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Significance of QSAR and molecular docking as an innovative approach in medicinal plant research

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The experimental evaluations of bioactive compounds in medicinal plants, their validation, clinical trials and commercial application together form a long process. To adopt such complete research usually takes lots of time and funding. Quantitative structure-activity relationship (QSAR) is the study based on the mathematical and statistical relations which uses software to predict the effect of chemicals on the biological system that helps us to know efficiency of the chemical compound on biological system. Molecular docking tells us the orientation affinity of ligand molecule (drug) when it is bound to a protein receptor or enzyme (target) using shape and physical interactions to quantify it (scoring function). In the present study QSAR and molecular docking is adopted to shortlist the most active compounds from the male anti-infertility medicinal plant. The result shows that out of the list of compounds obtained by LCMS analysis of plant extract, a few have stronger affinity towards the target molecules. This application reducing the time required for medicinal plant research to reach near to its final applicability. Thus, QSAR and molecular docking approach should be employed in medicinal plant research by botanists.

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Diversity and syconium-based identification of figs (*Ficus*, Moraceae) in Kerala

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Figs (*Ficus* L.) are some of the most complex plants among the angiosperms with their specialised inflorescence and infructescence condensed to the size of a normal small angiosperm fruit. The specialised features of the