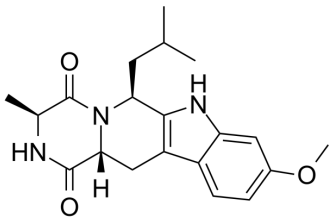
ML753286

Cat. No.:	HY-116494
CAS No.:	1699720-89-2
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 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (281.35 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / 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; Need ultrasonic
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; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (7.03 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

ML753286 is an orally active and selective BCRP (Breast cancer resistance protein) inhibitor with an IC_{50} of 0.6 μM. ML753286 has high permeability and low to medium clearance in rodent and human liver S9 fractions, and is stable in plasma cross species[1].

IC_{50} & Target

IC50: 0.6 μM (BCRP)[1]

In Vitro

ML753286 has IC_{50} values of >30, 0.6, and 39.0 μM for the inhibition of P-gp-, BCRP-, and OATP mediated transport,

	respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ML753286 (25- or 50-mg/kg (PO); 10 or 20 mg/kg (IV); 0.083-24 hours) appears to completely inhibit Bcrp functions in rats at 25 mg/kg PO or at 20 mg/kg IV. The t_{max} values in plasma were 1.4, 4.0, and 4.1 hours in Bcrp KO rats, WT rats pre-administered 25-mg/kg ML753286, and WT rats pre-administered 50-mg/kg ML753286, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Bcrp KO (Abcg2−/−) and WT (Wistar) Rats[1]
Dosage:	25- or 50-mg/kg (PO); 10 or 20 mg/kg (IV) (Pharmacokinetic Study)
Administration:	PO or IV; 0.083, 0.25, 0.5, 1, 2, 4, 6, 8, and 24 hours
Result:	The t_{max} values in plasma were 1.4, 4.0, and 4.1 hours in Bcrp KO rats, WT rats pre-administered 25-mg/kg ML753286, and WT rats pre-administered 50-mg/kg ML753286, respectively.

CUSTOMER VALIDATION

- Crit Rev Anal Chem. 2021 Mar 10;1-15.

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REFERENCES

[1]. Liao M, et al. Preclinical absorption, distribution, metabolism, excretion and pharmacokinetics of a novelselective inhibitor of breast cancer resistance protein (BCRP). Xenobiotica. 2018 May;48(5):467-477.

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