INTISARI

Sitotoksisitas ekstrak dan minyak atsiri rimpang *Curcuma mangga* Val. telah terbukti berpotensi sebagai anti kanker payudara. Secara *in silico,* kandungan minyak atsiri *C. mangga* Val. terbukti sebagai inhibitor reseptor ER-α. Tetapi belum ada peneliti yang membandingkan sitotoksisitas ekstrak dan minyak atsirinya secara *in vitro* terhadap T-47D dan MCF-7; serta afinitas senyawa aktif dalam ekstrak dan minyak atsiri tersebut terhadap protein reseptor ER-α. Oleh karena itu, penelitian ini bertujuan untuk membandingkan sitotoksisitas ekstrak *n*-heksan dan minyak atsiri terhadap sel T-47D dan MCF-7, serta afinitas beberapa senyawa aktif yang terkandung dalam sampel terhadap reseptor ER-α secara *in silico*.

Senyawa aktif rimpang *C. mangga* Val. (segar maupun kering) dimaserasi menggunakan *n*-heksan dan di-destilasi uap air untuk mendapatkan ekstrak *n*-heksan dan minyak atsiri. Selanjutnya, semua sampel diuji sitotoksisitasnya secara *MTT assay* terhadap sel T-47D dan MCF-7. Kandungan sampel diidentifikasi menggunakan GC-MS. Ligan *molecular docking* diseleksi berdasarkan *similarity index* (SI) $\geq$ 850 dan kelimpahan relatif $\geq$1% untuk menentukan *docking score* terhadap protein reseptor ER-α dengan ligan antagonis 4-hidroksi tamoxifen serta ligan agonis estradiol, estriol dan estron; menggunakan metode MOE 2015.10.

Uji sitotoksisitas menunjukkan ekstrak *n*-heksan rimpang segar *C. mangga* Val. memiliki potensi sitotoksik terbaik dengan IC_{50} 36,308 µg/ml terhadap T-47D; dan 68,077 µg/ml terhadap sel MCF-7. Identifikasi menggunakan GC-MS memperlihatkan perbedaan kandungan senyawa terbesar pada ekstrak *n*-heksan dan minyak atsiri rimpang *C. mangga* Val.; yaitu dalam ekstrak adalah golongan diterpenoid dengan senyawa (E)-labda-8(17),12-diene-15,16-dial (rimpang kering 41,61%; rimpang segar 83,84%); sedangkan dalam minyak atsiri adalah golongan monoterpenoid dengan senyawa β-myrcene (rimpang kering 18,30%; rimpang segar 26,28%). Delapan belas ligan uji terseleksi dari hasil identifikasi kandungan ekstrak *n*-heksan dan 26 ligan uji dari minyak atsiri. *Docking score* senyawa ekstrak *n*-heksan dan minyak atsiri yang paling baik dibanding skor estradiol (-6,1074) adalah *m*-Camphorene (-7,3390). Isolat ekstrak *n*-heksan lebih sitotoksik terhadap sel kanker payudara daripada minyak atsiri rimpang *C. mangga* Val.

Kata Kunci: *Curcuma mangga* Val., terpenoid, T-47D, MCF-7, ER-α.

ABSTRACT

Cytotoxicity studies of the extract and essential oil *Curcuma mangga* Val. rhizomes showed they are potential as anti-breast cancer. *In silico* studies proved that the active compounds of the essential oil were inhibitor of ERα. There is no researcher has compared the cytotoxicity of the extract and essential oil towards T-47D and MCF; and also the affinity of the active compounds contained in the extract and essential oil towards ERα. So that, this study is to compare the cytotoxicity against T-47D and MCF-7 cells of the *n*-hexane extract and essential oil of *C. mangga* Val. rhizomes, as well as *in silico* affinity of the active compounds contained in the samples towards ER-α.

Compounds of the *C. mangga* Val. rhizomes (either fresh or dry) were *n*-hexane macerated and water steam distillated to get the *n*-hexane extract and essential oil. All samples were then cytotoxicity tested using MTT assay towards T-47D and MCF-7. The samples compounds were identified using GC-MS. Compounds with similarity index (SI) $\geq$ 850 and relative area $\geq$1% then were used for molecular docking studies using MOE 2015.10 to determine the *docking score* towards ERα with antagonist ligand 4-hydroxy tamoxifen and agonist ligands of estradiol, estriol dan estron.

Cytotoxicity studies showed that the fresh-rhizome-extract of *C. mangga Val.* was the most cytotoxic with IC_{50} 36,308 µg/ml towards T-47D and 68,077 µg/ml towards MCF-7. GC-MS identification showed different biggest contents between the *n*-hexane extract and its essential oil of *C. mangga* Val. rhizomes; which was a diterpenoid of E)-labda-8(17),12-diene-15,16-dial (from the dry-rhizomes 41,61%; fresh-rhizomes 83,84%) in the extract; while in the essential oil was a monoterpenoid of β-myrcene (from the dry-rhizomes 18,30%; fresh-rhizomes 26,28%). Eighteen substances were selected from the identification of the *n*-hexane extract contents, and 26 substances were selected from the essential oil to became the test ligands. The best *docking score* of the *n*-hexane extract and the essential oil substances comparing to that of estradiol (-6,1074) was *m*-Camphorene (-7,3390). Isolate *n*-hexane extract was more cytotoxic towards breast cancer cells comparing to the essential oil of the *C. mangga* Val. rhizome.

Keywords: *Curcuma mangga* Val., terpenoid, T-47D, MCF-7, ER-α.