

BindForge Docking Analysis Report

Generated on 2025-04-27 14:32:23

Protein Information

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

Identified Cysteines

Chain	Residue Number	Residue Name
A	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	<chem>CC(=O)OC1=CC=CC=C1C(=O)O</chem>

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

Analysis and Recommendations

No specific recommendations available.