

# **DOCKING STUDIES OF FEBUXOSTAT BY USING MOLDOCK SOFTWARE**

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## **ABSTRACT:**

Febuxostat is a selective, novel, non-purine analog xanthine oxidase (XO) inhibitor for the treatment of chronic hyperuricemia in patients with gout. This enzyme is involved in oxidation of Hypoxanthine and Xanthine to uric acid. Febuxostat is the compound that inhibits the action of xanthine oxidase enzyme and helps in lowering the production of uric acid in the body. In this study, molecular docking of Febuxostat has been performed against XO (PDB ID: 3NVY) by using Moldock software and found that the amino acids Glu802, Ala1079 and Arg880 in the active site of XO are involved in the hydrogen bond formation with Febuxostat. The best conformation of this compound is reported here in which it is active as XO inhibitor and lower the production of Uric acid in body effectively and thus can be used for the treatment of Gout.

Key words: Febuxostat, Molecular Docking, MolDock, Xanthine Oxidase