pharmaceutics

Supplementary Materials: Resveratrol Encapsulation and Release from Pristine and Functionalized Mesoporous Silica Carriers

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Characterization of materials

Nitrogen adsorption - desorption isotherms

Nitrogen adsorption – desorption isotherms were recorded for all samples and the corresponding pore size distribution curves were determined from corresponding isotherm (Figure S1).

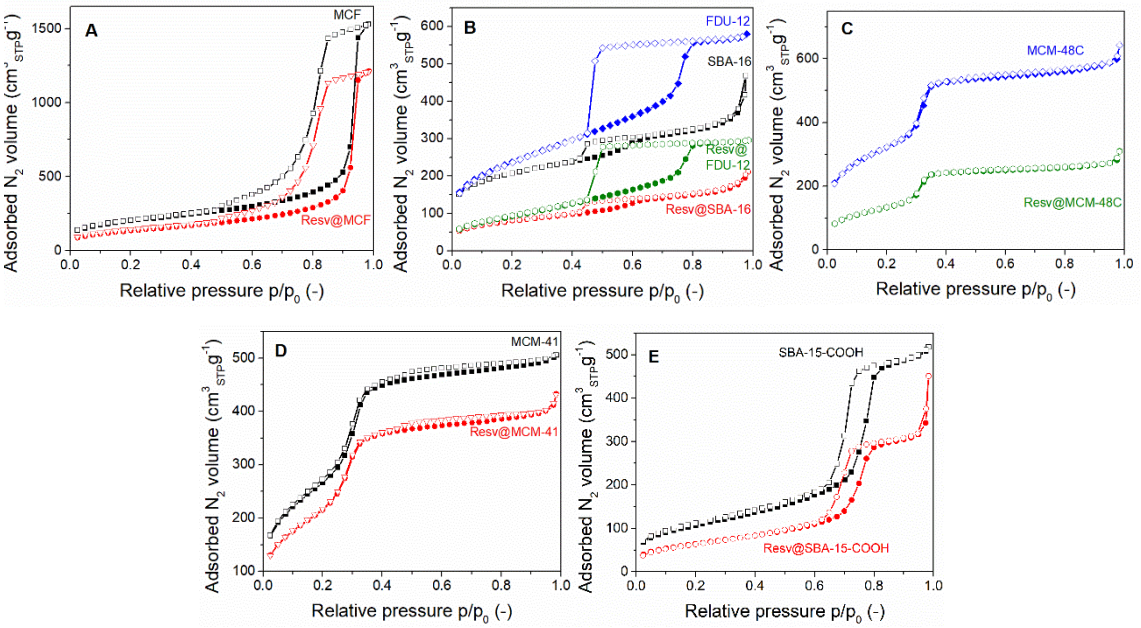

Figure S1. Nitrogen adsorption-desorption isotherms of mesoporous carriers and resveratrol-loaded carriers: MCF and Resv@MCF (A); FDU-12, SBA-16 and Resv@FDU-12, Resv@SBA-16 (B); MCM-48 and Resv@MCM-48 (C); MCM-41 and Resv@MCM-41 (D); SBA-15-COOH and Resv@SBA-15-COOH (E).

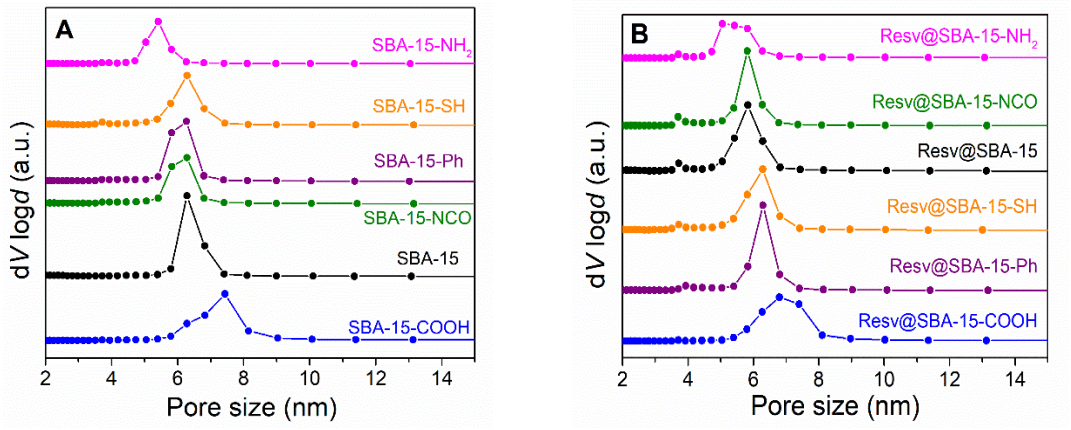

Figure S2. Pore size distribution curves determined from nitrogen adsorption-desorption isotherms for SBA-15-type carriers (**A**) and resveratrol-loaded SBA-15-type carriers (**B**).

