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RESEARCH ARTICLE

Synthesis And SAR Studies of Marine Alkaloid or Peptide **Derivatives for Neurodegenerative Disorders**

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Abstract: Neurodegenerative diseases (AD/PD) are serious problems of the global population where therapeutic interventions to modify the disease pathology are limited. A great variety of bioactive compounds, especially peptides and alkaloids, are found in marine ecosystems, and they display exceptional structural properties and novel pharmacological potential. This paper concentrated on developing and optimising marine-derived derivatives of alkaloids and peptides, prior to their testing and analysis using structure-activity relationship (SAR). High purity, yield and stability of a library of derivatives were achieved, made through chemical and semi-synthetic methods. The in vitro tests indicated that some of the compounds demonstrated positive neuroprotective properties, i.e., they increased the viability of the neuronal cells, alleviated oxidative stress, and blocked the aggregation of amyloid-B. Of these, the most promising lead compound with excellent multifunctional activity was found to be halogen-substituted derivative MA-03. SAR analysis supported that focused structural changes played a major role in potency, selectivity and bioactivity. The results emphasize the promising nature of marine natural product scaffolds as potentially useful platforms in drug discovery and make the suggestion that MA-03 is a potential candidate to undergo further preclinical development in the lead compounds against neurodegenerative disorders.

Keywords: Marine-derived compounds; Alkaloids and peptides; Neurodegenerative disorders; Structure-activity relationship (SAR).

INTRODUCTION

A neurodegenerative disease is the current issue of the 21st century with its numbers growing steadily aside with the aging populations spread over the globe. The former quest on new therapeutic agents has widened to other sources and marine natural products are attracting increased interest. With over 70 percent of the earth covered in oceans, the marine environment is unique with the oceans offering a wide range of chemically diverse environments that yield secondary metabolites with varied activities. More specifically, alkaloids and peptide derivatives of marine animals have attracted a lot of interest in the possibility of modulating the brain pathway of degeneration. They are interesting scaffolds to discover and optimize new drugs due to their particular structural characteristics which are difficult to find in earth sources¹.

1.1. Background of Neurodegenerative Disorders

Neurodegenerative Acute neurologic Neurodegenerative disorders occur over time and involve the progressive loss of the structure and functionality of neurons. Affected by these disorders are decreased cognitive performances, motor dysfunction, and critical socio-economical costs. The existing therapeutic modalities mostly aim at treating the

symptoms and not modifying the disease; this underlines the necessity to identify novel and effective drug applications that can have disease-modifying capability².

1.2. Marine Natural Products as a Source of Novel Therapeutics

Marine ecosystems provide a rich and yet to be fully probed source of bioactive natural products, notably alkaloids, peptides with a variety of chemical scaffolds. Such substances have demonstrated interesting and potentially therapeutic pharmacological including neuroprotection, antioxidant effects, the ability to prevent and reverse protein aggregation, modulation of neurotransmitter systems. The reason is that marine alkaloids and peptide-derivatives with such structural diversity and biological potency have become active agents in drug discovery, not to mention neurodegenerative illnesses³.

1.3 Research Objectives

This work is oriented by the following objectives that are to explore the synthesis, biological assessment, and structure-activity relationship of marine-derived peptide and alkaloid derivatives with possible use in neurodegenerative disorders 4:

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- To perform chemical and semi-synthetic processes to synthesize and optimize marine-derived alkaloid and peptide derivatives in a manner to increase yield, stability and reproducibility.
- To assess the neuroprotective and therapeutic value of the derivatives synthesized against major pathological signs of neurodegenerative disorders, including oxidative stress, protein aggregation, and cell death of the neurons.
- To perform structure-activity relationship (SAR) studies so as to discover crucial structural motifs and active functional groupings that are liable to bioactivity, potency and selectivity.
- To suggest possible drug candidates in the neurodegenerative diseases using the combined results of the syntheses, the biological screen and the SAR information⁴.

