Prediction of Mefenamic Acid Solubility and Molecular Interaction Energies in Different Classes of Organic Solvents and Water

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Abstract

Determination of solubility data either through experimental- or model-based approaches becomes a necessity in the crystallization of pharmaceutical compounds. The current work predicts the mefenamic acid solubility and molecular interaction energy, namely electrostatic (H-MF), hydrogen bonding (H-HB), and van der Waals (H-vdW), in different solvents at temperatures from 298 to 323 K using the conductor like screening model for real solvents (COSMO-RS). The solvents used were N,N-dimethylacetamide, N,N-dimethylformamide, acetone, ethyl acetate, ethanol, iso-propyl alcohol, n-hexane, n-heptane, cyclohexane, and water. The Gibbs free energy of fusion required in COSMO-RS computation was determined using differential scanning calorimetry and reference solubility method. The accuracy of methods employed in prediction of solubility were evaluated using mean squared quadratic error (MSE). The mefenamic acid solubility predicted using COSMO-RS with reference solubility method showed a small MSE value of less than 2%. The predicted solubility also follows the same trend as the experimental values and increases with temperature. The predicted H-HB energy and Gibbs free energy changes of mefenamic acid dissolution in the solvents studied highly influence the solubility data. Therefore, COSMO-RS with reference solubility method is a promising approach to predict the solubility and intermolecular interaction energy of mefenamic acid in different solvents.

Keywords

KeyWords Plus: DISSOLUTION THERMODYNAMIC DATA; COSMO-RS; IONIC LIQUIDS; COMPUTATIONAL PREDICTION; SYSTEMS; MODEL; ANDROSTENEDIONE; COEFFICIENTS; EQUILIBRIUM; EXPRESSION

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