Abstract

The present Thesis employs solution and solid state NMR experiments to elucidate relevant structural and dynamic properties of supramolecular (cyclodextrins), polymeric (PLGA) and nanoparticles (ZnO) based drug delivery systems (DDSs). Intermolecular interactions of a selected set of drug molecules in presence of the drug carriers have been highlighted by exploiting NMR chemical shifts, relaxation rate, magnetization transfer due to Nuclear Overhauser Effect (NOE) and chemical exchange, translational diffusion and cross polarization.

In the first part of the thesis, we have demonstrated applicability of 1D selective NMR relaxation methods quantifying molecular mobility and intermolecular proton distances in drug_cyclodextrin inclusion complexes. NMR relaxation experiments are presented as cost effective and time efficient compared to 2D NOE in reveling the mode of insertion. Also, we have identified that in case of inclusion complexes with severe spectral overlap 1D selective NOE is an efficient alternative.

In the subsequent part of the Thesis, solution dynamics of fluorinated drugs have been investigated inside polymeric PLGA microsphere using ^{1}H and ^{19}F NMR. Quantification of drug proton transfer rate within the cavity educated about the interior of PLGA exhibiting different kinds of water population. Further, ZnO nanoparticles were characterized as carrier for various anticancer drugs. ZnO surface, band gap and crystallite size of free and drug loaded ZnO were investigated by FTIR, UV-DRS and XRD measurements. ^{13}C CP-MAS and relaxation times analysis revealed the restricted mobility and rigid adsorption of 5-FU on ZnO surface.

Applicability of 1D NMR methods resulting speedy data acquisition has been highlighted throughout.

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