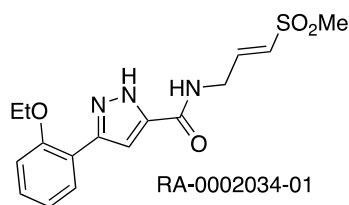


READDI-AC Compound CV

Compound IDs

Investigator or Origin	Ken Pearce (CICBDD)
Investigator ID	Z3017953696
READDI-AC ID	RA-0002034-01
SMILES	<chem>CCOc1cccc1c2cc(n[nH]2)C(=O)NCC=CS(=O)(=O)C</chem>

Hit properties:



Viral Family	CHIKV	Notes
Target	NSP2 Protease	
In-vitro Potency (Protease, CHIKV)	0.04-0.2	μM
In-vitro Binding NMR	Chem shifts obs	
Cellular Anti-viral activity (CHIKV/VEEV/Mayaro nLuc IC ₅₀)	133/458/23	nM
MW	349.41	
cLogP	1.76	
Ligand Efficiency	0.404	
PSA	101	A ²
Permeability/ Efflux Ratio		Papp x 10 ⁶ (cm/sec)
Calcd. Solubility	>70	μM