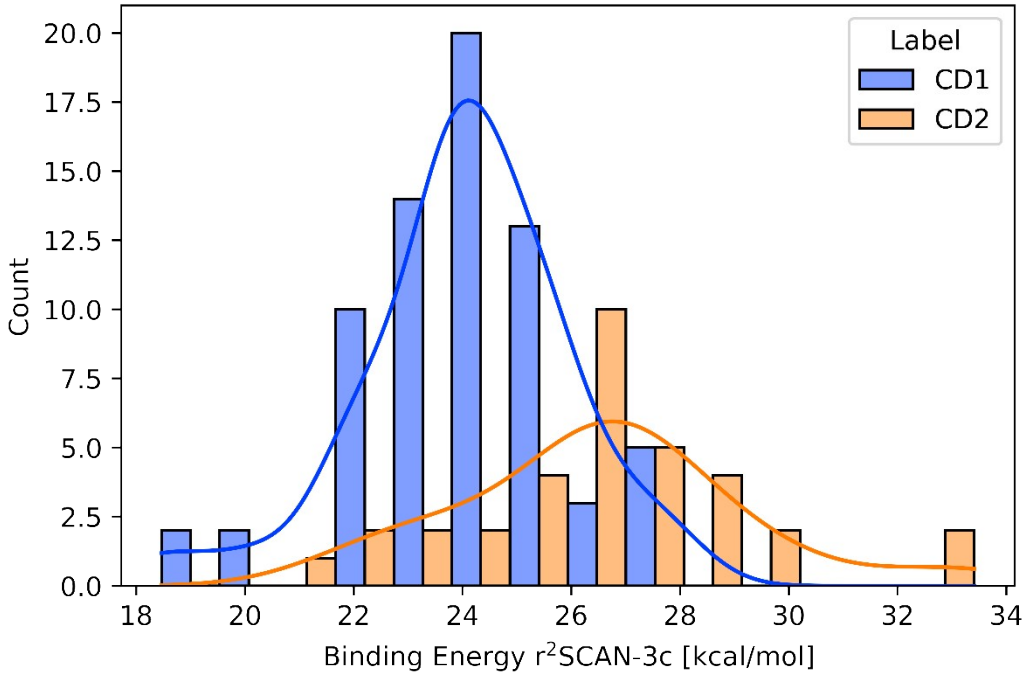
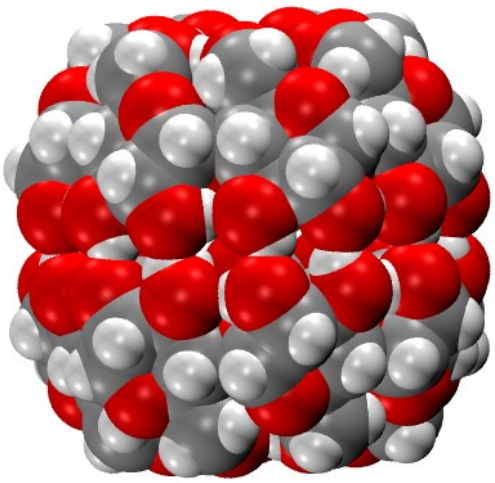
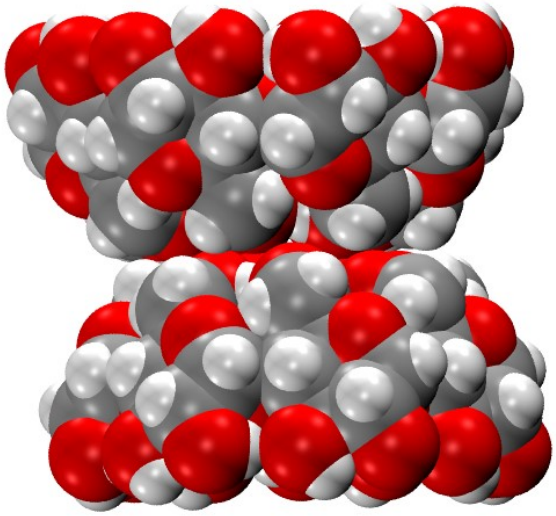


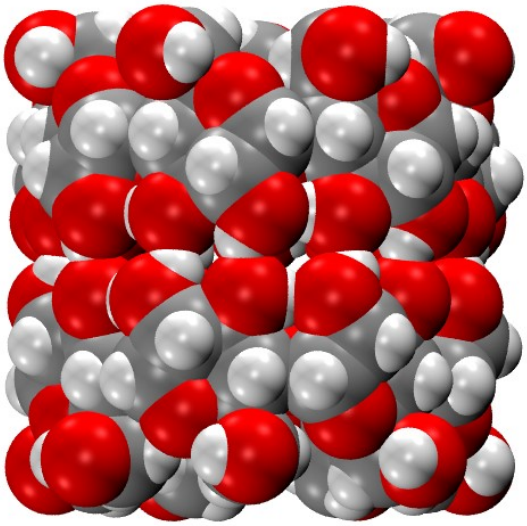
Figure S3: r^2SCAN-3c binding energy (kcal/mol) distribution of MT/β-CD complex in gas phase, in which the contributions given by CD1 and CD2 are separated.



