

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan penelitian perhitungan energi bebas menggunakan metode *umbrella sampling* dari protein MIP dengan ligan *rapamycin* memberikan kesimpulan sebagai berikut:

1. Perubahan energi bebas dengan empat variasi selisih dan jarak awal memiliki hasil perhitungan ΔG masing-masing pada jarak awal dan selisihnya:
 - a. Jarak awal 1,249(0) selisih 0,057 nm hasil ΔG -39,234 kJ/mol,
 - b. Jarak awal 1,249(0) selisih 0,118nm hasil ΔG -37,833 kJ/mol,
 - c. Jarak awal 1,249(0) selisih 0,119nm hasil ΔG -45,817 kJ/mol,
 - d. Jarak awal 1,275(1) selisih 0,176nm hasil ΔG -32,653 kJ/mol.
2. Celah yang terjadi pada grafik histogram dari trayektori menunjukkan pada trayektori 5 dan 6 kemudian 12 dan 13. Celah ini menunjukkan adanya pemutusan interaksi protein MIP dan ligan *rapamycin* yang terjadi secara bertahap.

5.2 Saran

Penelitian ini dapat dilanjutkan lebih lanjut lagi untuk mengetahui jenis interaksi apa yang terlibat dalam pemutusan interaksi protein MIP dengan ligan *rapamycin*.

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