

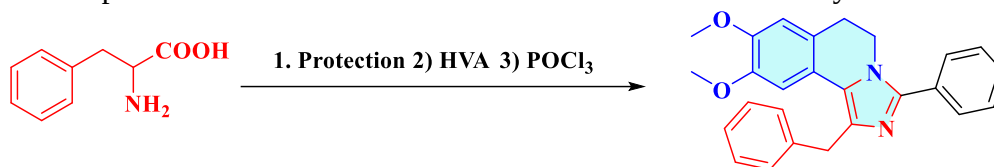
SYNTHESIS AND MOLECULAR DOCKING STUDY OF 1-BENZYL-8,9-DIMETHOXY-3-PHENYL-5,6-DIHYDROIMIDAZO[5,1-A]ISOQUINOLINE

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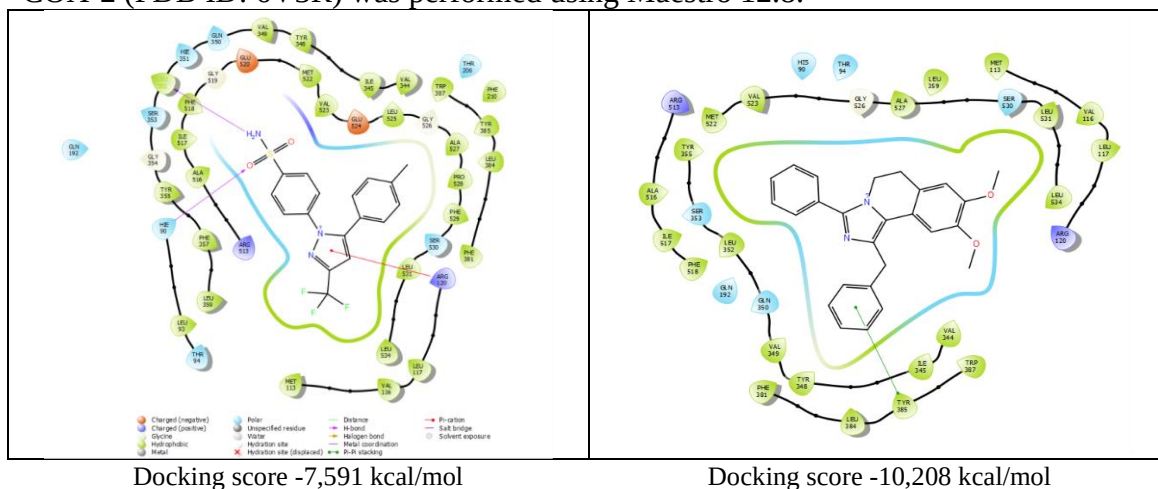
Samarkand State University named after Sharof Rashidov

In this study, an imidazo[5,1-*a*]isoquinoline derivative was synthesized, and its potential interaction with cyclooxygenase-2 (COX-2) was evaluated using molecular docking and compared with the reference inhibitor celecoxib.

Cyclooxygenase-2 (COX-2), an enzyme that plays an important role in pathological processes associated with inflammation and cancer, is considered a promising molecular target for the development of new biologically active ligands. Cribrostatin 6, isolated from a marine sponge, contains the imidazo[5,1-*a*]isoquinoline scaffold and exhibits anticancer and potent antimicrobial activities. Therefore, the development of novel imidazoisquinoline-based COX-2 inhibitors and the evaluation of their molecular properties represent a relevant direction in current medicinal chemistry research.



Molecular docking of the imidazoisquinoline derivative against the active site of COX-2 (PDB ID: 6V3R) was performed using Maestro 12.8.



Docking score -7,591 kcal/mol

Docking score -10,208 kcal/mol

The ligand showed a docking score of -10.208 kcal/mol, while the standard selective COX-2 inhibitor celecoxib showed a score of -7.593 kcal/mol. The lower docking score of the ligand indicates a higher predicted binding affinity for the COX-2 active site compared with celecoxib. These findings suggest that the synthesized imidazo[5,1-*a*]isoquinoline derivative may serve as a promising COX-2 inhibitor candidate for further biological investigation.

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