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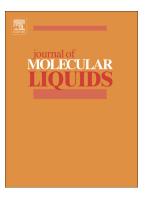
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ACCEPTED MANUSCRIPT

Prediction of Solubility of Active Pharmaceutical Ingredients by Semi-

Predictive Flory Huggins/Hansen model

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Abstract

In this work, solubility of four Active Pharmaceutical Ingredients (APIs) including Butyl

Paraben, Fenoxycarb, Fenofibrate and Risperidone were predicted using Hansen Flory

Huggins model using two different scenarios. In the first method, activity coefficient of APIs

were obtained through fitting the experimental activity coefficients of solvents at particular

temperature of 293 K, then components solubility in entire temperature range of study was

predicted. In the second scenario, the model parameters were adjusted using experimental

data of two selected solvents, then components solubility were predicted in other solvents. In

order to check the physical meanings of obtained values, Molecular Dynamic (MD)

simulations was utilized and the results were compared. Finally the predictive capabilities of

two Hansen Flory Huggins models were compared to temperature-dependent NRTL-SAC

model.

Keywords: Pharmaceuticals, Solubility prediction, Activity coefficient, Hansen Flory

Huggins model

1

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