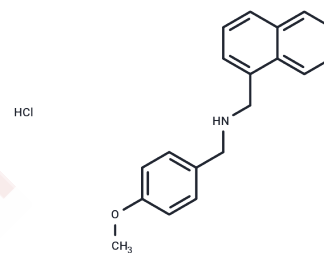


## ML133 hydrochloride

## Chemical Properties

CAS No. :	1222781-70-5
Formula:	C <sub>19</sub> H <sub>19</sub> NO·HCl
Molecular Weight:	313.82
Storage:	Powder: -20°C for 3 years   In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



## Biological Description

Description	ML133 hydrochloride (ML133 HCl) is a selective potassium channel inhibitor for Kir2.1 with IC <sub>50</sub> of 1.8 μM (pH 7.4) and 290 nM (pH 8.5), has no effect on Kir1.1 and weak activity for Kir4.1 and Kir7.1.
Targets(IC <sub>50</sub> )	Potassium Channel
In vitro	The ratio of total concentration of extracellular ML133 versus intracellular ML133 is 1: 0.13 at pH 6.5, 1:9.09 at pH 8.5. ML133 is clean against 3A4 and 2C9 (IC <sub>50</sub> >30 μM), displays moderate inhibition of 1A2 (IC <sub>50</sub> = 3.3 μM) but proves to be a potent inhibitor of 2D6 (IC <sub>50</sub> = 0.13 μM) in CYP450 assay. ML133 is highly protein bound (>99%) in both human and rat and also displays high intrinsic clearance in both species. ML133 (10 μM) is not displaced by K <sup>+</sup> influx from the wild-type Kir2.1 in HEK 293 cells. M1 and/or M2 transmembrane domains contain the critical molecular determinant for ML133 inhibition of Kir2.1, especially D172 and I176. [1]

## Solubility Information

Solubility	DMSO: 255 mg/mL (812.57 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: 10 mg/mL (31.87 mM), Solution. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (6.37 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

### Preparing Stock Solutions

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	1mg	5mg	10mg
1 mM	3.1865 mL	15.9327 mL	31.8654 mL
5 mM	0.6373 mL	3.1865 mL	6.3731 mL
10 mM	0.3187 mL	1.5933 mL	3.1865 mL
50 mM	0.0637 mL	0.3187 mL	0.6373 mL

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Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

#### Reference

Wang HR, et al. ACS Chem Biol, 2011, 6(8), 845-856.

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