

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian yang telah dilakukan, maka dapat diambil kesimpulan yaitu:

1. Simulasi dinamika molekul yang dilakukan selama 40 ns menghasilkan rata-rata nilai perhitungan RMSD untuk semua atom protein FKBP12 sebesar 0,15 nm dan untuk semua atom penyusun tulang belakang protein FKBP12 sebesar 0,08 nm.
2. Hasil perhitungan RMSF menunjukkan sub bagian nomor 2, 4, 6, dan 13 memiliki fleksibilitas yang tinggi. Pada sub bagian nomor 2, 4, dan 6 tidak terdapat residu asam amino, sedangkan pada sub bagian nomor 13 terdapat residu asam amino sisi aktif yaitu Y82, H87, dan I90.
3. Residu asam amino sisi aktif Y82 dan H87 terlibat dalam interaksi hidrogen dengan ligan.
4. Interaksi ikatan hidrofobik menjadi interaksi dominan antara protein FKBP12 dan ligan yang melibatkan residu Y26, F36, F37, P45, F46, Q53, E54, V55, I56, W59, Y82, I90, I91, L97, dan F99.

5.2 Saran

Berdasarkan hasil penelitian yang diperoleh maka disarankan agar dilakukan simulasi dinamika molekul protein FKBP12 dengan ligan turunan lainnya.

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