

Exploring therapeutic potential of *Acorus Calamus*: An in silico approach



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ABSTRACT

Background: In Asian sub-continent *Acorus Calamus* or sweet flag or Indian Vacha was used for long time in ayurvedic and folklore medicine for the treatment of various ailments ranging from asthma, cough, rheumatoid arthritis, high blood pressure, diarrhea, treatment of memory loss, bronchospasm, bronchitis, ulcer, problems related to central nervous system and many others. Several active compounds from *Acorus Calamus* were reported in some literatures, however, systemic study was lacking on it. The objective of this study was to identify anti-allergic activities of the secondary metabolites of *Acorus calamus* in silico.

Methodology: The active compounds were listed from several literatures. The structures of some of these compounds were retrieved from ZINC database and others were created in Discovery Studio (version 3.0) using SMILE notation. The structures of IL-4, IL-13 and H1 receptor were retrieved from PDB. Docking study was performed between the active compounds of *Acorus calamus* and IL-4, IL-13 and H1 receptor using SWISSDOCK. On the basis of binding affinity 4 compounds were selected. The binding sites of these compounds were studied extensively using Autodock Vina software.

Result: More than 30 active compounds were reported in the literatures of which 4 compounds (Eugenol, Acoric Acid, Malonyl-CoA and aserone) showed highest affinity against IL-4, IL-13 and H1 receptor. Study of active sites revealed that eugenol, acoric acid and aserone were potent antagonist of H1 receptor. They were also interacting strongly with IL-4 and IL-13.

Conclusion: Eugenol, acoric acid and aserone will be promising therapeutic agent against allergy and asthma.

BIOGRAPHY

Nandini Ghosh is working on allergen identification and development of therapeutic strategies. She has expertise in immunology, proteomics, molecular biology and bioinformatics. She has published many papers in internationally reputed journals, such as Scientific Reports (Nature), Plos One, BMC public health etc. She was selected as a Fellow of Indian Aerobiological Society. She has received P.H. Gregory Young Scientist Award, Abstract Award from European Academy of Allergy and Clinical Immunology etc.

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