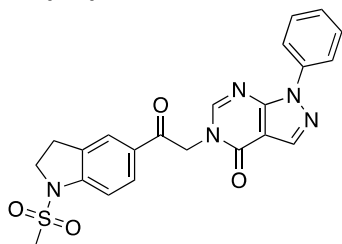


READDI-AC Compound CV

Compound IDs

Investigator or Origin	Jim Sattchettini
Investigator ID	SACC-0098346 (Z73832553)
READDI-AC ID	RA-0010660-01
SMILES	<chem>CS(=O)(=O)N1CCC2=CC(=CC=C12)C(=O)CN1C=NC2=C(C=NN2C2=CC=CC=C2)C1=O</chem>

Hit properties:



Viral Family	Coronavirus	Notes
Target	NSP12 (RdRp)	
Site		
PicoGreen Assay (CoV-2 RdRp)	35	μM (IC_{50}) PicoGreen assay
PicoGreen Assay (LASV RdRp)	NT	
In-vitro Potency (RdRp, CoV-2)	43	μM (IC_{50}) Gel-based assay
In-vitro Potency (h-mtRNAP)	1473	μM (IC_{50}) Gel-based assay
Cellular Anti-viral activity	2.88	μM (EC_{50}) SARS
Cellular Anti-viral activity	3.48	μM (EC_{50}) MERS
MW	449.5	
cLogP	1.79	
Ligand Efficiency	0.195	
PSA	107	Å^2
Permeability/ Efflux Ratio		$\text{P}_{\text{app}} \times 10^6$ (cm/sec)
Solubility	5	μM