

Product Information

Raf inhibitor ML 786 dihydrochloride, Purity $\geq 98\%$

Cat. No.: X23-10-ZQ960

Size: 5 mg; 10 mg; 25 mg; 50 mg; 100 mg

CAS Number: 1237536-18-3

Compound CID: 90488999

Synonym: ML 786 dihydrochloride; 1237536-18-3; MLN786 Dihydrochloride; ML786

(dihydrochloride); BGB659;

3-(1-Amino-1-methyl-ethyl)-N-[7-(7-oxo

-5,6,7,8

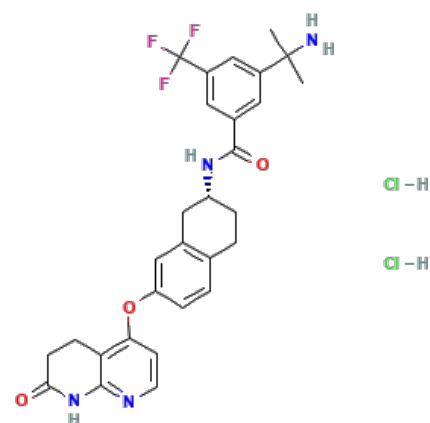
-tetrahydro-[1,8

]naphthyridin-4-yloxy)-1,2,3,4-t

etrahydro-naphthalen-2(R)-yl]-5-trifluoromethyl-benzamide dihydrochloride; Raf

inhibitor

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	ML 786 dihydrochloride blocks a MAPK/ERK signaling pathway. It targets Abl1, DDR2, EPHA2, and KDR.
Molecular Weight	611.48
Molecular Formula	C ₂₉ H ₂₉ F ₃ N ₄ O ₃ ·2HCl
Targets	Abl1: <0.5 nM; DDR2: 7.0 nM; EPHA2: 11 nM; KDR: 6.2 nM
IUPAC Name	3-(2-Aminopropan-2-yl)-N-[(2R)-7-[(7-oxo-6,8-dihydro-5H-1,8-naphthyridin-4-yl)oxy]-1,2,3,4-tetrahydronaphthalen-2-yl]-5-(trifluoromethyl)benzamide;dihydrochloride
InChI	InChI=1S/C29H29F3N4O3.2ClH/c1-28(2,33)19-11-18(12-20(15-19)29(30,31)32)27(38)35-21-5-3-16-4-6-22(14-17(16)13-21)39-24-9-10-34-26-23(24)7-8-25(37)36-26;;/h4,6,9-12,14-15,21H,3,5,7-8,13,33H2,1-2H3,(H,35,38)(H,34,36,37);2*1H/t21-;/m1../s1
InChI Key	DNMWHXHMDZCGEX-GHVWMZMZA-N
Canonical SMILES	CC(C)(C1=CC(=CC(=C1)C(=O)NC2CCC3=C(C2)C=C(C=C3)OC4=C5CCC(=O)NC5=NC=C4)C(F)(F)F)N.Cl.Cl
Isomeric SMILES	CC(C)(C1=CC(=CC(=C1)C(=O)N[C@@H]2CCC3=C(C2)C=C(C=C3)OC4=C5CCC(=O)NC5=NC=C4)C(F)(F)F)N.Cl.Cl



Form	Lyophilized powder
Purity	≥98%
Identity	Confirmed by NMR/HPLC/MS.
Stability	The product is stable for three years when stored at the recommended temperature in lyophilized powder.
Applications	ML 786 dihydrochloride can be utilized to investigate the inhibition of specific protein kinases in cellular processes.
Storage	Store at -20°C.
