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Pharmacophoric Studies Of Marine Cardioactive Biomolecules (MCBS) On The Theoretical Basis

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Abstract:
Marine novel chemical entities have great potential for the therapeutical exploration. Their intelligent screening and application gifted pharmaceutical innovations in biomedications. We made a pioneer approach for designing the hypothetical pharmacophoric model for MCBs. This provides insight of various binding sites at cardiovascular receptors.

1.Introduction

The biofunctional moieties of MCBs were elucidated through structural chemistry of MCBs (1-Methylisoguanosine[1], Aaptamine[2], Anthopleurine[3], Autonomium Chloride[4], Dieckol[5], Doridosine[1], Eckol[5], Eledoisin[6], Halenaquinol[7], Hymenin[8], Laminine[9], Octopamine[10], Phlorofucofuroeckol[5], Saxitoxin[11], Spongosine[12], Spongouridine[13], Tetrodotoxin[14], and Xestoquinone[15]).

They exhibited antianginal, antiarrhythmic, antihyperlipidemic, antihypertensive and cardiotonic types of bioactivities and followed the basic cardiopharmacological drug actions .We designed the basic pharmacophoric model of their possible binding sites.

2.Theoretical Methodology-

The pharmacophoric studies analyse the biofunctional moieties of MCBs which are responsible for the biological action. The biofunctional moieties are of two types.

- Essential- They interact with receptor to give response and have high structural specificity. They cannot be structurally modified at great extent.
- Nonessential- They do not involve in drug –receptor complexation, therefore they can tolerate great chemical variability.

To elucidate essential moieties of MCBs, their mode of actions were interpreted in the terms of structural requirements for the cardiovascular activities. Such chemical functionalities contribute to receptor binding through various types of bondings and interactions.

Five types of essential moieties of MCBs were characterised by appropriate structural functionalities (Table One).

S.No	Types of essential moieties	Structural functionalities	Types of bondings
1.	Cationic	guanidium	Ionic or Electrostatic
2.	Anionic	carboxylic/phenolic	
3.	H-donor	Amino group	H- bonding
4.	H-acceptor	Hydroxyl or heteroatoms	
5.	Hydrophobic	Aryl or alkyl groups	Hydrophobic vander waal interactions

Table 1:Essential moieties of MCBs and their roles in receptor interaction

3.Result And Conclusion

This knowledge of chemopharmacological aspects allowed to propose a hypothetical pharmacophoric model for MCBs, which is composed of ionic, H-bonding, and hydrophobic sites.

The most striking finding is that MCBs have mimetic / isosteric moieties of neurotransmitters (acetylcholine/ norepinepherine) e.g. - Octopamine and Autonomium chloride, DNA (bases/sugars) e.g. - marine nucleosides and neuropeptides e.g. - Anthopleurines.

This study concluded that MCBs have promising cardioactive potential at therapeutical front.

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