BAB 5
KESIMPULAN DAN SARAN

5.1. Kesimpulan

Berdasarkan hasil penelitian dari simulasi dinamika molekul MIP-Rapamycin dengan menggunakan metode *umbrella sampling* selama 450 ns, maka disimpulkan bahwa :

1. Semakin besar jarak COM, maka ikatan hidrogen yang lebih dahulu terputus adalah ikatan antara gugus karboksil pada rantai samping residu D66 dengan gugus hidroksil pada gugus piranosil dari ligan rapamycin kemudian diikuti oleh ikatan hidrogen antara gugus hidroksil pada rantai samping residu Y109 dengan gugus hidroksil dari ligan rapamycin, selanjutnya ikatan hidrogen yang terlepas adalah residu I83 dengan gugus amina dari ligan rapamycin, dan dan residu Q78 dengan gugus amida dari protein MIP terputus paling akhir.
2. Semakin besar jarak COM, maka interaksi ikatan hidrofobik antara residu W86 dengan gugus pipekolil dari ligan rapamycin terlepas bersamaan dengan ikatan hidrogen antara residu Q78 dengan gugus amida dari protein MIP.
3. Meskipun secara energi kekuatan hidrogen lebih kuat, ikatan hidrofobik juga cukup dominan dalam mempertahankan interaksi antara ligan rapamycin dengan protein MIP.

5.2. Saran

Berdasarkan hasil penelitian dan kesimpulan yang diperoleh, maka dapat disarankan untuk dilanjutkan dengan perhitungan bebas dengan ligan lain dan dilanjutkan dengan metode *umbrella sampling.*

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