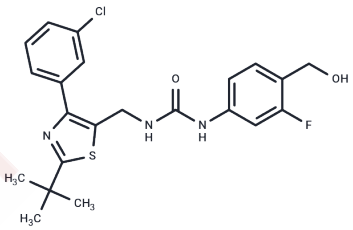
# Data Sheet (Cat.No.T22360)

TargetMol

MDR-652

## Chemical Properties



CAS No. : 1933528-96-1

Formula: C22H23ClFN3O2S

Molecular Weight: 447.95

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

## Biological Description

| | |
|---|---|
| Description | MDR-652 is a highly specific and efficacious agonist of nonpungent transient receptor potential vanilloid 1 (TRPV1), with Ki values of 11.4 nM and 23.8 nM for hTRPV1 and rTRPV1, respectively, and EC50s of 5.05 nM and 93 nM for hTRPV1 and rTRPV1, respectively. MDR-652 is a potent topical analgesic. |
| Targets(IC50) | TRP/TRPV Channel |
| In vivo | MDR-652 (0.5 and 5 mg/kg) demonstrates a dose-dependent decrease in body temperature, indicating TRPV1 agonism in intact animals[1]. It exhibits potent analgesic activity in neuropathic pain models and blocks capsaicin-induced allodynia, with dermal accumulation and minimal transdermal absorption. At 5-10 mg/kg (i.p. and s.c.), MDR-652 completely inhibits neuropathic pain, achieving 100% maximum possible effect (MPE)[1]. MDR-652 has a promising topical pharmacokinetic profile, shows weak systemic toxicity, and is negative in genotoxicity assays. In a single-dose toxicity study, the LD50 of MDR-652 exceeds 200 mg/kg (i.p.) and 2000 mg/kg (p.o.)[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 (555.87 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (11.16 mM),Sonication is recommended.<br>*Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.* |

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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

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.