BAB 5
KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan penelitian perhitungan perubahan energi bebas menggunakan metode *Umbrella Sampling* dari protein MIP-Rapamycin memberikan kesimpulan sebagai berikut :

1. Perubahan energi bebas dengan empat variasi selisih jarak COM dan jarak awalnya : (A) Jarak awal 1,238 nm dan selisih 0,047 nm hasil perhitungan ΔG -38,802 kJ/mol, (B) Jarak awal 1,238 nm dan selisih 0,094 nm hasil perhitungan ΔG -28,449 kJ/mol , (C) Jarak awal 1,285 nm dan selisih 0,082 nm hasil perhitungan ΔG -48,531 kJ/mol, (D) Jarak awal 1,238 nm dan selisih 0,128 nm hasil perhitungan ΔG -52,736 kJ/mol.
2. Selisih jarak COM dari empat variasi menggunakan kecepatan tarikan dikurangi menjadi 0,005 nm ps^{-1} semuanya menunjukkan adanya celah. Celah kecil menyebabkan perhitungan perubahan energi bebas menjadi naik, tetapi bila celahnya lebih besar perhitungan perubahan energi bebas menjadi turun dilihat pada (Tabel 4.3)

5.2 Saran

Penelitian untuk kompleks MIP-Rapamycin perlu dilakukan penelitian lebih lanjut untuk interaksi antara protein dan ligan pada kecepatan tarikan 0,005 nm ps^{-1}.

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