BindForge Docking Analysis Report

Generated on 2025-04-27 12:18:41

Protein Information

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

Identified Cysteines

Chain	Residue Number	Residue Name
А	3	CYS

Molecule Information

Parameter	Value	
Name	molecule_8216	
SMILES	CC(=O)OC1=CC=CC=C1C(=O)O	

Docking Results

Summary

Metric	Value
Best Binding Affinity	-7 kcal/mol
Covalent Binding Potential	Low

Warhead Distance	3.5 Å
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Docking Poses

Pose	Affinity (kcal/mol)	RMSD LB	RMSD UB
1	-7	0	0

Analysis and Recommendations

No specific recommendations available.

Generated by BindForge - Al-Enhanced Covalent Docking Prediction Tool