



University of Zabol

Graduate school

Faculty of Sciences

Department of Bioinformatics

The Thesis Submitted for the Degree of M.Sc (in the field of Bioinformatic)

**Evaluation of stations drugs solubility in supercritical
fluid with use of multilayer perceptron neural network**

Supervisor:

Dr. M. Khajeh

Advisors:

Dr. M. Bohluli

Dr. M. Ghafari-Moghadam

By:

R. Afrasiabi

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Abstract

Drug solubility is a critical parameter in the pharmaceutical industry for developing efficient processes for production of nanomedicine at industrial scale. Several attempts have been made in recent years to investigate and obtain this parameter using various data mining methods, including neural networks. In this study, to reduce the error rate in predicting solubility, methods including Multi-layer Perceptron (MLP). It have been applied to 32 rows of experimental data collected for solubility of a model drug in supercritical CO₂. Afterwards, the results of these models are examined and compared with measured data to calibrate and validate the developed models. The results showed that the estimated accuracy using the multi-layer perceptron method for all data, training, validation and testing was 0.9326, 0.9274, 0.9563 and 0.9173 respectively, which indicates the existence of a good relationship between the results It is experimental and results obtained from prediction. In general, the method used showed high accuracy of predicted values and actual values.

Keywords: Supercritical, Supercritical fluid, Carbon dioxide, Artificial Neural Network (MLP), statin drug