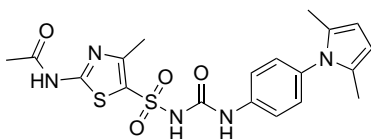


READDI-AC Compound CV

Compound IDs

Investigator or Origin	Anwar Hossain
Investigator ID	
READDI-AC ID	RA-0002243-01
SMILES	<chem>CC1=CC=C(C)N1C1=CC=C(NC(NS(C2=C(C)N=C(NC(C)=O)S2)(=O)=O)=O)C=C1</chem>

Hit properties:



Viral Family	Coronavirus	Notes
Target	NSP13 (Helicas)	
Site		
Gel-based Assay (CoV-2 RdRp)		Inhibition (100 μ M)
Gel-based Assay (LASV RdRp)		Inhibition (100 μ M)
In-vitro Potency (nsp13)	10	μ M (IC ₅₀) ADP-Glo
Gel-based Assay (h-mtRNAP)		Inhibition (100 μ M)
In-vitro Potency (RdRp, CoV-2)		μ M (IC ₅₀) PicoGreen
Cellular Anti-viral activity	100	SARS2 positive (20 μ M)
MW	447	
cLogP	3.5	
Ligand Efficiency		
PSA	122	A ²
Permeability/ Efflux Ratio		Papp x 10 ⁶ (cm/sec)
Solubility	495	μ M