

ABSTRAK

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Program Studi : Farmasi
Judul Skripsi : Kombinasi *Molecular Docking* Inhibitor *Human Epidermal Growth Factor Receptor 2* (HER2) dengan Senyawa Aktif Daun Pucuk Merah (*Syzygium myrtifolium* Walp.) sebagai Antikanker Serviks

Kanker serviks adalah pertumbuhan jaringan epitel mulut rahim yang abnormal. Daun pucuk merah (*Syzygium myrtifolium* Walp.) merupakan tanaman yang memiliki aktivitas antibakteri, antijamur, antioksidan dan antikanker. Penelitian ini bertujuan untuk mengetahui potensi senyawa aktif daun pucuk merah (*Syzygium myrtifolium* Walp.) sebagai inhibitor *Human Epidermal Growth Factor Receptor 2* (HER-2) kode PDB : 3PP0 terhadap antikanker serviks dengan metode *molecular docking*. Penelitian diawali dengan preparasi struktur protein, ligan asli dan ligan pembanding (trastuzumab dan pertuzumab) menggunakan YASARA, kemudian dilakukan validasi metode yang didapatkan nilai RMSD sebesar 1,3480 Å. Penelitian dilakukan pada senyawa aktif daun pucuk merah yang memenuhi aturan Lipinski. Hasil penelitian kombinasi *molecular docking* menggunakan PLANTS menunjukkan skor lebih rendah dari *molecular docking* sederhana, terdapat tiga senyawa yang menjadi kandidat obat yaitu bis 2-ethylhexyl hexanedioat, bis 2-ethylhexyl phthalate dan 1-octadecene. Skor *molecular docking* yang menggunakan trastuzumab berurutan -111,2550; -102,9830; -96,5067. Skor *molecular docking* yang menggunakan pertuzumab berurutan -111,3540; -101,3144; -96,9593. Setelah dilakukan *molecular docking* senyawa kandidat obat dilakukan visualisasi menggunakan Discovery Studio dan prediksi ADMET menggunakan *website* pkCSM. Ketiga senyawa tidak bersifat hepatotoksik dan karsinogenik, sehingga berpotensi sebagai kandidat obat kanker serviks.

Kata kunci : Kanker serviks, *Syzygium myrtifolium* Walp., kombinasi *molecular docking*, HER-2, trastuzumab, pertuzumab ADMET.

ABSTRACT

Name : Morani Fauziyah
Major : Pharmacy
Title : Combination of *Molecular Docking* Inhibitor *Human Epidermal Growth Factor Receptor 2* (HER2) on Active Compound Pucuk Merah Leaves (*Syzygium myrtifolium* Walp.) as Cervical Anticancer

Cervical cancer is an abnormal growth of cervical epithelial tissue. *Syzygium myrtifolium* Walp. is a plant that has antibacterial, antifungal, antioxidant and anticancer activities. This study aims to determine the potential of the active compound of *Syzygium myrtifolium* Walp. as inhibitor Human Epidermal Growth Factor Receptor 2 (HER-2) PDB code : 3PP0 as anti cervical cancer by molecular docking method. The study began with the preparation chemical structure of protein, original ligand and standard of ligand (trastuzumab and pertuzumab) using YASARA, then method validation was carried out which obtained an RMSD value of 1.3480 Å. The research on active compounds of *Syzygium myrtifolium* Walp. leaves that complied with Lipinski's rule. The results of a combined molecular docking study using PLANTS showed a lower score than simple molecular docking. There were three compounds as drug candidates, the names are bis 2-ethylhexyl hexanedioate, bis 2-ethylhexyl phthalate and 1-octadecene. The molecular docking scores using trastuzumab were -111.2550; -102.9830; -96.5067. Molecular docking scores using pertuzumab were -111.3540; -101.3144; -96.9593. After molecular docking of drug candidate compounds, visualization was carried out using Discovery Studio and ADMET prediction using the pkCSM website. The three compounds are not hepatotoxic and carcinogenic, so they are potential candidates for cervical cancer drugs.

Keywords : Cervical cancer, *Syzygium myrtifolium* Walp., combination molecular docking, HER-2, trastuzumab, pertuzumab ADMET.