Quantitative structure-activity relationship (QSAR) study of newly synthesized carbonyl thiourea derivatives on *Acanthamoeba* sp.

Maizatul Akma Ibrahim*[a], Nor Hafizah Zakaria[a], and Mohd Sukeri Mohd Yusof[b]

[a]Department of Plant Science, Kulliyyah of Science, International Islamic University Malaysia, 25200 Kuantan, Pahang
[b]Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu.

Corresponding author
maizatulakma@iium.edu.my

Abstract

In this study, the effort was to predict and elucidate the molecular structure of newly-synthesized carbonyl thiourea derivatives with their anti-amoebic activities. Therefore, inhibition concentration of 50% the cells population (IC_{50}) was determined for 44 carbonyl thiourea derivatives on a pathogenic *Acanthamoeba* sp. (Hospital Kuala Lumpur isolate). Then, quantitative structure-activity relationship (QSAR) analysis was conducted using three QSAR models, namely stepwise-MLR, GA-MLR and GA-PLS. Results showed that these thiourea derivatives are positively active against the *Acanthamoeba* sp. HKL isolate with IC_{50} values ranging from 2.56 to 7.81 µg.mL^{-1}. From the evaluation of all QSAR models built in this study GA-PLS technique is found to be the best model due to its best predictive ability. The final equation of GA-PLS model gave good statistical output with r^2 = 0.827, and r^2_{cv} = 0.682 *RMSEC*=0.047, *RMSECV*=0.064, r^2_{test} =0.790 and *RMSEP*=0.051. Y-randomization confirmed that the model did not occur from chances of correlation with r^2 = 0.015-0.372. Small residual with values less than 0.25 from prediction in the test set explains robustness of the model. The wealth of information in this study will provide an insight to designing a new thiourea compound with anti-amoebic activity.

Keywords: Thiourea, *Acanthamoeba* sp., IC_{50}, anti-amoebic activity, QSAR