(S)-ML753286

Cat. No.: HY-100390

CAS No.: 1699720-85-8

Molecular Formula: $C_{20}H_{25}N_3O_3$

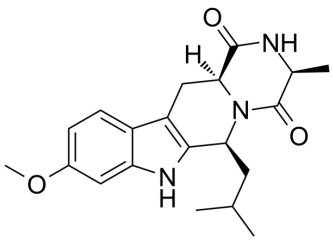
Molecular Weight: 355.43

Target: BCRP

Pathway: Membrane Transporter/Ion Channel

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (140.67 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8135 mL	14.0675 mL	28.1349 mL
	5 mM	0.5627 mL	2.8135 mL	5.6270 mL
	10 mM	0.2813 mL	1.4067 mL	2.8135 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: ≥ 2.5 mg/mL (7.03 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.03 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.03 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(S)-ML753286 is a breast cancer resistance protein (BCRP) inhibitor with an IC_{50} of 0.6 μM on BCRP efflux transporter.

IC_{50} & Target

IC50: 0.6 μM (BCRP efflux transporter)[1]

In Vivo

(S)-ML753286 (Compound A) shows the potency and a potent pharmacokinetic (PK) profile in rats (lower clearance [1.54 L/h/kg] and higher bioavailability [123%]). XL388 has moderate terminal elimination half-life with $t_{1/2}$s of 0.9 h and 2.0 h for 2

mg/kg (iv) and 20 mg/kg (po) in rats, respectively[1].

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

PROTOCOL

Animal Administration [1]

Mice[1]

To determine pharmacokinetic profile of (S)-ML753286 and Ko143 in vivo, Sprague-Dawley rats are administered 2.0 mg/kg or 20 mg/kg (S)-ML753286 or 2.0 mg/kg or 50 mg/kg Ko143, formulated in 0.5% HPMC/0.2% Tween80, via iv or po, respectively. After administration of (S)-ML753286 or Ko143, blood is obtained from all animals at predose and at 0.083, 0.25, 0.5, 1, 4, 8, and 24 h postdose. Approximately 200 μL of whole blood is collected from the jugular vein catheter of each animal into tubes containing the anticoagulant dipotassium ethylenediaminetetraacetic acid (K2EDTA) and is further processed into plasma at approximately 4°C[1].

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

REFERENCES

[1]. Li Y, et al. Synthesis of a new inhibitor of breast cancer resistance protein with significantly improved pharmacokinetic profiles. Bioorg Med Chem Lett. 2016 Jan 15;26(2):551-555.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA