

ABSTRAK

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

Oleh

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Kanker kolorektal merupakan salah satu jenis kanker dengan jumlah kasus dimortalitas yang semakin tinggi di Indonesia dan dunia. Upaya penemuan obat antikanker baru terus dikembangkan, salah satunya melalui eksplorasi biota laut seperti spons *Stylissa massa* yang diketahui menghasilkan berbagai senyawa bioaktif. Penelitian ini bertujuan untuk mengidentifikasi potensi senyawa aktif dari *Stylissa massa* sebagai agen antikanker kolorektal melalui pendekatan *in silico* dengan metode *molecular docking*. Senyawa diperoleh melalui data LC-HRMS dan database KNApSACk, kemudian diseleksi berdasarkan aktivitas sitotoksik menggunakan CLC-Pred. Prediksi target protein dilakukan dengan SEA Search Server dan Therapeutic Target Database (TTD), yang dilanjutkan dengan analisis Protein-Protein Interactions menggunakan STRING-DB. Hasil tahap tumpang tindih menunjukkan dua senyawa potensial (Asam flufenamat dan MFCD00135810) dengan sepuluh target protein kanker kolorektal. *Molecular docking* menunjukkan afinitas ikatan yang kuat antara senyawa dan protein target, terutama asam flufenamat terhadap reseptor KIT, NTRK1 dan RET. Hasil ini menunjukkan bahwa senyawa aktif dari spons *S. massa* memiliki potensi sebagai kandidat agen antikanker kolorektal dan dapat dikembangkan lebih lanjut melalui uji eksperimental lanjutan.

Kata kunci: *In Silico*, Kanker Kolorektal, *Molecular Docking*, *Stylissa massa*.

ABSTRACT

IN SILICO TEST OF THE ACTIVITY SOLUTION OF SPONS *Stylissa Massa* (CARTER, 1887) AGAINST COLORECTAL CANCER CELL PROTEIN

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Colorectal cancer is one of the most common cancer types with an increasing number of mortality cases in Indonesia and the world. The discovery of new anti-cancer drugs continues to be pursued, including through the exploration of marine biota such as the sponge *Stylissa massa*, known for producing various bioactive compounds. This study aims to identify the potential of active compounds from *S. massa* as colorectal anticancer agents using an in silico approach with molecular docking methods. Compounds were obtained through LC-HRMS analysis and the KNApSAcK database, and screened for cytotoxic activity using CLC-Pred. Protein target prediction was conducted via the SEA Search Server and the Therapeutic Target Database (TTD), followed by protein-protein *interactions* (PPI) analysis using STRING-DB. The overlapping results revealed two potential compounds (Flufenamic acid and MFCD00135810) with ten colorectal cancer-related target proteins. Molecular docking demonstrated strong binding affinities, particularly flufenamic acid with KIT, NTRK1, and RET receptors. These findings indicate that active compounds from *S. massa* show potential as candidate colorectal anti-cancer agents and need more experimental investigation.

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