BAB 5
KESIMPULAN DAN SARAN

5.1. Kesimpulan

Berdasarkan hasil penelitian yang telah dilakukan maka dapat disimpulkan hasil dari Simulasi dinamika kompleks MIP-*rapamycin* pada konsentrasi garam fisiologis yang dilakukan selama 400 ns, dapat dipaparkan sebagai berikut :

1. Simulasi dinamika kompleks yang dilakukan selama waktu 400 ns menghasilkan nilai rata-rata dari perhitungan RMSD untuk semua atom protein 0,2745 nm dan nilai rata-rata untuk atom tulang belakang 0,1983 nm.
2. Hasil nilai rata-rata dari perhitungan RMSF untuk semua atom protein 0,1444 nm dan nilai rata-rata untuk atom tulang belakang 0,0964 nm. Pada RMSF sub bagian 6 dan 13 berfluktuasi lebih rendah.
3. Interaksi ikatan hidrogen yang terbentuk selama waktu 400 ns, yaitu pada residu Q78, I83, Y109, dan D66.
4. Interaksi ikatan hidrofobik antara residu W86 dengan gugus pipekolil dari ligan *rapamycin* stabil dengan jarak rata-rata 0,4661 nm.

5.2. Saran

Pada penelitian simulasi dinamika kompleks MIP-*rapamycin* pada konsentrasi garam fisiologis dapat dilanjutkan dengan perhitungan energi bebas.

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