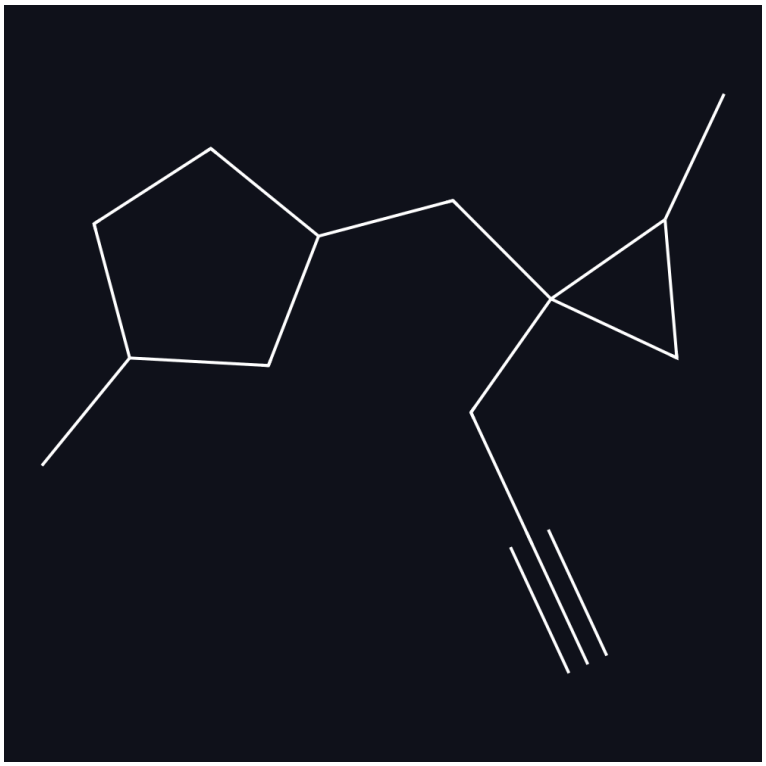
MUG: Computational Drug Discovery Report

Candidate: MUG-Candidate-Batch...

Date: 2025-12-31 03:50

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 -6.93 kcal/mol. The calculated drug-likeness (QED) score is 0.59, suggesting favorable oral bioavailability characteristics. The compound has a molecular weight of 190.3 Da.



2. Physicochemical Profile

MW: 190.3 Da	LogP: 3.86	TPSA: 0.0 A^2	QED: 0.59
SMILES: C#CCC1(CC1C)CC2CC(C)CC2...			

3. Safety & Synthesis

Toxicology: Clean (No structural alerts detected)

Synthesis Route:
Strategy: _Convergent Assembly_
Feasibility: _Moderate_

Complexity: _Low_
Key Building Blocks identified: 4