Abstract

Marine fungi represent a largely untapped source of bioactive natural products with significant potential for novel drug discovery, particularly as antiviral, anti-inflammatory, and anticancer agents. This study aimed to identify and characterize bioactive compounds from marine fungi and assess their pharmacological potential using in silico methods. Metabolite extraction from marine fungi followed by chromatographic separation yielded several fractions, with one pure compound, (3S)-6-hydroxy-8-methoxy-3,5-dimethylisochroman (DMD), successfully isolated and structurally elucidated using open column chromatography, HPLC, and NMR. Molecular docking demonstrated that DMD could interact with several target proteins, particularly those involved in antiviral and anti-inflammatory pathways, through hydrogen bonding and non-covalent interactions, indicating potential inhibitory effects. However, DMD exhibited weaker binding affinities compared to known inhibitors and showed limited interaction with some cancer protein-related targets. These findings suggest that marine fungi-derived DMD holds promise as a lead compound for developing new antiviral and anti-inflammatory agents, though further investigation and validation are required.

Keywords: marine fungi, bioactive natural products, drug discovery, molecular docking