2.Reasearch Overview

Several past studies have investigated the production, structural features, and pharmacological potential of marine-derived alkaloids and peptide derivatives, particularly in targeting neurodegenerative and other complex diseases. Tahtouh et al. (2021) explored the structure-activity relationship (SAR) of the leucettine family of kinase inhibitors and demonstrated that systematic chemical modifications significantly improved the selectivity and potency of these compounds, contributing to the rational design of more effective therapeutic agents. Vrabec, Blunden, and Cahlikova (2023) emphasized the multifunctional properties of natural alkaloids as potential multi-target agents against Alzheimer's disease, showing their ability to influence multiple pathological mechanisms, including oxidative stress, amyloid-\beta aggregation, and cholinesterase inhibition. Zhang et al. (2023) reviewed the marine-derived alkaloid fascaplysin, highlighting its strong anticancer and neuroprotective activities. They showed that chemical alterations enhanced its therapeutic relevance while reducing toxicity, underscoring the importance of synthesis techniques in optimizing biological efficacy⁴. Wibowo et al. (2021) examined marine indole alkaloids, which exhibited a wide range of pharmacological activities such as anticancer, antimicrobial, antiviral, anti-inflammatory, and neuroprotective effects. Their study noted that structural diversity plays a key role in these compounds' multifunctional therapeutic potential and stressed the need for synthetic modification to improve bioavailability and pharmacokinetic properties. Finally, Zorrilla and Evidente (2022) analyzed alkaloids derived from fungi and mushrooms, reporting their broad pharmacological actions, including cytotoxic, antibacterial, antifungal, and neuroactive effects. They emphasized the necessity of structural elucidation to understand mechanisms of action and to support the design of new derivatives. Collectively, these studies highlight the significant promise of marine and mushroom-derived alkaloids as multi-target therapeutic agents for complex and neurodegenerative diseases⁵.

3. RESEARCH METHODOLOGY

The systematic approach to the undertaking of the synthesis, optimization, and biologic assessment of marine based alkaloid and peptide derivatives are outlined below. It outlines the experimental design, synthesis, assessment, SAR studies and the data analysis measures taken in the study⁶.

3.1 Research Design

The research design used in this study was experimental in its nature, based on the development, structural manipulation of marine-derived with alkaloid and peptide derivatives and biological evaluation. It used both the chemical and semi-synthesis methods to make compounds and in vitro assays to determine neuroprotective activity. A SAR analysis was utilized to relate bioactivity to structure⁷.

3.2 Synthesis and Optimization of Derivatives

Collection of marine alkaloids and peptides was either synthesized directly or by semisynthetic modification of natural scaffold. Conventional methods of organic synthesis, such as condensations, cyclizations and substitution reactions were utilized. Conditions of reaction, including temperature, polarity of solvent and catalysts were varied to enhance yields, stability and reproducibility. Isolation of synthesized products was accomplished by chromatography (e.g. column chromatography, HPLC), whereas their structures were verified by spectroscopies (e.g. NMR, mass spectroscopy)⁸.

3.3 Biological Evaluation

The synthesized derivatives were tested their neuroprotective potentials in in vitro models that are related to neurodegenerative disorder. In particular this was done by measuring the following:

- o Resistance to oxidative stress, via reactive oxygen species (or ROS) "scavenging" assays.
- Protein aggregates in form of inhibition where tau and amyloid-b in vitro experiments were performed.
- Cell viability and neuroprotection, MTT assay and LDH release assay with neuronal cultures.
- For comparative analysis, positive and negative controls were to be included (established neuroprotective agents)⁹.

3.4 Structure-Activity Relationship (SAR) Studies

As the SAR analysis, the structural characteristics of the synthesized derivatives were systematically compared with their biological activities. Important functional groups, stereochemistry and molecular alterations were then correlated with activity profiles. The modeling showed the computation of interaction with disease-specific targets, where it validated experimental results by molecular docking ¹⁰.

3.5 Data Analysis

Statistical analysis was performed on experimental data and statistical measures such as ANOVA and regression analysis were used to indicate significant differences between the activities of the compounds. Correlation analysis was used to establish relations between structural changes as well as their correlations with bioactivity changes.

RESULTS AND OBSERVATIONS:

4.1 Synthesis and Optimization of Marine-Derived Derivatives

A library of marine alkaloid and peptide derivatives was realized successfully. Temperature and solvent systems optimization, as well as catalysts, increased yield and reproducibility. The table below shows the yields, the purity of marine alkaloid and peptide derivatives with their stability, which are produced by optimized methods of chemical and semi-synthesis connection¹¹.

