Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Webinar

Development of selective proton recoupling at fast magic angle spinning and the structural characterization of Dabrafenib pseudopolymorphs, an anti-cancer drug

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The first part of the presentation would dwell on development and characterization of selective recoupling of protons at fast Magic angle spinning. Two particular recoupling sequences, namely Selective Recoupling of Protons (SERP) and symmetry based C sequence will be discussed. A theoretical model has been used to explain the origin of SERP recoupling conditions while detailed numerical simulation has been used to explain the origin of errors in the measured 1H-1H distances. We have also tailored well established C symmetry class of sequences to allow selective recoupling of protons with higher transfer efficiencies and low rf power requirements than SERP recouping. In the second part of the presentation, we discuss spectral differences and location of solvent molecules as observed by solid-state NMR in the isostructural hydrate/perhydrate pseudopolymomrphs of Dabrafenib.

Wednesday, Jun 17th 2020

2:30 PM