Certificate of Analysis

Product Name: **ML 418** **Catalog No.: 6889** **Batch No.: 1**

CAS Number: 1928763-08-9

IUPAC Name: Isopropyl (1-((5-chloro-8-hydroxyquinolin-7-yl)methyl)piperidin-4-yl)carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{24}ClN_3O_3$

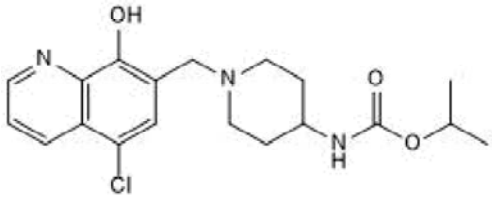
Batch Molecular Weight: 377.87

Physical Appearance: White solid

Solubility: DMSO to 20 mM
ethanol to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.21 (Dichloromethane:Methanol:Triethylamine [89:10:1])

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.39	6.4	11.12
Found	60.55	6.4	11.08

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Description:

$K_{ir}7.1$ inhibitor (IC_{50} = 0.31 µM). Also inhibits $K_{ir}6.2$ with similar potency. Displays >17-fold selectivity for $K_{ir}7.1$ over $K_{ir}1.1$, $K_{ir}2.1$, $K_{ir}2.2$, $K_{ir}2.3$, $K_{ir}3.1/3.2$ and $K_{ir}4.1$. Active in vivo.

Physical and Chemical Properties:

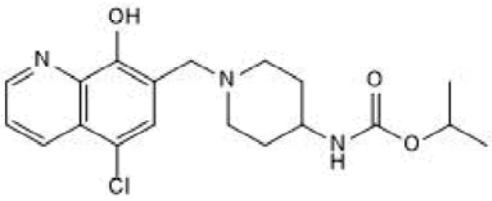
Batch Molecular Formula: $C_{19}H_{24}ClN_3O_3$

Batch Molecular Weight: 377.87

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM
ethanol to 5 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:

Kharade (2017) Pore polarity and charge determine differential block of $K_{ir}1.1$ and $K_{ir}7.1$ potassium channels by small-molecule inhibitor VU590. Mol.Pharmacol. ***92*** 338. PMID: 28619748.

Swale *et al* (2016) ML418: the first selective, sub-micromolar pore blocker of $K_{ir}7.1$ potassium channels. ACS Chem.Neurosci. ***7*** 1013. PMID: 27184474.