

BAB 5

KESIMPULAN

5.1 Kesimpulan

Berdasarkan penelitian perhitungan energi bebas menggunakan metode *Umbrella Sampling* dari protein Mip dan ligan turunan s35dt menghasilkan kesimpulan sebagai berikut:

1. Pada perhitungan perubahan energi bebas dengan menggunakan variasi jumlah trayektori 35 didapatkan hasil sebesar -15,3144 kJ/mol. Perubahan nilai energi bebas pada trayektori 35 terhadap 45 sebesar -0,251%.
2. Pada perhitungan perubahan energi bebas dengan menggunakan variasi jumlah trayektori 40 didapatkan hasil sebesar -15,3216 kJ/mol. Perubahan nilai energi bebas pada trayektori 40 terhadap 45 sebesar 0,205%.
3. Pada perhitungan perubahan energi bebas dengan menggunakan variasi jumlah trayektori 45 didapatkan hasil sebesar -15,353 kJ/mol.
4. Pada protein Mip dengan ligan s35dt menunjukkan bahwa semakin besar jumlah trayektori selisih ΔG akan semakin menurun, sedangkan pada protein Mip dan ligan rapamisin menunjukkan bahwa semakin kecil jumlah trayektori selisih ΔG akan semakin menurun.

5.2 Saran

Pada metode *Umbrella Sampling* disarankan menggunakan jumlah trayektori 35, karena dengan jumlah trayektori 35 sudah dapat digunakan untuk menghitung energi bebas.

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