

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Penelitian Berdasarkan penelitian simulasi dinamika molekul bentuk apo dari imunofilin FKBP12, telah diperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan tersebut dipaparkan sebagai berikut :

1. Simulasi dinamika molekul selama 200 ns menghasilkan perhitungan RMSD yang cukup stabil dengan rata-rata nilai perhitungan RMSD untuk semua atom protein memiliki rata-rata 0,15 nm, sedangkan dan untuk atom penyusun tulang punggung protein memiliki rata-rata 0,08 nm.
2. Residu yang bersifat paling fleksibel berdasarkan hasil perhitungan RMSF dan dikonfirmasi oleh perubahan struktur dPCA adalah I90.
3. Analisa dPCA dari 20000 konformasi menghasilkan lima struktur dan kelima konformasi protein FKBP12 mengalami perubahan posisi residu yang signifikan.

5.2 Saran

Penelitian Penelitian ini dapat dilanjutkan dengan:

1. Simulasi dinamika molekul protein FKBP12 dengan ligan yang lain.

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