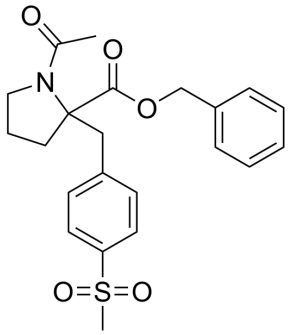
KCC2 blocker 1

Cat. No.:	HY-18172
CAS No.:	1228439-36-8
Molecular Formula:	$C_{22}H_{25}NO_5S$
Molecular Weight:	415.5
Target:	Potassium Channel
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 : 250 mg/mL (601.68 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4067 mL	12.0337 mL	24.0674 mL
	5 mM	0.4813 mL	2.4067 mL	4.8135 mL
	10 mM	0.2407 mL	1.2034 mL	2.4067 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 (5.01 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.01 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.01 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

KCC2 blocker 1 is an orally active and selective K^+-Cl^- cotransporter KCC2 blocker with an IC_{50} of 1 μM. KCC2 blocker 1 is a benzyl prolinate[1].

IC_{50} & Target

IC50: 1 μM (KCC2)[1]

In Vitro

KCC2 blocker 1 (compound 13; 100 μM) inhibits NKCC1 with 35%.

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

In Vivo

KCC2 blocker 1 (compound 13; 1 mg/kg iv and 6 mg/kg po) has a $t_{1/2}$ of 0.3 hours, a CL of 26 mL/min/kg, a C_{max} of 457 ng/mL and a AUC of 726 ng•h/mL for male Wistar rats[1].

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

Animal Model:	Male Wistar rats[1]
Dosage:	1 mg/kg or 6 mg/kg (Pharmacokinetic Analysis)
Administration:	IV (1 mg/kg) and PO (6 mg/kg)
Result:	Had a $t_{1/2}$ of 0.3 hours, a CL of 26 mL/min/kg, a C_{max} of 457 ng/mL and a AUC of 726 ng•h/mL.

REFERENCES

[1]. Pégurier C, et al. Benzyl prolinate derivatives as novel selective KCC2 blockers. Bioorg Med Chem Lett. 2010 Apr 15;20(8):2542-5.

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