

BAB 5

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian pengaruh jarak COM pada kompleks protein MIP-Rapamycin terhadap interaksi non kovalen menggunakan metode umbrella sampling dengan kecepatan tarikan $0,001 \text{ nm ps}^{-1}$ memberikan kesimpulan sebagai berikut:

1. Semakin besar jarak COM, dari ketujuh ikatan hidrogen yang terbentuk, ikatan yang paling lama terlepas adalah residu Q78 dan Q81 pada waktu 131 ns. Di lain pihak, dari kelima interaksi hidrofobik yang terbentuk, interaksi yang paling lama terlepas adalah residu F77 pada waktu 141 ns.
2. Berdasarkan lama interaksi non kovalen terlepas, maka yang menstabilkan protein MIP dan ligan rapamycin adalah interaksi hidrofobik daripada ikatan hidrogen.

5.2 Saran

Bersadarkan hasil penelitian yang telah diperoleh, maka dapat disarankan untuk desain ligan lain dengan mempertahankan gugus sikloheksil, piranosil dan pipekolil.

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