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MARINE-INSPIRED DRUG DESIGN: A NEW APPROACH TO PHARMACEUTICAL DEVELOPMENT

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Abstract
Cone snails, cyanobacteria, fungi, bacteria, and halophytes are just a few of the marine creatures that have produced the bioactive chemicals needed for therapeutic development. More than 90% of oceanic biomass comes from these sources, which have exceptional chemical qualities and a wealth of potential applications, especially in the treatment of cancer. The review emphasizes how marine natural materials' unique chemical structures and bioactivity have historically led to successful medication discovery.It clarifies the elements that led to these findings, including sophisticated isolation and characterisation methods, knowledge of marine ecological niches, and multidisciplinary study by marine biologists, chemists, and pharmacologists. The difficulty of chemical synthesis, restricted distribution, and environmental considerations all cause constraints. Preclinical research, clinical testing, and extensive testing are necessary to turn medications originating from marine sources into effective medicines. Future scientific and technological developments like metagenomics and synthetic biology present excellent opportunities for better discovery and quicker development of medications derived from marine sources.There is a lot of room for the development of new drugs, and continued research into marine natural products could greatly enhance medical knowledge while accounting for sustainability and environmental effects.
Keywords: Pharmaceutical Development, great potential, continued exploration

1. INTRODUCTION

In addition to their significance as food sources, transportation channels, oxygen manufacturers, and tourist destinations, our oceans provide an unparalleled wealth of options [1]. The field of using computer-aided ligand and structure-based approaches to find new therapeutic leads is constantly evolving[11]. By aiding in the structure elucidation of secondary metabolites, repurposing known marine natural products (MNPs) for new therapeutic applications, and identifying new hits or leads against particular therapeutic targets, computational methods and chemistry simulation tools can be used effectively in the discovery, design, and development of new chemical agents for therapeutic purposes[2]. As a result of the very popular marine (blue) biotechnology field's rising international recognition across a variety of related research fields, numerous legislative, infrastructure, and scientific collaboration networks have been formed[13].Since computer-aided approaches have been crucial to the advancement of this scientific field, computational resources have the potential to be a significant driver of

economic development, the creation of innovative biotechnological solutions, and the realization of sustainable drug discovery approaches worldwide[16].
The Special Issue "Marine Drug Discovery through Computer-Aided Approaches" was created to highlight the current scientific actors in the field of computer-aided approaches for blue biotechnology and to give a broad overview of the many innovative computer-aided methodologies for identifying and characterizing molecular agents with enhanced value and health-promoting properties for the preparation of medicinal and biotechnology applications[4].The objective was also to build a "guidebook" for maximizing the impact of marine biotechnology development by sharing information, professional contacts, and their knowledge[6]. Through computing methodologies, this guidebook would be used to start, strengthen, and expand partnerships between related and complementary scientific fields, which will both directly and indirectly promote the discovery and innovation of blue biotechnology and boost the blue bioeconomy. [3].

2. REVIEW OF LITERATURE

The "Marine Drug Discovery through Computer-Aided Approaches" special issue has nine original research pieces. Their spectrum of applications includes computer software, machine learning, molecular docking, in silico modelling, animal modelling for dereplication, and aiding in the clarification of MNPs' structure, bioactivities, and protein binding target prediction[8]. Anyone interested in beginning to use computer approaches in marine biotechnology research should read this Special Issue[15]. Below is a list of the nine contributions, arranged by publication date. A CADD method utilizing ligand- and structure-based methodologies was used to predict MNPs' antifouling ability[9]. All solitary natural products (NPs) from the sponge order collected between 1960 and May 2020 were surveyed in order to compile a wealth of data on their physical-geographical features[12].
From physio-chemical data, the pharmacokinetic properties of Veronica NPs and their possible medicinal applications were inferred[17]. In order to identify differences and correlations within a dataset and to thoroughly examine the chemical space interactions between taxonomy, secondary metabolites, and drug score components, network analysis was applied to NPs obtained from Veronica sponges. Bipartite networks of association and scaffold networks enabled the investigation of chemical diversity and chemical similarity networks that link pharmacokinetic factors with structural analogs. These networks can be expanded to various sponge orders or families.RKIP is aberrantly expressed in a number of disorders, such as diabetes mellitus, Alzheimer's disease, and cancer. Since RKIP also suppresses tumors, it is a valuable therapeutic target. It has been demonstrated that only few tiny compounds can change RKIP activity[19]. To investigate the properties of loco statin, the best RKIP modulator, a pharmacophore model was developed. Following a screening process that screened the intended model, a library of MNPs was later obtained [5].
The in-silico hits interfere with interactions with RKIP binding proteins and are potent RKIP modulators. One of the most common joint illnesses in both humans and animals, osteoarthritis is more common in older people.Dogs with osteoarthritis were used to investigate the bioactivities of collagen hydrolysates, sulphated glucosamine, and certain dog diets fortified with fatty acids as potential treatment agents. The used collagen hydrolysates and the sulphated glucosamine molecules of marine species were thoroughly confirmed by molecular modelling and an animal model for the intermolecular interactions of the receptor proteins MMP-3, TIMP-1, and ADAMTS-5.

