

## IDENTIFIKASI SENYAWA POTENSIAL ANTIKANKER DARI EKSTRAK ETIL ASETAT SPONS *Amphimedon paraviridis* ASAL PANTAI WATU KARUNG PACITAN BERDASARKAN UJI TOKSISITAS

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### INTISARI

Telah dilakukan isolasi, identifikasi, dan *molecular docking* senyawa potensial antikanker dari ekstrak etil asetat spons *Amphimedon paraviridis* asal Pantai Watu Karung berdasarkan uji toksisitas. Penelitian ini bertujuan untuk mengetahui toksisitas ekstrak etil asetat spons *Amphimedon paraviridis* asal Pantai Watu Karung dengan metode *Brine Shrimp Lethality Test* (BSLT) dan memperoleh senyawa bioaktif dari fraksi toksik serta mengetahui interaksinya terhadap protein target antikanker. Ekstraksi senyawa dilakukan dengan maserasi menggunakan pelarut metanol dan diklorometana, kemudian fase diklorometana dipartisi dengan etil asetat dan air. Ekstrak etil asetat diuji toksisitas dengan metode BSLT. Ekstrak etil asetat dipisahkan menggunakan kromatografi kolom. Fraksi kromatografi kolom diuji BSLT untuk mencari fraksi yang paling toksik. Fraksi paling toksik diidentifikasi senyawa menggunakan *Liquid Chromatography-High Resolution Mass Spectrometry* (LC-HRMS). Senyawa hasil identifikasi dianalisis interaksinya terhadap protein target CDK-6 dengan *molecular docking*.

Hasil uji toksisitas menunjukkan ekstrak etil asetat bersifat toksik dengan nilai *Lethality Concentration 50%* ( $LC_{50}$ ) sebesar 330,45  $\mu\text{g/mL}$ . Dari hasil pemisahan dengan kromatografi kolom, diperoleh enam fraksi, yang mana fraksi 1 merupakan fraksi paling toksik dengan nilai  $LC_{50}$  sebesar 155,88  $\mu\text{g/mL}$ . Fraksi 1 diidentifikasi dengan LC-HRMS yang menyatakan mengandung senyawa nebrosteroid M, conicasterol B, aspewentin A, minabeolide-2, dan erectusfuranone A. Dari hasil *molecular docking* terhadap protein CDK-6 dengan *native ligand* palbociclib, kelima senyawa menunjukkan interaksi kuat terhadap CDK-6 dengan energi ikatan berturut-turut sebesar -11,6; -11,5; -10,4; -10,3; dan -9,2 kkal  $\text{mol}^{-1}$ .

Kata kunci: *Amphimedon paraviridis*, BSLT, Spons, toksisitas

**IDENTIFICATION OF POTENTIAL ANTICANCER COMPOUNDS  
FROM ETHYL ACETATE EXTRACT OF *Amphimedon paraviridis*  
SPONGE FROM WATU KARUNG BEACH PACITAN BASED ON  
TOXICITY TEST**

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**ABSTRACT**

Isolation, identification, and molecular docking of potential anticancer compounds from ethyl acetate extracts of *Amphimedon paraviridis* sponges from Watu Karung Beach have been conducted based on toxicity tests. This study aims to determine the toxicity of ethyl acetate extracts from *Amphimedon paraviridis* sponges from Watu Karung Beach using the Brine Shrimp Lethality Test (BSLT) method and to obtain bioactive compounds from toxic fractions and determine their interaction with anticancer target proteins. Compound extraction was performed by maceration using methanol and dichloromethane solvents, then the dichloromethane phase was partitioned with ethyl acetate and water. The ethyl acetate extract was tested for toxicity using the BSLT method. The ethyl acetate extract was separated using column chromatography. The column chromatography fractions were tested using BSLT to find the most toxic fraction. The most toxic fraction was identified using Liquid Chromatography-High Resolution Mass Spectrometry (LC-HRMS). The identified compounds were analyzed for their interaction with the target protein CDK-6 using molecular docking.

The toxicity test results showed that the ethyl acetate extract was toxic with a Lethality Concentration 50% (LC<sub>50</sub>) value of 330.45 µg/mL. From the column chromatography separation results, six fractions were obtained, of which fraction 1 was the most toxic fraction with an LC<sub>50</sub> value of 155.88 µg/mL. Fraction 1 was identified by LC-HRMS as containing the compounds nebrosteroid M, Conicasterol B, Aspewentin A, Minabeolide-2, and erectusfuranone A. From the results of molecular docking of the CDK-6 protein with the native ligand palbociclib, the five compounds showed strong interactions with CDK-6 with bond energies of -11.6, -11.5, -10.4, -10.3, and -9.2 kcal mol<sup>-1</sup>, respectively.

**Keywords:** *Amphimedon paraviridis*, BSLT, sponge, toxicity