MUG: Computational Drug Discovery Report

Candidate: MUG-Candidate-Batch...

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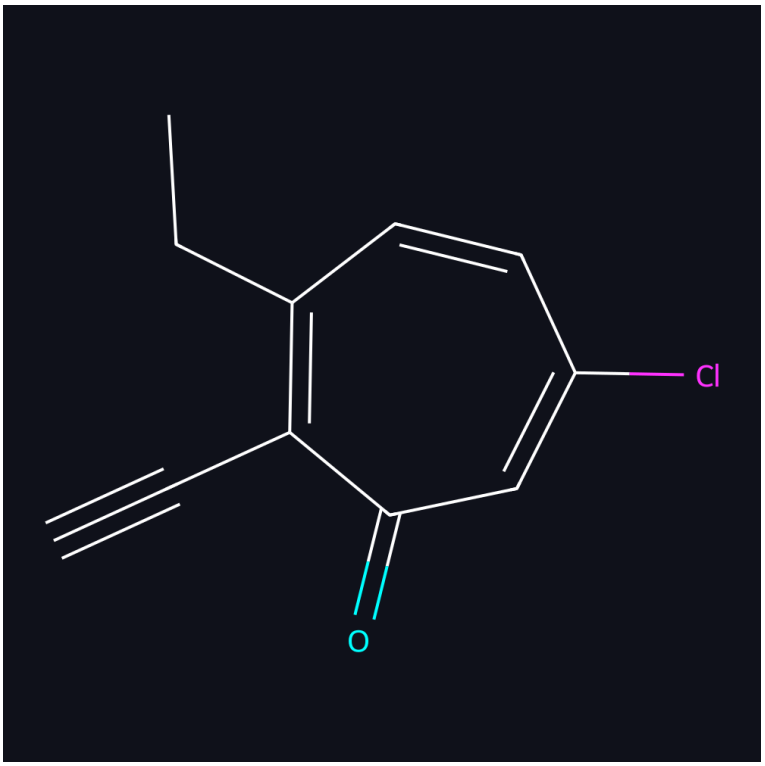
1. Abstract Analysis

The proposed chemical entity represents a de novo generated scaffold targeting specific protein binding pockets. In silico evaluation predicts a binding affinity of -6.12 kcal/mol. The calculated drug-likeness (QED) score is 0.62, suggesting favorable oral bioavailability characteristics. The compound has a molecular weight of 192.6 Da.



2. Physicochemical Profile

MW: 192.6 Da	LogP: 2.24	TPSA: 17.1 A^2	QED: 0.62
SMILES: C#CC=1C(=O)C=C(Cl)C=CC=1CC...			

3. Safety & Synthesis

Toxicology Flags: Alerts: Halogen

Synthesis Route:
Strategy: _Simple Derivatization / Coupling_
Feasibility: _High_
Complexity: _Low_

Key Building Blocks identified: 2