

BAB V

KESIMPULAN DAN SARAN

5.1 Kesimpulan penelitian

Berdasarkan penelitian simulasi dinamika molekul FKBP12 dengan ligan rapamycin, telah diperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan tersebut dipaparkan sebagai berikut :

1. Simulasi dinamika molekul selama 40 ns menghasilkan lima konformasi protein FKBP12.
2. Pada kelima konformasi protein FKBP12 struktur rapamycin mengalami lekukan.
3. Interaksi ikatan hidrogen memiliki pengaruh yang lebih dominan daripada interaksi hidrofobik dalam stabilitas interaksi ligan rapamycin dan residu protein FKBP12 pada sisi aktifnya.

5.2 Saran Penelitian

Penelitian ini dapat dilanjutkan dengan:

1. Simulasi dinamika molekul untuk struktur apo dari protein FKBP12 untuk memahami peranan ligan rapamycin terhadap struktur protein FKBP.
2. Perhitungan energi bebas ikatan rapamycin dengan protein FKBP12 yang dibandingkan dengan protein FKBP yang lain.

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