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A combinatorial methodology for the discovery of new agents with insect repellent properties

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Mosquitoes and other hematophagous arthropods, the primary vectors of multiple parasites and viruses, are responsible for the transmission of serious diseases to humans such as malaria, dengue fever, West Nile fever, leishmaniasis etc. Today, the growing resistance of vectors to existing repellents render them as ineffective. The interest is focused on the development of novel repellents with advanced properties to the existing ones in the fields of duration of the protection, minimum effective dose, efficacy against a wide variety of insects' bites and safety. Towards this direction, the present study attempts the discovery of novel hit compounds which may evolve as insect repellents. To fulfill this goal, a combination of computational and analytical approaches were implemented and proposed scaffolds were tested in vivo with behavioral assays in female mosquitoes. Particularly, a pharmacophore-based virtual screening of databases focusing on natural products and molecular docking studies were performed to identify novel compounds which present binding affinity to Odorant Binding Proteins (OBPs) and physicochemical properties associated with insect repellency. In total, 6 compounds were picked and tested for their insect repellent activity against female mosquitoes (*Aedes albopictus*). Results revealed that all the examined compounds present insect repellent activity (35-57,9%) compared to naked hand.

Biography

Eftychia Kritsi is a postgraduate student at the Institute of Biology, Medicinal Chemistry and Biotechnology (IBMCB) of National Hellenic Research Foundation (NHRF). She is a chemist with experience in Computational Drug Design. She earned her Bachelor's and master's degree from the Department of Chemistry at the University of Athens and she has completed her PhD thesis at the School of Chemical Engineering of National Technological University of Athens (NTUA). She has published 7 papers in scientific journals and she has 11 poster presentations at International Conferences. Furthermore, she has been co-organizer of 1 workshop (2013, NHRF). During her PhD studies, she has received a fellowship for the University of Patras, "C. Caratheodory program", in 2013-2014. Also, she was participated to the research project KPIPIS - GSRT, "Targeted therapeutic approaches against degenerative diseases-conditions with emphasis in cancer and aging" (2015, NHRF). In 2017, she was awarded a postgraduate fellowship from the program "IKY FELLOWSHIPS OF EXCELLENCE FOR POSTGRADUATE STUDIES IN GREECE-SIEMENS PROGRAMM". The main field of her interest is the design of novel bioactive compounds using Nuclear Magnetic Resonance (NMR) Spectroscopy and in silico applications.

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