ABSTRAK

UJI *IN SILICO* SENYAWA AKTIF SPONS *Stylissa massa* (Carter, 1887) TERHADAP PROTEIN SEL KANKER PARU-PARU

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Kanker paru-paru merupakan penyebab utama kematian akibat kanker di Indonesia dan dunia. Efek samping dari kemoterapi yang berat mendorong pencarian alternatif terapi yang lebih aman, salah satunya melalui pemanfaatan senyawa bioaktif dari organisme laut seperti spons *Stylissa massa*. Penelitian tersebut bertujuan untuk mengidentifikasi senyawa bioaktif aktif dari spons *Stylissa massa* yang berpotensi sebagai antikanker paru-paru dan menguji aktivitasnya secara *in silico* terhadap protein sel kanker paru-paru. Berdasarkan hasil ana-lisis LC-HRMS, diperoleh 28 senyawa yang kemudian dilakukan penapisan menggunakan CLC-Pred, menghasilkan 4 senyawa potensial. Selanjutnya, dilakukan prediksi protein target menggunakan SEA *Search Server* dan *Therapeutic Target Database*, menghasilkan 12 protein target yang relevan dengan kanker paru-paru. Proses *docking* menunjukkan bahwa senyawa asam flufenamat dari ekstrak spons *Stylissa massa* memiliki afinitas ikatan yang kuat dan interaksi stabil terhadap protein target seperti RET dan CDK2. Prediksi profil fisikokimia dan farmakokinetika juga mendukung potensi asam flufenamat sebagai kandidat obat. Hasil tersebut menunjukkan bahwa senyawa bioaktif dari ekstrak spons *Stylissa massa* berpotensi dikembangkan sebagai agen antikanker alami. Studi lebih lanjut secara *in vitro* dan *in vivo* diperlukan untuk memastikan efektivitas dan keamanannya.

Kata Kunci: *In Silico,* Kanker Paru-Paru, *Molecular Docking, Stylissa massa*.

ABSTRACT

IN SILICO TEST OF THE ACTIVITY SOLUTION OF SPONS *Stylissa massa* (Carter, 1887) AGAINST LUNG CANCER CELL PROTEINS

By

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Lung cancer is the leading cause of cancer-related deaths in Indonesia and worldwide. The severe side effects of chemotherapy have prompted the search for safer alternative therapies, one of which involves the use of bioactive compounds from marine organisms such as the *Stylissa massa* sponge. This study was aimed to identify bioactive compounds from the sponge *Stylissa massa* that have potential as lung cancer anticancer agents and to test their activity in silico against lung cancer cell proteints. Based on LC-HRMS analysis results, 28 compounds were obtained and then screened using CLC-Pred, yielding 4 potential compounds. Next, protein target prediction was performed using SEA Search Server and Therapeutic Target Database, yielding in 12 relevant protein targets associated with lung cancer. Docking result showed that flufenamic acid from *Stylissa massa* sponge extract exhibits strong binding affinity and stabel interactions with target proteins such as RET and CDK2. Physicochemical and pharmacokinetic predictions also support the potential of flufenamic acid as a drug candidate. These results indicate that bioactive compounds from *Stylissa massa* sponge extract have the potential to be development as natural anticancer agents. Further in vitro and in vivo studies are needed to confirm their efficacy and safety.

Keywords: In Silico, Lung Cancer, Molecular Docking, *Stylissa massa.*