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Therapeutic importance of capsanthin against urinary disorder: Bioactivity through dynamical simulation for xanthine oxidase and other anti-oxidant enzymes

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Objectives: Xanthine oxidase and anti-oxidant enzymes play an important role in various forms of kidney disorders. Capsanthin is a red color crystalline pigment mostly synthesized and accumulated in the *Capsicum annuum* fruits.

Methods: In order to know the therapeutic importance of Capsanthin for the treatment of kidney disease, experimental studies have been performed and data were collected from scientific sources. To explore the possible mechanism of action of capsanthin for the treatment of urinary disorder, their inhibitory potential against xanthine oxidase and other anti-oxidant enzymes have been investigated. Molecular docking study was performed to the binding sites of xanthine oxidase and other anti-oxidant enzymes to explore their potential for the treatment of kidney disorders. *In-silico* ADME parameter of capsanthin was evaluated in order to estimate their drug likeness behavior.

Results: From the analysis of various databases, it was found that capsanthin attenuates inflammation and could be used for the treatment of kidney disorders. Molecular docking study was performed in order to understand the binding interaction of the compounds in the active site of enzyme. The molecular docking studies showed that capsanthin well accommodate in the active site of the xanthine oxidase enzyme by interacting with key amino acids. In order to get more insight into the binding mode of capsanthin to xanthine oxidase, a molecular docking study was also carried out and the best binding affinities were unveiled. Capsanthin exhibited favorable ADME profiles with good predicted oral bioavailability. Capsanthin was found to be effective in kidney disorder.

Conclusions: Molecular simulation study suggests that capsanthin is a potent molecule that interfere enzymes and other inflammatory mediators by binding to a novel site. The findings of the present study have revealed the therapeutic importance of capsanthin against kidney disorders with their molecular mechanism.