ORIGINAL RESEARCH ARTICLES

COMPUTATIONAL ANALYSIS OF A MEDIUM-CHAIN FATTY ACID REFINED FROM MARINE BACTERIAL CRUDE EXTRACT

Jeyameenakshi Annamalai[a], Ravikumar Sundaram[b*] and Nachammai Kathiresan[c]

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ABSTRACT

The current study investigates the *in silico* molecular interaction behavior of octanoic acid derived from the metabolite of a marine bacterium against targeted bacterial virulence factors and cancer-associated protein structures. Liquid Chromatography-Tandem Mass Spectrometry analysis was carried out to confirm and identify the derived metabolite. *In silico* analysis was performed to assess the binding affinity and interaction profiles of the ligand with structurally resolved targets obtained from existing protein databases. The findings indicated that the analysis has favorable binding interactions, with the ligand forming a stable conformational fit and establishing key stabilizing contacts within the active sites of all the selected targets. Additionally, the pharmacokinetic and toxicity profile of the ligand revealed promising ADMET characteristics, indicative of acceptable drug-likeness and toxicity profile. In summary, the results from the present study supply preliminary computational evidence validating the dual-target potential of the chosen ligand and emphasize its relevance for subsequent experimental studies in the discovery of novel anti-infective and anticancer therapeutic approaches.