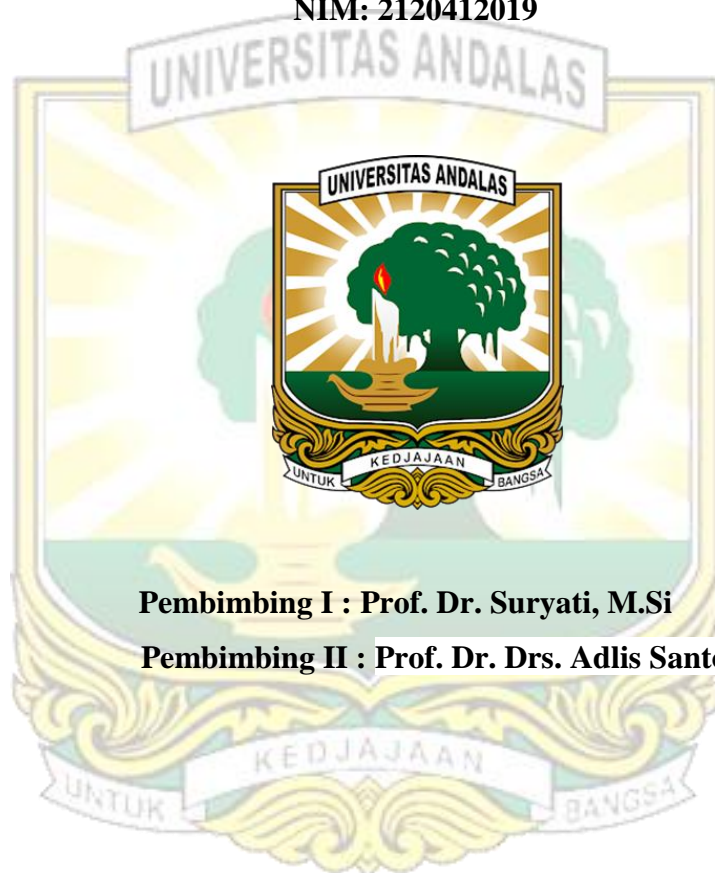


**POTENSI ANTIKANKER DAN STUDI *MOLECULAR DOCKING*  
MINYAK ATSIRI DAUN *Citrus×taitensis* Risso DAN *Citrus×limon* (L)  
Osbeck TERHADAP SEL KANKER SERVIKS**

**TESIS**

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**Potensi Antikanker Dan Studi *Molecular Docking* Minyak Atsiri Daun  
*Citrus×taitensis* Risso Dan *Citrus×limon* (L.) Osbeck Terhadap Sel Kanker  
Serviks**

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**Abstrak**

Kanker serviks merupakan salah satu penyebab utama kematian pada wanita diseluruh dunia. Salah satu tumbuhan obat yang sering digunakan sebagai antikanker adalah tumbuhan dari genus *Citrus*. Genus *Citrus* memiliki spesies diantaranya *Citrus×taitensis* Risso dan *Citrus×limon* (L.) Osbeck. Penelitian ini bertujuan untuk menganalisis komponen kimia penyusun minyak atsiri dari daun *C×taitensis* dan *C×limon*, serta menentukan potensinya sebagai antikanker serviks secara *in vitro* dan *in silico*. Minyak atsiri hasil isolasi dari daun *C×taitensis* dan *C×limon* dengan metode hidrodistilasi dianalisis menggunakan GC-MS yang kemudian dilakukan uji toksisitas awal dengan metode BSLT, selanjutnya dilakukan uji sitotoksik dengan *molecular docking* dan metode MTT. Hasil penelitian diperoleh kedua minyak atsiri berupa cairan berwarna kuning dengan massa jenis minyak atsiri daun *C×taitensis* sebesar 0,8901 g/mL dan randemen 0,223%, sedangkan minyak atsiri daun *C×limon* memiliki massa jenis sebesar 0,8684 g/mL dan randemen 0,181%. Berdasarkan analisis GC-MS, diketahui minyak atsiri daun *C×taitensis* memiliki 56 komponen senyawa kimia dengan senyawa utama yaitu (-)-limonen (18,88%), geranial (6,82%), β-citral (5,7%), *caryophyllene* (5,11%) dan nerol (5,05%). Sedangkan minyak atsiri daun *C×limon* terdapat 60 komponen kimia dengan senyawa utama yaitu (-)-β-pinen (7,32%), (-)-limonen (28,40%), geranial (5,54%), dan *caryophyllene* (5,22%). Berdasarkan uji BSLT diketahui kedua minyak atsiri menunjukkan aktivitas sangat toksik terhadap larva udang *Artemia salina* L. dengan nilai LC<sub>50</sub> sebesar 6,570 μg/mL (*C×taitensis*) dan 3,697 μg/mL (*C×limon*). Melalui *molecular docking* diketahui RMSD senyawa utama kedua minyak atsiri ini yaitu (-)-limonen (1,6203), geranial (1,6574), β-citral (1,5591), *caryophyllene* (1,6932), nerol (1,4107) dan (-)β-pinen (1,3259). Nilai *docking score* (kcal.mol<sup>-1</sup>) senyawa utama minyak atsiri yang mendekati senyawa doxorubicin (-8,3309) sebagai kontrol positif yaitu *caryophyllene* (-5,9714), nerol (-5,5400), β-citral (-5,2961), geranial (-5,2415), (-)-limonen (-4,9753), (-)β-pinen (-4,5313). Uji MTT menunjukkan minyak atsiri memiliki aktivitas sitotoksik yang lemah terhadap sel HeLa dengan nilai IC<sub>50</sub> yaitu 260,4 μg/mL (*C×taitensis*) dan 218,9 μg/mL (*C×limon*).

