BAB 5
SIMPULAN

5.1 Simpulan

Simulasi selama 20 ns menghasilkan dua klaster Ago yang berada dalam kesetimbangan. Interaksi Ago-siRNA bersifat dinamis dan didominasi oleh interaksi elektrostatik dari ikatan hidrogen. Hanya dua dari sembilan ikatan hidrogen yang dipertahankan. Tiga ikatan hidrogen tidak tampak sama sekali, dua ikatan hidrogen berada dalam kesetimbangan, sedangkan dua lainnya bertahan kira-kira selama 10 ns. Fleksibilitas sisi aktif terutama disebabkan oleh residu 128GLN tetapi tidak terjadi penyimpangan pada rotasi sudut dihedral rantai utama residu tersebut.

5.2 Alur Penelitian Selanjutnya

Perlu adanya analisa sampling konformasi lebih lanjut untuk struktur siRNA selama simulasi.

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