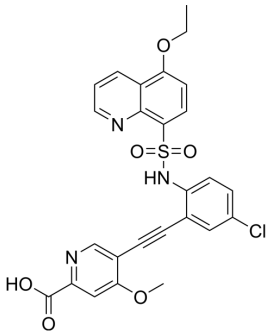
MSC-4381

Cat. No.:	HY-132301
CAS No.:	2445185-57-7
Molecular Formula:	$C_{26}H_{20}ClN_3O_6S$
Molecular Weight:	537.97
Target:	Monocarboxylate Transporter
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 : 83.33 mg/mL (154.90 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8588 mL	9.2942 mL	18.5884 mL
	5 mM	0.3718 mL	1.8588 mL	3.7177 mL
	10 mM	0.1859 mL	0.9294 mL	1.8588 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 (3.87 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MSC-4381 (MCT4-IN-1) is an orally active and selective monocarboxylate transporter 4 (MCT4/SLC16A3) inhibitor with an IC_{50} of 77 nM and a K_i of 11 nM. MSC-4381 targets to the cytosolic domain of MCT4. MSC-4381 results in lactate efflux inhibition and reduction of cellular viability in MCT4 high expressing cells. MSC-4381 has the potential for MCT4 transporter inhibition research[1]. MSC-4381 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target		
	MCT4 77 nM (IC_{50})	MCT4 11 nM (Ki)

In Vitro

MSC-4381 (compound 18n) inhibits lactate efflux in the MDA-MB-231 cell line with an IC_{50} of 1 nM. The on-target activity is confirmed with a K_i of 11 nM by fluorescence cross-correlation spectroscopy (FCCS)[1].
MSC-4381 does not inhibit lactate efflux to a similar extent in SNU-398 and MiaPaca2, and only 600-fold less in RT-4 cell lines

[1].

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

In Vivo

MSC-4381 (compound 18n; 30 mg/kg; PO; single dose) only combined with MCT1/2 inhibitor exhibits a significant tumoral intracellular lactate accumulation[1].

MSC-4381 (30 mg/kg/day; for 15 days) shows no significant antitumor activity[1].

MSC-4381 (0.2 mg/kg; iv) has a $T_{1/2}$ of 1 hours, a CL of 0.33 L/h kg, a C_{max} of 489 ng/mL and a V_{ss} of 0.4 L/kg for mice[1].

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

Animal Model:	MC38 tumor-bearing C57/BL6 mice[1]
Dosage:	30 mg/kg
Administration:	PO; single dose
Result:	Only combined with MCT1/2 inhibitor exhibited a significant tumoral intracellular lactate accumulation.

Animal Model:	Mice[1]
Dosage:	0.2 mg/kg (Pharmacokinetic Analysis)
Administration:	IV
Result:	Had a $T_{1/2}$ of 1 hours, a CL of 0.33 L/h•kg, a C_{max} of 489 ng/mL and a V_{ss} of 0.4 L/kg for mice.

REFERENCES

[1]. Timo Heinrich, et al. Discovery of 5-{2-[5-Chloro-2-(5-ethoxyquinoline-8-sulfonamido)phenyl]ethynyl}-4-methoxypyridine-2-carboxylic Acid, a Highly Selective in Vivo Useable Chemical Probe to Dissect MCT4 Biology. J Med Chem. 2021 Aug 26;64(16):11904-11933.

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