ABSTRACT

ANTICANCER ACTIVITY PREDICTION AGAINST SIRT1 RECEPTOR AND CYTOTOXIC ACTIVITY ASSAY AGAINST T47D CELL OF N-2,4-DICHLOROBENZOYL-N’-(4-FLUOROPHENYL)THIOUREA

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Cancer is the second largest cause of death in the world, with a mortality rate of around 9.6 million in 2018 based on WHO. Of these cases, breast cancer is the highest mortality due to cancer in Indonesia. This high rate of death encourages drug researchers to develop more efficient anticancer drugs. One of the studies that are often done is on urea derivatives. N-2,4-dichlorobenzoyl-N’-(4-fluorophenyl)thiourea is one of the thiourea derivatives which is developed from parent compound N-benzoyl-N’-(4-fluorophenyl)thiourea with additional 2 chloro group within the benzoyl group. In silico study against the SIRT1 receptor (PDB ID: 4I5I) shows a low rerank score -100,521 kcal/mol for N-2,4-dichlorobenzoyl-N’-(4-fluorophenyl)thiourea and -96,893 kcal/mol for N-benzoyl-N’-(4-fluorophenyl)thiourea, which indicates they low bond energy and a more stable in drug-receptor interaction. Next, its cytotoxic activity was determined through in vitro study by using the MTT assay method against T47D cell culture. N-2,4-dichlorobenzoyl-N’-(4-fluorophenyl)thiourea show to have 5 times cytotoxic activity than those in N-benzoyl-N’-(4-fluorophenyl)thiourea, because it has lower IC50 value (479,988 μM) in comparison to those in N-benzoyl-N’-(4-fluorophenyl)thiourea (1514,986 μM).

Keywords : in silico study, N-2,4-dichlorobenzoyl-N’-(4-fluorophenyl)thiourea, cytotoxic activity