BAB 5
KESIMPULAN & SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian ini dapat disimpulkan bahwa:

1. Simulasi dinamika molekul selama 40ns menghasilkan rata-rata nilai perhitungan RMSD untuk semua atom protein memiliki rata-rata 0,39 nm, sedangkan untuk atom penyusun tulang punggung protein memiliki rata-rata 0,33 nm.
2. Adanya potensial *flooding* mengakibatkan perubahan konformasi pada sisi aktif protein FKBP12 namun ligan tetap berada pada kantong pengikatan.
3. Residu yang bersifat paling fleksibel berdasarkan penomoran sub bagian pada RMSF adalah pada sub bagian nomor 2 yang tidak memiliki residu sisi aktif, sub bagian nomor 4 yang tidak memiliki residu sisi aktif, E54, V55, I56 pada sub bagian nomor 8 dan Y82, H87, I90 pada sub bagian nomor 13.
4. Interaksi antara FKBP12 dan ligan turunan asam pipekolat terjadi melalui interaksi ikatan hidrogen antara I56 dengan oksigen karbonil pada gugus karboksilat dan interaksi hidrofobik yaitu Y26, T27, G28, M29, L30, K35, F36, D37, S38, F46, F48, Q54, V55, W59, ILE76, PRO 78, TYR80, A81, Y82, H87, I90, I91, L97, V98, F99, D100 dan V101.
5. Interaksi yang dominan antara protein FKBP12 dengan ligan adalah interaksi hidrofobik.

5.2 Saran

Berdasarkan hasil yang diperoleh maka disarankan:

1. Simulasi dinamika molekul FKBP12 dengan turunan lainnya.

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