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Computational studies of derivatives of selected marine organisms on acute myeloid leukemia

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Acute myeloid leukemia (AML) is the most common subtype of leukemia cancer that produces an uncontrolled number of muted blood cells in the bone marrow. AML is common among adults, and it affects red blood cells, white blood cells and platelets. The anticancer activity of marine organisms has been proven in several *in vitro* and *in vivo* preclinical and clinical studies. Amongst several Marine ecosystems, Marine sponges are the richest source of anticancer compounds, because they are endowed with natural compounds that can act against AML by targeting active protein sites. This study highlights the investigation of binding interaction between the natural Marine derivatives and the proteins associated with AML and comparing the values with a reference drug using a computational chemistry platform. The natural Marine derivatives which are selected for the present study are lacking information about the drug potency against AML. The main proteins that are targets for this study are Receptor tyrosine kinase (C-Kit), FMS-like tyrosine kinase 3 (FLT3), Myeloid leukemia (MCL1), Glycogen synthase kinase (GSK3), Casein kinase 2 (CK2), while the derivatives of Marine sponges are Gracillin J, Gracillin K, Gracillin L and 3-norspongio. ARA-which is also known as Cytarabine is a Food and Drug Administration (FDA) approved drug for chemotherapy and it was used as a reference drug for this research. A molecular docking study was conducted to determine the binding energies of the interaction of selected proteins and ligand using Auto Dock 4.2 software in which the derivatives of Marine sponge's act as ligands for the active binding sites of proteins associated with AML. Further, Root Mean Square Deviation (RMSD) was calculated for the protein-ligand complexes to discover the stability of the protein-ligand complexes. The computational studies revealed that the natural derivatives of Marine sponges have the potential to act against the AML cancer cells due to the relatively high binding energies compared to that of ARA-C drug.

Keywords: Acute myeloid leukemia, Marine sponges, Derivatives, Molecular docking