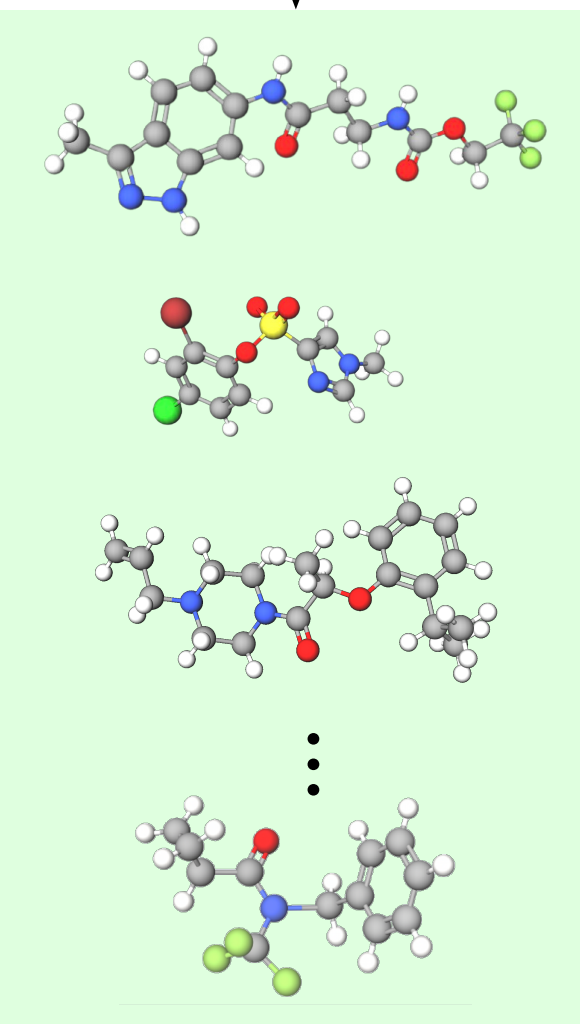


Reference Retrieval

Query

Please help me generate a new valid molecule with **qed=0.75**, **logp =2.7**, **molecular weight=330**.

Retrieved Results



Stage I: Prototype Generation

Retrieved Molecule Analysis

Start by analyzing the retrieved molecules to identify common fragments and potential starting points.

Edit Plan

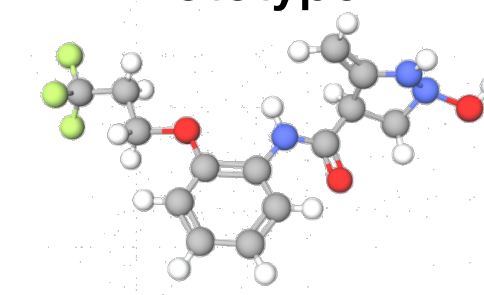
Select the scaffold "C1CC1", which appears in several retrieved structures, Add an amide group "NC(=O)" Add a trifluoromethyl group "C(F)(F)F" to increase the LogP and molecular weight. Attach the trifluoromethyl group "C(F)(F)F" Add a phenyl group "c1ccccc1"

Feedback

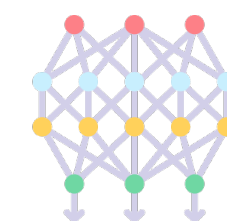
The generated molecule's QED is 0.747, 0.002 lower than the constraint, LogP is 2.945, 0.245 higher than the constraint. Molecular Weight 243.228 is 86.772 less than the constraint.

Stage II: Multi-hop Optimization

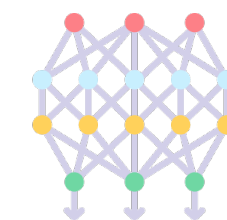
Prototype



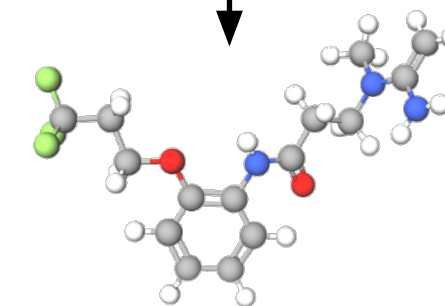
1-hop



⋮



n-hop



Final Result