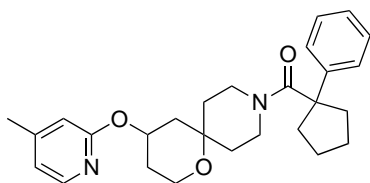


READDI-AC Compound CV

Compound IDs

Investigator or Origin	HTS at NCCU
Investigator ID	
READDI-AC ID	RA-0001821-01
SMILES	<chem>O=C(C1(CCCC1)C2=CC=CC=C2)N(CC3)CCC43OCCC(OC5=NC=CC(C)=C5)C4</chem>

Hit properties:



Viral Family	Alphavirus CHIKV	Notes
Target	nsp2 (helicase)	
Site		
In-vitro Potency FRET UW	21	μM (IC_{50})
In-vitro Potency ADP Glo	14	μM (IC_{50})
Cellular Anti-viral activity	9.7	μM (EC_{50}) CHIKV
Cellular Anti-viral activity	73	μM (EC_{50}) VEEV
Cell Tox	>100	μM (CC_{50})
MW	434	
cLogP	4.3	
Ligand Efficiency		
PSA	52	\AA^2
Permeability/ Efflux Ratio		$P_{\text{app}} \times 10^6$ (cm/sec)
Solubility	14	μM