X-ray diffraction

The small-angle XRD patterns of pristine and functionalized SBA-15 carriers exhibit the characteristic (110) and (200) Bragg reflections of the *P6mm* hexagonal space group (Figure S3).

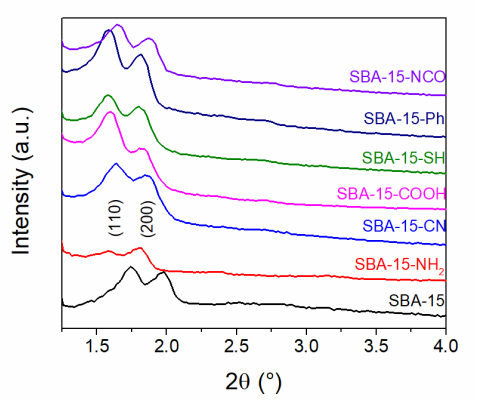

Figure S3. Small–angle XRD patterns of pristine and functionalized SBA-15 carriers.

DSC analysis

The DSC traces of resveratrol–loaded functionalized SBA-15 carriers are presented in Figure S4.

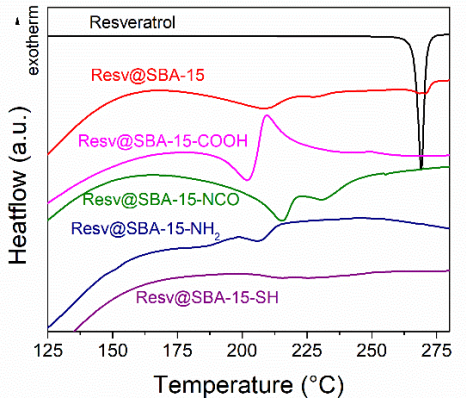

Figure S4. DSC traces of resveratrol – loaded samples containing functionalized carriers.

Release profiles

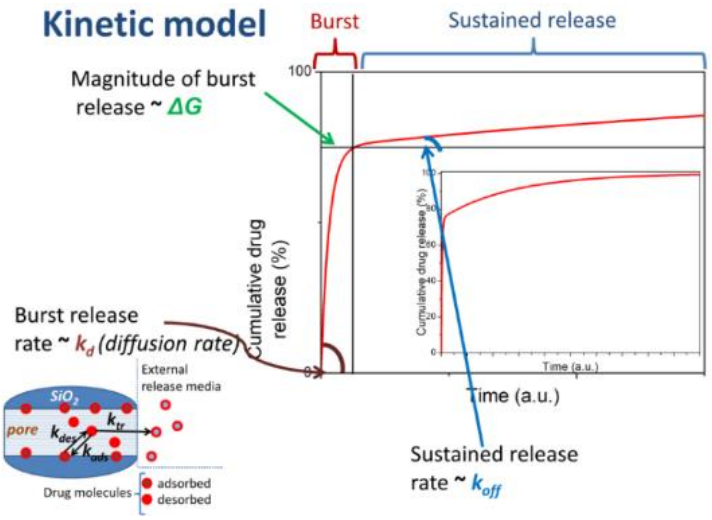

Figure S5. Representation of the three-parameter model.

Correlation of model parameters to textural properties

Two correlation studies between the fitted parameters of the theoretical kinetics model and the physico-chemical parameters of the carriers and resveratrol-loaded samples have been performed using Microsoft Excel. The two correlation studies were carried out on the materials containing pristine mesoporous silica (MCM-41, MCM-48C, SBA-16, FDU-12, MCF, SBA-15) or on the functionalized samples, including the parent SBA-15 (SBA-15, SBA-15-COOH, SBA-15-NCO, SBA-15-NH_2, SBA-15-Ph, SBA-15-SH). The correlation coefficients *r* take values between -1 and 1, with values close to 1 indicating direct correlation and values close to -1 indicating inverse correlation (Table S1, Table S2). The *p*-values were computed for each pair of model parameter – physico-chemical property.

