BAB V

KESIMPULAN

5.1. Kesimpulan

1. Berdasarkan hasil simulasi *Molecular Docking* dan *Molecular Dynamic*, senyawa *3-hidroxylup-20(29)-en* turunan triterpenoid dapat menghambat aktivitas sel kanker payudara Estrogen Reseptor-α secara *in silico* yang bisa dilihat dari *binding affinity* yang dihasilkan. Hasil simulasi *Molecular Docking* menunjukkan energi ikatan yang terbentuk sebesar -9,7 kkal/mol dan hasil simulasi *Molecular Dynamic* sebesar -27.1 kkal/mol.
2. Berdasarkan analisis interaksi senyawa *3-hidroxylup-20(29)-en* turunan triterpenoid dengan residu-residu aktif menunjukkan bahwa kontribusi residu penentu interaksi yang paling besar pada komplekas ERα-lupeol adalah pada residu *Leusin 346, Metionin 388* dan *Metionin 421*.

5.2. Saran

Perlu dilakukan penelitian selanjutnya untuk melakukan simulasi *MD* menggunakan variasi waktu simulasi untuk mengetahui kondisi interaksi senyawa *3-hidroxylup-20(29)-en* yang lebih baik dan juga dapat melakukan uji secara *in vivo* dan *in vitro* sebagai kandidat obat anti kanker payudara.

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