BAB 5

KESIMPULAN DAN SARAN

5.1.   Kesimpulan

Berdasarkan penelitian Perhitungan Energi Bebas Mip-ligan (2-[4-((2*R*)-2-(3*S*,5*S*)-3-5dimetilsikloheksil)-2-hidroksietil)-2,6-dioxopiperidin-1-il)-N-((1*R*,5*R*,7*R*)1,7-dimetiltrisiklo[3.3.1.1^{3,7}]dekan-3-il)asetamida dengan metode MMPBSA memberikan kesimpulan sebagai berikut :

1.   Perubahan energi bebas antara ikatan Mip-ligan (2-[4-((2*R*)-2-(3*S*,5*S*)-3-5dimetilsikloheksil)-2-hidroksietil)-2,6-dioxopiperidin-1-il)-N-((1*R*,5*R*,7*R*)1,7-dimetiltrisiklo[3.3.1.1^{3,7}]dekan-3-il)asetamida menggunakan metode MMPBSA (*Molecular mechanics Poisson-Boltzmann surface area*) mendapatkan hasil rata-rata -147,325 kJ/mol.

2.   Residu yang memberikan kontribusi energi bebas pada interaksi protein Mip-ligan (2-[4-((2*R*)-2-(3*S*,5*S*)-3-5dimetilsikloheksil)-2-hidroksietil)-2,6-dioxopiperidin-1-il)-N-((1*R*,5*R*,7*R*)1,7-dimetiltrisiklo[3.3.1.1^{3,7}]dekan-3-il)asetamida, terutama pada sisi pengikatan adalah Y55, F65, D66, F77, Q81, V82, I83, W86, Y109, S113, V114, G116, P117, I118, L124, F126.

5.2.   Saran

Penelitian ini dapat dilanjutkan dengan perhitungan energi bebas Mip dengan ligan lain menggunakan metode MMPBSA (*Molecular mechanics Poisson-Boltzmann surface area*).

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