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

Influence of microporosity in SBA-15 on the release properties of anticancer drug Dasatinib

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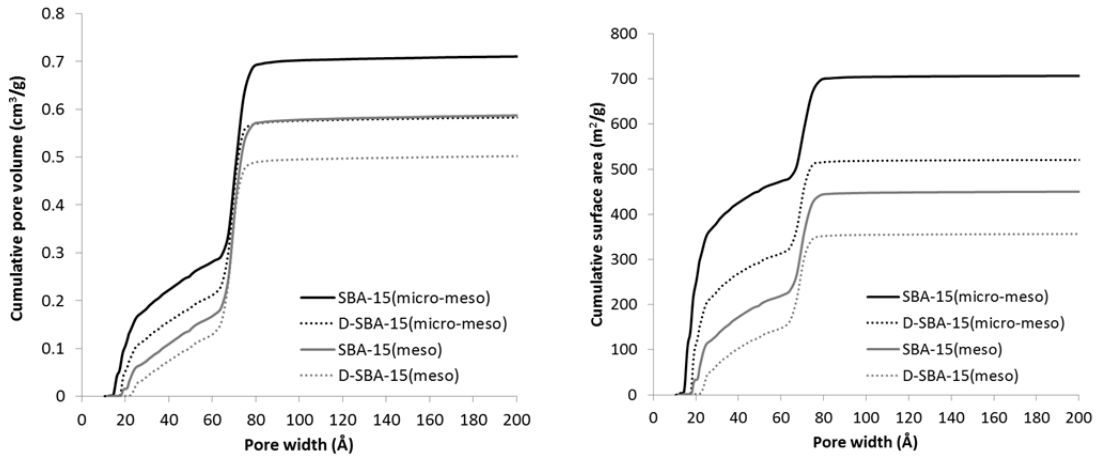
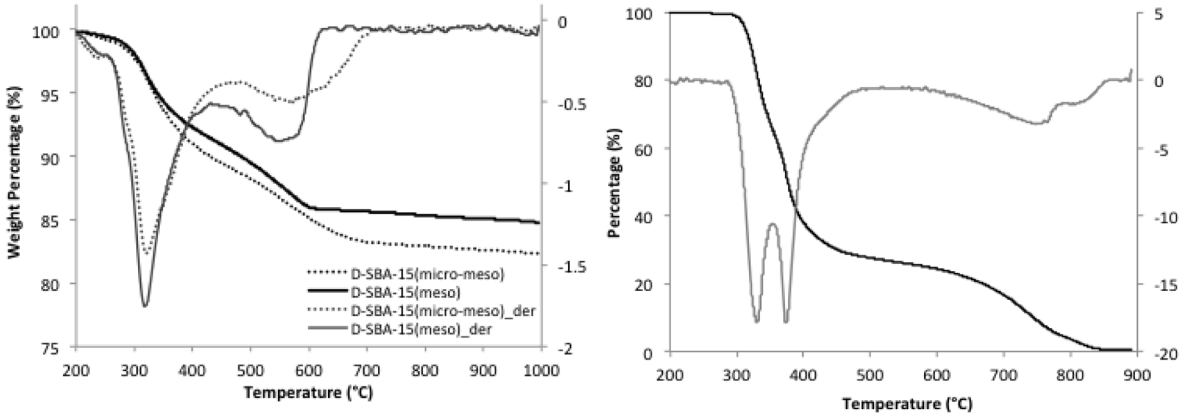
Electronic Supplementary Information:

ESI-1. Cumulative surface area (a) and Cumulative pore volume curves of calcined and loaded SBA-$15_{(micro\text{-}meso)}$ and SBA-$15_{(meso)}$ derived from density functional theory (DFT) model using a cylindrical pore geometry.



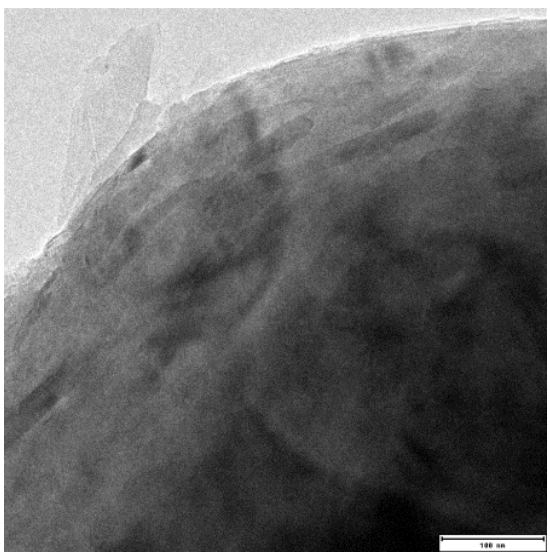
(a) (b)

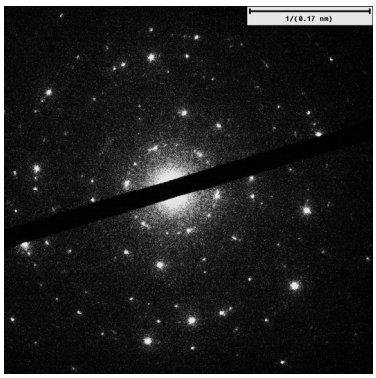
ESI-2 (a)TGA weight loss and its derivative curves of D-SBA-$15_{(micro\text{-}meso)}$and D-SBA-$15_{(meso)}$. (b) TGA weight loss and its derivative curve of Dasatinib.



