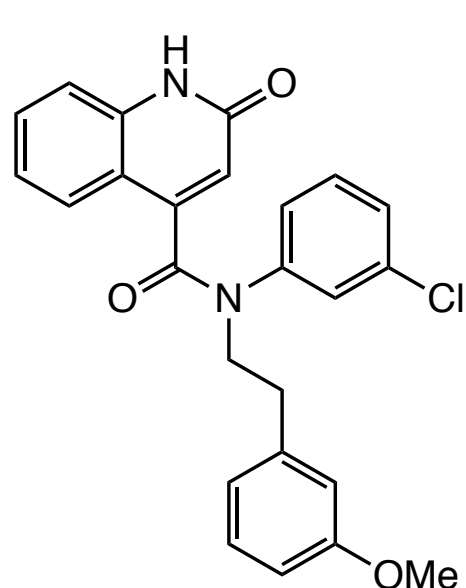
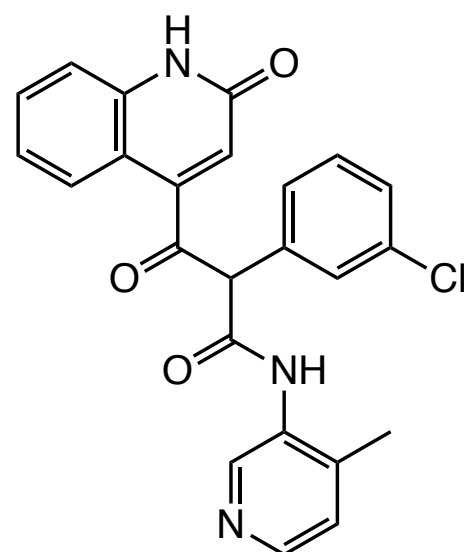


Top 5 compound predictions

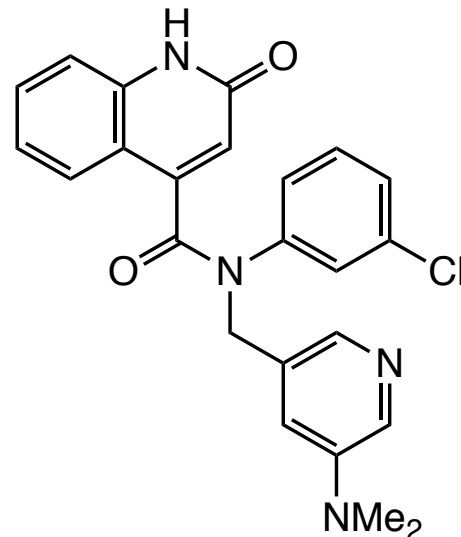
A



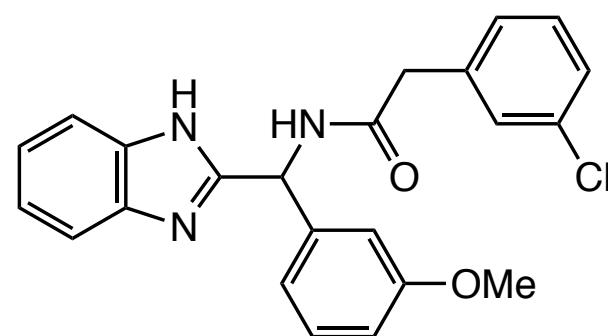
1



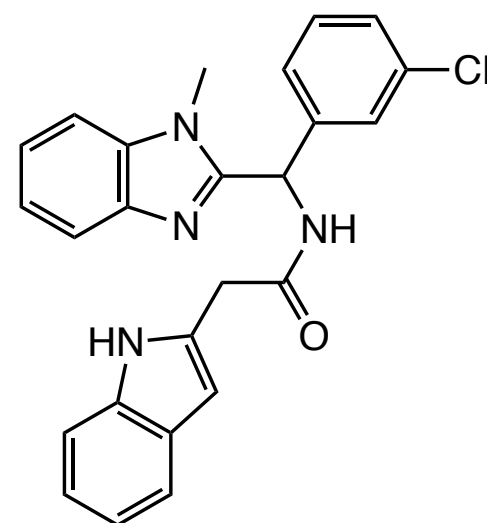
2



3



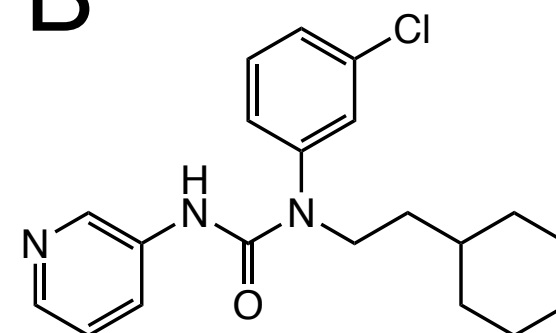
4



5

Top 3 training set compounds

B

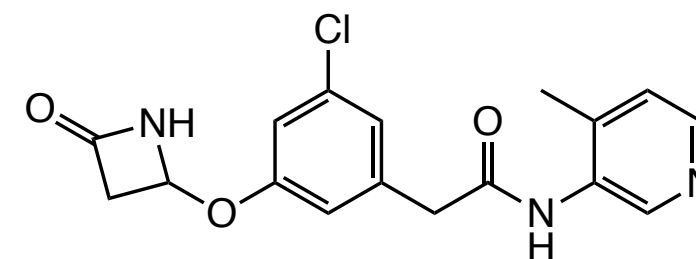


JOR-UNI-2fc98d0b-12

$IC_{50} = 3.06 \mu M$

CC_{50} (Calu 3) = 18.2 μM

CC_{50} (A549) = 14.1 μM

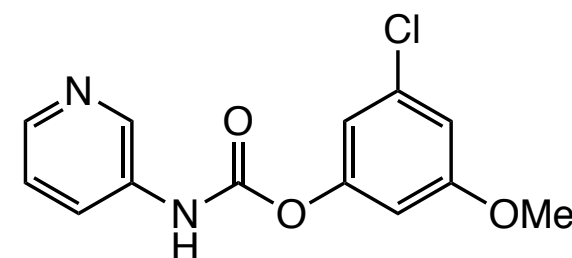


TRY-UNI-2eddb1ff-7

$IC_{50} = 3.61 \mu M$

CC_{50} (Calu 3) = 63.5 μM

CC_{50} (A549) > 100 μM



AGN-NEW-891393a6-1

$IC_{50} = 6.68 \mu M$

CC_{50} (Calu 3) > 100 μM