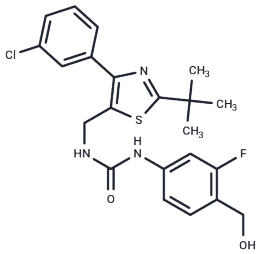
Data Sheet (Cat.No.T22360)

TargetMol
YOUR TARGET MOLECULES

MDR-652

Chemical Properties



CAS No. : 1933528-96-1

Formula: C22H23ClFN3O2S

Molecular Weight: 447.95

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	MDR-652 is a highly specific and efficacious agonist of nonpungent transient receptor potential vanilloid 1 (TRPV1) with Ki value of 11.4 nM and 23.8 nM for hTRPV1 and rTRPV1 respectively and EC50s for hTRPV1 and rTRPV1 are 5.05 and 93 nM respectively. MDR-652 is a potent topical analgesic.
Targets(IC50)	TRP/TRPV Channel
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]. Potent analgesic activity was observed in models of neuropathic pain, and MDR-652 blocked capsaicin induced allodynia, showing dermal accumulation with little transdermal absorption. 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 displays weak systemic toxicity and is negative in assays of genotoxicity. In a single-dose toxicity study, the LD50 of MDR-652 is higher than 200 and 2000 mg/kg in i.p. and p.o. administration, respectively[1].
Animal Research	MDR-652 (0.5 and 5 mg/kg; Administered intraperitoneally; 7 hours; ICR mouse) decreased body temperature in a dose-dependent manner. MDR-652 (1, 2, 5, and 10 mg/kg; Administered intraperitoneally and subcutaneously; 24 hours; Rats with spinal nerve ligation (SNL) model)The i.p. administration exhibited an excellent and dose dependent analgesic profile with an ED50 of 0.5-2 mg/kg. The subcutaneous injection (sc) also displayed an excellent analgesic outcome with maximum effect at 30 min after administration.

Solubility Information

Solubility	DMSO: 249 mg/mL (555.86 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2324 mL	11.162 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
50 mM	0.0446 mL	0.2232 mL	0.4465 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

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.