Product Data Sheet

Product Name: NKL 22
Cat. No.: GC32964

Chemical Properties

Cas. No.	537034-15-4		
SMILES	O=C(NC1=CC=CC=C1N)CCCCCC(NC2=CC=CC=C2)=O		
Formula	$C_{19}H_{23}N_3O_2$	M.Wt	325.4
Solubility	DMSO : ≥ 29 mg/mL (89.12 mM)	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	NKL 22		

Background

PAOA is a selective histone deacetylase (HDAC) inhibitor with IC_{50} values of 199 and 69 nM for HDAC1 and HDAC3, respectively.[1] It is selective for HDAC1 and HDAC3, having IC_{50} values greater than 1.59 μM for HDAC2, 4, 5, 7, and 8 in a cell-free enzyme assay. *In vitro*, PAOA induces histone H3 and H4 hyperacetylation.[2] PAOA improves the metabolic deficit exhibited by murine striatal cells isolated from Hdh^{Q111} knock-in mice in a dose-dependent manner and reduces eye neurodegeneration in a *D. melanogaster* model of Huntington's disease.[1] *In vivo*, PAOA prevents formation of Huntingtin (Htt) protein aggregates in the brain and reduces the cognitive deficits in the N171-82Q mouse model of Huntington's disease.[3]

1.Jia, H., Pallos, J., Jacques, V., et al.Histone deacetylase (HDAC) inhibitors targeting HDAC3 and HDAC1 ameliorate polyglutamine-elicited phenotypes in model systems of Huntington's diseaseNeurobiol. Dis.46(2)351-361(2012) 2.Mai, A., Perrone, A., Nebbioso, A., et al.Novel uracil-based 2-aminoanilide and 2-aminoanilide-like derivatives: Histone deacetylase inhibition and in-cell activitiesBioorg. Med. Chem. Lett.18(8)2530-

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2535(2008) 3.Jia, H., Kast, R.J., Steffan, J.S., et al.Selective histone deacetylase (HDAC) inhibition imparts beneficial effects in Huntington's disease mice: Implications for the ubiquitin-proteasomal and autophagy systemsHum. Mol. Genet.21(24)5280-5293(2012)

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