ABSTRAK

KAJIAN KOMPONEN AKTIF EKSTRAK *Lasiodiplodia theobromae* SEBAGAI ANTIJAMUR *Botrytis cinerea* MELALUI PENDEKATAN *IN SILICO*

Oleh

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Ekstrak *Lasiodiplodia theobromae* menghasilkan senyawa metabolit sekunder seperti, sikloheksena, jasmonat, indol dan lainnya sehingga berpotensi sebagai agen antijamur terhadap *Botrytis cinerea*, penyebab busuk abu-abu pada buah stroberi selama pascapanen. Penelitian ini bertujuan mengidentifikasi komponen aktif kultur *L. theobromae* yang berpotensi sebagai antijamur *B. cinerea* secara *In silico.* Penelitian ini menggunakan metode deskriptif meliputi hasil fraksi terbaik dan diuji LC-MS. Data yang diperoleh dilanjutkan dengan uji *In silico* dalam bentuk gambar dan tabel. Hasil uji *In silico* terhadap senyawa hasil LC-MS menggunakan *molecular docking* dengan protein target ribosom biogenis Ytm1 dan ATP-dependent RNA helicase Dbp5 dari *B. cinerea*, senyawa O-(1,2,3,4,4,5,5,6,6-nonaaminocyclohex-2-en-1-yl)hydroxylamine dari *L. theobromae* menghambat protein target ribosom biogenesis Ytm1 dengan nilai *binding affinity* -7,3 kcal/mol melalui ikatan hidrogen dengan residu Lys168A, Lys171A, Ser218A, Ile219A, Ser378A, Ser377A, Asp447A, Phe446A, serta menghambat protein target ATP-dependent RNA helicase Dbp5 dengan *binding affinity* -6,9 kcal/mol melalui ikatan hidrogen dengan residu Tyr181A, Thr221A, dan Gln292A. Hasil penelitian menunjukkan bahwa senyawa O-(1,2,3,4,4,5,5,6,6-nonaaminocyclohex-2-en-1-yl)hydroxylamine dari kultur *L. theobromae* berpotensi sebagai antijamur alami terhadap *B. cinerea.*

Kata kunci: antijamur**,** *Botrytis cinerea*, *docking molekuler, in silico, Lasiodiplodia theobromae*

ABSTRACT

STUDY OF ACTIVE COMPONENTS IN *Lasiodiplodia theobromae* EXTRACT AS ANTIFUNGAL AGAINTS *Botrytis cinerea* THROUGH AN *IN SILICO* APPROACH

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Extracts of *Lasiodiplodia theobromae* produced secondary metabolites such as cyclohexene, jasmonate, indole, and others, making it a potential antifungal agent against *Botrytis cinerea*, the cause of gray mold on strawberries during post-harvest. This study aimed to identify the active components of *L. theobromae* culture that had potential as an antifungal agents against *B. cinerea In silico*. The study used a descriptive method covering the results of the best fraction, wich was analyzed using LC-MS. The data obtained were then evaluated through *In silico* analysis presented in the form of images and tables. *In silico* testing of the LC-MS compounds using *molecular docking* with the ribosom biogenesis Ytm1 and ATP-dependent RNA helicase Dbp5 from *B. cinerea,* the compound O-(1,2,3,4,4,5,5,6,6-nonaaminocyclohex-2-en-1-yl)hydroxylamine from *L. theobromae* inhibited the ribosom biogenesis Ytm1 with a *binding affinity* value of -7.3 kcal/mol through hydrogen bonds with residues Lys168A, Lys171A, Ser218A, Ile219A, Ser378A, Ser377A, Asp447A, Phe446A and inhibited the target protein ATP-dependent RNA helicase Dbp5 with a *binding affinity* of -6.9 kcal/mol through hydrogen bonding with residues Tyr181A, Thr221A, and Gln292A. These results of the study indicated that the compound O-(1,2,3,4,4,5,5,6,6-nonaaminocyclohex-2-en-1-yl)hydroxylamine from *L. theobromae* culture had potential as a natural antifungal agent against *B. cinerea*.

Keywords: antifungal, *Botrytis cinerea*, *in silico, Lasiodiplodia theobromae*, *moleculer docking*