3. MATERIALS AND METHODS

To further assess how well collagen peptides and glucosamines interact with protein receptor structures, molecular modelling simulations were also used. In food supplements for human and veterinary medicine, lipids—particularly eicosapentaenoic acid from fish oil, sulphated glycans (like sulphated glucosamine isolated from crab and mussel tissues), and hydrolysed collagen—have the potential to improve biochemical and physiological processes. Mycelium from filamentous microorganisms, including fungi and actinomycetes, could be physically separated in situ thanks to the novel solid-phase extraction embedded dialysis (SPEED) approach. The released specialized metabolites were captured by the XAD-16 resin. The components of SPEED include an internal dialysis tube filled with XAD resin and a nylon cloth covering it.The encapsulated compounds' molecular weight is selected via barrier dialysis, which also prevents biomass or macromolecules from precipitating out to the XAD beads. In order to facilitate the SPEED culture process, the outer nylon encourages the development of a bacterial biofilm. Marine Streptomyces 19-S21 isolated from an underwater Kopara core removed from the shoreline of a saltwater pond at a depth of 20 meters were treated using SPEED technology [16]. Using deep chemical profiling and dereplication techniques from molecular networking, the strain's chemical space was thoroughly examined, revealing how support culture affected the molecular fingerprint of Streptomyces secondary metabolites.Compared to land-based sources and non-marine microorganisms, marine creatures have a high and diverse concentration of bioactive compounds, making them the most lucrative natural product sources. The vast oceans, which cover more than 70% of the earth's surface, are home to a multitude of biological resources.

Significant variations in temperature, pH, light, pressure, salinity, and nutrient availability are among the dynamic environmental factors of the ocean that propel the formation of an extraordinary diversity of secondary metabolites in marine creatures. Because the chemical structures and biological activities of the compounds in the marine ecosystem are diverse, it is a particularly appealing site to search for new compounds that might be applied in a range of fields, including medication research. Since ancient times, people all over the world have used a variety of natural items derived from animal, vegetable, and mineral sources as medicine. Although some of these cures were really effective, others weren't so good.Before the printing press was developed in the 15th century, which made it possible to publish herbal remedies in large quantities, there was little information available on such ancient disease remedies. Natural products have been essential in the fight against infectious diseases for more than 50 years. The main factors that doubled our life expectancy, decreased treatment expenses, and revolutionized medicine in the 20th century were secondary metabolites of bacteria and plants. Resistance to well-known antibacterial, antifungal, and anticancer medications prompted theoretical and experimental chemists to look for alternate sources of treatment for diseases that are difficult to cure. Novel pharmacophores and innovative frameworks for drug development are still mostly derived from natural products (NPs)[7].

4. RESULT AND DISCUSSION

Although research into the specialized niches that support specialized bacteria in water ecosystems is still in its early stages, it will undoubtedly be an even more fruitful endeavor. For instance, using ecological logic and guidelines, it has been discovered that a shipworm obligate bacterial symbiont produces antibiotic compounds that are useful in treating resistant human diseases like Acinetobacter baumannii.

