

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian mengenai perhitungan perubahan energi bebas kompleks Mip-*rapamycin* menggunakan metode *umbrella sampling* pada kecepatan tarikan $0,001 \text{ nm ps}^{-1}$, dapat diperoleh kesimpulan sebagai berikut:

1. Nilai perubahan energi bebas (ΔG) pengikatan Mip-*rapamycin* dengan menggunakan metode *Umbrella Sampling* dengan jumlah trayektori 35, 40, dan 45 masing-masing adalah sebesar -43,219 kJ/mol, -43,42 kJ/mol, dan -43,395 kJ/mol.
2. Perubahan jumlah trayektori tidak menyebabkan perubahan perhitungan energi bebas yang cukup besar, dengan perbedaan kurang dari 1% terhadap perhitungan perubahan energi bebas dengan jumlah trayektori 45.

5.2 Saran

Untuk memahami secara lebih rinci penyebabnya, diperlukan penelitian lanjutan untuk menelaah interaksi yang terjadi antara protein Mip dan *rapamycin*, khususnya pada jarak COM 1,26 nm dan 1,46 nm.

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