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GC-MS analysis of marine invertebrate from sea urchin (*Diadema savignyi*) and identification of potential anti-cancer activity against colorectal cancer

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Colorectal cancer is the second most common chronic disease in the world that affecting almost 1.9 million people in 2020. Till now, no specific drug candidates have been developed or yet available that can treat this cancer. Therefore, it is an urgent need to discover a novel anticancer drug against the diseases from the marine invertebrate. However, Importin-11 is a protein that is responsible for transporting β-catenin to the cell nucleus and acts as a cell proliferation of colorectal cancers. The blocking of Importin-11 can block the β-catenin from entering the nucleus. It may act as a precursor to inhibit the growth of colorectal cancer formed by APC mutant. Therefore, the study aims to identify potential natural anticancer agents that can inhibit the activity of Impotrin-11, subsequently blocking the progression of colorectal cancer. Initially, a total of 15 compounds from the Sea Urchin invertebrates were identified through the gas chromatography-mass spectrometry (GC-MS) analytical method. Consequently, the compounds were screened through molecular docking, absorption, distribution, metabolism, excretion (ADME), toxicity (T), and molecular dynamics (MD) simulation approach. The molecular docking method initially identified four molecules having PubChem CID: 304, CID: 6432458, CID: 605775 and, CID: 11955 with a good binding affinity. All the selected compounds exhibit good pharmacokinetics and toxicity properties. Finally, the four compounds were further evaluated based on the MD simulation methods that confirmed the binding stability of the compounds to the targeted protein. The computational approaches identified the best four compounds CID: 304, CID: 6432458, CID: 605775, and, CID: 11955 that can be developed as a treatment option that has a better binding affinity to the target protein. To sum up, marine animal sea urchin showed better anticancer activity against an importein-11 protein that can be further developed as an anti-CRC drug. Although, experimental validation is suggested for further evaluation of the work.

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