

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan penelitian Perhitungan Energi Bebas Mip-Rapamycin dengan metode MMPBSA telah diperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan tersebut dapat dipaparkan sebagai berikut:

1. Perubahan energi bebas antara ikatan Mip-Rapamycin menggunakan metode MMPBSA mendapatkan hasil rata-rata -229,737 kJ/mol yang menunjukan bahwa perubahan energi bebas pengikatan.
2. Residu yang memberikan kontribusi energi bebas besar pada interaksi dengan protein Mip adalah F77, Q81, V82, I83 dan Y109.

5.2 Saran

Penelitian ini dapat dilanjutkan dengan :

Perhitungan energi bebas ikatan Rapamycin dengan protein FKBP12 untuk dibandingkan dengan ikatan kompleks Mip-Rapamycin dengan menggunakan metode MMPBSA.

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