

ABSTRAK

Yudha Syahrul Fadillah. B.17110607. *Potential extract compounds of celery (Apium graveolens) as inhibitors of angiotensin-converting enzyme 2 by in silico. Supervised by M. Fakhri Kurniawan and Titi Rohmayanti.*

Covid-19 occurs due to the entry of Severe Acute Respiratory Syndrome Corona Virus 2 (SARS CoV2) into the human body using spike protein (S) which is able to interact with Angiotensin-converting enzyme 2 (ACE2) receptors. This viral interaction can be prevented by inhibiting the activity of ACE2. This research was designed to study the potential of celery extract as an ACE2 inhibitor using the Lipinski test and molecular anchoring method based on the value of Gibbs free energy (ΔG), the value of RMSD (Root Mean Square Deviation), and the interaction of amino acid residues. Of the 20 celery extract compounds, 14 compounds were found that complied with Lipinski's 5 rules including -ionone, apigenin, Caryophyllene, -selinene, nerol, Cis-Carveol, linalool, Cis-Dihydrocarvone, P-Mentha-2,8-dien-1-ol, P-Mentha-trans-2,8-dien-1-ol, Limonene, P-Cymene, -Myrcene, Trans-Caryophyllene. After performing 14 compounds of celery extract, 6 compounds were found that have the potential as ACE2 inhibitors that have Gibbs free energy (ΔG), RMSD and amino residues that play a role in the formation of hydrophobic and hydrogen interactions that approach better ligand validation 4, including Limonene, Apigenin, Cis-Carveol, P-Mentha-trans-2,8-dien-1-ol, -Ionone and P-Mentha-2,8-dien-1-ol. And the best celery extract compound selected as an ACE2 inhibitor was Limonene. It can be concluded that celery extract compounds can inhibit the interaction between ACE2 and SARS CoV2.

Keywords : COVID-19, Molecular docking, Celery, ACE2, in silico.

ABSTRAK

Yudha Syahrul Fadillah. B.1710607. Potensi senyawa ekstrak tanaman seledri (*Apium graveolens*) sebagai inhibitor angiotensin-converting enzyme 2 secara *in silico*. Dibawah bimbingan M. Fakhri Kurniawan dan Titi Rohmayanti.

Covid-19 terjadi karena masuknya *Severe Acute Respiratory Syndrome CoronaVirus 2* (SARS CoV2) kedalam tubuh manusia dengan menggunakan protein *spike* (S) yang mampu berinteraksi dengan reseptor *Angiotensin-converting enzyme 2* (ACE2). Interaksi virus ini dapat dicegah dengan cara menghambat aktivitas ACE2. Penelitian ini dirancang untuk mempelajari potensi ekstrak seledri sebagai inhibitor ACE2 dengan uji lipinski dan metode penambatan molekul berdasarkan nilai energi ikatan bebas gibbs (ΔG), nilai RMSD (*Root Mean Square Deviation*) serta interaksi residu asam amino. Dari 20 senyawa ekstrak seledri didapatkan 14 senyawa yang memenuhi ke 5 aturan lipinski diantaranya *α -ionone*, *apigenin*, *Caryophyllene*, *β -selinene*, *nerol*, *Cis-Carveol*, *linalool*, *Cis-Dihydrocarvone*, *P-Mentha-2,8-dien-1-ol*, *P-Mentha-trans-2,8-dien-1-ol*, *Limonene*, *P-Cymene*, *β -Myrcene*, *Trans-Caryophyllene*. Setelah dilakukan penambatan terhadap 14 senyawa ekstrak seledri, didapatkan 6 senyawa yang berpotensi sebagai inhibitor ACE2 yang memiliki energi ikatan bebas Gibbs (ΔG), nilai RMSD dan Residu asam amino yang berperan dalam pembentukan interaksi hidrofobik dan ikatan hidrogen yang mendekati bahkan lebih baik ligan 4 validasi, diantaranya yaitu *Limonene*, *Apigenin*, *Cis-Carveol*, *P-Mentha-trans-2,8-dien-1-ol*, *α -Ionone* dan *P-Mentha-2,8-dien-1-ol*. Dan terpilih senyawa ekstrak seledri terbaik sebagai inhibitor ACE2 adalah *Limonene*. Dapat ditarik kesimpulan bahwa senyawa ekstrak seledri berpotensi dalam menghambat interaksi antara ACE2 dengan SARS CoV2.

Kata Kunci: COVID-19, penambatan molekul, Seledri, ACE2, *in silico*.