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Analisis Penambatan Molekuler Senyawa Turunan Benzimidazol Mannich Terhadap Siklooksigenase Menggunakan Autodock 4 dan Autodock Vina = Molecular Docking Analysis of Mannich Benzimidazole Derivatives into Cyclooxygenase by Autodock 4 and Autodock Vina

Figel Ilham, author

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Abstrak

Inflamasi merupakan respon fisiologis terhadap cedera jaringan dan infeksi. Inflamasi dapat ditangani dengan sejumlah obat seperti obat anti-inflamasi nonsteroida inhibitor selektif COX-2. Benzimidazol merupakan senyawa penuntun yang memiliki berbagai aktivitas farmakologis, salah satunya sebagai anti-inflamasi. Penelitian ini dilakukan secara in silico dengan metode penambatan molekuler senyawa turunan benzimidazol Mannich terhadap COX-1 dan COX-2 untuk mengetahui potensi anti-inflamasi senyawa menggunakan Autodock 4 dan Autodock Vina. Hasil validasi menunjukkan bahwa nilai RMSD Autodock 4 dan Autodock Vina dibawah 2 Ã sehingga penambatan molekuler dilakukan pada kedua perangkat lunak. Pada penambatan molekuler menggunakan Autodock 4, turunan benzimidazol substituen vanilin 2,6-dimetilmorfolin diprediksi paling selektif terhadap COX-2 yaitu rasio Ki COX-1/2 senilai 162,79. Pada penambatan molekuler menggunakan Autodock Vina, turunan benzimidazol substituen vanilin dietilamina diprediksi paling selektif terhadap COX-2 yaitu rasio Ki COX-1/2 senilai 112,88. Visualisasi interaksi pada Autodock 4 dan Autodock Vina juga menunjukkan hasil yang sedikit berbeda. Dengan demikian terdapat dua buah kesimpulan yang diperoleh: senyawa turunan benzimidazol Mannich memiliki potensi anti-inflamasi inhibitor selektif COX-2, dan terdapat perbedaan interaksi yang muncul di antara penambatan molekuler terhadap Autodock 4 dan Autodock Vina.

.....Inflammation is a physiological response occurred by tissue injury and infection. Inflammation can be treated with drugs such as COX-2 selective NSAID. Benzimidazole is a leading compound that has many pharmacological activities such as anti-inflammation. In this study, in silico testing is carried out with molecular docking into Mannich benzimidazole derivatives against COX-1 and COX-2 using Autodock 4 and Autodock Vina to determine the anti-inflammatory potential of the test compounds. Validation result shows that both the RMSD value of both Autodock 4 and Autodock Vina are below 2 Ã. Hence, molecular docking is conducted with both programs. Autodock 4 result shows that benzimidazole derivative with vanillin 2,6-dimethylmorpholine substitution is predicted to be the most selective against COX-2 with the Ki COX-1/2 ratio of 162.79. Autodock Vina result shows that benzimidazole derivative with vanillin diethylamine substitution is predicted to be the most selective against COX-2 with the Ki COX1/2 ratio of 112.88. Interaction visualization of Autodock 4 and Autodock Vina also shows few differences, yielding two conclusions from the study: Mannich benzimidazole derivatives have anti-inflammatory potential selective to COX-2 and there are few differences appeared in molecular docking with Autodock 4 and Autodock Vina.