

# Sintesis ester sitronelol dan geraniol serta uji aktivitas sitotoksik secara *in silico* terhadap murine leukimia dan *in vitro* terhadap sel kanker murine leukimia P388 dan payudara MCF7 = Synthesis of citronelol and geraniol esters and *in silico* cytotoxic activity test against murine leukimia and *in vitro* against murine leukemia P388 cancer cells and MCF7 breast cancer cells

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## Abstrak

Sitronelol dan geraniol dilaporkan mempunyai aktivitas antibakteri, antiinflamasi dan sitotoksik terhadap beberapa sel kanker. Hasil uji sitotoksik sitronelol dan geraniol terhadap sel kanker murine leukimia P388 menunjukkan bahwa, sitronelol dan geraniol mempunyai aktivitas sitotoksik terhadap sel kanker tersebut. Untuk meningkatkan aktivitas sitotoksik, kedua senyawa tersebut dirancang menjadi sejumlah senyawa ester dan diskriminasi virtual terhadap reseptor protein proviral insertion site in Moloney murine leukemia virus-1 Pim1 kinase dengan perangkat lunak Molegro Virtual Docker MVD. Hasil skrining virtual menunjukkan bahwa senyawa ester hasil rancangan mempunyai potensi sebagai antikanker dan disintesis 8 senyawa ester terpilih yaitu sitronelil kaproat, geraniol kaproat, sitronelil isobutirat, geraniol isobutirat, sitronelil 2,2-dimetil butirat, geraniol 2,2-dimetil butirat, sitronelil kaprilat dan geraniol kaprilat. Senyawa ester hasil sintesis dianalisis awal menggunakan KLT, dimurnikan menggunakan kolom kromatografi, diidentifikasi strukturnya menggunakan FTIR dan NMR serta dianalisis spektrometri massa menggunakan GCMS. Analisis toksisitas senyawa ester hasil sintesis dengan metode BSLT menunjukkan bahwa, ester sitronelol dan geraniol hasil sintesis toksik terhadap larva udang *Artemia salina* dengan nilai LC<sub>50</sub> 1,21-1,96 µg/mL, sehingga berpotensi sebagai senyawa antikanker. Hasil uji aktivitas sitotoksik terhadap sel murine leukimia P388 secara *in vitro* dengan metode MTT menunjukkan bahwa, ester sitronelol dan geraniol hasil sintesis sitotoksik terhadap P388 dengan nilai IC<sub>50</sub> 10,63-37,69 µg/mL. Aktivitas sitotoksik ester sitronelil kaproat yang disintesis dari asam kaproat minyak inti sawit sekitar 4 kali lebih kuat daripada sitronelol. Senyawa yang aktivitas sitotoksiknya lebih tinggi daripada senyawa induk, selanjutnya diuji sitotoksik terhadap sel kanker payudara MCF7 dengan metode alamar blue. Hasil uji sitotoksik ini menunjukkan bahwa senyawa ester sitronelil isobutirat, sitronelil 2,2-dimetil butirat, geraniol isobutirat dan geraniol 2,2-dimetil butirat sitotoksik terhadap MCF7 dengan nilai IC<sub>50</sub> 1,32-4,83 µg/mL. Hidrofobisitas log P senyawa berpengaruh terhadap aktivitas sitotoksik.

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Citronellol and geraniol have been reported as an antibacterial, anti-inflammatory and cytotoxic against some cancer cells. The cytotoxic test result both of citronellol and geraniol against murine leukemia P388 cancer cells showed that citronellol and geraniol have cytotoxic activity against the cancer cells. To enhance the cytotoxic activity both of the compounds, the compounds were designed into a number of ester compounds and virtual screened against the target receptor of proviral insertion site in Moloney murine leukemia virus 1 Pim1 kinase using Molegro Virtual Docker MVD software. The virtual screening result showed that citronellol and geraniol esters have potential as anticancer and 8 ester compounds selected that are citronellyl caproate, geranyl caproate, citronellyl isobutyrate, geranyl isobutyrate, citronellyl 2,2 dimethyl

butyrate, geranyl 2,2 dimethyl butyrate, citronellyl caprylate and geranylcaprylate further synthesized. The synthesized ester compounds were preliminary analyzed by TLC, purified by column chromatography, elucidated the molecular structure using FTIR and NMR and analyzed the mass spectra using GCMS. Toxicity analysis of ester compounds by BSLT method showed that, citronellol and geraniol esters toxic against *Artemia salina* Leach shrimp larvae with LC50 values of 1.21-1.96 mg mL, thereby potentially as anticancer compound. The result of in vitro cytotoxic activity of esters against murine leukemia P388 cancer cells by MTT method showed that, citronellol and geraniol esters cytotoxic against P388 cancer cells with IC50 values of 10.63-37.69 g mL. The cytotoxic activity of citronellyl caproate that synthesized from caproic acid of palm kernel oil was about 4 more active than citronellol. Ester compounds that have higher cytotoxic activity than starting compound, then were tested for cytotoxic activity against breast MCF7 cancer cells by alamar blue method, The result showed that citronellyl isobutyrate, citronellyl 2,2 dimethyl butyrate, geranyl isobutyrate and geranyl 2,2 dimethyl butyrate active against MCF7 cancer cells with IC50 values of 1.32-4.83 g mL. Hydrophobicity logP of ester compounds effect on the cytotoxic activity.