BAB 5
KESIMPULAN DAN SARAN

5.1 Kesimpulan Penelitian

Berdasarkan hasil penelitian ini dapat disimpulkan bahwa:

1. Simulasi dinamika molekul yang dilakukan selama 200 ns yang menghasilkan perhitungan rata-rata RMSD yang cukup stabil untuk semua atom protein 0,26 nm dan untuk atom penyusun tulang belakang 0,18 nm.
2. Hasil perhitungan RMSF menunjukkan bahwa pada bagian 7, 6, 8 dan 13 bersifat fleksibel dan pada masing-masing bagian terdapat residu asam amino yaitu F77, Q81, V82, Y109, P117 dan I118.
3. Hasil analisa dPCA dari 20000 konformasi menghasilkan enam struktur yang mengalami perubahan konformasi yang signifikan.
4. Interaksi yang dominan antara protein MIP dengan ligan adalah interaksi hidrofobik.
5. Interaksi antara protein MIP dengan ligan berubah selama simulasi dengan jumlah 4 struktur.

5.2 Saran Penelitian

Berdasarkan hasil yang diperoleh maka dapat disarankan:

1. Perhitungan energi bebas untuk mengetahui afinitas antara protein MIP dengan ligan (2-[2-(3,5-dimetil-2-oksosikloheksil)-2-hidroksietil-2,6-piperidindion-N-(3,5-dimetiladamantan-1 il)etanamida).

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