MDR-652

Cat. No.: HY-136363

CAS No.: 1933528-96-1

Molecular Formula: $C_{22}H_{23}ClFN_3O_2S$

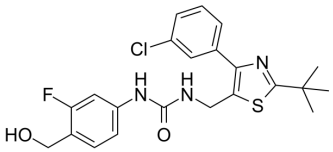
Molecular Weight: 447.95

Target: TRP Channel

Pathway: Membrane Transporter/Ion Channel; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (558.10 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2324 mL	11.1620 mL	22.3239 mL
5 mM	0.4465 mL	2.2324 mL	4.4648 mL
10 mM	0.2232 mL	1.1162 mL	2.2324 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: ≥ 6.25 mg/mL (13.95 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 6.25 mg/mL (13.95 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MDR-652 is a highly specific and efficacious transient receptor potential vanilloid 1 (TRPV1) ligand with agonist activity. The K_is are 11.4 and 23.8 nM for hTRPV1 and rTRPV1, respectively. The EC_{50}s are 5.05 and 93 nM for hTRPV1 and rTRPV1, respectively. Potent topical analgesic activity[1].

IC_{50} & Target

hTRPV1	rTRPV1	hTRPV1	rTRPV1
11.4 nM (Ki)	23.8 nM (Ki)	5.05 nM (EC50)	93 nM (EC50)

In Vivo

MDR-652 (0.5 and 5 mg/kg) displays a dose-dependent decrease of body temperature, supporting that MDR-652 displays TRPV1 agonism in the intact animal[1].

MDR-652 (5-10 mg/kg; i.p. and s.c.) blocks the neuropathic pain completely, indicating 100% maximum possible effect (MPE)

[1].

MDR-652 has a promising topical pharmacokinetic profile[1].

MDR-652 has no significant toxicity. In a single-dose toxicity study, the LD_{50} of MDR-652 is higher than 200 and 2000 mg/kg in i.p. and p.o. administration, respectively[1].

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

Animal Model:	ICR mouse[1]
Dosage:	0.5 and 5 mg/kg
Administration:	Administered intraperitoneally; 7 hours
Result:	Decreased body temperature in a dose-dependent manner.

Animal Model:	Rats with spinal nerve ligation (SNL) model[1]
Dosage:	1, 2, 5, and 10 mg/kg
Administration:	Administered intraperitoneally and subcutaneously; 24 hours
Result:	The i.p. administration exhibited an excellent and dose dependent analgesic profile with an ED_{50} of 0.5-2 mg/kg. The subcutaneous injection (sc) also displayed an excellent analgesic outcome with maximum effect at 30 min after administration.

REFERENCES

[1]. Jihyae Ann, et al. Discovery of Nonpungent Transient Receptor Potential Vanilloid 1 (TRPV1) Agonist as Strong Topical Analgesic. J Med Chem. 2020 Jan 9;63(1):418-424.

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