**Kata Kunci:** BSLT, *Citrus×taitensis* Risso, *Citrus×limon* (L.) Osbeck, Kanker serviks, Minyak atsiri, *Molecular docking*, MTT

## Anticancer Potential and Molecular Docking Study of Essential Oils of *Citrus×taitensis* Risso and *Citrus×limon* (L) Osbeck Leaves Against Cervical Cancer Cells

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### Abstract

Cervical cancer is one of the leading causes of death in women around the world. One of the medicinal plants that are often used as anticancer is plants from the genus *Citrus*. The genus *Citrus* has species including *Citrus×taitensis* Risso and *Citrus×limon* (L.) Osbeck. This study aims to analyse the chemical components of essential oils from the leaves of *C×taitensis* and *C×limon*, and determine their potential as cervical anticancer in vitro and in silico. Essential oils isolated from the leaves of *C×taitensis* and *C×limon* by hydrodistillation method were analysed using GC-MS which was then carried out initial toxicity test with BSLT method, then cytotoxic test with molecular docking and MTT method. The results showed that both essential oils were yellow liquid with a density of 0,8901 g/mL and a yield of 0,223%, while the essential oil of *C×limon* leaves had a density of 0,8684 g/mL and a yield of 0,181%. Based on GC-MS analysis, it is known that *C×taitensis* leaf essential oil has 56 chemical compound components with the main compounds being (-)-limonen (18,88%), geranial (6,82%),  $\beta$ -citral (5,7%), caryophyllene (5,11%) and nerol (5,05%). While the essential oil of *C×limon* leaves contained 60 chemical components with the main compounds being (-)- $\beta$ -pinen (7,32%), (-)-limonen (28,40%), geranial (5,54%), and caryophyllene (5,22%). Based on BSLT test, both essential oils showed highly toxic activity against *Artemia salina* L. shrimp larvae with  $LC_{50}$  values of 6,570  $\mu$ g/mL (*C×taitensis*) and 3,697  $\mu$ g/mL (*C×limon*). Through molecular docking, the RMSD of the main compounds of these two essential oils are (-)-limonen (1,6203), geranial (1,6574),  $\beta$ -citral (1,5591), caryophyllene (1,6932), nerol (1,4107) and (-)- $\beta$ -pinen (1,3259). The docking score (kcal.mol<sup>-1</sup>) of the main compounds of essential oil that are close to doxorubicin (-8,3309) as a positive control are caryophyllene (-5,9714), nerol (-5,5400),  $\beta$ -citral (-5,2961), geranial (-5,2415), (-)-limonen (-4,9753), (-)- $\beta$ -pinen (-4,5313). MTT assay showed that essential oils have weak cytotoxic activity against HeLa cells with  $IC_{50}$  values of 260,4  $\mu$ g/mL (*C×taitensis*) and 218,9  $\mu$ g/mL (*C×limon*).

Keywords: BSLT, *Citrus×taitensis* Risso, *Citrus×limon* (L.) Osbeck, Cervical cancer, Essential oil, Molecular docking, MTT