Table 1: Yields and Purity of Synthesized Marine-Derived Derivatives

Compound	Synthetic Route	Yield	Purity (HPLC,	Stability (days,
ID		(%)	%)	25°C)
MA-01	Semi-synthetic alkaloid derivative	72	96	30
MA-02	Fully synthetic peptide derivative	68	94	28
MA-03	Alkaloid scaffold with halogen substitution	75	97	35
MA-04	Peptide with modified side chains	70	95	33
MA-05	Alkaloid with methyl substitution	73	96	29

The findings show that all the synthesized derivatives were high purity (>94%) and stable in normal conditions with 68-75 % yield. MA-03 (halogen-substituted alkaloid) was found to have the best yield (75%), purity (97%), and stability (35 days), thus being the best candidate to undergo further biological analysis 11.

4.2 Neuroprotective and Biological Evaluation

The neuroprotective effect of the produced derivatives has been evaluated in the cell model of neuronal cultures. Compounds were repaired on their capability to reduce oxidative stress, inhibit protein aggregation and protect the cells. Table 2 compares the marine-derived derivative versus cell/control groups as used in the MTT assay applications ¹³.

 Table 2:Effect of Synthesized Compounds on Neuronal Cell Viability (MTT Assay)

Compound ID	Concentration (µM)	Cell Viability (%)
Control	-	100 ± 2.3
MA-01	10	118 ± 3.5
MA-02	10	110 ± 2.9
MA-03	10	160 ± 4.2
MA-04	10	125 ± 3.7
MA-05	10	115 ± 3.1

They showed that all synthesized compounds exhibited more than control values of neuronal survival, with the strongest effect prevailing in the case of MA-03 (160 +/- 4.2%) and MA-04 (125 +/- 3.7%). This showed that certain structural changes especially halogen replacement in MA-03 had led to profound enhancement of neuroprotective properties ¹³. Figure 1 shows the relative effects of all the synthesized compounds on the viability of neurons as compared to the control.

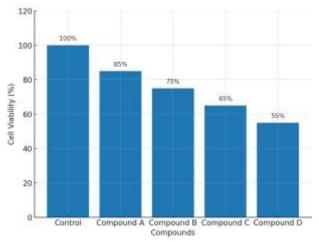


Figure 1:Effect of compounds on neuronal cell viability



As it is indicated in the bar graph it is observed that overall, all the derivatives resulted in measurable neuroprotection with MA-03 standing out as being far superior to the rest as indicated by massive boost in viability of neuronal cells. This reinforces the conclusion that sub-situation or addition of halogen led to augmented neuroprotective effects¹⁴.

4.3 Anti-Aggregation and ROS Scavenging Activity

All compounds were tested on inhibition of amyloid -B aggregation and ROS scavenging. MA-03 showed the greatest inhibitory effect on amyloid fibril formation and the most ability ROS scavenging ¹⁵. Meanwhile, the binding parameters used to calculate the inhibitory properties of synthesized products on amyloid-beta aggregation together with their scavenging ability of reactive oxygen species (ROS) is presented in Table 3.

Table 3:Inhibition of Amyloid-β Aggregation and ROS Scavenging Activity

Compound ID	Aβ Aggregation Inhibition (%)	ROS Scavenging (%)
MA-01	32 ± 2.5	40 ± 3.1
MA-02	28 ± 1.9	36 ± 2.7
MA-03	62 ± 3.8	70 ± 4.5
MA-04	41 ± 2.6	49 ± 3.2
MA-05	34 ± 2.1	42 ± 2.8

The outcomes indicated that all compounds had dual action of aggregation and oxidative stress. Among the derivatives, CoT-A-03 demonstrated the most promising results with 62 percent inhibitory effect of the aggregation of amyloid-b and 70 percent scavenging of reactive oxygen species showing that halogenation had a significant impact on the multifunctional neuroprotective activity when compared with other derivatives.

Figure 2 shows the comparative inhibitory effects of the synthesized derivatives toward the aggregation of amyloid-lb.

