

Muharromah, S., 2018, Sintesis 2,4-dimetoksi-2'-hidroksicalkon dan 4-N,N-dimetil-2'-hidroksicalkon serta Uji *In Silico* Terhadap Protein MDM2 dan P53. Skripsi di bawah bimbingan Dr. Alfinda Novi Kristanti, DEA. dan Dr. Hery Suwito, M. Si., Departemen Kimia, Fakultas Sains dan Teknologi, Universitas Airlangga, Surabaya.

ABSTRAK

Senyawa (*E*)-2,4-dimetoksi-2'-hidroksicalkon dan (*E*)-4-N,N-dimetil-2'-hidroksicalkon telah berhasil disintesis melalui reaksi kondensasi Claisen Schmidh dengan mereaksikan 2-hidroksiasetofenon dan benzaldehid tersubstitusi gugus -OCH₃ dan -N(CH₃)₂ dalam katalis NaOH. Subtituen pada benzaldehid mempengaruhi hasil sintesis, dimana subtituen -OCH₃ yang lebih elektronegatif menunjukkan rendemen yang lebih tinggi (93%) dibanding subtituen -N(CH₃)₂ (82%). Karakterisasi senyawa 2-hidroksicalkon dilakukan menggunakan spektroskopi UV-Vis, FTIR, dan NMR. Senyawa hasil sintesis kemudian dilakukan uji *in silico* untuk mengetahui aktivitas inhibisi terhadap protein MDM2 dan p53. Protein MDM2 dan p53 merupakan suatu makromolekul yang berperan pada regulasi proses proliferasi sel kanker. Hasil analisis secara *in silico* menunjukkan kompleks 2-hidroksicalkon-MDM2 memberikan interaksi yang lebih stabil dibandingkan dengan kompleks 2-hidroksicalkon-p53. Senyawa 2-hidroksicalkon mampu menghalangi interaksi MDM2-p53 dengan berikatan pada sisi aktif MDM2 sehingga diharapkan aktivitas protein p53 sebagai *suppressor* tumor dapat kembali.

***Kata kunci* :** 2-hidroksicalkon, reaksi Claisen-Schmidh, *in silico*, antikanker.

Muharromah, S., 2018, Synthesis and *In Silico* Evaluation of 2,4-dimethoxy-2'-hydroxychalcone and 4-N,N-dimethyl-2'-hydroxychalcone on MDM2 and P53 proteins. Scription is under advisement of Dr. Alfinda Novi Kristanti, DEA. and Dr. Hery Suwito, M. Si, Department of Chemistry, Faculty of Science and Technology, Universitas Airlangga, Surabaya.

ABSTRACT

2,4-dimethoxy-2'-hydroxychalcone and 4-N,N-dimethyl-2'-hydroxychalcone have been synthesized via Claisen Schmidt condensation from 2-hydroxyacetophenone and benzaldehyde substituted -OCH₃ and -N(CH₃)₂ group using NaOH catalyst. Substituents in benzaldehyde affect the product yield, in which the more electronegative -OCH₃ substituent exhibits higher yield (93%) than -N(CH₃)₂ substituent (82%). Characterization of 2-hydroxychalcone compounds was performed using UV-Vis spectroscopy, FTIR, and NMR. The compounds were then tested *in silico* to determine the inhibition activity of MDM2 and p53 proteins. MDM2 and p53 are a macromolecule that plays a role in regulation of cancer cell poliferation process. The results of *In-silico* analysis show that the 2-hydroxychalcone-MDM2 complex provides a more stable interaction than the 2-hydroxychalcone-p53 complex. The 2-hydroxychalcones are able to inhibit the interaction of MDM2-p53 by binding in active site of MDM2 so activity of p53 protein as tumor suppressor can be reactivate.

Keyword : *2-hydroxychalcone, Claisen-Schmidt reaction, in silico, anticancer.*