

**ISOLASI, IDENTIFIKASI, DAN PENAMBATAN MOLEKUL SENYAWA  
POTENSIAL ANTIKANKER DARI EKSTRAK ETIL ASETAT SPONS  
*Sphaciospongia inconstans* ASAL PANTAI WATU KARUNG  
BERDASARKAN UJI TOKSISITAS**

Rusdian  
21/477231/PA/20641

**INTISARI**

Telah dilakukan penelitian terkait isolasi, identifikasi, dan penambatan molekul senyawa potensial antikanker dari ekstrak etil asetat spons *Sphaciospongia inconstans* asal Pantai Watu Karung berdasarkan uji toksisitas. Penelitian ini bertujuan untuk mengetahui toksisitas ekstrak etil asetat spons *Sphaciospongia inconstans* asal Pantai Watu Karung, Pacitan dengan metode BSLT, memperoleh senyawa bioaktif dari fraksi toksik, dan mengetahui interaksinya terhadap protein target antikanker melalui *molecular docking*. Ekstraksi dilakukan dengan metode maserasi menggunakan pelarut metanol dan diklorometana, kemudian ekstrak diklorometana dipartisi dengan etil asetat dan aquades. Ekstrak etil asetat diuji toksisitasnya menggunakan metode *Brine Shrimp Lethality Test* (BSLT). Ekstrak etil asetat dipisahkan menggunakan kromatografi kolom, lalu fraksi kromatografi kolom juga diuji dengan metode BSLT. Setelah uji BSLT, fraksi paling toksik diidentifikasi senyawanya menggunakan *Liquid Chromatography-High Resolution Mass Spectrometry* (LC-HRMS). Senyawa hasil identifikasi dianalisis interaksinya terhadap protein target CDK-6 dengan metode *molecular docking*.

Hasil uji toksisitas menunjukkan ekstrak etil asetat bersifat toksik dengan nilai *Lethal Concentration 50%* (LC<sub>50</sub>) sebesar 373,41 µg/mL. Dari hasil pemisahan diperoleh enam fraksi, dimana fraksi 1 sebagai fraksi paling toksik dengan nilai LC<sub>50</sub> sebesar 84,59 µg/mL. Identifikasi senyawa dengan LC-HRMS mengindikasikan fraksi 1 mengandung senyawa ergosta-5,7,22E-trien-3β-ol, ergosta-5,7,22,24(28)-tetraen-3β-ol, ximaosteroid E, (24R,24'R)-fucosterol epoksida, dan conicasterol B. Dari hasil *molecular docking* terhadap protein CDK-6 dengan palbociclib sebagai *native ligand*, kelima senyawa teridentifikasi menunjukkan interaksi yang kuat terhadap CDK-6 dengan energi ikatan sebesar -10,2; -9,8; -9,8; -9,6; dan -9,3 kkal/mol serta pola interaksi yang mirip dengan *native ligand*.

Kata kunci: antikanker, ekstrak, *Sphaciospongia inconstans*, spons, toksisitas

**ISOLATION, IDENTIFICATION, AND MOLECULAR DOCKING OF  
POTENTIAL ANTICANCER COMPOUNDS FROM ETHYL ACETATE  
EXTRACT OF *Spheciospongia inconstans* SPONGE FROM WATU  
KARUNG BEACH BASED ON TOXICITY ASSAY**

Rusdian  
21/477231/PA/20641

**ABSTRACT**

Research has been conducted on the isolation, identification, and molecular docking of potential anticancer compounds from ethyl acetate extracts of *Spheciospongia inconstans* sponges from Watu Karung Beach based on toxicity assay. This study aims to determine the toxicity of ethyl acetate extracts from *Spheciospongia inconstans* sponges from Watu Karung Beach, Pacitan, using the BSLT method, to obtain bioactive compounds from toxic fractions, and to determine their interaction with anticancer target proteins through molecular docking. Extraction was performed using the maceration method with methanol and dichloromethane as solvents, then the dichloromethane extract was partitioned with ethyl acetate and aquadest. The ethyl acetate extract was tested for toxicity using the Brine Shrimp Lethality Test (BSLT) method. The ethyl acetate extract was separated using column chromatography, and the column chromatography fractions were also tested using the BSLT method. After the BSLT test, 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 CDK-6 target protein using the molecular docking method.

The toxicity assay results showed that the ethyl acetate extract was toxic with a Lethal Concentration 50% (LC<sub>50</sub>) value of 373.41 µg/mL. Six fractions were obtained from the separation, with fraction 1 being the most toxic with an LC<sub>50</sub> value of 84.59 µg/mL. Compound identification using LC-HRMS indicated that fraction 1 contains ergosta-5,7,22E-trien-3β-ol, ergosta-5,7,22,24(28)-tetraen-3β-ol, ximaosteroid E, (24R,24'R)-fucosterol epoxide, and conicasterol B. From the results of molecular docking of the CDK-6 protein with the palbociclib as the native ligand, the five identified compounds showed strong interactions with CDK-6 with bond energies of -10.2; -9.8; -9.8; -9.6; and -9.3 kcal/mol and interaction patterns like the native ligand.

Keywords: anticancer, extract, *Spheciospongia inconstans*, sponge, toxicity