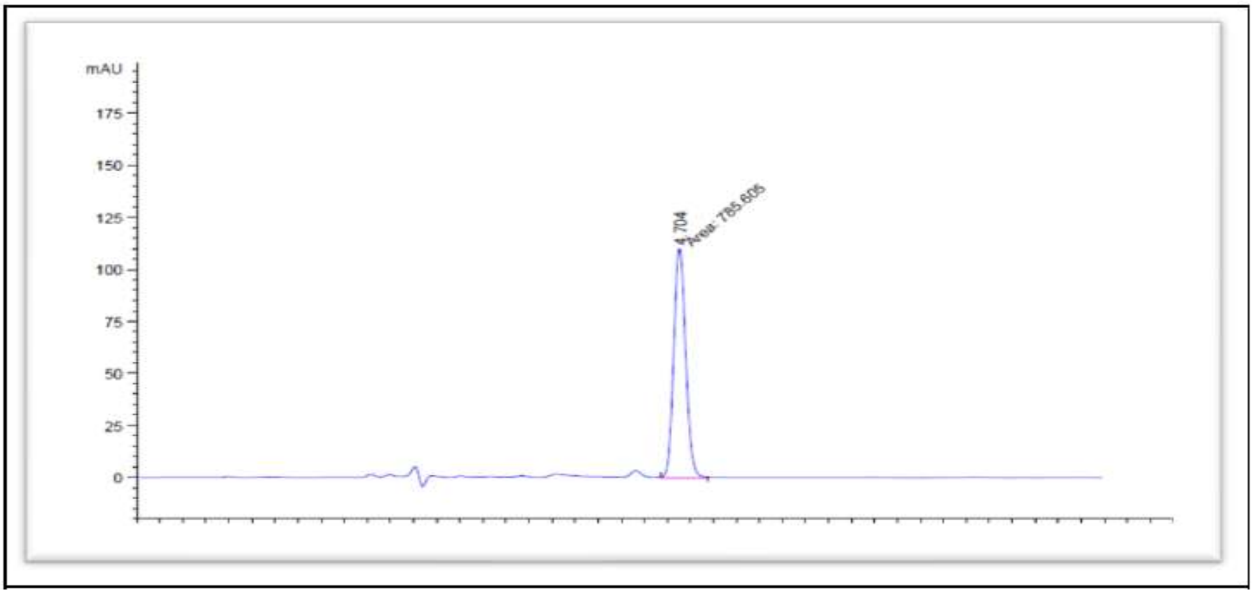

Figure 1: Chromatogram of sample

Most of the bioactive substances collected from larger marine creatures like sponges, tunicates, and sea slugs are actually secondary products of microbial metabolism, whether they are symbiotic or consumed bacteria of some kind. Another innovative method for finding normally resistant bacterial metabolites is the in-situ recovery of expressed and released NPs. The following describes the developments in analytical and informatic technologies that have contributed to this process. Because environmental cues are believed to induce expression of otherwise repressed NPs under standard culture conditions, the recovery and characterization of in-situ metabolites support traditional laboratory culture techniques and offer new insights into the natural activities of marine microbial NPs[14].

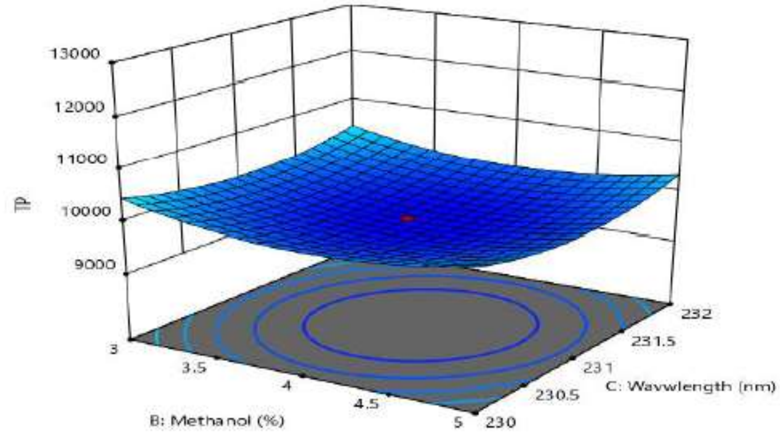

Figure 2: 3D Contour plot

Consequently, HP20 resin bags that were buried shallowly in tropical marine sediments have yielded numerous characterized marine bacterial metabolites as well as unknown molecular species. The sample methods outlined above are being utilized in combination with more intricate bioassays for NPs that are good for human health.

