

Investigation of the Impact of the Ionic Liquid on the Solubility of Acyclovir Derivative through Computational Analysis

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Acyclovir derivative is one of the most nucleoside analogs used as an antiviral drug for treatment of chickenpox, simplex virus infection and shingles. Acyclovir derivative like other analogs facing with poor solubility in water and organic solvent hindering its bioavailability and membrane permeation. To deal with this problem, Ionic liquid emerged to be potential candidate with the ability to improve the solubility of these drugs. To understand this, solvation mechanism was identified computationally. The findings shows that, Ionic liquid has high ability to improve the solubility of these drugs. From the results various factors that contribute to increase in the solubility of the drug was discussed including the contribution of van der waals and electrostatic interaction.

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