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Targeting liposomal drug delivery for anti-protozoal drugs: A systems biology approach

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Lipid bilayers which govern and mediate various biologically relevant processes on the microscopic level is one of the great challenges in biology. To investigate the characteristics of the membranes and to obtain the intriguing physicochemical aspects of membranes systems many experiments have been and are still being performed. A full understanding of biological function emerges only if we are able to integrate all relevant information at multiple levels and recreate molecular dynamic interactions. These dynamic interactions involves force field parametrization on the basis of extended QM calculations mainly structures, energetics and phase transitions. Atomistic level simulation was performed to examine the partitioning and nature of interactions of anti-protozoal drug emetine in bilayers of dipalmitoylphosphatidylcholine. Neutral and anionic states of the drug were simulated to understand the effect of protonation or pH on drug partitioning. It is observed that the charged forms were found to permeate fully and prediction of structural changes, phase transition in particular, may have potential therapeutic applications.

Biography

Dr. Shailza Singh has completed her Ph.D in the area of Bioinformatics from IIT Delhi and presently working as Scientist C at National Centre for Cell Science, Pune. She is the recipient of DST Young Scientist Award and International Travel Award by DBT and CSIR. She has published more than 15 papers in reputed international journals and serving as reviewer for international journals such as Current Medicinal Chemistry, Acta Crystallographica (Section F) and Computers in Biology and Medicine. She has guided several project students and MSc. students in bioinformatics.