

In-Silico Evaluation and Antihyperglycemic Potential of Leucas Cephalotes

Authors : Anjali Verma, Mahesh Pal, Veena Pande, Dalip Kumar Upreti

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 anti-hyperglycemic activity. The present study indicated that, ethanolic extract of fruit and leaves have shown significant α -amylase inhibitory activity with IC₅₀ value of $92.86 \pm 0.89 \mu\text{g/mL}$ and $98.09 \pm 0.69 \mu\text{g/mL}$ respectively. Two known compounds β -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 $55.73 \pm 0.47 \mu\text{g/mL}$ and the results were verified by docking study of these compounds with mammalian α -amylase was carried out on its active site. It was concluded from the study that β -sitosterol and lupeol form one H-bond interactions with the active site residues either Asp212 or Thr21. The estimated free energy binding of β -sitosterol was found to be $-9.47 \text{ kcal mol}^{-1}$ with an estimated inhibition constant (K_i) of 558.94 nmol whereas the estimated free energy binding of lupeol was $-11.73 \text{ kcal mol}^{-1}$ with an estimated inhibition constant (K_i) of 476.71 pmmol. The present study clearly showed that lupeol is more potent in comparison to β -sitosterol. The study indicates that *L. cephalotes* have significant potential to inhibit α -amylase enzyme.

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

Conference Title : ICNPDD 2017 : International Conference on Natural Products and Drug Discovery

Conference Location : London, United Kingdom

Conference Dates : February 16-17, 2017