QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) OF *N'*-ETHYL-*N'*-PHENYL-*N*-BENZOYLTHIOUREA AND ITS DERIVATIVES AS ANTICANCER COMPOUNDS BY IN SILICO STUDY

D. Kesuma[1]*, Siswandono[2], and H. Santosa [1]
[1]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Surabaya
Jalan Raya Kalirungkut, Surabaya 60293, Indonesia
[2]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Airlangga
Jalan Dharmawangsa Dalam, Surabaya 60286, Indonesia
Email : dinikesuma@gmail.com

ABSTRACT

Quantitative Structure Activity Relationship (QSAR) has important role in drug development that is improving efficiency on next research to determine new derivatives which are more potent, safer, and have good absorption when consumed. In this research we used *N'*-Ethyl-*N'*-Phenyl-*N*-Benzoylthiourea and 12 derivatives which have anticancer activity based on *in silico* test. Then, we conducted their relationship analysis of physicochemical properties (lipophilic, electronic, and steric) to *in silico* prediction of activity, toxicity, and bioavailability to obtain the best QSAR equation. QSAR equation was determined by linear and non linier regression using statistic program of SPSS 20.0. The result showed that activity prediction (Log 1/RS, from docking on RR receptor PDB ID: 2EUD) with the best QSAR equation: Log 1/RS = 0,118 Mw + 22,994 pKa + 0,022 $tPSA^2$ – 2,590 tPSA -270,960 (n = 13; R = 0,949; SE = 2,054; F = 18,150; Sig = 0,000), toxicity prediction (Log 1/LD-50, ACD/I-Lab prediction) with the best QSAR equation: Log 1/(LD-50 Mouse oral) = - 4,527 Mw – 0,496 $tPSA^2$ + 57,150 tPSA + 744,724 (n = 13; R = 0,925; SE = 61,569; F = 17,846; Sig = 0,000), and bioavailability prediction (Log1/F, ACD/I-Lab prediction) with the best QSAR equation: Log 1/F = - 0,006 Mw - 0,003 tPSA – 2,554 (n = 13; R = 0,802; SE = 0,132; F = 9,006; Sig = 0,006). Furthermore, all of the best equation can be used to develop new compounds as anticancer agent.

Keywords: QSAR, *N'*-Ethyl-*N'*-Phenyl-*N*-Benzoylthiourea, Anticancer, In Silico