Table S1. Correlation coefficients, *r* and *p*-values for the drug-loaded samples obtained using pristine silica carriers.

					Carriers				Resveratrol-loaded samples			
	ΔH (J g-1)	*Crystalline* (% wt.)	*Amorphous* (% wt.)	S_{BET} (m^2g^{-1})	V_p (cm^3g^{-1})	*d des* (nm)	*d ads* (nm)	S_{BET} (m^2g^{-1})	V_p (cm^3g^{-1})	*d des* (nm)	*d ads* (nm)
	-0.75	0.75	-0.75	-0.15	0.71	0.65	0.69	0.26	0.73	0.65	0.69
	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =
ΔG	0.084)	0.085)	0.085)	0.778)	0.114)	0.163)	0.129)	0.615)	0.099)	0.166)	0.132)
	0.6	-0.62	0.62	-0.01	-0.38	-0.36	-0.35	-0.43	-0.43	-0.34	-0.34
	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =
k_{tr}	0.205)	0.192)	0.192)	0.983)	0.461)	0.489)	0.493)	0.399)	0.394)	0.516)	0.504)
	0.78	-0.78	0.78	**0.91**	-0.7	**-0.83**	-0.78	0.17	-0.7	**-0.82**	-0.77
	(p =	(p =	(p =	**(p =**	(p =	**(p =**	(p =	(p =	(p =	**(p =**	(p =
k_{des}	0.069)	0.068)	0.068)	**0.012)**	0.123)	**0.042)**	0.069)	0.749)	0.118)	**0.045)**	0.073)
	0.83	**-0.84**	**0.84**	0.28	-0.69	-0.69	-0.69	-0.25	-0.72	-0.67	-0.68
	(p =	**(p =**	**(p =**	(p =	(p =	(p =	(p =	(p =	(p =	(p =	(p =
k_{ads}	**0.039)**	**0.039)**	**0.039)**	0.586)	0.129)	0.132)	0.132)	0.627)	0.108)	0.143)	0.139)

Crystalline (% wt.)	-	-	-	**-0.52 (p = 0.034)**	**0.85 (p = 0.016)**	**0.90 (p = 0.044)**	0.82 (p = 0.658)	**0.23 (p = 0.023)**	**0.87 (p = 0.022)**	**0.88 (p = 0.05)**	0.81 (p = 0.085)

Table S2. Correlation coefficients, *r* and *p*-values for the drug-loaded samples obtained using functionalized silica carriers.

			Carriers				Resveratrol-loaded samples			
	Resv.(% wt.)	SiO_2/OG (mol)	S_{BET} (m^2g^{-1})	V_p (cm^3g^{-1})	*d des (nm)*	*d ads (nm)*	S_{BET} (m^2g^{-1})	V_p (cm^3g^{-1})	*d des (nm)*	*d ads (nm)*
ΔG	**-0.87 (p = 0.025)**	0.27 (p = 0.6)	-0.26 (p = 0.614)	0.1 (p = 0.857)	0.56 (p = 0.246)	0.41 (p = 0.423)	-0.24 (p = 0.651)	0.08 (p = 0.875)	0.47 (p = 0.343)	0.53 (p = 0.278)
k_{tr}	0.30 (p = 0.568)	-0.7 (p = 0.119)	-0.43 (p = 0.399)	-0.72 (p = 0.107)	-0.74 (p = 0.089)	-0.64 (p = 0.174)	-0.66 (p = 0.152)	**-0.92 (p = 0.009)**	-0.77 (p = 0.071)	-0.65 (p = 0.164)
k_{des}	-0.52 (p = 0.289)	0.05 (p = 0.92)	-0.63 (p = 0.178)	-0.22 (p = 0.67)	**0.84 (p = 0.034)**	0.81 (p = 0.052)	-0.44 (p = 0.388)	0.03 (p = 0.958)	0.67 (p = 0.144)	0.74 (p = 0.091)
k_{ads}	-0.16 (p = 0.757)	-0.05 (p = 0.928)	-0.63 (p = 0.181)	-0.35 (p = 0.502)	0.65 (p = 0.159)	0.67 (p = 0.147)	-0.34 (p = 0.516)	0 (p = 0.994)	0.46 (p = 0.364)	0.48 (p = 0.339)