## **In-Silico Evaluation and Antihyperglycemic Potential of Leucas Cephalotes**

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Abstract : The present study is carried out to explore the anti-hyperglycemic activity of Leucas cephalotes plant parts. A fruit, leaves, stems, and roots part of the Leucas cephalotes has been extracted in ethanol and have been evaluated for antihyperglycemic activity. The present study indicated that, ethanolic extract of fruit and leaves have shown significant  $\alpha$ - amylase inhibitory activity with IC50 value of 92.86 ± 0.89 µg/mL and 98.09 ± 0.69 µg/mL respectively. Two known compounds  $\beta$ -sitosterol and lupeol were isolated from ethanolic extract of L. cephalotes leaves and were subjected to anti-hyperglycemic activity. Lupeol shows the best activity with IC50 55.73 ± 0.47 µg/mL and the results were verified by docking study of these compounds with mammalian  $\alpha$ -amylase was carried out on its active site. It was concluded from the study that  $\beta$ -sitosterol and lupeol form one H-bond interactions with the active site residues either Asp212 or Thr21. The estimated free energy binding of  $\beta$ -sitosterol was found to be -9.47 kcal mol-1 with an estimated inhibition constant (Ki) of 558.94 nmol whereas the estimated free energy binding of lupeol was -11.73 kcal mol-1 with an estimated inhibition constant (Ki) of 476.71pmmol. The present study clearly showed that lupeol is more potent in comparison to  $\beta$ -sitosterol. The study indicates that L. cephalotes have significant potential to inhibit  $\alpha$ -amylase enzyme.

Keywords : alpha-amylase, beta-sitosterol, hyperglycemia, lupeol

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