

**ANALISIS *IN SILICO* SENYAWA MINYAK ATSIRI PADA
Cymbopogon citratus TERHADAP MAIN PROTEASE SARS-COV-2**

SKRIPSI



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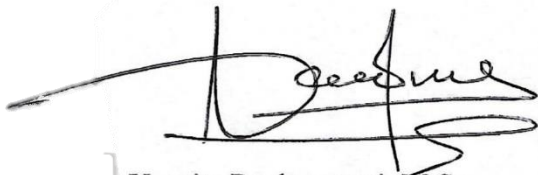
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Terhadap Main Protease SARS-COV-2

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ABSTRAK
ANALISIS *IN SILICO* SENYAWA MINYAK ATSIRI PADA *Cymbopogon citratus*
TERHADAP MAIN PROTEASE SARS-COV-2

Pandemi COVID-19 akibat virus SARS-COV-2 mendorong pencarian obat antivirus yang efektif. Salah satu target terapinya adalah enzim Main Protease (Mpro), yang berperan penting dalam replikasi virus dan tidak memiliki homolog pada sel manusia. *Cymbopogon citratus* (serai dapur) diketahui mengandung senyawa minyak atsiri yang bersifat antimikroba dan antivirus. Penelitian ini bertujuan mengevaluasi potensi interaksi senyawa minyak atsiri *C. citratus* terhadap protein Mpro SARS-COV-2 dengan metode *in silico*. Sebanyak sembilan senyawa diuji, yaitu: Citral, Isoneral, Isogeranial, Geraniol, Geranil asetat, Citronellal, Citronellol, Germacrene-D, dan Elemol, dengan Nirmatrelvir sebagai kontrol. Prosedur penelitian meliputi skrining toksisitas dan kelayakan berdasarkan Hukum 5 Lipinski. Preparasi protein target dan penambatan molekuler dilakukan menggunakan *AutoDockTools* lalu visualisasi interaksi dengan *Discovery Studio Visualizer*. Setiap ligan ditambatkan sebanyak 50 kali untuk memperoleh rerata dan standar deviasi nilai afinitas. Hasil menunjukkan Germacrene-D memiliki nilai afinitas terbaik (-6,3 kcal/mol), diikuti oleh Elemol (-5,6 kcal/mol) dan Isoneral (-5,2 kcal/mol). Isoneral dan Elemol berinteraksi langsung dengan residu katalitik His41 dan Cys145 Mpro, dengan standar deviasi rendah (0,178 dan 0,234), menunjukkan interaksi yang stabil. Dengan demikian, senyawa minyak atsiri dari *C. citratus* yaitu Isoneral dan Elemol, menunjukkan potensi sebagai kandidat inhibitor Mpro SARS-COV-2 dan layak ditindaklanjuti melalui studi *in vitro* dan *in vivo*.

Kata kunci: SARS-COV-2, Main Protease (Mpro), *Cymbopogon citratus*, minyak atsiri, *in silico*, penambatan molekuler

ABSTRACT
IN SILICO ANALYSIS OF ESSENTIAL OIL COMPOUNDS FROM
***Cymbopogon citratus* AGAINST THE MAIN PROTEASE OF SARS-COV-2**

The COVID-19 pandemic caused by the SARS-COV-2 virus has driven the search for effective antiviral drugs. One of the therapeutic targets is the Main Protease (Mpro) enzyme, which plays a key role in viral replication and has no human homolog. *Cymbopogon citratus* (lemongrass) is known to contain essential oil compounds with antimicrobial and antiviral properties. This study aims to evaluate the potential interaction of *C. citratus* essential oil compounds with the SARS-CoV-2 Mpro protein using in silico methods. Nine compounds were tested: Citral, Isoneral, Isogeranial, Geraniol, Geranyl acetate, Citronellal, Citronellol, Germacrene-D, and Elemol, with Nirmatrelvir used as a control. The research procedure included toxicity screening and evaluation based on Lipinski's Rule of Five, followed by protein preparation and molecular docking using AutoDockTools, with interaction visualization performed using Discovery Studio Visualizer. Each ligand was docked 50 times to obtain the mean and standard deviation of binding affinity values. Results showed that Germacrene-D had the best binding affinity (-6.3 kcal/mol), followed by Elemol (-5.6 kcal/mol) and Isoneral (-5.2 kcal/mol). Isoneral and Elemol interacted directly with the Mpro catalytic residues His41 and Cys145, with low standard deviations (0.178 and 0.234), indicating stable interactions. In conclusion, essential oil compounds from *C. citratus*, particularly Isoneral and Elemol, show potential as candidate inhibitors of SARS-COV-2 Mpro and are worth further investigation through *in vitro* and *in vivo* studies.

