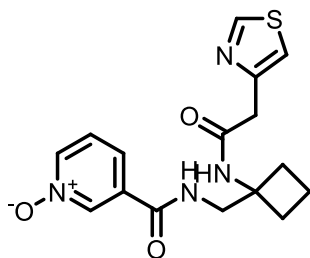


READDI-AC Compound CV

Compound IDs

Investigator or Origin	Konstantin Popov
Investigator ID	Z6661338119
READDI-AC ID	RA-0001264-01
SMILES	[O-][N+]=1C=CC=C(C1)C(=O)NCC2(CCC2)NC(=O)CC3=CSC=N3

Hit properties:



Viral Family	Coronavirus	Notes
Target	NSP13	
Site	C-terminus-B	
In-vitro Potency (ATPase, CoV-2)	48	μM
In-vitro Potency (SPR, CoV-2)	6	μM
In-vitro Potency (SPR, MERS)	5	μM
Cellular Anti-viral activity	NA	
MW	346.41	
cLogP	-1.28	
Ligand Efficiency	0.298	
PSA	98.03	A ²
Permeability/ Efflux Ratio		Papp x 10 ⁶ (cm/sec)
Solubility	>180	μM