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Molecular Modeling and Docking analysis of URAT1 and XOD with Chemotherapeutic compounds for Inherited Kidney Disease: An Insilico approach.

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Objectives: The furthermost of the Kidney Diseases Hospital, patients can see a nephrologist with definite expertise in genetics, then access other experts in genetics, urology and pathology to help address the special issues that ascend in adults with genetically-determined kidney disease. Uric acid transporter 1 (URAT1) and xanthine oxidase (XOD) protein elaborate in uric acid reabsorption has been linked to pathogenesis of hyperuricemia. Hence, targeting this protein is essential for successful drug design and preventing adversative interactions. The present study was aimed to build URAT1 and XOD 3D structures by homology modeling and to examine chemotherapeutic drugs binding with the interactions therein.

Methods: The BLAST results, glucose transporter GLUT1 (PDB ID: 5EQG) and XOD crystal structure (PDB ID:1FIQ) was considered as a template for homology modeling. Homology models were constructed and polished using MODELLER program and the generated model validated using SAVES analysis in which PROCHECK showing the Ramachandran plots. The response of proteins toward various inhibitors, molecular docking study was carried out and binding affinities was evaluated between -3.04 to -11.22 kcal/mol using AutoDock software method.

Results: Homology modelling was accomplished using knowledge-based model build method in Modeller. After a model generated, the both proteins docked with following ligand compounds like Benzbromarone, Probeinecid, Benzarone, 2,4-Dihydroxybenzylamine, Orcylaldehyde and it shows good ligand energy. Constructed structure of URAT1 and XOD has more than 95% of residues in the favoured regions of the Ramachandran plots, suggesting high quality of it.

Conclusions: The identification of binding modes for various inhibitive molecules will guide us designing molecular tools for therapeutic intervention that may prove useful in numerous diseases associated with uric acid levels. The molecular docking has been able to identify promising compounds that might represent future solutions in critical areas of human health.