

## BAB 5

### KESIMPULAN DAN SARAN

#### 5.1. Kesimpulan

Penelitian Berdasarkan penelitian perhitungan energi FKBP12-Rapamycin dengan metode Integrasi Termodinamika, telah diperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan berikut adalah:

Perhitungan  $\Delta G$  dan  $\Delta G_{\text{kumulatif}}$  pada kondisi  $\lambda = 10$  sampai  $\lambda = 13$ , kenaikan nilai parameter  $\lambda_{\text{coul}}$  tidak menyebabkan perubahan  $\Delta G$ . Tetapi ketika  $\lambda = 14$ , yaitu parameter  $\lambda_{\text{coul}} = 1$  terjadi kenaikan  $\Delta G$  sebesar 10,69 kJ/mol. Nilai ini menunjukkan bahwa tidak ada interaksi antara protein FKBP12 dan ligan rapamycin. Hal ini bertentangan dengan hasil eksperimen dari van Duyne dkk (1991) Oleh karena itu hasil perhitungan perubahan energi bebas dengan menggunakan metode integrasi termodinamika. tidak sesuai dengan hasil percobaan. Hal ini disebabkan oleh interval perubahan parameter interaksi elektrostatik yang terlalu besar.

#### 5.2. Saran

Penelitian ini dapat dilanjutkan dengan:  
Pada penelitian ini kondisi parameter  $\lambda_{\text{coul}}$  harus diperkecil.

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