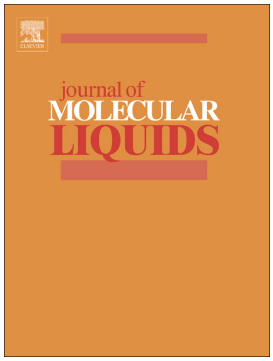

Prediction of solubility of active pharmaceutical ingredients by semi- predictive Flory Huggins/Hansen model

Masood Valavi, Marko Ukrainczyk, Mohammad Reza Dehghani

PII: S0167-7322(17)32573-4
DOI: doi: 10.1016/j.molliq.2017.09.073
Reference: MOLLIQ 7910

To appear in: *Journal of Molecular Liquids*

Received date: 12 June 2017
Revised date: 11 September 2017
Accepted date: 19 September 2017

Please cite this article as: Masood Valavi, Marko Ukrainczyk, Mohammad Reza Dehghani , Prediction of solubility of active pharmaceutical ingredients by semi- predictive Flory Huggins/Hansen model, *Journal of Molecular Liquids* (2017), doi: 10.1016/j.molliq.2017.09.073

Prediction of Solubility of Active Pharmaceutical Ingredients by Semi-Predictive Flory Huggins/Hansen model

Masood Valavi[1], Marko Ukrainczyk[1], Mohammad Reza Dehghani[2]*

[1] Synthesis and Solid State Pharmaceutical Centre, Bernal Institute, University of Limerick, Limerick, Ireland

[2]Chemical engineering Department, Iran University of science and technology, Tehran, Iran

* Corresponding author; m_dehghani@iust.ac.ir

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