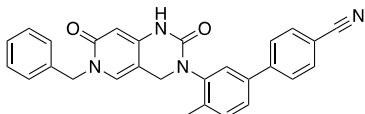


READDI-AC Compound CV

Compound IDs

Investigator or Origin	Peter Brown
Investigator ID	RAC-1-7
READDI-AC ID	RA-0001313-01
SMILES	<chem>O=C(N(C1=C(C)C=CC(C2=CC=C(C#N)C=C2)=C1)CC3=CN4CC5=CC=CC=C5)NC3=CC4=O</chem>

Hit properties:



Viral Family	SARS CoV-2	Notes
Target	Nsp13	
Site	helicase	
In-vitro Potency (assay 1)	ATPase IC ₅₀ 83 μM	ADPglo assay
In-vitro Potency (assay 2)	SPR K _d 3 μM	
Cellular Anti-viral activity	IC ₅₀ 8 μM	
MW	446.2	
cLogP	5.3	
Ligand Efficiency	0.17	
PSA	78.13	A ²
Permeability/ Efflux Ratio		Papp x 10 ⁶ (cm/sec)
Solubility	2.1	μM
Aggregation	Signif @ 50 μM	