BAB 5
KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian dari simulasi dinamika molekul maka disimpulkan bahwa:

1. Berdasarkan hasil simulasi, semakin tinggi kecepatan tarikan maka jarak COM, semakin cepat interaksi FKBP12-s35dt terlepas. Interaksi FKBP12-s35dt terlepas pada waktu 50, 113 dan 279 ps masing-masing untuk kecepatan tarikan 0,01, 0,005 dan 0,001 nm ps^{-1}.
2. Berdasarkan hasil simulasi, semakin tinggi kecepatan tarikan maka gaya tarik menarik antara protein dan ligan yang melawan gaya luar semakin besar. Gaya interaksi untuk kecepatan tarikan 0,01, 0,005, 0,001 nm ps^{-1}, masing-masing adalah 540, 450, 350 kJ $mol^{-1}nm^{-1}$.
3. Ikatan hidrogen dan interaksi hidrofobik melibatkan residu D37, E54, I90 dan yang terakhir lepas D37.

5.2 Saran

Berdasarkan hasil penelitian yang diperoleh, dapat disarankan agar dilakukan simulasi lanjutan *umbrella sampling* dengan perhitungan energi bebas.

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