BAB 5
KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan penelitian yang telah dilakukan terkait perhitungan perubahan energi bebas menggunakan metode *Umbrella sampling* dari kompleks protein FKBP12-Rapamycin diperoleh kesimpulan sebagai berikut:

1. Dengan selisih jarak COM 0,031 nm, dan jarak COM awal 1,119 nm menghasilkan ΔG sebesar -64,811 kJ/mol.
2. Dengan selisih jarak COM 0,062 nm dan jarak COM awal 1,119 nm menghasilkan ΔG sebesar -58,892 kJ/mol, sedangkan dengan selisih jarak COM 0,062 nm dan jarak COM awal 1,135 nm menghasilkan ΔG sebesar -65,588 kJ/mol.
3. Dengan selisih jarak COM 0,093 nm dan jarak COM awal 1,119 nm menghasilkan ΔG sebesar -57,543.

5.2 Saran

Penelitian ini dapat dilanjutkan dengan mengamati interaksi yang terjadi dengan simulasi dinamika molekul pada jarak COM awal 1,524 nm dan 1,580 nm.

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