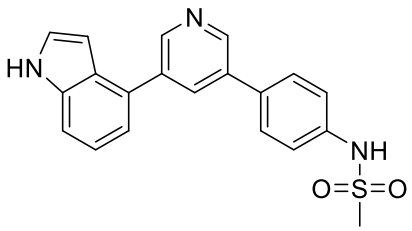
TM-04-176-01



Chemical Formula: $C_{20}H_{17}N_3O_2S$
Molecular Weight: 363.4350

Category	Parameter	Description
Compound	Name	TM-04-176-01
	Citation	J. Med. Chem. 2020, 63, 4880−4895 https://doi.org/10.1021/acs.jmedchem.0c00227
	Chemical descriptors	CS(=O)(=O)NC1=CC=C(C=C1)C1=CC(=CN=C1)C1=C2C=CNC2=CC=C1
	Chemical name	N-(4-(5-(1H-indol-4-yl)pyridin-3-yl)phenyl)methanesulfonamide
	Entries in chemical databases	N/A
	Availability	N/A
	Papers that use the compounds	N/A
	Additional comments	Close analog CVM-05-002 is also available
In vitro profiling	Target (potency)	PI5P4K2A: 2.0 µM (ADP Glo)
	Target (potency)	PI5P4K2B: 9.4 µM (Transcreener)
	Target (potency)	PI5P4K2C: 3.4 nM (K_D; Invitrogen)
	Selectivity	Ambit KINOMEscan at 1 µM (PI5P4K2C < 10%)
	Potential reactivity	None to our knowledge
	SAR	Described in this paper
	Mechanism of inhibition	ATP-competitive
	Structure of target-probe complex	N/A
	Additional comments	N/A
Cellular profiling	Validation of cellular target	Isothermal CETSA
	Validation of cellular specificity	N/A
	Additional comments	N/A
Pharmacodynamics		N/A
Pharmacokinetics		N/A

Synthetic scheme