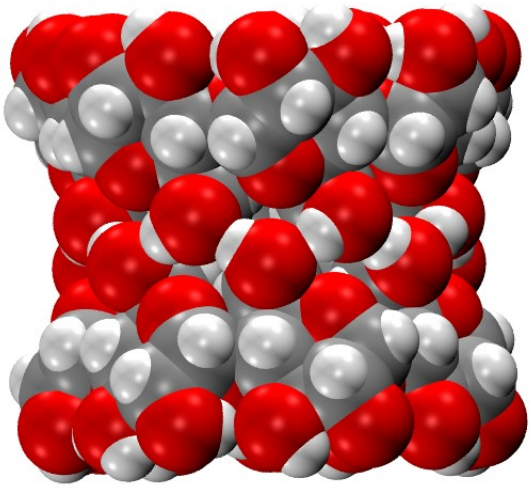
a) β-CD1-HH (0.0) [9.2]



b) β-CD1-TT (48.1) [41.3]



c) β-CD2-HH (8.3) [0.0]



d) β-CD2-TT (29.7) [8.3]

Figure S4: r^{2}SCAN-3c optimized structures of the β-CD dimers in the gas phase. Numbers in round parenthesis correspond to the relative energy in the gas phase, in square parenthesis to the relative energy in water C-PCM (in kcal/mol). H and T stand for Head and Tail sides. Color code: H in white, C in grey, O in red.

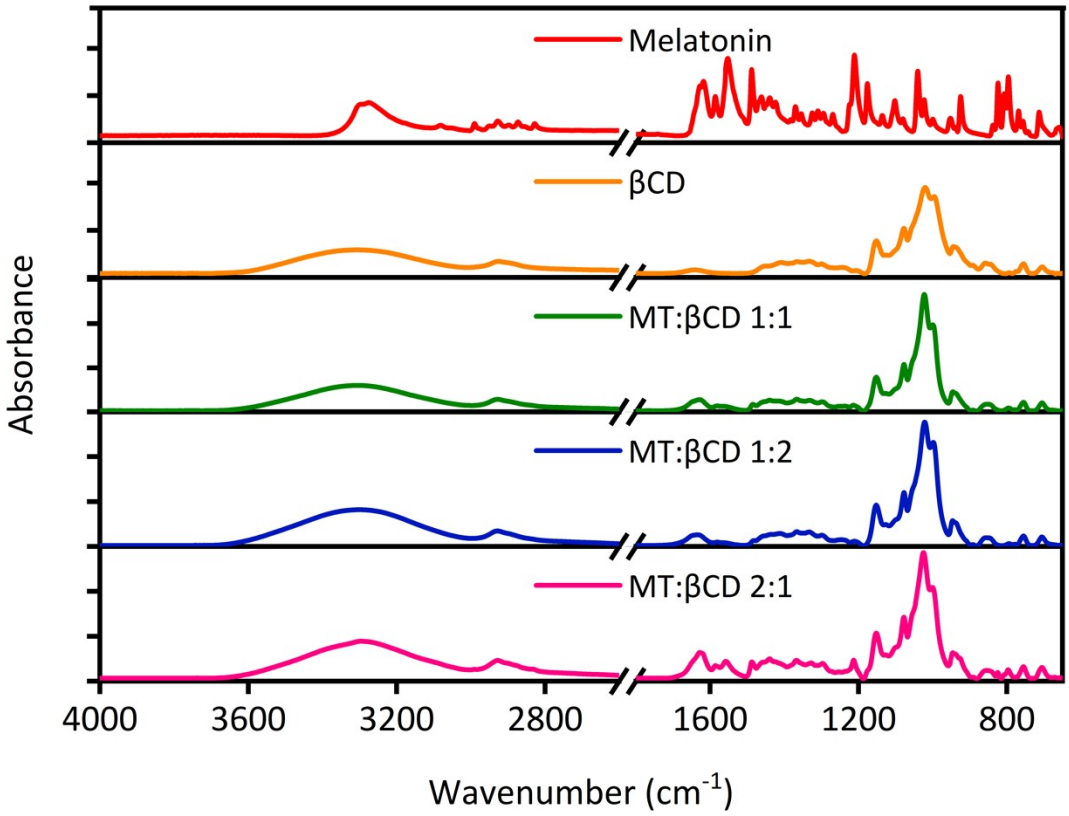


Figure S5: Experimental FTIR spectra of pure molecules (MT in red, β-CD in orange) and of the inclusion complexes in the three molar ratio proposed.

Gas				Water			
GFN2		r^{2}SCAN-3c		GFN2		r^{2}SCAN-3c	
Structures	ΔE	Structures	ΔE	Structures	ΔE	Structures	ΔE
x10	0.00	x00	0.00	x06	0.00	x04	0.00
x11	0.00	x01	0.83	x05	0.10	x00	0.34
x07	0.01	x03	1.40	x15	0.10	x03	0.65
x04	0.06	x02	1.73	x00	0.81	x01	0.68
x15	0.07	x04	2.09	x11	0.89	x11	1.06
x05	0.08	x15	2.36	x10	0.90	x07	1.07
x00	0.12	x05	2.37	x07	0.90	x10	1.08
x06	0.17	x10	2.70	x04	0.90	x02	1.27
x09	0.65	x11	2.70	x09	1.04	x09	1.72
x02	0.93	x07	2.71	x01	1.19	x06	1.77
x18	0.98	x09	2.88	x02	1.26	x05	2.38
x21	0.98	x06	2.90	x18	1.50	x15	2.40
x22	1.01	x18	3.61	x22	1.51	x18	2.57
x01	1.15	x21	3.63	x21	1.53	x21	2.61
x03	1.53	x22	3.63	x03	1.80	x22	2.63

Table S1: GFN2 and r^{2}SCAN-3c energetic ranking of melatonin conformers in gas and implicit water phases.