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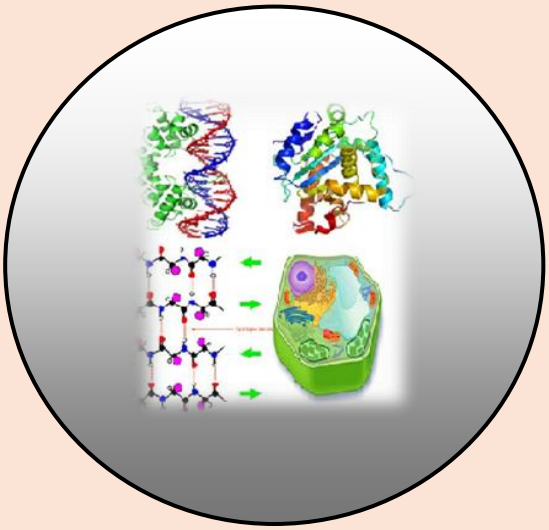

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RESEARCH PAPER

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Consensus Pharmacophore Model for Larvicidal activity against *Plutella xylostella* for Nortopsentin Alkaloids

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ABSTRACT

Developing a common pharmacophore is a highly helpful approach to find out structural features that sway the biological profile of lead compound. In the present work, an attempt has been made to develop a consensus pharmacophore model for larvicidal activity against Diamond Back Moth (Plutella xylostella) for Nortopsentin Alkaloids. The developed model points out that H-bond donor/acceptor and lipophilic regions are necessary to have prominent larvicidal activity against Diamond Back Moth (Plutella xylostella) for Nortopsentin Alkaloids. The developed model could be beneficial to medicinal chemists to derive a better derivative with significant augmented activity.
Keywords: Pharmacophore modeling, Plutella xylostella, Nortopsentin Alkaloids and Larvicidal activity.

INTRODUCTION

Natural products are chemical compounds produced by living organisms. Throughout history, diverse types of natural products have been used in multifarious roles, such as insecticidal, fungicidal, medicines, coloring agents, a few to mention. The marine environment is massively complex, consisting of extreme variations in pressure, salinity, temperature, and biological habitats that have led to the production of several novel structures with unique biological properties, which may not be found in terrestrial natural products for example Nortopsentin Alkaloids. In addition, they can also be amalgamated with synthetic compounds to develop type of semi-synthetic compounds, which are aimed to improve effectiveness beyond those of the natural products. Nitrogen containing rings such as pyrrole, pyridine, etc. are widely abundant in nature with promising biological and chemical profiles to be explored as novel utilities (Ji et al., 2018; Dayan et al., 2009; Cantrell et al., 2012).

Recently Ji et al. (2018) reported larvicidal activity against Diamond Back Moth (*Plutellaxyl ostella*) for Nortopsentin Alkaloids. They discussed SAR (Structure-Activity Relationships) in good details, however no attempt was instigated by them to generate a consensus pharmacophore model. Pharmacophore modeling is a structure-based approach to develop new compounds possessing desired activity. Therefore, the present work is intended to attain development of such pharmacophore model.

Experimental Methodology

1. Selection of Dataset: The consensus pharmacophore model is developed using a dataset of twenty-six molecules Ji et al. (2018). The molecules were screened for their activity and selectivity for larvicidal activity against Diamond Back Moth (*Plutella xylostella*) at a concentration of 200 and 600 µg/mL.

2. Development of pharmacophore model: The complete method involves four main steps Masand, and Rastija, (2017), Masand et al (2017), Masand et al (2017):

1. Structure drawing: The task of structure drawing was accomplished using Chem Sketch 12 freeware (www.acdlab.com).
2. Structure optimization: In second step, Avogadro 1.2 was employed to optimize the 3D- structure of twenty-six derivatives using semi-empirical method (MMFF94).
3. Alignment of molecules: This step was accomplished using Open3Dalign.
4. Model generation: Lastly, top five active aligned molecules were introduced in PyMOL 2.0. Then, PyMOL plugin 'LIQUID' was employed to generate consensus model using default settings.

RESULT AND DISCUSSIONS

The present pharmacophore-oriented analysis unveils that the larvicidal activity against Diamond Back Moth (*Plutella xylostella*) for Nortopsentin Alkaloids selected in the present work has good correlation with one high-volume and another small lipophilic, two H-Bond donor and two H-bond acceptor groups.

