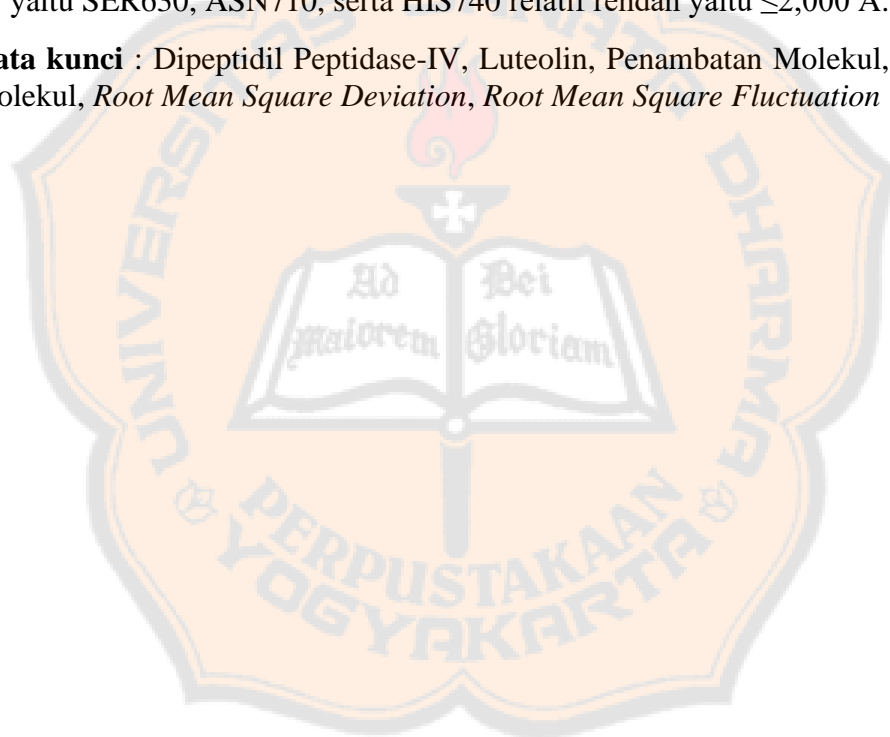


ABSTRAK

Penghambatan enzim Dipeptidil Peptidase IV (DPP-IV) merupakan salah satu obat mengatasi DM tipe 2. Penghambatan DPP-IV serta meningkatkan sekresi insulin. Luteolin dilaporkan memiliki aktivitas penghambatan enzim DPP-IV. Tujuan penelitian ini untuk mengetahui stabilitas kompleks Dipeptidil Peptidase IV (DPP-IV) dan luteolin pada simulasi dinamika molekul dalam waktu 15 ns. Jenis penelitian ini adalah teoritis deskriptif eksploratif dengan parameter yang digunakan adalah nilai RMSD atom-atom *backbone* DPP-IV dan *ligand move* $\leq 2,000 \text{ \AA}$, dan nilai RMSF $\geq 0,5 \text{ \AA}$. Hasil penelitian ini Δ RMSD atom-atom *backbone* yang diperoleh pada 5 ns terakhir pada luteolin pose 1 (0,762 \AA), pose 2 (0,655 \AA), dan pose 3 (0,717 \AA). Selanjutnya, Δ RMSD *ligand move* luteolin pose 1 (1,354 \AA), pose 2 (2,286 \AA), dan pose 3 (5,427 \AA). Berdasarkan hasil tersebut maka luteolin membentuk kompleks yang tidak stabil. Nilai RMSF pada sisi katalitik dari DPP-IV yaitu SER630, ASN710, serta HIS740 relatif rendah yaitu $\leq 2,000 \text{ \AA}$.

Kata kunci : Dipeptidil Peptidase-IV, Luteolin, Penambatan Molekul, Dinamika Molekul, *Root Mean Square Deviation*, *Root Mean Square Fluctuation*



ABSTRACT

Inhibition of the enzyme Dipeptidyl Peptidase IV (DPP-IV) is one of the drugs to treat type 2 DM. DPP-IV inhibits and increases insulin secretion. Luteolin is reported to have inhibitory activity on the DPP-IV enzyme. This study aimed to determine the stability of the Dipeptidyl Peptidase IV (DPP-IV) complex and luteolin in molecular dynamics simulations within 15 ns. This type of research is theoretical exploratory descriptive with the parameters used are RMSD values of DPP-IV backbone atoms and ligand move $\leq 2,000\text{\AA}$ and RMSF values $\geq 0,5\text{\AA}$. The results of this study Δ RMSD backbone atoms obtained in the last 5 ns in luteolin pose 1 (0.762\AA), pose 2 (0.655\AA), and pose 3 (0.717\AA). Next, Δ RMSD ligand move luteolin poses 1 ($1,354\text{\AA}$), pose 2 ($2,286\text{\AA}$), and pose 3 ($5,427\text{\AA}$). Based on these results, luteolin forms an unstable complex. RMSF values on the catalytic site of DPP-IV, namely SER630, ASN710, and HIS740, were relatively low, namely $\leq 2,000\text{\AA}$.

Keywords: *Dipeptidyl Peptidase-IV, Luteolin, Molecular Docking, Molecular Dynamics, Root Mean Square Deviation, Root Mean Square Fluctuation*

