Evaluation of efficacy of selected *Bryophyllum pinnatum* phytochemicals in hepatocarcinogenic therapy through *in silico* approach

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One of the worst diseases in the world, hepatic carcinoma requires expensive medical care upfront. Around the world, *Bryophyllum pinnatum* is a plant that is used in folk medicine to treat a variety of illnesses. Because of its abundance of active therapeutic compounds, the plant is employed for its major pharmacological effects. As a result, it aids in the treatment of liver cancer, and *Bryophyllum pinnatum* can be used in place of more expensive medications. In hepatocarcinogenesis disease, the Pi3k-Akt pathway, downstream signalling pathway, MAPK pathway, and PDGF pathway in the liver is engaged in the invasion and spread of malignant cells. Methanolic, ethanolic, and aqueous extracts of the phytochemicals of *Bryophyllum pinnatum* were subjected to qualitative analysis, the results indicated that the yield of phytochemicals in the ethanolic extracts was higher than in the other two extracts. The bufadienolides, β-sitosterol and bryophyllin A, which possess chemotherapeutic potential, were chosen for our computational investigation to assess their ability to interact with key signalling molecules such as VEGFR2, IGFR, C-KIT, RET, Pi3K, C-Met, MEK-inhibitor, and PDGFR. UCSF Chimera X was utilised to optimise the recovered molecules and by using data from the protein databank. The interaction of bryophyllin A and β-sitosterol, of the plant with the selected signalling molecules was investigated using the molecular docking tool, CB-Dock. According to the docking analysis, Bryophillin A strongly interacted with Pi3K than the other proteins whereas β-sitosterol showed stronger interaction with C-met.

Keywords: Bryophyllin A, β-sitosterol, Down-stream signalling pathway, MAPK pathway, Molecular docking, PDGF pathway, Pi3k-Akt pathway