Product Data Sheet

Product Name: Nilotinib D6
Cat. No.: GC60270

Chemical Properties

Cas. No.	1268356-17-7		
SMILES	O=C(NC1=CC(C(F)(F)F)=CC(N2C=C(C)N=C2)=C1)C3=C([2H])C(NC4=NC=CC(C5=CC=CN=C5)=N4)=C(C([2H])([2H])[2H])C([2H])=C3[2H]		
Formula	$C_{28}H_{16}D_6F_3N_7O$	M.Wt	535.55
Solubility	DMF: 3 mg/ml,DMSO: 10 mg/ml	Storage	
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	Nilotinib D6		

Background

Nilotinib-d_6 is intended for use as an internal standard for the quantification of nilotinib by GC- or LC-MS. Nilotinib is an inhibitor of wild-type and mutant Bcr-Abl (IC_{50}s = 15 and 9-400 nM, respectively).[1] It is selective for wild-type and mutant Bcr-Abl over Src and LYN (IC_{50}s = >5,000 nM for both). Nilotinib inhibits Bcr-Abl autophosphorylation and cell proliferation in Ba/F3 cells expressing wild-type or mutant Bcr-Abl (IC_{50}s = 7-155 and 13-51 nM, respectively). *In vivo*, nilotinib (1 mg/kg) reduces midbrain Bcr-Abl autophosphorylation, amyloid-β levels, and neuronal loss, as well as improves autophagosome clearance and reverses cognitive deficits in the Tg2576 transgenic mouse model of Alzheimer's disease.[2] It also reduces serum creatine levels, renal profibrotic gene expression, and tubulointerstitial damage, as well as increases survival in a rat model of 5/6 nephrectomy-induced chronic kidney disease.[3] Formulations containing nilotinib have been used in the treatment of leukemia.

1.O'Hare, T., Walters, D.K., Stoffregen, E.P., et al.In vitro activity of Bcr-Abl inhibitors AMN107 and BMS-354825 against clinically relevant imatinib-resistant Abl kinase domain mutantsCancer Res.65(11)4500-4505(2005) 2.La Barbera, L., Vedele, F., Nobili, A., et al.Nilotinib restores memory function by preventing dopaminergic neuron degeneration in a mouse model of Alzheimer's DiseaseProg. Neurobiol.202102031(2021) 3.Iyoda, M., Shibata, T., Hirai, Y., et al.Nilotinib attenuates renal injury and prolongs survival in chronic kidney diseaseJ. Am. Soc. Nephrol.22(8)1486-1496(2011)

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