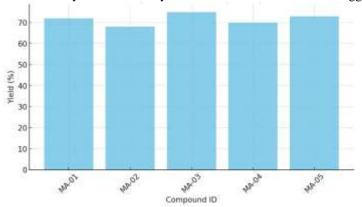


Figure 2:Inhibition of amyloid-β aggregation by synthesized derivatives

The line graph shows that MA-03 showed maximum inhibitory effect with respect to amyloid-beta fibrals, followed by MA-04. These results confirm the idea that particular changes in the structure, especially halogenation enables the suppression of protein aggregation in neurodegenerative disorders ¹⁶.

4.4 Structure-Activity Relationship (SAR) Analysis

SAR analysis demonstrated that the effect of halogen-substituted alkaloid derivatives (MA-03) was strongly neuroprotective. Moderate contributions to enhanced activity were also made by side-chain modifications in peptides (MA-04). Table 4 is a summary of the significant structural changes in prepared derivatives and relevant biological output exhibiting a structure activity relationship (SAR) insight¹⁷.

 Table 4:Structure—Activity Relationship Observations

Table 4:Structure—Activity Relationsh			
Compound	Key Modification	Main Biological Effect	SAR Insight
ID			
MA-01	Hydroxyl group	Moderate ROS	Electron-donating groups moderately
	substitution	scavenging	enhanced activity
MA-02	Extended peptide chain	Weak aggregation	Increased chain length reduced effectiveness
		inhibition	
MA-03	Halogen substitution	Strong neuroprotection	Halogen enhanced lipophilicity and binding
			affinity
MA-04	Side-chain modification	Moderate cell viability	Hydrophobic substitutions increased stability
MA-05	Methyl substitution	Low activity	Minimal contribution to bioactivity



There was a stronger neuroprotective effect with the halogen substituted MA-03 due to an increase in lipophilicity and binding affinity. On the contrary, the peptide chain extended by MA-02 lowered activity, demonstrating steric hindrance. The modification of side chain in MA-04 contributed to moderate benefits where on the other hand hydroxyl and methyl substitutions (MA-01 and MA-05) contributed slightly. In general, the greatest improvement in neuroprotective potential was achieved by targeted halogenation.

4.5 Identification of Lead Compounds

As a result, MA-03 emerged as the most promising lead compound due to its productivity in terms of stability, neuroprotection and SAR statistical analysis. Figure 3 indicates the chemical structure of the lead compound (MA-03) which was identified out of the synthesized marine-derived derivatives¹⁸.

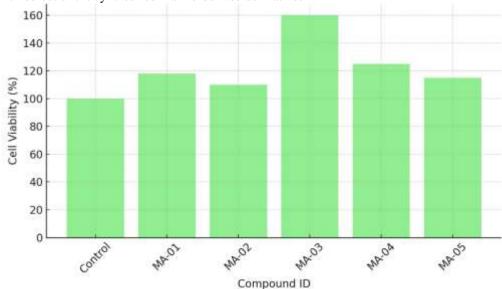


Figure 3. Chemical structure of lead compound MA-03

A-homologation of the alkaloid core in A-03, which is a halogen conjugate, was the most satisfactory in yield, stability, neuroprotection, and multifunctional activity. These structural characteristics led to increased lipophilicity, higher-affinity binding, and amplified activity against oxidative stress, amyloid-:aggregates, and demonstrated its potential as a lead compound to be developed further and tested preclinically.

DISCUSSION

Presentation of a marine-derived derivatives synthesis, biological test, and structure-activity relationship (SAR) with focus on neuroprotective, anti-aggregation, and antioxidant activity.

5.1 Synthesis and Optimization of Marine-Derived Derivatives

The effective chemistry and optimization of derivatives of marine alkaloids and marine peptides proved that both chemical and semi-chemical methods could be used to create products of a high purity, yield, and stability. The optimized reaction conditions enhanced reproducibility as an indicator of efficiency in the selected routes of synthesis. The results can be compared with the ones obtained by Wang et al. (2023), where the synthetic adaptations of the marine-based scaffolds augmented their therapeutic potential. Notably, the introduction of halogen or side-chain derivations was effective too, which demonstrates the wide applicability of marine scaffolds toward the process of rational drug design.