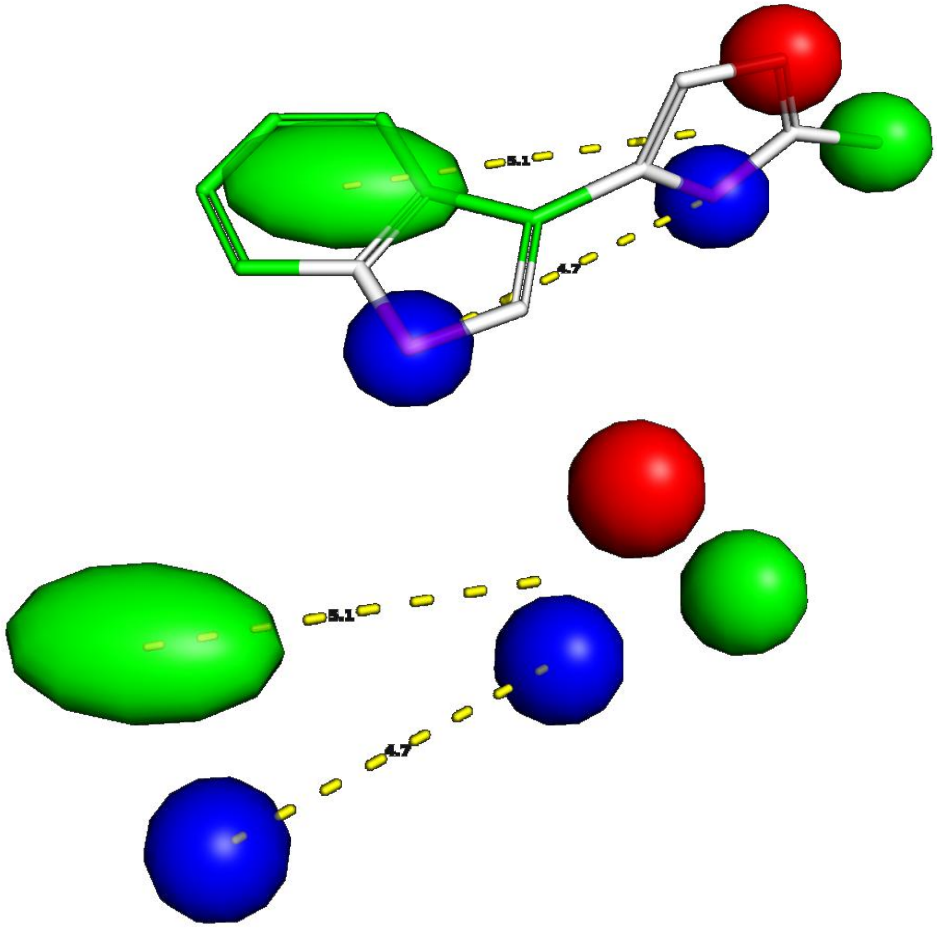

Figure 1. Consensus pharmacophore model with and without molecule and contours for different regions (Green: Lipophilic, Blue: H-Bond donor and Red: H-Bond acceptor region).

A closure inspection of figure 1 reveals that the larvicidal activity against Diamond Back Moth (*Plutella xylostella*) for Nortopsentin Alkaloids is due to lipophilic nature of bi-cyclic ring and methyl group attached to imidazole ring. The nitrogen atoms of imidazole ring and indole ring act as H-bond acceptor. The second nitrogen of imidazole ring acts as a H-bond acceptor. Therefore, a good strategy to retain the activity is to give good importance to these regions.

CONCLUSIONS

The larvicidal activity against Diamond Back Moth (*Plutella xylostella*) for Nortopsentin Alkaloids which is associated with lipophilic nature of bi-cyclic ring and methyl group attached to imidazole ring. The nitrogen atoms of imidazole ring and indole ring. Therefore, such a combination of these moieties must be retained in future optimization to have good activity. The present study was effective in discovering useful structural features for future optimizations.

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REFERENCES

Ji, X., Guo, J., Liu, Y., Lu, A., Wang, Z., Li, Y., Yang, S. and Wang, Q. (2018). Marine-Natural-Product Development: First Discovery of Nortopsentin Alkaloids as Novel Antiviral, Anti-phytopathogenic-Fungus, and Insecticidal Agents, *J Agric Food Chem*., 66(16): 4062-4072.

Dayan, F. E., Cantrell, C. L. and Duke, S. O. (2009). Natural products in crop protection. *Bioorg. Med. Chem*., 17, 4022−4034.

3. Cantrell, C. L., Dayan, F. E. and Duke, S.O. (2012). Natural products as source for new pesticides. *J. Nat. Prod.*, 75, 1231−1242.

Masand, V. H. and Rastija, V. (2017). Py Descriptor: A new PyMOL plugin for calculating thousands of easily understandable molecular descriptors. *Chemometrics and Intelligent Laboratory Systems, 169*, 12-18.

Masand, V. H., El-Sayed, N. N. E., Mahajan, D. T. and Rastija, V. (2017). QSAR analysis for 6-arylpyrazine-2-carboxamides as *Trypanosoma brucei* inhibitors. *SAR and QSAR in Environmental Research, 28*(2), 165-177.

Masand, V. H., El-Sayed, N. N. E., Mahajan, D. T., Mercader, A. G., Alafeefy, A. M. and Shibi, I. G. (2017). QSAR modeling for anti-human African trypanosomiasis activity of substituted 2-Phenylimidazopyridines. *Journal of Molecular Structure, 1130*, 711-718.

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