Product Data Sheet

Product Name: IKKε-IN-1
Cat. No.: GC13278

Chemical Properties

Cas. No.	1292310-49-6		
Chemical Name	5-(2-((4-morpholinophenyl)amino)pyrimidin-4-yl)-2-((tetrahydro-2H-pyran-4-yl)oxy)benzonitrile		
SMILES	N#CC1=CC(C2=NC(NC3=CC=C(C=C3)N4CCOCC4)=NC=C2)=CC=C1OC5CCOCC5		
Formula	$C_{26}H_{27}N_5O_3$	M.Wt	457.52
Solubility	DMSO : 21.5 mg/mL (46.99 mM; Need ultrasonic and warming)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	IKKε-IN-1		

Protocol

Cell experiment:

Cell proliferation experiments are carried out in a 96-well format (6 replicates), Panc 02.13 cells are plated at a density of 2,000 to 5,000 cells per well. At 24 hours following cell seeding, the cells are treated with the tool inhibitor titrations (e.g., TBK1/IKKε-IN-2, 1 nM, 10 nM, 100 nM, 1 μM and 10 μM) for 4 days at 37°C and then assayed by using the ATP CellTiter-Glo luminescent cell viability assay[1].

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References:

[1]. Muvaffak A, et al. Evaluating TBK1 as a therapeutic target in cancers with activated IRF3. Mol Cancer Res. 2014 Jul;12(7):1055-66.

Background

TBK1/IKKε-IN-2 is a dual TBK1 and IKKε inhibitor.

TBK1/IKKε-IN-2 (Cmpound #1) inhibits TBK1 biochemical function in Ulight kinase assay at 5 and 250 μM ATP concentration with IC50s of 0.6 and 2.6 nM, rsespectively. TBK1/IKKε-IN-2 inhibits IKKε biochemical function in Ulight kinase assay at 10 μM ATP with an IC50 of 3.9 nM. The IC50 of TBK1/IKKε-IN-2 in the Panc 02.13 proliferation assay is 5 μM[1].

References:
[1]. Muvaffak A, et al. Evaluating TBK1 as a therapeutic target in cancers with activated IRF3. Mol Cancer Res. 2014 Jul;12(7):1055-66.

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