(a) (b)

ESI-3. (a) Transmission Electron microscopy images of Dasatinib crystals in the exterior of SBA-15 particles and corresponding Selected Area Electron diffraction pattern confirming the crystallinity originating from drug particles outside the pores.

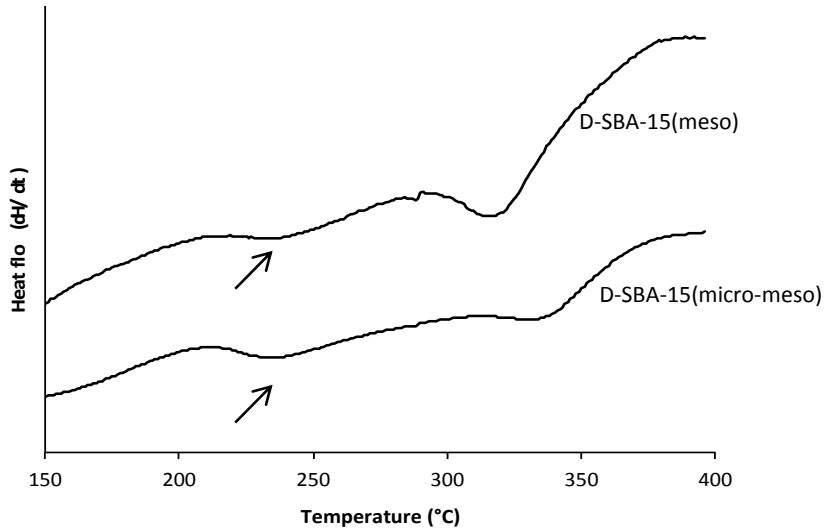




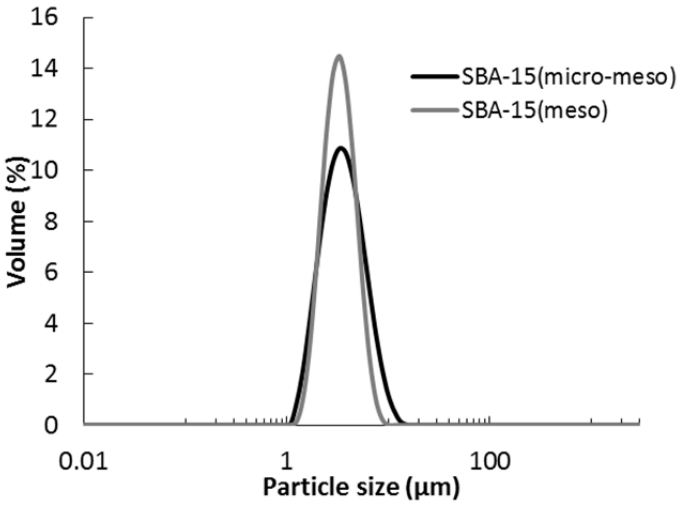
(b) Diffraction peaks shown in Figure 4 were analysed further by using the Scherrer equation in order to obtain a value for the crystallite size, and resulting in the following values.

	°2Theta Peak position	Peak Width	Dp (nm)
Free Dasatinib	16.73	0.20	41.95
D-SBA-15(meso)	16.60	0.17	49.34
D-SBA-15(micro-meso)	16.68	0.18	46.61

ESI-4. Enlarged differential scanning calorimetry curves of D-SBA-15$_{(micro.meso)}$ and D-SBA-15$_{(meso)}$. Arrows point to broad peaks corresponding to crystalline phase on the exterior of the particles.



ESI-5. Dynamic light scattering profiles of SBA-15 samples prepared in this work with particle size distributions centred around 3.3 microns.



ESI-6. Kinetic release profiles of dasainib, D-SBA-15$_{meso}$ and D-SBA-15$_{meso-micro}$ conducted at different dose (5, 10 and 20 mg/L denoted as L, M and H). Additionally, all curves for D-SBA-15$_{meso-micro}$ are plotted together for comparison reasons.

Note that at the lowest dose (L) the D-SBA-15$_{meso}$ achieves the highest release of all three samples, due to its faster release kinetics. Since the total concentration released is below that required for re-crystallization the curve does not decrease.

When the doses are increased (H) all formulations lead to a higher initial released concentration, and all curves decrease due to the high concentration. However, the D-SBA-15$_{meso-micro}$ formulation results in the most stable supersaturation state at the higher dose of 20 mg/L.

As can be seen for the comparison with the three doses for D-SBA-15$_{meso-micro}$, the highest attainable supersaturation state for Dasatinib using the sample containing micropores should be attainable at doses between 10-20 mg/L.