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MARINE-DERIVED COMPOUNDS FOR THE TREATMENT OF RESPIRATORY DISEASES

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Abstract
Coronavirus disease 2019 (COVID-19) is a modern pandemic. SARS-CoV-2, the virus that causes the disease, typically targets the respiratory system, which can lead to pneumonia and, in extreme situations, death. Many marine chemicals that have shown great medical potential have been approved by the Food and Drug Administration, and some are currently undergoing clinical research. Using a variety of sophisticated computational approaches, we repurposed several marine compounds against SARS-CoV-2 in the current work by focusing on the primary protease and comparing them to the model drug, co-crystallized ligand. Two compounds outperformed the reference medication in terms of docking scores based on the findings of the binding affinity studies. Using molecular dynamics modelling, these compounds showed stable binding to the binding pocket of the target protein. Throughout the simulation experiment, the systems occupied the binding pocket and showed constant values for the radius of gyration and root mean square deviation. Additionally, the protein had passed through a low-energy basin and had a favourable shape while binding to the suggested inhibitors, according to the analysis of the free energy landscape and critical dynamics. All things considered, our research indicates that two marine compounds and sob are promising primary protease inhibitors.
Keywords: COVID-19, Essential dynamics, respiratory diseases

1. INTRODUCTION

and animals from the sea contain approximately half of all terrestrial life on Earth and are the most precious natural resource that humanity can use. Marine environments, with their diverse biodiversity encompassing changes in temperature, pressure, salinity, and light intensity, are not only rich in essential amino acids and high in protein, but they are also a significant source of many bioactive compounds that can be used as agents to promote health[13]. The severity of the disease is significantly correlated with the level of inflammatory markers, and it has been established that COPD is a systemic chronic inflammatory disorder [1]. Skeletal muscle weakness in people with COPD may be caused by the "spillover" of inflammatory substances from the lungs into the systemic circulation[2]. Previous research has shown that high levels of pro-inflammatory cytokines such interleukin and tumor necrosis factor-alpha (TNF-α) cause inflammation in the skeletal muscles and systemic circulation in the surrounding parts of the body in people with COPD. Furthermore, by altering the metabolic

types of muscles and mitochondria, inflammation can also have an indirect effect on the function of skeletal muscles [11]. Conversely, acute inflammation brought on by physical activity or an injury promotes muscle repair by activating anabolic pathways[6].

