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Development of herbal mosquito repellent nanopatch

P D Juyal¹, Amit K Goyal² and G Rath²

¹Nanjaji Deshmukh Veterinary Science University, India

²ISF College of Pharmacy, India

There were considerable efforts made to promote the use of environment friendly and biodegradable natural insecticides and repellents, particularly from botanical sources. However, limited period of effect is the major drawback of these products. There is a need in art for a safe, cost effective and highly efficient carriers/absorbent composition of matter that provides for a controlled time release of an aromatic substance, such as an essential oil or a combination of essential oils. The objective of research project relates to wearable insect repellent patch comprised of nanopatch intended to provide personal protection from insect bites particularly from mosquitoes. The repellent action is attributable to a one or mixture of essential oils including eucalyptus oil, citronella oil, geranium oil, rosemary oil, lemongrass oil and neem oil. Resultant nanopatch have shown enhanced surface-to-volume ratio, high porosity, numerous active sites and controlled release of encapsulated oils. The developed nanopatch serve as matrix for essential oils, enclosed in a perforated backing substrate and further with a release liner to protect the volatile component from the external environment. The resulting patch provides an effective means of personal protection against flying insects and safe for use in children.

juyalpd54@rediffmail.com

NMDA-Chemometric analyses to explore essential structural and physicochemical requirement of small molecules to inhibit NMDA functionality

Tabassum Hossain and Achintya Saha

University of Calcutta, India

The N-methyl-D-aspartate (NMDA) is a glutamate receptor, an important target for controlling synaptic plasticity and memory function, but over activation resulting in an excess of intracellular calcium formation, triggers neuronal injury and is involved in numerous pathologies. The present study has been emphasized to explore both ligand and structure-based QSAR, pharmacophore, docking and simulation studies on a set of structurally diverse inhibitors to optimize prime structural features responsible for selective binding to NMDA, and vis-à-vis inhibiting enzyme activity. The pharmacophore model showed the importance of HB acceptor, and hydrophobic features of the molecule for effective binding. Structure-based docking and simulation study adjudged the significance of the features obtained from ligand-based QSAR (ROC score=0.917), HQSAR (Q2=0.812, R2pred=0.772) and pharmacophore models (R2=0.927). Both docking and simulation studies confirmed the stable interaction with the catalytic residue Glu106. Presence of electronegative groups, aromatic rings and methyl chains in 3D space of molecular scaffold depict their importance in NMDA inhibition.

tabu0910@rediffmail.com