Product Data Sheet

Product Name: ML 786 dihydrochloride
Cat. No.: GC15296

Chemical Properties

Cas. No.	1237536-18-3		
Chemical Name	(R,Z)-3-(2-aminopropan-2-yl)-N-(7-((7-hydroxy-5,6-dihydro-1,8-naphthyridin-4-yl)oxy)-1,2,3,4-tetrahydronaphthalen-2-yl)-5-(trifluoromethyl)benzimidic acid dihydrochloride		
SMILES	CC(C1=CC(C(F)(F)F)=CC(/C(O)=N/[C@]2([H])CCC3=CC=C(OC4=C5CCC(O)=NC5=NC=C4)C=C3C2)=C1)(N)C.Cl.Cl		
Formula	$C_{29}H_{29}F_3N_4O_3.2HCl$	M.Wt	611.48
Solubility	<61.15mg/ml in DMSO; <61.15mg/ml in Water	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	ML 786 dihydrochloride		

Background

IC50: 2.1, 2.5 and 4.2 nM for B-RafV600E, C-Raf and wild-type B-Raf, respectively

ML 786 is a potent Raf kinase inhibitor.

As one component of MAPK signal transduction pathway, the Raf isoform B-Raf has a high rate of activating mutation in melanoma (50-70%) and other cancers including papillary thyroid, ovarian, and colorectal. Inhibition of mutant B-Raf signaling, via either direct inhibition of the enzyme or inhibition of MEK, which is the direct substrate of Raf, has been demonstrated preclinically to inhibit tumor growth.

In vitro: ML 786 and its analog had been found to inhibit a significant number of kinases and were inhibitors of wild-type B-Raf and C-Raf. Although ML 786 and its analog displayed significant receptor tyrosine kinase activity, it was likely that such additional activity would not significantly contribute to pERK inhibition in melanoma tumors with constituitively activated B-Raf [1].

In vivo: ML 786 and its analog were found to have activity in vivo, as demonstrated by the fact that both compounds strongly inhibited the in vivo Raf pathway following a 75 or 100 mg/kg oral dose [1].

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Clinical trial: N/A

Reference:
[1] Gould AE,Adams R,Adhikari S. Design and optimization of potent and orally bioavailable tetrahydronaphthalene Raf inhibitors. J Med Chem.2011 Mar 24;54(6):1836-46.

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