Product Data Sheet

Product Name: BRD6688
Cat. No.: GC13088

Chemical Properties

Cas. No.	1404562-17-9		
Chemical Name	N-[2-amino-5-(4-pyridinyl)phenyl]-1-pyrrolidinecarboxamide		
SMILES	O=C(N1CCCC1)NC2=CC(C3=CC=NC=C3)=CC=C2N		
Formula	$C_{16}H_{18}N_4O$	M.Wt	282.3
Solubility	≤2mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide	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	BRD6688		

Background

IC50: 21 nM, 100 nM, and 11.48 μM for HDAC1, 2, and 3, respectively

BRD6688 is an HDAC inhibitor.

A few chromatin modifying enzymes have been implicated in the neurobiology of learning and memory, especially, histone deacetylases (HDACs). HDACs are responsible for catalyzing the posttranslational hydrolysis of acetyl groups from the 3-nitrogen of lysine residues of histone and non-histone proteins.

In vitro: BRD6688 was found to demonstrate kinetic selectivity for HDAC2 against HDAC1, an isoform with 95% similarity within the catalytic binding domain. Moreover, BRD6688 could increase histone acetylation (H4K12 and H3K9) in primary mouse neuronal cultures [1].

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In vivo: Mouse in-vivo study showed that BRD6688 was able to increase the histone acetylation (H4K12 and H3K9) in hippocampal CA1 neurons of CK-p25 mice. Moreove, the increased histone acetylation in brain served as a surrogate pharmacodynamic marker of HDAC engagement and was consistent with previously observed brain pharmacokinetic properties. In addition, BRD6688 rescued the cognitive deficits in CK-p25 mice, a model of neurodegeneration, in a Pavlovian fear conditioning behavioral assay [1].

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Wagner, F. F.,Zhang, Y.-L.,Fass, D.M., et al. Kinetically selective inhibitors of histone deacetylase 2 (HDAC2) as cognition enhancers. Chem.Sci. 6(1), 804-815 (2015).

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