Title:	Drug Dynamics Study in the Ionic-liquid Environment using PFG-Diffusion, Relaxation NMR and Computational Calculations
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Abstract:	The pharma industries are facing many challenges in the drug delivery of newly discovered drug molecules due to their low bioavailability, solubility, polymorphic conversion, and stability. Such limitations further got intensified if a drug is partially soluble or insoluble in water or any other pharmaceutically approved organic solvents. In the pharmaceutical sciences, innovation is needed to overcome these barriers for the formulation of drugs and systems for efficient drug delivery. In this work, we focused on investigating the dissolution mechanism and hydrogen-bonding interactions between 5-Fluorouracil (A pyrimidine nucleic acid-base) and IL, 1-Butyl-3- methylimidazolium bromide using the combined application of 19 F, 1 H NMR, and 1 H– 1 H NOESY NMR spectroscopy along with quantum chemical calculations using Gaussian 09. The bifunctional dissolution nature of IL can be deduced via the presence of interactions between both ions of the [BMIM] + [Br] - and 5-Furacil that is responsible for the dissolution mechanism, which involves hydrogen bonding between the drug-cation and anion of IL. The location of these interaction sites is attempted to unveil using the relaxation and diffusion NMR experiments, complemented by Gaussian calculations, which provided additional evidence concerning the cation-5-Furacil interactions.
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