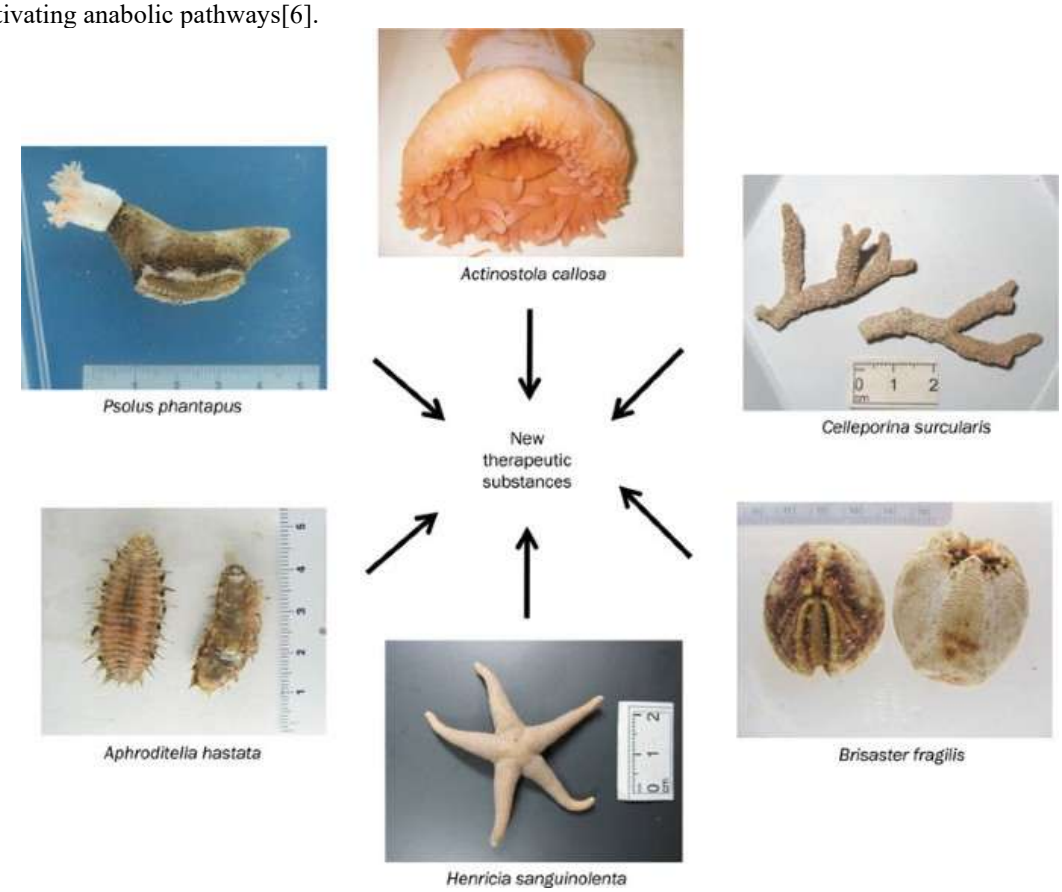


Figure 1: Application of marine derived compounds

To sum up, persistent low-grade inflammation is one of the primary pathogenic processes generating skeletal muscle dysfunction in COPD. It impacts the structure and function of skeletal muscles through a variety of pathways before eventually leading to the development of skeletal muscle dysfunction.

2. REVIEW OF LITERATURE

Muscle groups all over the body are affected by skeletal muscle dysfunction, which impairs respiratory function and exercise tolerance and ultimately results in physical inactivity. Regardless of other variables, this dysfunction predicts quality of life, hospitalization, survival, and rates of cachexia in individuals with COPD[5]. Studies have shown that individuals with COPD have 20% to 30% less muscle strength and are more prone to tiredness. As skeletal muscular endurance tends to decline before muscle strength, it is possible for endurance impairment to occur before strength impairment [3]. Different muscle groups have varying degrees of skeletal muscle failure[14]. Although it can happen to adults with normal or even higher body weight, skeletal muscle dysfunction is more prevalent and more severe in COPD patients with low fat-free mass index (FFMI) and cachexia[17]. Skeletal muscle dysfunction can be considerably improved, which could improve daily living activities, exercise ability, and survival rates for COPD patients[8]. Therefore, treating skeletal muscle weakness is essential to managing COPD patients overall and has significant effects on COPD treatment and rehabilitation[7].

3. MATERIALS AND METHODS

When oxidants and antioxidants are out of balance, oxidative stress results, which causes reactive oxygen species (ROS) to build up. Low amounts of ROS are necessary for appropriate force generation in skeletal muscle and are involved in regulating cellular signalling mechanisms. However, the mechanisms become disorganized in certain diseased circumstances [16]. The structure and function of muscle tissue may be harmed as a result of this equilibrium, which can start oxidative changes in DNA, lipids, proteins, and carbohydrates. There is broad consensus among researchers that skeletal muscle dysfunction development in COPD is largely caused by

systemic and local muscle oxidative stress[4]. Autophagy, inflammation, and impaired mitochondrial activity can all be functionally impacted by oxidative stress. This activation is the basis for long-term activity that raises oxidative stress in COPD skeletal muscle[12]. Generally speaking, oxidative stress and other pathologic reactions interact to cause skeletal muscle loss in COPD[5-8].

4. RESULT AND DISCUSSION

The coactivator of peroxisome proliferator-activated receptor γ is the main regulator of mitochondrial biogenesis. PGC-1α increases the expression of mitochondrial transcription factor A (TFAM) via activating multiple nuclear transcription factors, which in turn promotes DNA transcription and replication, which governs mitochondrial development and function. In the skeletal muscles of COPD patients, prior research has revealed decreased levels of mRNA expression and mitochondrial density[9].

