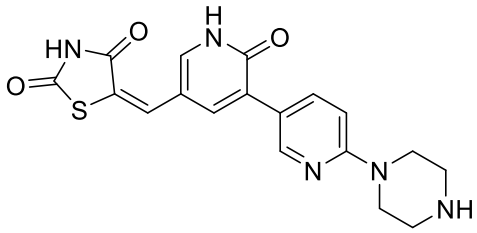
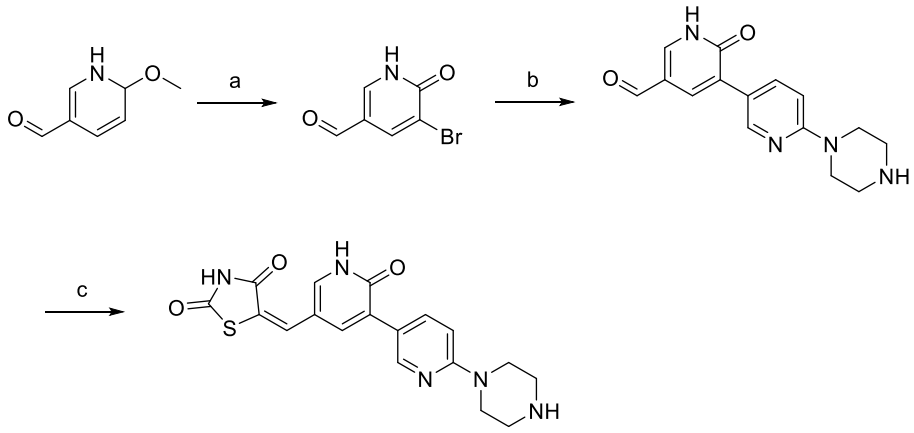
CVM-6-139-1



Chemical Formula: $C_{18}H_{17}N_5O_3S$
Molecular Weight: 383.43

Category	Parameter	Description
Compound	Name	CVM-6-139-1
	Citation	*Neuron.* ***2016****,* 91(1), 41-55. *Chem Biol.* **2011**, 18(7), 868-79 (compound A64).
	Chemical descriptors	O=C1NC(=O)\C(S1)=C/C1=CNC(=O)C(=C1)C1=CC=C(N=C1)N1CCNCC1
	Chemical name	(5E)-5-{[2-oxo-6'-(piperazin-1-yl)-1,2-dihydro-[3,3'-bipyridin]-5-yl]methylidene}-1,3-thiazolidine-2,4-dione
	Entries in chemical databases	CAS# 1365986-44-2
	Availability	no commercial source
In vitro profiling	Target (potency)	HIPK2 (96.3 nM, Invitrogen Z-lyte)
	Selectivity	S-Score(10) = 0.12 (Ambit)
	Potential reactivity	Type 1
	SAR	
	Mechanism of inhibition	reversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	CVM-6-139-1 blocked HIPK2 phosphorylation on S359/T360 and JNK activation in HEK293 cells, and blocked tunicamycin-induced cell death with an EC50 of 0.403 uM. CVM-6-139-1 blocked p-HIPK2 [S359/T360] in primary spinal motor neurons and protected >60% of these neurons from tunicamycin- and SOD1G93A-induced cell death.
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		

Synthetic scheme



Reagents and conditions: (a) 1) Conc. HCl, dioxane, 100 ^{o}C, 2) Br_2, H_2O, 0 ^{o}C to r.t.; (b) *tert*-butyl 4-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)piperazine-1-carboxylate, $Pd(PPh_3)_2Cl_2$, Cs_2CO_3, Dioxane/H_2O, 100 ^{o}C; (c) thiazolidine-2,4-dione, beta-alanine, AcOH, 100 ^{o}C.