Rahmah, Nia, N., 2015, Sintesis dan Analisis Inhibisi Senyawa Turunan Amida Calkon terhadap Enzim FNR (feredoksin-NADP$^+$ reduktase) pada Plasmodium falciparum secara in silico. Skripsi di bawah bimbingan Prof. Dr. Ni Nyoman Tri P., M.Si dan Dr. Hery Suwito, M.Si., Departemen Kimia, Fakultas Sains dan Teknologi, Universitas Airlangga

ABSTRAK

Feredoksin-NADP$^+$ reduktase (FNR) mempunyai peran penting dalam jalur respirasi *Plasmodim falciparum* yang bertanggungjawab dalam proses transfer elektron menuju ferredoksin. Penelitian ini bertujuan untuk mensintesis senyama turunan amida calkon sebagai inhibitor enzim *Pf*FNR disertai dengan analisis *in silico*. Tiga senyawa turunan amida calkon disintesis menggunakan reaksi kondensasi Claisen-Schmidt yakni senyawa asam 4-(4-(3-(4-metoksi-fenil)akriloil)fenilamino)-4-oksobutanoat **(1)**, senyawa asam 4-(4-(3-(2,5-dimetoksi-fenil)akriloil)fenilamino)-4-oksobutanoat **(2)** dan senyawa asam 4-(4-sinamoil-fenil-amino)-4-oksobutanoat **(3).** Analisis struktur senyawa hasil sintesis menggunakan metode spektroskopi FTIR, HRESI-MS serta NMR. Analisis secara *in silico* dengan *Autodock4* menunjukkan ikatan hidrogen, ikatan Van Der Waals dan interaksi elektrostatis antara senyawa hasil sintesis dengan residu asam amino enzim *Pf*FNR. Berdasarkan hasil analisis tersebut dapat diketahui senyawa asam 4-(4-sinamoil-fenil-amino)-4-oksobutanoat **(3)** berperan sebagai inhibitor terbaik *Pf*FNR.

Kata Kunci : *amida-calkon, Plasmodium falciparum, FNR, inhibisi, in silico*

Rahmah, Nia, N., 2015, Synthesis and Inhibition in silico Analysis of Amide Derivatives Compounds Against FNR Enzyme (ferredoxin-NADP$^+$ reductase) for Plasmodium falciparum. Final project under guidance Prof. Dr. Ni Nyoman Tri P., M.Si and Dr. Hery Suwito, M.Si., Department of Chemistry, Faculty of Science and Technology, Universitas Airlangga

ABSTRACT

Ferredoksin-NADP+ reductase (FNR) has an important role in *Plasmodium falciparum's* respiration pathway which is involved in the electron transfer to ferredoxin. The purpose of this study is to synthesized amide-chalcone derivatives, followed by in silico analysis. The three of amide-chalcone derivatives were synthesized by Claisen-Schmidt condensation reaction is 4-(4-(3--(4-methoxyphenyl)acryloyl)phenylamino)-4-oxobutanoic acid **(1)**, 4-(4-(3-(2,5-dimethoxyphenyl)acryloyl)phenylamino)-4-oxobutanoic acid **(2)**,and 4-(4-cinnamoylphenylamino)-4-oxobutanoic acid **(3)**. Those compounds synthesized was analyzed using spectroscopy methods such as FTIR, HRESI-MS and NMR. In silico analysis by Autodock4 showed that hydrogen bonding, Van Der Waals bonding, and electrostatic interaction between the compounds and residues of *Pf*FNR enzymes. The results of the in silico analysis assumed that the best compound of act as inhibitor *Pf*FNR.

Keywords : *amide-chalcone, Plasmodium falciparum, FNR, inhibition, in silico*