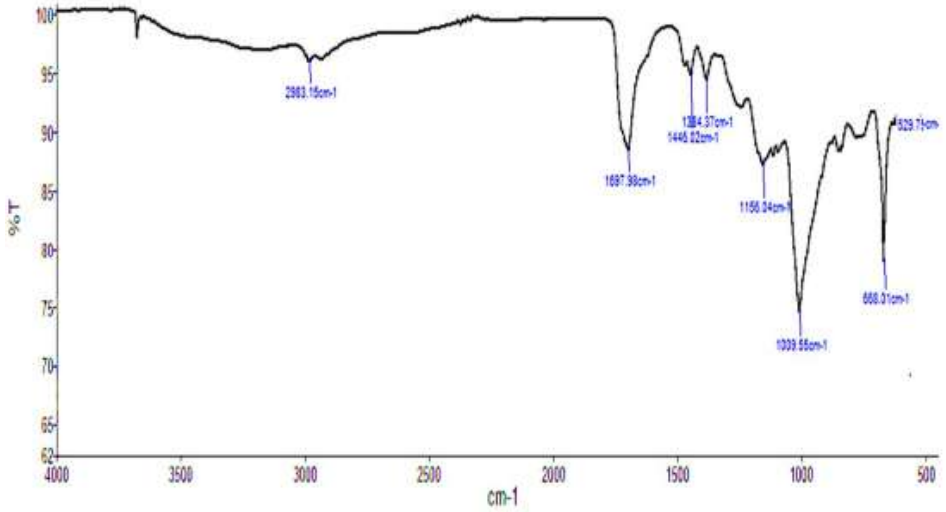
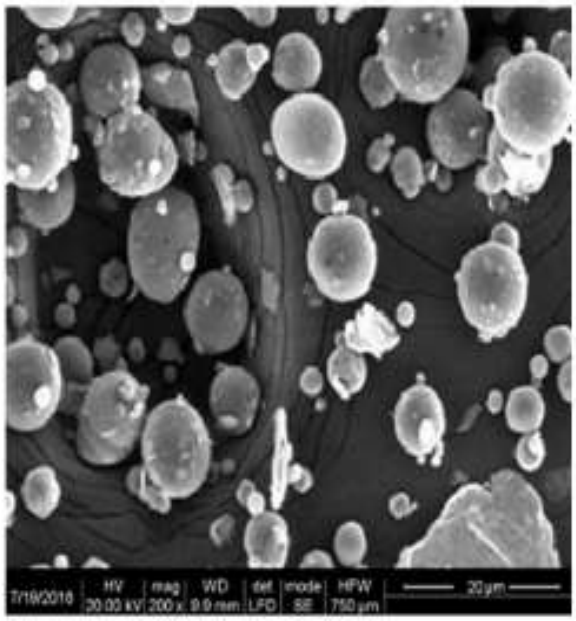
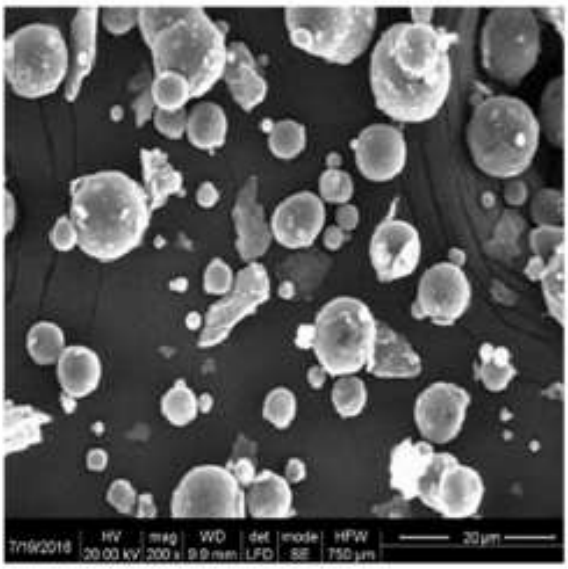


Figure 1: Fourier Transform Infrared Spectra graph

Mitochondrial biogenesis is the process of generating new mitochondria from preexisting ones by means of DNA replication, transcription, and translation, as well as mitochondrial fission, fusion, and quality control.



(a)



(b)

Figure 2: SEM results

Therefore, even though it is advised to exercise caution when interpreting the available data, it is evident that more research is necessary given the anomalies [15]. Skeletal muscle dysfunction could occur more quickly as a result of the interaction if there is an imbalance in the synthesis and degradation of muscle proteins[10]. In the skeletal muscle of individuals with COPD, oxidative stress has two functions: acute exercise-induced oxidative stress triggers the body's antioxidant defences, while pathological oxidative stress damages the skeletal muscle structurally and functionally.

5. CONCLUSION

The pathophysiology of COPD skeletal muscle failure is briefly discussed in this article, which also identifies bioactive chemicals originating from marine sources that may be useful as treatments for the illness. There is currently evidence that certain bioactive chemicals obtained from marine sources, including crude and refined extracts of marine plants and animals, have the ability to promote the health of skeletal muscles. Some marine-derived bioactive compounds, such as fucoidan, n-3 LC-PUFAs, MOPs, AST, lutein, and zeaxanthin, have advanced to the clinical-phase level of inquiry and have demonstrated promise in improving the health of skeletal muscle, even though the majority of investigations are still in the early exploratory phase. Of them, only n-3 LC-PUFAs have been extensively studied in clinical settings for the treatment of COPD skeletal muscle dysfunction as well as for enhancing skeletal muscle health. However, it is necessary to determine their maximal safe and effective supplementation dosages. The published results of current studies that demonstrate supplementation intervals ranging from days to six months emphasize the necessity of long-term follow-up studies to fully assess safety profiles. Current research' mechanistic evaluations are still crude and rely more on observational data than on complex causality validation. Combining bioactive substances from the sea is a viable supplemental approach for the future that could improve efficacy without causing toxicity or drug resistance. Multidisciplinary teams will be vitally needed in the future to define underlying mechanisms, optimize dose regimes, and support clinical translation in patients with COPD.

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