Ummah, Khoirotul, 2013, Sintesis dan Uji Aktivitas Senyawa Turunan Amino-Calkon dan Analognya sebagai Inhibitor Dihidrofolat Reduktase (DHFR) serta Analisis *In Silico.* Skripsi di bawah bimbingan Drs. Hery Suwito, M.Si dan Dr. Alfinda Novi Kristanti, DEA, Departemen Kimia, Fakultas Sains dan Teknologi, Universitas Airlangga.

ABSTRAK

Dihidrofolat reduktase (DHFR) adalah enzim yang mereduksi dihidrofolat menjadi tetrahidrofolat yang merupakan prekusor penting dalam biosintesis DNA dan pertumbuhan sel, yang biasanya digunakan sebagai target untuk obat-obat antifolat. Penelitian ini bertujuan untuk mensintesis senyawa turunan amino-calkon dan analognya sebagai inhibitor enzim DHFR, disertai dengan analisis secara *in silico.* Molekul target 1-(4-amino-fenil)-3-furanil-prop-2-en-1-on **(1)**, molekul target 4'-amino calkon **(2)**, dan molekul target 4'-amino-2,3-dimetoksi calkon **(3)** disintesis dari 4-amino-asetofenon dengan beberapa turunan benzaldehid. Identifikasi senyawa hasil sintesis dilakukan menggunakan spektroskopi meliputi UV-Vis, FTIR, NMR dan MS. Hasil analisis *in vitro* menunjukkan ketiga senyawa hasil sintesis mempunyai aktivitas inhibitor terhadap enzim DHFR dengan nilai IC_{50} molekul target **(1)** sebesar 45,992 ppm, molekul target **(2)** sebesar 83,221 ppm dan molekul target **(3)** sebesar 61,289 ppm. Analisis secara *in silico* dengan *Autodock4* menunjukkan bahwa terjadi ikatan hidrogen, interaksi π-π *stacking*, dan interaksi van der Waals antara molekul target dengan residu aktif pada enzim DHFR.

***Kata Kunci**: amino-calkon, DHFR, in silico*

Ummah, Khoirotul, 2013, Synthesis and Activity Assay of Amino-Chalcone Derivatives and its analog as Inhibitor of Dihydrofolate Reductase (DHFR) with In Silico Analysis, Final project under guidance Drs. Hery Suwito, M.Si and Dr. Alfinda Novi Kristanti, DEA, Department of Chemistry, Faculty Science and Technology, Airlangga University

ABSTRACT

Dihydrofolate reductase (DHFR) is an enzyme that reduces dihydrofolate into tetrahydrofolate which is an important precursor in the biosynthesis of DNA and cell growth, therefore it is usually used as target protein in drug desaign. The objectives of this study is to synthesize amino-calkon derivatives and its analog as inhibitor of DHFR, followed by in silico analysis. Target molecule 1-(4-amino-phenyl)-3-furanyl-prop-2-en-1-one **(1)**, 4'-amino chalcone **(2)**, and 4'-amino-2,3-dimethoxy-chalcone **(3)** was synthesized from 4-amino-acetophenone and aldehyde derivatives. The structure of the target molecule was identified by spectroscopy methods, such as UV-Vis, FTIR, NMR and MS. The result of in vitro analysis showed that all of target molecules can inhibit the DHFR with IC_{50} value of the target molecule (1) was 45.992 ppm, the target molecule (2) was 83.221 ppm and the target molecule (3) was 61.289 ppm. In silico analysis by Autodock4, showed that occur hydrogen bonding, π-π stacking, and van der Waals interaction between the target molecules and active residues of DHFR.

Keywords: amino-calkon, DHFR, in silico