

MS37-P02 | TOWARDS UNDERSTANDING PHASE TRANSITIONS OF CONFINED

PHARMACEUTICALS

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The change in the phases of matter has been extensively studied; from simplistic thermal changes of liquids, solids and gases to more the complex transitions of the different forms of the same material, namely polymorphism. This is important for pharmaceuticals as different crystalline forms of the same drug have different intrinsic properties such as solubility, which may in turn affect bioavailability.

Isolation of different phases of matter in early stages of crystallisation is difficult due to limited lifetime and possible interchange of these transitional phases. Therefore stopping/slowing microscale crystallisation in order to observe the early stages is the aim of this project. This is achieved by encapsulating the pharmaceutical into a host with confined nanoscale geometry, in this case a mesoporous silica host. This allows for an indirect route into understanding relationships between different phases and motilities of pharmaceutical materials.

The cocrystal of flufenamic acid and nicotinamide was encapsulated into the mesoporous silica pores using melt loading method. The loading of cocrystal at different ratios inside the pores was confirmed using DSC and nitrogen adsorption isotherms. Subsequent ^1H , ^{13}C and ^{19}F environments of encapsulated pharmaceuticals was completed by different correlation analyses using solid-state NMR methods under MAS conditions. Previous investigation of these materials enabled detection of separate phase peaks using ^{19}F NMR; surface, crystalline and amorphous peaks. Using ^{19}F - ^{19}F NOESY NMR, interactions between two out of three coexisting phases were observed giving insight into spatial distribution between the different phases of material.