Product Data Sheet

ML133 hydrochloride

Cat. No.: HY-100230A **CAS No.:** 1222781-70-5

Molecular Formula: C₁₉H₂₀ClNO Molecular Weight: 313.82

Target: Potassium Channel

Pathway: Membrane Transporter/Ion Channel

Storage: 4°C, sealed storage, away from moisture

* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)

SOLVENT & SOLUBILITY

In Vitro DMSO: 100 mg/mL (318.65 mM; ultrasonic and warming and heat to 60°C)

H₂O: < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (6.63 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- β -CD in saline) Solubility: \geq 2.08 mg/mL (6.63 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (6.63 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	ML133 hydrochloride is a selective K_{ir} 2 family channels inhibitor, with an IC $_{50}$ of 1.8 μ M at pH 7.4 and 290 nM at pH 8.5 $^{[1]}$.
IC ₅₀ & Target	IC50: 1.8 μ M (K $_{ir}$ 2 at pH 7.4), 290 nM (K $_{ir}$ 2 at pH 8.5) $^{[1]}$.
In Vitro	ML133, which inhibits $K_{ir}2.1$ with IC_{50} of $1.8~\mu\text{M}$ at pH 7.4 and 290 nM at pH 8.5, but exhibits little selectivity against other members of $K_{ir}2.x$ family channels ^[1] . ML133 has no effect on $K_{ir}1.1$ ($IC_{50} > 300~\mu\text{M}$), and displays weak activity for $K_{ir}4.1$ ($76~\mu\text{M}$) and $K_{ir}7.1$ ($33~\mu\text{M}$), making ML133 the most selective small molecule inhibitor of the Kir family reported to date ^[1] .

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Metab. 2022 Sep 7;S1550-4131(22)00359-X.
- Pharmacol Res. 2022 Feb 2;177:106112.

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REFERENCES

[1]. Wang HR, et al. Selective inhibition of the K(ir)2 family of inward rectifier potassium channels by a small molecule probe: the discovery, SAR, and pharmacological characterization of ML133. ACS Chem Biol. 2011 Aug 19;6(8):845-56.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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