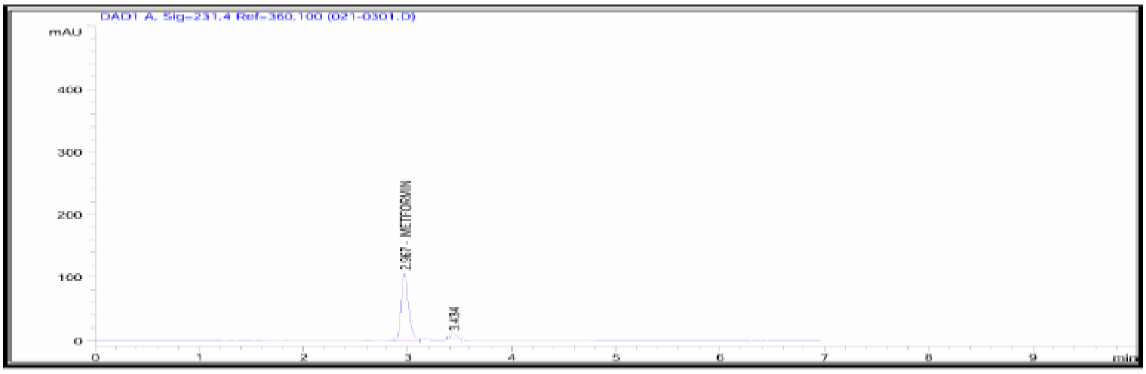

Figure 3: Chromatogram of Metformin HCl

For instance, even with primary screening of crude fractions, cytological screening for the presence of cancer cells utilizing vital stains and high content microscopy yields important information on mechanisms of action [10]. The search for important macromolecules in marine life has also been generally avoided because of the whims of associated methodologies. Marine animals are taking advantage of recent advancements in sampling techniques, genetic data and molecular biology techniques, advancements in synthetic organic chemistry, and computational approaches that include artificial intelligence, despite still being relatively understudied in these areas.Out of the 39,238 documented sea NPs, 23 sea-inspired medications have already entered clinical use. Compared to the industry ratio of conventional methods, which screen 15,000 compounds in an effort to locate an approved agent, this is a far higher success rate. As a result, marine NPs are offering beneficial drugs that promote human health. Large, easily observable creatures including sponges, corals, tunicates, and macroalgae have been the focus of most prior marine drug discovery attempts. Even though the study of marine microbes is relatively new, it has been quite successful in finding bioactive compounds.

5. CONCLUSION

Marine nanoparticles are a great source of compounds that can inspire therapeutic innovation. Compared to other sources of chemicals, marine NPs have a higher chance of yielding clinically effective medicines. Improved sample methods (e.g., slow-growing bacteria and microbial symbionts from oligotrophic sites) and sampling from new environments (e.g., the deep sea) are revealing new forms of understudied NPs.New methods of discovering marine NPs based on genetic and biosynthetic processes are being facilitated by interdisciplinary connections among chemists, biologists, and bioinformaticians. Finding new marine NPs is being prioritized by effective dereplication techniques.All things considered, these cutting-edge techniques and approaches are optimizing the success of drug discovery from the sea. The application of synthetic biology techniques to chemical availability issues is rapidly progressing. Whole chemical synthesis or semi-synthesis can also address the low-abundance NPs supply problem. Another issue with medications produced from the sea is that they are mostly peptides, which may not be the greatest pharmacological agents because of issues with metabolism. To enhance their pharmacological and pharmacokinetic qualities, synthetic medicinal chemistry techniques can be used to modify these peptide traits. Developing antibody drug conjugates to precisely deliver extremely powerful cytotoxic payloads to cancer cells is another effective application of medicinal chemistry in the development of marine NP medications.

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