(1S,2S)-ML-SI3

Cat. No.: HY-134819

CAS No.: 2563870-87-9

Molecular Formula: $C_{23}H_{31}N_3O_3S$

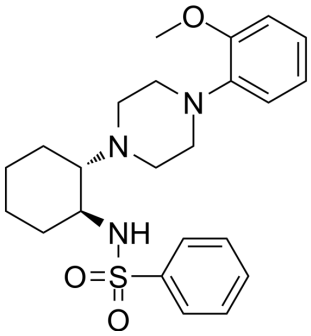
Molecular Weight: 429.58

Target: TRP Channel

Pathway: Membrane Transporter/Ion Channel; Neuronal Signaling

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (232.79 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3279 mL	11.6393 mL	23.2786 mL
	5 mM	0.4656 mL	2.3279 mL	4.6557 mL
	10 mM	0.2328 mL	1.1639 mL	2.3279 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 (5.82 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.82 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.82 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(1S,2S)-ML-SI3 is the trans-isomer of ML-SI3, a TRPML inhibitor. The (-)-isomer is a potent inhibitor of TRPML1 and TRPML2 (IC_{50}=1.6 μM/2.3 μM) and a weak inhibitor of TRPML3 (IC_{50}=12.5 μM), whereas the (+)-enantiomer is an inhibitor on TRPML1 (IC_{50}=5.9 μM), but an activator on TRPML 2 and 3 (EC_{50}=2.7 μM/10.8 μM)[1].

IC_{50} & Target	TRPML1	TRPML2	TRPML3
	5.9 μM (IC_{50})	2.7 μM (EC50)	10.8 μM (EC50)

REFERENCES

[1]. Leser C, et al. Chemical and pharmacological characterization of the TRPML calcium channel blockers ML-SI1 and ML-SI3. Eur J Med Chem. 2021 Jan 15;210:112966.

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