SUPPLEMENTARY MATERIAL, File 1

For the manuscript

Inclusion of the Phytoalexin *trans*-Resveratrol in Native Cyclodextrins: A Thermal, Spectroscopic, and X-Ray Structural Study

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Table S1. Solvents and volumes used in the recrystallizations of commercial RSV with thermal data from DSC of samples isolated. (Standard deviation in parentheses (n = 3)).

Solvent	mL per 1 g RSV	$T_{onset,m}$ (°C)	$T_{peak,m}$ (°C)	H_m J g^{-1}
Water	$2.8 \cdot 10^3$	262(2)	263(2)	265(8)
Methanol	17	262(1)	264(1)	237(6)
Methanol/water 7:3 (*v*/*v*)	23	263(2)	265(3)	265(9)
Ethanol	15	262(1)	264(1)	269(7)
Ethanol/water 1:1 (*v*/*v*)	9	263(1)	265(1)	314(8)
Ethanol/water 4:1 (*v*/*v*)	5	263(2)	266(1)	253(6)
Ethanol/water 7:3 (*v*/*v*)	5	263(1)	264(2)	288(9)
Acetone	8	264(1)	265(2)	272(3)
Isopropanol	7	263(1)	265(1)	288(5)
n-propanol	7	261(3)	264(3)	272(4)
Tetrahydrofuran	4	263(2)	265(1)	274(5)
Methylene chloride	$3.7 \cdot 10^3$	263(1)	265(2)	243(5)
Ethyl acetate	37	262(2)	264(2)	269(6)

Table S2. Peak assignments and integrations for host-guest stoichiometry.

Proton (CD/G) [Total no. of protons]	δ (ppm)	Peak integrations	Scale factor 8 x integration value	Experimental peak integral /theoretical proton. No.	Convert to integers
8 x H**1** (CD) – [8]	4.88	1.000*	8	1	3
8 x O-H**6**(CD) –[8]	4.38	0.95	8	1	3
8 x O-H**2**(CD) –[8]; 8 x O-H**3 (CD)**–[8]	5.62	1.98	16	1	3
H**10** and H**14** (G) – [2]	6.36	0.33	2.6	1.3	4
H**3** and H**5**(G) – [2]	7.36	0.35	2.8	1.3	4

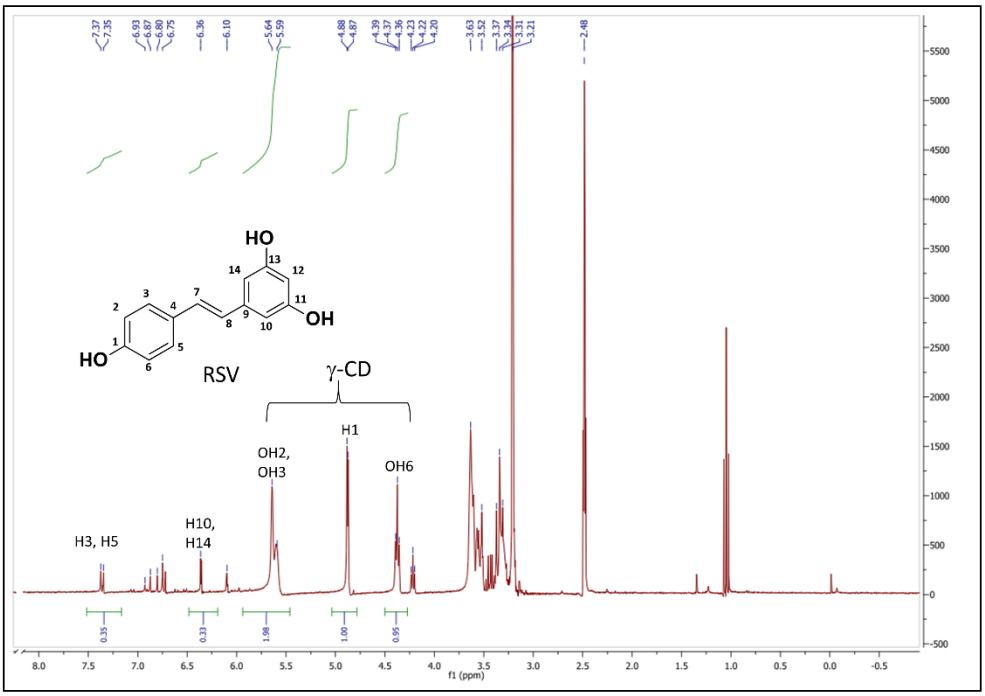

Figure S1. 1H NMR spectrum for γ-CD·RSV stoichiometry determination.

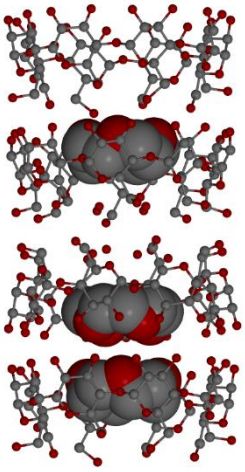

Figure S2. Inclusion of an ordered guest (12-crown-4) within the channel formed by γ-CD host molecules (CSD refcode DOCYID [31]). .

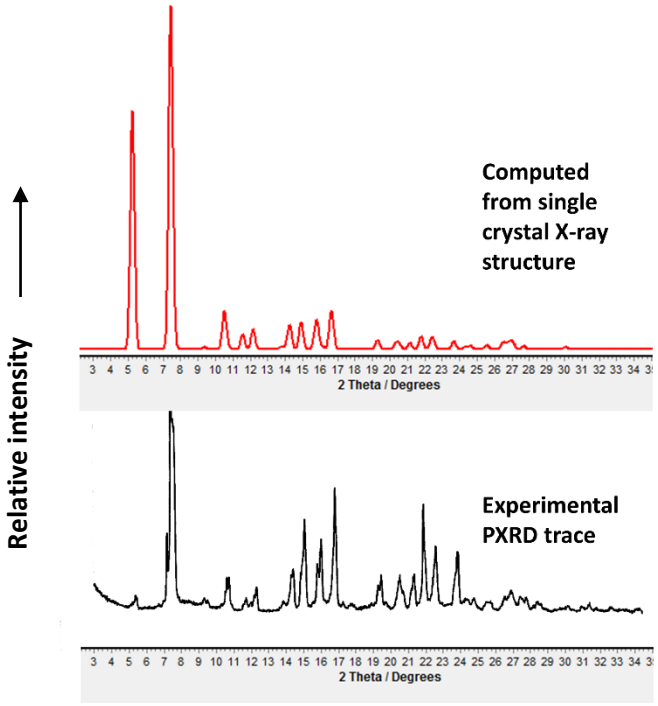

Figure S3. The simulated and experimental PXRD patterns of the γ-CD·RSV hydrate complex.