Abstract

The Thesis aims to explore the potential of ligand-based one dimensional (1D) ^{19}F NMR methods (with ^{1}H, ^{2}H NMR and ODNP: Overhauser Dynamic Nuclear Polarization whenever required) to provide the qualitative and quantitative description of molecular interactions in solutions, for a selected (a) Ligand-Protein (b) Agrochemicals-Humic Acid and (c) Solute-Solvent type fluorinated systems in *in vitro* fashion.

The Thesis illustrates the application of ^{19}F transverse relaxation and diffusion analysis unravelling interaction of organofluorines with (a) serum and digestive proteins, (b) humic acid (HA). Extraction of exchange rate between the free and bound state of the organofluorine is accomplished through ^{19}F constant time fast pulsing CPMG experiments allowing determination of the lifetime of the complex. ^{19}F diffusion measurements are found to be more reliable leading to easier interpretation of kinetic parameters using suitable binding isotherms. ^{19}F-^{1}H and ^{1}H-^{1}H Saturation Transfer Difference measurements enabled prediction of the binding mode. ^{19}F spectral analysis in addition to ^{1}H NMR highlighted the influence of HA on photo-degradation of a fluorinated agrochemical.

Further a successful attempt is made to establish a new approach to investigate the trifluoroethanol solvation dynamics inducing structural transition of melittin employing a combination of solvent detected low field ^{19}F relaxation and ^{19}F ODNP. A direct determination of molecular correlation times from low field ^{19}F longitudinal relaxation simplifies the analysis. Further, the preferential solvation of carbohydrates is also investigated in TFE: D_2O cosolvent mixture to benchmark the high field ^{2}H and low field ^{19}F NMR relaxation measurements for investigating such processes.

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