Icenticaftor

Cat. No.: HY-109177

CAS No.: 1334546-77-8

Molecular Formula: $C_{12}H_{13}F_6N_3O_3$

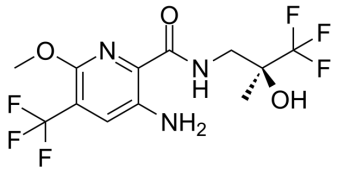
Molecular Weight: 361.24

Target: CFTR

Pathway: Membrane Transporter/Ion Channel

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 150 mg/mL (415.24 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7682 mL	13.8412 mL	27.6824 mL
	5 mM	0.5536 mL	2.7682 mL	5.5365 mL
	10 mM	0.2768 mL	1.3841 mL	2.7682 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: 4.25 mg/mL (11.77 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 4.25 mg/mL (11.77 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 4.25 mg/mL (11.77 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Icenticaftor (QBW251) is an orally active CFTR channel potentiator, with EC_{50}s of 79 nM and 497 nM for F508del and G551D CFTR, respectively. Icenticaftor can be used for chronic obstructive pulmonary disease (COPD) and cystic fibrosis research[1].

IC_{50} & Target

EC50: 79 nM (F508del CFTR) and 497 nM (G551D CFTR)[1]

In Vitro

Icenticaftor (QBW251), an orally bioavailable small molecule CFTR potentiator, can restore CFTR function in specific CFTR genotypes as well as wild-type CFTR[2].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	In Sprague-Dawley rats, the pharmacokinetic profile of Icenticaftor is established. After oral administration at a dose of 3 mg/kg, the oral bioavailability is 90%, and AUC_{last} is 20 635 nmol/L•h[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Darren Le Grand, et al. Discovery of Icenticaftor (QBW251), a Cystic Fibrosis Transmembrane Conductance Regulator Potentiator with Clinical Efficacy in Cystic Fibrosis and Chronic Obstructive Pulmonary Disease. J Med Chem. 2021 Jun 10;64(11):7241-7260.

[2]. Steven M Rowe, et al. Efficacy and Safety of the CFTR Potentiator Icenticaftor (QBW251) in COPD: Results from a Phase 2 Randomized Trial. Int J Chron Obstruct Pulmon Dis. 2020 Oct 5;15:2399-2409.

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