



Comparison of Four Models to Predict Intrinsic Solubility of Drugs

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SUMMARY. The aqueous solubility of drugs/drug candidates (S_w) is one of the crucial physicochemical parameters in drug discovery studies and any computational method to predict the solubility is highly in demand in the pharmaceutical industry. This work is aimed to compare the accuracy of a recently proposed model ($\log S_w = -1.120E - 0.599ClogP$) composed of two computational descriptors; excess molar refraction (E) and calculated partition coefficient of octanol to water ($ClogP$) with the accuracies of the Hansch model, general solubility equation and linear solvation energy relationship model. These results showed that the prediction capability of the proposed model is better than those of three famous models and the E is a crucial descriptor for aqueous solubility prediction of drugs and drug-like molecules.

KEY WORDS: Drug and drug-like molecules, Excess molar refraction (E), Intrinsic solubility, Prediction.

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