

SINTESIS SENYAWA TURUNAN KALKON DENGAN METODE *MICROWAVE-ASSISTED ORGANIC SYNTHESIS* SERTA UJI AKTIVITASNYA SEBAGAI ANTIVIRUS COVID-19 SECARA *IN SILICO*

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INTISARI

Sejak tahun 2019, dunia telah dilanda pandemi Covid-19 yang kemudian menarik perhatian untuk melakukan sintesis senyawa baru yang dapat dijadikan sebagai antivirus Covid-19. Senyawa kalkon menjadi salah satu kandidat yang berpotensi menjadi antivirus Covid-19 karena memiliki berbagai aktivitas biologis, termasuk sebagai antivirus. Penelitian ini berfokus pada sintesis senyawa turunan kalkon serta uji aktivitasnya sebagai antivirus Covid-19 secara *in silico*. Pada penelitian ini, sintesis turunan senyawa kalkon dilakukan dengan metode konvensional dan metode *Microwave-Assisted Organic Synthesis* (MAOS) melalui kondensasi Claisen-Schmidt antara senyawa aseton dengan tiga senyawa turunan benzaldehida, yaitu benzaldehida, 4-metoksibenzaldehida, dan 3,4-dimetoksibenzaldehida. Sintesis dengan kedua metode dilakukan menggunakan pelarut etanol dan katalis berupa NaOH 30%. Karakterisasi senyawa produk yang dihasilkan dilakukan dengan GC-MS, FTIR, ¹H-NMR, dan ¹³C-NMR. Uji aktivitas kalkon tidak tersubstitusi (kalkon **A**), kalkon dengan satu substituen metoksi (kalkon **B**), dan kalkon dengan dua substituen metoksi (kalkon **C**) dilakukan secara *in silico* terhadap protein SARS-CoV-2 Mpro dan SARS-CoV-2 NSP 10-NSP 16.

Hasil penelitian menunjukkan bahwa senyawa kalkon **A**, **B**, dan **C** memiliki karakteristik berupa padatan berwarna kekuningan. Kalkon **A**, **B**, dan **C** hasil sintesis dengan metode konvensional memiliki kemurnian berturut-turut 94,87%; 95,30%; dan 95,30% serta persen hasil sebesar 85%; 70,47%; dan 91,77%. Produk hasil sintesis dengan metode MAOS untuk kalkon **A**, **B**, dan **C** memiliki kemurnian berturut-turut 99,39%; 99,43%; dan 96,73% serta persen hasil sebesar 62,47%; 83,55%; dan 64,49%. Hasil penambatan molekul menunjukkan senyawa kalkon **C** merupakan senyawa usulan dengan interaksi terbaik dengan reseptor protein SARS-CoV-2 Mpro dan SARS-CoV-2 NSP 10-NSP 16.

kata kunci : antivirus, covid-19, kalkon, kondensasi Claisen-Schmidt, *microwave*

SYNTHESIS OF CHALCONE DERIVATIVES WITH MICROWAVE-ASSISTED ORGANIC SYNTHESIS METHOD AND THEIR ACTIVITIES AS COVID-19 ANTIVIRUS

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ABSTRACT

Since 2019, the world has been hit by the Covid-19 pandemic which has attracted attention to synthesize new compounds that can be used as antiviral drugs for Covid-19. Chalcone is a compound that has potential as an anti-Covid drug as it is a compound with various biological activities, including as an antiviral. This research was focused on synthesis of chalcone derivatives and their activities as Covid-19 antivirus agents. In this study, synthesis of chalcone derivatives were carried out by conventional and Microwave-Assisted Organic Synthesis (MAOS) method through Claisen-Schmidt condensation reaction between acetophenone and benzaldehyde derivatives, namely benzaldehyde, 4-methoxybenzaldehyde, and 3,4-dimethoxybenzaldehyde using ethanol as solvent and NaOH 30% as catalyst. Characterization of resulting products were carried out using GC-MS, FTIR, ¹³C-NMR, and ¹H-NMR spectrometers. Antiviral activity of unsubstituted chalcone (chalcone **A**), chalcone with one methoxy substituent (chalcone **B**), and chalcone with one methoxy substituent (chalcone **C**) were carried out in silico against SARS-CoV-2 Mpro and SARS-CoV-2 NSP 10-NSP 16.

The results showed that chalcones **A**, **B**, and **C** had the characteristics of yellow solid. Chalcones **A**, **B**, and **C** synthesized by conventional method has the purity of 94.87%; 95.30%; and 95.30% and the yield of 85%; 70.47%; and 91.77% respectively. The products synthesized by MAOS method respectively for chalcones **A**, **B**, and **C** has the purity of 99.39%; 99.43%; and 96.73% and the yield of 62.47%; 83.55%; and 64.49%. The results of molecular docking of chalcone **C** produced best interaction, both with SARS-CoV-2 Mpro and NSP 10-NSP 16.

keyword : antivirus, chalcone, Claisen-Schmidt condensation, covid-19, microwave