

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

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

1. Perubahan energi bebas dengan variasi interval jarak COM beserta jarak COM awal yang digunakan: (A). Jarak awal yang digunakan adalah 1,238 nm dan interval jarak COM 0,050 nm didapatkan perhitungan perubahan energi bebas -43,395 kJ/mol, (B). Jarak awal yang digunakan adalah 1,238 nm dan interval jarak COM 0,098 nm didapatkan perhitungan perubahan energi bebas -51,280 kJ/mol, (C). Jarak awal yang digunakan adalah 1,281 nm dan interval jarak COM 0,098 nm didapatkan perhitungan perubahan energi bebas -37,062 kJ/mol, (D). Jarak awal yang digunakan adalah 1,238 nm dan interval jarak COM 0,147 nm didapatkan perhitungan perubahan energi bebas -46,498 kJ/mol.
2. Pada variasi interval jarak COM menggunakan kecepatan tarikan yang diperlambat menjadi 0,001 nm ps⁻¹ menunjukkan adanya celah. Namun pada celah kecil atau celah besar nilai perubahan energi bebasnya berbeda.

5.2 Saran

Penelitian untuk kompleks protein MIP dan ligan Rapamycin perlu dilakukan penelitian selanjutnya untuk mengamati celah pada jarak COM berapa supaya mengetahui interaksi apa yang terjadi.

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