



University of Zabol
Graduate school
Faculty of Agriculture
Department of Basic Sciences

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

**Estimation of solubility
Anastasol(Arimidex),Exemestane
(Aromasin),Letrozole (Femara) drugs
dioxide in supercritical fluid of carbon
using artificial intelligence**

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Abstract

Today, the supercritical fluid method is widely accepted in various industries due to its environmental friendliness and high efficiency. The main advantage of using supercritical fluid is not to use organic solvent. In this Science China Technological Sciencesogy, a solvent is used in supercritical conditions for separation. The most important supercritical solvent known in this process is CO₂. In this research, perceptron neural network has been used to estimate the solubility of Anastazole (Arimidex), Exemestane (Aromasin), Letrozole (Femara) aromatase inhibitors using carbon dioxide supercritical fluid. The data in different conditions of temperature, pressure and density have been used in modeling. The intermediate layer neurons use sigmoid tangent transformation functions and the output layer neurons use linear transformation functions for the activity function, and for training and optimizing the neural network, Lunberg-Marquardt algorithm is chosen as the neural network training method. Mean square error (MSE) and correlation coefficient (R²) have been used to evaluate the network. In this research, the mean square error (MSE) is 0.078295 and the correlation coefficient (R²) is 0.9764, which are favorable numbers that show that this network provides the expected results.