Abstract

World Health Organization (WHO) predict that cancer will be the main cause of death around the world. One of the method that can be used to overcome cancer is chemo. In the beginning, cancer cell could respond to chemo activity, but as the time goes on the cell become resistant to chemo therapy. Because of that, an effort is needed in development of new anti-cancer drugs. This research objective is to predict indenopyrazole derivative as anti-cancer drugs with Ant Colony Optimization (ACO) as feature selection and Artificial Neural Network (ANN) as prediction model. In previous researchs, declare that indenopyrazole have correlative and predictive ability as anti-cancer agent. The physiochemistry, toxicity and the biology characteristic of the anti-cancer drug must be predicted in advance with Quantitive Structure and Activity Relationships (QSAR) method. In this research 93 Indenopyrazole derivative is used with 1876 descriptor. Then, the descriptor is selected with PCC to acquire 100 descriptor with high number of correlation againts the target. The 100 selected descriptor is then selected again with ACO to acquire relevant feature. The sum of best descriptor ACO selection is 10 descriptor. ANN prediction model is build with 3 topology that is a model with 1, 2 and 3 hidden layer. Accrording to ANN prediction, the model with 3 hidden layer is better because it has R^2_{test} score of 0.882, while the score of 1 and 2 hidden layer in sequence is 0.5218 and 0.6591.

Keywords: Cancer, *indenopyrazole, Quantitive Structure and Activity Relationships, Ant Colony Optimization, Artificial Neural Network.*