

Reference Retrieval

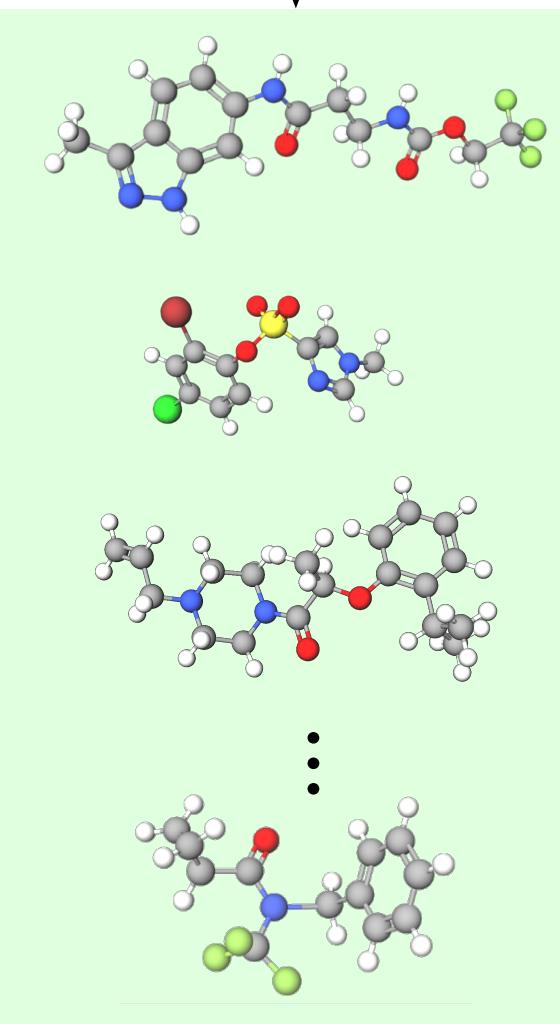


Query

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.

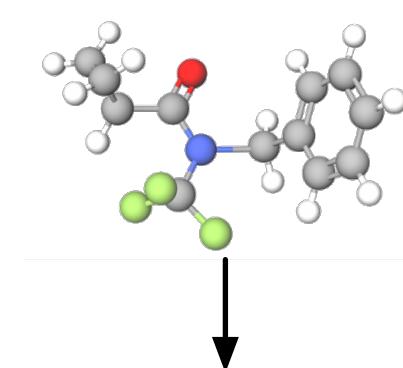
Edit Plan



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"



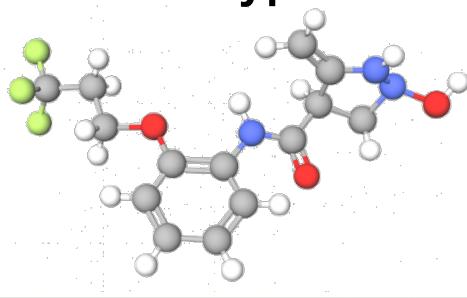
Feedback



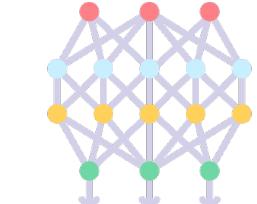
The generated molecule's QED is 0.747, 0.002 lower than the constraint, LogP is 2.945, 0.245 higher than the constraint. Molecular Weight 243.228 is 86.772 less than the constraint.

Stage II: Multi-hop Optimization

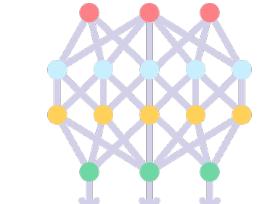
Prototype



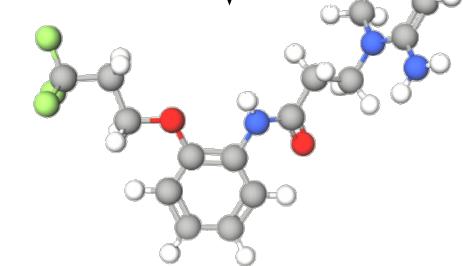
1-hop



⋮



n-hop



Final Result