BindForge Docking Analysis Report

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Protein Information

Parameter	Value
Name	Target Protein
PDB ID	Unknown
Number of Cysteines	1

Identified Cysteines

Chain	Residue Number	Residue Name
Α	114	CYS

Molecule Information

Parameter	Value	
Name	molecule_1785	
Molecular_weight	~200-300 Da	
Molecular_formula		
Has_warhead	False	
Source	User uploaded molecule	
Logp	-0.67	
Druglikeness	0.55	
Synthetic_accessibility	1.25	
SMILES	CC(=O)OC1=CC=CC=C1C(=O)O	

Docking Results

Summary

Metric	Value
Best Binding Affinity	-10 kcal/mol
Covalent Binding Potential	Low
Warhead Distance	3.5 Å

Docking Poses

Pose	Affinity (kcal/mol)	RMSD LB	RMSD UB
1	-10	0	0
2	-10	0	0
3	-10	0	0
4	-10	0	0
5	-10	0	0

Analysis and Recommendations

No specific recommendations available.

Generated by BindForge - Al-Enhanced Covalent Docking Prediction Tool