

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan Penelitian

Berdasarkan hasil penelitian ini dapat disimpulkan bahwa:

1. Simulasi dinamika molekul selama 200 ns menghasilkan rata-rata nilai perhitungan RMSD untuk semua atom protein memiliki 0,16 nm, dan untuk atom penyusun tulang belakang protein memiliki rata-rata 0,08 nm.
2. Hasil rata-rata nilai perhitungan RMSF untuk semua atom protein memiliki rata-rata 0,11 nm, dan untuk atom penyusun tulang belakang protein memiliki rata-rata 0,05 nm.
3. Residu yang bersifat paling fleksibel berdasarkan penomoran sub bagian pada RMSF adalah E54, V55, I56 (sub bagian 8) dan Y82, H87, I90 (sub bagian 13).
4. Residu yang berinteraksi ikatan hidrogen dengan ligan adalah Y26, R42, dan Y82.
5. Interaksi yang dominan antara protein FKBP12 dengan ligan adalah interaksi hidrofobik.

5.2 Saran

Berdasarkan hasil yang diperoleh maka dapat disarankan:

1. Simulasi dinamika molekul FKBP12 dengan turunan sikloheksimida lainnya.

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