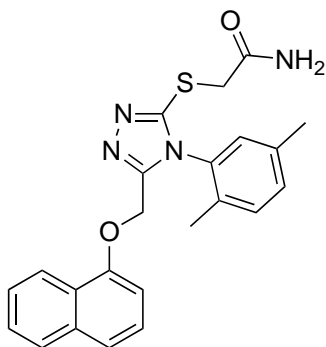


READDI-AC Compound CV

Compound IDs

Investigator or Origin	UNC HTS
Investigator ID	
READDI-AC ID	RA-0020031-01
SMILES	<chem>CC1=CC=C(C)C=C1N1C(COC2=CC=CC3=CC=CC=C23)=NN=C1SCC(N)=O</chem>

Hit properties:



Viral Family	CHIKV	Notes
Target	NSP2 (Helicase)	
Site		
In-vitro Potency (nsp2 ATPase)	10	μM (IC_{50}) ADP-Glo
In-vitro Potency (nsp2 Unwind)	>200	μM (IC_{50}) Unwindase
Cellular Anti-viral activity	>40	IC_{50} μM CHIKV
MW	418	
cLogP	4.8	
Ligand Efficiency		
PSA	83	A^2
Permeability/ Efflux Ratio		$\text{Papp} \times 10^6$ (cm/sec)
Solubility		μM