

In Silico Anti- HIV Analysis of FTIR identified Bioactive compounds present in *Vitex altissima* L and *Vitex leucoxylon* L

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Abstract : The knowledge of the traditional plants in India is a collection over millennia by our ancient people. The Siddha System of Medicine (Traditional Tamil System of medicine) is the foremost of all other medical systems in the world which provide service to the humanity for more than 5000 years in combating diseases and also in maintaining its physical, mental and moral health. *Vitex* species were used in siddha for its anti- viral activity for several years. However, the present study deals with the Human Immunodeficiency Virus because of its complexity and killing effects. FTIR analysis of *Vitex altissima* L and *Vitex leucoxylon* L revealed the presence of 21 and 17 bioactive compounds respectively. These compounds were analysed further for its binding affinity mechanism against one of the virulence causing protein, reverse transcriptase (target protein) of Human Immunodeficiency Virus (HIV) by using molecular docking and bioinformatics tools. Interaction rate was determined between bioactive compounds against the protein target based on binding free energy requirements. Molecular docking was also made to the commercially available drugs (Zidovudine, Stavudine, and Nevirapine) against the target protein. By comparing the results between bioactive compounds in the *Vitex* species and the commercially available drugs, it was clear that the bioactive compounds were much more effective than the commercially available drugs, thereby suitable for the treatment of AIDS. Hence, this study will form the basis for promoting therapeutic lead molecules from the traditional plants which restore the tradition and also eliminates the harmful side effects.

Keywords : FTIR analysis, *Vitex altissima* L, *Vitex leucoxylon* L, Zidovudine, Stavudine, Nevirapine, Binding free energy, Molecular docking.

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