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Medicinal importance and mechanism of hispidulin in xanthine oxidase and nuclear factor kappa B (NF- κ B) for the treatment of kidney disease: A molecular base integrated study and docking analysis

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Objectives: Medicinal plants have been used as remedy for numerous disorders throughout world. Hispidulin is a naturally occurring flavone found in *Saussurea involucrate* is a rare traditional Chinese medicinal herb, several *Artemisia* and *Salvia* species.

Methods: To know the potential health beneficial aspects of hispidulin in kidney and related problem, effect of hispidulin on xanthine oxidase and nuclear factor kappa B (NF- κ B) through data base have been collected from various sources. Molecular docking study has been performed to know the interaction of hispidulin with xanthine oxidase and nuclear factor kappa B (NF- κ B) which plays an important role in the kidney function. Further interaction of molecule with different ligand for energy and type of attachment has been also investigated in the present investigation. However effect of hispidulin on superoxide dismutase (SOD), catalase and glutathione peroxidase (GPx) were also evaluated through different database to know their protective role against free radical injury in the kidney. Moreover all the data have been analyzed through statistical methods to reveal their significant activity for the treatment of kidney disorders.

Results: From the analyzed data, it was found that hispidulin have potent antioxidative and anti-inflammatory which play an important role in the protection and cure of kidney injury. Analysis of the different database also revealed that hispidulin is inhibitor of superoxide dismutase (SOD), catalase and glutathione peroxidase (GPx). Molecular docking study revealed that hispidulin could be potent substrate of xanthine oxidase and nuclear factor kappa B (NF- κ B) which would be responsible for the reduction of uric acid formation. Interaction between ligand and targeted molecule were found to be significant with minimum energy and better configuration.

Conclusions: Present study revealed the importance of hispidulin for the treatment of kidney disorders, which could be used for the development of better molecule against kidney disorders and peripheral artery disease.