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Understanding drug likeness of novel compound Fucoxanthin derivative isolated from *Chnoospora minima*

U. Bandaranayake[1], K. W. Samarakoon[3], P. Ranasinghe[4] and L. D. C. Peiris[2*]

[1]Department of Zoology/Genetics & Molecular Biology Unit (Center for Biotechnology), Faculty of Applied Sciences, University of Sri Jayewardenepura, Sri Lanka.
[2]Department of Zoology, Faculty of Applied, University of Sri Jayewardenepura, Sri Lanka
[3]Institute for Combinatorial Advanced Research and Education, General Sir John Kotelawala Defence University, Sri Lanka
[4]Industrial Technology Institute, Halbarawa Gardens, Malabe, Sri Lanka
dinithi@sci.sjp.ac.lk*

Non-communicable diseases pose an ever-increasing burden to many worldwide, regardless of gender, age, and nationality. In Sri Lanka, type 2 diabetes is prevalent due to the rapid transition of lifestyles, unhealthy dietary changes, and population demographic changes, which could be why the epidemic is escalating in South Asia. Advances in chemical biology have expanded the understanding of the marine environment as a diverse source of important bioactive compounds. These organisms include animals, microorganisms, and, most importantly, marine algae. Previously, a derivative of Fucoxanthin has been successfully isolated from Marine algae C*hnoospora minima*, and this study characterizes and studies the compound computationally using *in-silico* solubility, toxicity, and molecular docking studies. The compound was drawn using ChemDraw (version 12.0) and was energy minimized using Chem3Dpro (version 12.0). The energy-minimized structure was used in further analysis. Toxicity and aqueous solubility predictions were conducted using OSIRIS Property Explorer. The solubility was expressed in mol/l, and the value of the corresponding log was -6.17. Nearly 80% of the drugs on the market have an estimated logS value greater than -4. Therefore, the compound displays a lower solubility. The partition coefficient of the compound was predicted in cLogP value, which was -8.91. Chemical Property prediction such as half-life, AMES toxicity, and degradation patterns of the compound was made using the EPIsuite (version 4.11). The compound was deemed nontoxic and had a half-life of 14.603 Min. The compound was classified as recalcitrant in terms of bio-degradation. Auto dock tools (version 4.2.0) were used for molecular docking studies against human pancreatic α-amylase and α-glucosidase proteins, and the binding energies were -6.56 kcal/mol and -4.83 kcal/mol, respectively. The ligand formed hydrogen bonds with the protein residue of α-amylase, Arg92, and Asn250, and the residues Pro690, Arg696, and Leu811 were essential for α-glucosidase and ligand binding. The docking procedure was repeated for both proteins with the known drug Acarbose as the ligand. For α-amylase protein binding energy was -4.08 kcal/mol and for α-glucosidase protein binding energy was -3.40 kcal/mol. The data suggest that the novel ligand shows high suitability as a drug based on docking studies. The data suggest that the novel compound could be developed into a herbal supplement against type- 2 Diabetes Mellitus.

Keywords: Bioactive compounds, *Chnoospora minima*, Drug discovery, *In-silico* assays

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