Certificate of Analysis

Product Name: **ML 786 dihydrochloride** **Catalog No.: 5036** **Batch No.: 1**

CAS Number: 1237536-18-3

IUPAC Name: 3-(1-Amino-1-methylethyl)-*N*-[(2*R*)-1,2,3,4-tetrahydro-7-oxo-1,8-naphthryridin-4-yl)oxy]-2-naphthalenyl]-5-benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{29}F_3N_4O_3.2HCl.2H_2O$

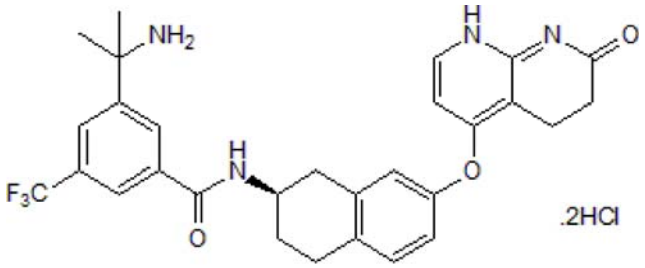
Batch Molecular Weight: 647.51

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Dichloromethane:Methanol [9:1] (V/V) 2M NH3)

HPLC: Shows >98.6% purity

Chiral HPLC: Shows >99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +17.7 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.79	5.45	8.65
Found	53.77	5.41	8.64

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

Product Name: **ML 786 dihydrochloride** **Catalog No.: 5036** **Batch No.: 1**

CAS Number: 1237536-18-3

IUPAC Name: 3-(1-Amino-1-methylethyl)-*N*-[(2*R*)-1,2,3,4-tetrahydro-7-oxo-1,8-naphthryridin-4-yl)oxy]-2-naphthalenyl]-5-benzamide dihydrochloride

Description:

Potent Raf kinase inhibitor (IC_{50} values are 2.1, 2.5 and 4.2 nM for B-Raf^{V600E}, C-Raf and wild-type B-Raf respectively). Also inhibits Abl-1, DDR2, EPHA2 and RET tyrosine kinase activity. Inhibits pERK formation and attenuates tumor growth in melanoma cell xenografts expressing the B-Raf^{V600E} mutation in vivo. Orally bioavailable.

Physical and Chemical Properties:

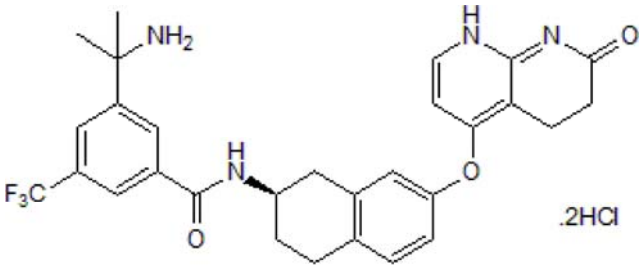
Batch Molecular Formula: $C_{29}H_{29}F_3N_4O_3.2HCl.2H_2O$

Batch Molecular Weight: 647.51

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Gould *et al* (2011) Design and optimization of potent and orally bioavailable tetrahydronaphthalene Raf inhibitors. J.Med.Chem. ***54*** 1836. PMID: 21341678.