BAB V
KESIMPULAN DAN SARAN

5.1 Kesimpulan Penelitian

Berdasarkan hasil penelitian ini dapat disimpulkan bahwa:

1. Simulasi dinamika molekul selama 40 ns memperlihatkan *domain motion* pada sisi aktif dan terjadinya *flipped state* dari ligan rapamycin.
2. Interaksi hidrofobik menstabilkan *flipped state* lebih dominan dari pada interaksi ikatan hidrogen.

5.2 Saran Penelitian

Berdasarkan hasil yang diperoleh maka dapat disarankan sebagai berikut:

1. Simulasi dinamika molekul untuk protein MIP pada struktur apo.
2. Simulasi dinamika molekul untuk protein yang mirip dengan protein MIP dan *family* FKBP dengan ligan rapamycin untuk mengetahui faktor yang berperan dalam selektivitas ligan.

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