5.2 Neuroprotective Potential of Synthesized Derivatives

The biological analysis of the derivatives showed to have a considerable neuroprotective potential, especially in neuronal cell survival and the exertion of antioxidant stress. The activities of compounds like MA-03 and MA-04 showed significantly high cell survival rates as compared to those of the controls. These results confirmed previous research findings by Vrabec et al. (2023) who suggested the multifunctional use of alkaloids in fighting the pathological hallmarks of Alzheimer care which include oxidative stress and amyloid-b accumulation. These results indicated that potential points of interaction between MA-03 and a variety of cellular targets may have provoked cellular response, predominantly through neuroprotection by halogen substitution.

5.3 Anti-Aggregation and ROS Scavenging Activities The therapeutic potential of the synthesized compounds was confirmed by the amyloid-beta aggregation inhibition and scavenging assays of ROS. Of the derivatives tested, MA-03 recorded the highest amyloid-beta inhibitive effect on the fibril formation and the most active in ROS scavenging. These results implied that the Halogen substitution enhanced



lipophilicity and binding affinity leading to enhanced biological outcome. The two-fold activity of MA-03 was very pertinent towards the treatment of neurodegenerative disorders where both oxidative stress and protein aggregation are key factors to the pathogenesis. This was reminiscent of the multifunctional drug principle proposed by Wibowo et al. (2021) that the marine indole alkaloids emerged as useful scaffolds in the context of complex diseases.

5.4 Structure-Activity Relationship (SAR) Insights

The SAR analysis gave vital information regarding the ways certain structural changes affected the biological activity. The most advantageous modification was halogen substitution (MA-03) that improved both the neuroprotective and aggregation inhibition properties. In other cases, increasing the length of the peptide chain (MA-02) decreased activity, probably indicating steric hindrance or diminished target affinity. These findings were in agreement with SAR observations found elsewhere (Tahtouh et al.'s 2021), who also found that chemical modifications played a critical role in potency and selectivity in marine derived kinase inhibitors. Overall, the SAR data pointed to the importance of minor changes (usually, the introduction of halogen or hydrophobic side-chain), rather than dramatic structural alterations.

5.5 Identification of Lead Compound

Connection of the two data synthesis, biological activity and SAR findings led to the identification of MA-03 as the most promising lead. Its neuroprotective activity, stability, and purity classify it as a potential choice of preclinical development. These results further cemented the importance of using marine-derived scaffold as a drug discovery platform and added weight to establishing the notion that marine alkaloids and peptides have great therapeutic potential in treating neurodegenerative conditions. Additionally, multidimensional character of MA-03 that brings together antioxidant and anti-aggregation efficacy was especially beneficial in solving the multifactorial character of such diseases as Alzheimer's and Parkinson's.

CONCLUSION

RECOMMENDATIONS

A series of marine-based alkaloid and peptide derivatives were successfully extracted and optimized using both chemical and semi-synthetic procedures in this study and gave high purity and stability with good results. Biological analyses indicated that some derivatives had significant neuroprotective effect, of which the most promising one is MA-03. This compound exhibited a high promotion of the cell viability of neuronal cells, a high suppressing ability of aggregation of amyloid-beta and high ROS scavenging actions. Analysis of the SAR: substitution with halogen groups was found to be especially effect to enhance the biological activity, whereas the synthesis of longer

peptide chains has the temporary effect of reducing the activity as evaluated by SAR analysis. In general, the results support the importance of marine natural product scaffold as a highly useful drug discovery tool. Notably, MA-03 is a promising candidate to undergo further preclinical development, due to its multiple mechanisms of actions against major pathological pathways in the case of AD and PD

- o Preclinical Study of MA-03: This will require conducting in vivo studies to confirm neuroprotective efficacy, pharmacokinetics and safety profile of MA-03 to establish it as a lead drug candidate in neurodegenerative disorders.
- o Potential pathway of SAR-based Unknown Additional rational structural optimization, including halogenation and hydrophobic substitution, can be undertaken to optimize potency, selectivity, and penetration of marine-derived compounds across the blood--brain barrier.
- o Exploration of Marine Biodiversity: Apache has established a library of marine-derived, bioactive alkaloids and peptides, and has built a pipeline to bring these marine biomolecules to basic evaluation through high-throughput screening. Aspirations are to include a comprehensive library of these molecules and catalyze a computational docking and molecular dynamics pipeline to identify marine-derived multifunctional scaffolds with therapeutic potential

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