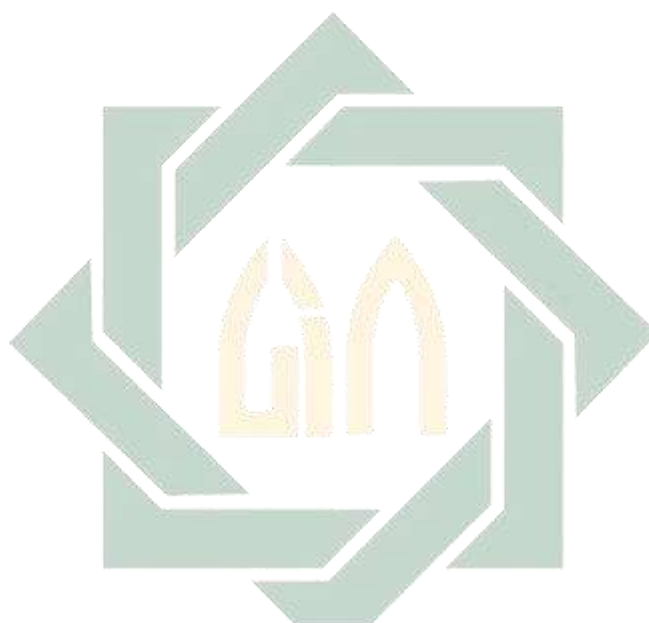
Key words: SARS-COV-2, Main Protease (Mpro), *Cymbopogon citratus*, essential oils, *in silico*, molecular docking.

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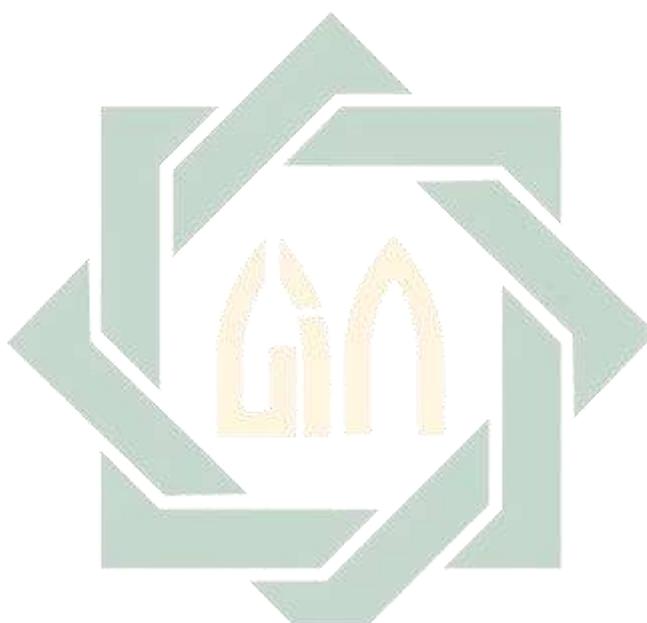
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DAFTAR SINGKATAN PENTING

ADMET	: Absorpsi, Distribusi, Metabolisme, Ekskresi, dan Toksisitas
COVID-19	: <i>Coronavirus Disease 2019</i>
Cys	: Sistein (Asam Amino)
DDBJ	: <i>DNA Data Bank of Japan</i>
DNA	: <i>Deoxyribonucleic Acid</i> (Asam Deoksiribonukleat)
FASTA	: <i>Format Aligned Sequence Text-based Alignment</i>
GC-MS	: <i>Gas Chromatography-Mass Spectrometry</i>
Glu	: Asam glutamat (Asam amino)
H	: Hidrogen
H-bond	: <i>Hydrogen Bond</i> (Ikatan Hidrogen)
His	: Histidin (Asam amino)
IC50	: <i>Inhibitory Concentration 50%</i>
MD	: <i>Molecular Dynamics</i>
N	: Nitrogen
NCBI	: <i>National Center for Biotechnology Information</i>
O	: Oksigen
ORF	: <i>Open Reading Frame</i>
PDB	: <i>Protein Data Bank</i>
PDBQT	: <i>Protein Data Bank, Partial Charges & Torsions</i>
Phe	: Fenilalanin (Asam amino)
PIR	: <i>Protein Information Resource</i>
PLpro	: <i>Papain-Like Protease</i>
PyMOL	: <i>Python-enhanced Molecular Graphics Tool</i>
PyRx	: <i>Python Prescription Docking Software</i>
RCSB	: <i>Research Collaboratory for Structural Bioinformatics</i>
RMSD	: <i>Root Mean Square Deviation</i>
RNA	: <i>Ribonucleic Acid</i> (Asam ribonukelat)
SARS-COV-2	: <i>Severe Acute Respiratory Syndrome Coronavirus 2</i>
SD	: <i>Standard Deviation</i> (Standar deviasi)
Ser	: Serin (Asam amino)
UniProt	: <i>Universal Protein Resource</i>
WHO	: <i>World Health Organization</i>

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