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QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) STUDY OF NEWLY SYNTHESIZED CARBONYL THIOUREA DERIVATIVES ON Acanthamoeba sp.

[Kajian Kuantitatif Hubungan Struktur-Aktiviti (QSAR) Terhadap Terbitan Karbonil Tiourea Hasilan Sintesis Baru Terhadap Acanthamoeba sp.]

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Abstract

This research aims to build a mathematical quantitative structure-activity relationship (QSAR) model, which could relate the relationship between newly-synthesized carbonyl thiourea derivatives with their anti-amoebic activities. Therefore, in this study, inhibition concentration of 50% cells population (IC50) was evaluated for 44 carbonyl thiourea derivatives on pathogenic Acanthamoeba sp. (Hospital Kuala Lumpur isolate). QSAR analysis was conducted using the obtained IC50 data with additional 4 thiourea compounds of the same group from our previous work by applying three linear regression techniques namely stepwise-MLR, GA-MLR, and GA-PLS. Results showed that these thiourea derivatives are positively active against the tested Acanthamoeba sp. with IC50 values ranging from 2.56 to 7.81 µg/mL. From the evaluation of the obtained models, the 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 values of $r^2 = 0.827$, $r^2cv = 0.682$ RMSEC=0.047, RMSECV=0.064, and $r^2test = 0.790$ and RMSEP=0.051. Y-randomization test has confirmed that the model did not occur from the chance of correlation with $r^2 = 0.015$-0.372. Small residual with values less than 0.25 from the prediction in the test set proves the robustness of the model. The information generated from this study will provide an insight into designing a new lead compound from carbonyl thiourea containing highly potential anti-amoebic properties. © 2022, Malaysian Society of Analytical Sciences. All rights reserved.
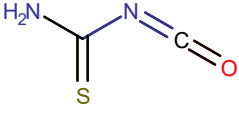
Author keywords

Acanthamoeba sp; anti-amoebic activity; IC50; QSAR models; thiourea derivatives
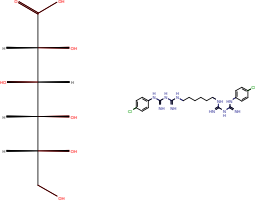
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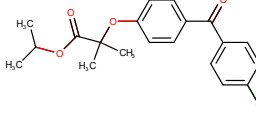
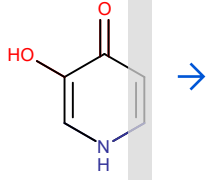**Substances**   View all substances (5)

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