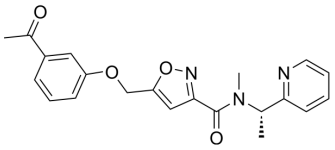
ML381

Cat. No.:	HY-101839
CAS No.:	1623481-80-0
Molecular Formula:	$C_{21}H_{21}N_3O_4$
Molecular Weight:	379.41
Target:	mAChR
Pathway:	GPCR/G Protein; Neuronal Signaling
Storage:	Pure form -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 (263.57 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6357 mL	13.1784 mL	26.3567 mL
	5 mM	0.5271 mL	2.6357 mL	5.2713 mL
	10 mM	0.2636 mL	1.3178 mL	2.6357 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 (6.59 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.59 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.59 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML381 (VU0488130) is a highly selective, central nervous system penetrant mAChR M5 orthogonal antagonist (IC_{50} = 450 nM; Ki = 340 nM). ML381 is unstable in rat plasma and can be mainly used as a molecular probe for in vitro and electrophysiological studies[1][2].

IC_{50} & Target

IC50: 450 nM (mAChR M5)[1].

In Vivo

ML381 (0.2 mg/kg; i.v.; single) possesses an overall acceptable DMPK profile for pharmacodynamic studies in rat, with the

exception of poor metabolic stability and a potential for amide hydrolysis in plasma; as such, ML381 is best suited to use as an in vitro/electrophysiological probe[1].

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

Animal Model:	Sprague-Dawley rat[1].
Dosage:	0.2 mg/kg
Administration:	Intravenous injection; single.
Result:	Pharmacokinetic Parameters of ML381 in Sprague-Dawley rat[1].

	IV (0.2 mg/kg)
Hepatic microsomal CL_{int} (mL min^{-1} kg^{-1})	770
Predicted CL_{hep} (mL min^{-1} kg^{-1})	64
fu_{brain}	0.14
C_{brain}/C_{plasma} (K_p*)	0.58

*K_p value was determined at 0.25 h following a 0.2 mg/kg IV dose (n=2).

REFERENCES

[1]. Gentry PR, et al. Discovery, synthesis and characterization of a highly muscarinic acetylcholine receptor (mAChR)-selective M5-orthosteric antagonist, VU0488130 (ML381): a novel molecular probe. ChemMedChem. 2014 Aug;9(8):1677-82.

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