

Product data sheet



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| MedKoo Cat#: 465015 Name: MDR-652 CAS: 1933528-96-1 Chemical Formula: C ₂₂ H ₂₃ ClFN ₃ O ₂ S Exact Mass: 447.1184 Molecular Weight: 447.9534 | |
| Product supplied as: Powder | |
| Purity (by HPLC): ≥ 98% | |
| Shipping conditions: Ambient temperature | |
| Storage conditions: Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks. | |

1. Product description:

MDR-652 is a nonpungent transient receptor potential vanilloid 1 (TRPV1) agonist discovered to be a strong topical analgesic.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

| Solvent | Max Conc. mg/mL | Max Conc. mM |
|---------|-----------------|--------------|
| DMSO | 170.0 | 379.50 |
| Ethanol | 90.0 | 200.91 |

4. Stock solution preparation table:

| Concentration / Solvent Volume / Mass | 1 mg | 5 mg | 10 mg |
|---------------------------------------|---------|----------|----------|
| 1 mM | 2.23 mL | 11.16 mL | 22.32 mL |
| 5 mM | 0.45 mL | 2.23 mL | 4.46 mL |
| 10 mM | 0.22 mL | 1.12 mL | 2.23 mL |
| 50 mM | 0.05 mL | 0.22 mL | 0.45 mL |

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

TBD

In vivo study

Ann J, Kim HS, Thorat SA, Kim H, Ha HJ, Choi K, Kim YH, Kim M, Hwang SW, Pearce LV, Esch TE, Turcios NA, Blumberg PM, Lee J. Discovery of Nonpungent Transient Receptor Potential Vanilloid 1 (TRPV1) Agonist as Strong Topical Analgesic. J Med Chem. 2020 Jan 9;63(1):418-424. doi: 10.1021/acs.jmedchem.9b01046. Epub 2019 Nov 26. PMID: 31702924.

7. Bioactivity

Biological target:

MDR-652 is a highly specific and efficacious transient receptor potential vanilloid 1 (TRPV1) ligand with agonist activity.

In vitro activity

TBD

In vivo activity

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Here, this study describes the scaled-up synthesis and characterization in mouse models of a novel, nonpungent vanilloid. Potent analgesic activity was observed in models of neuropathic pain, and the compound blocked capsaicin induced allodynia, showing dermal accumulation with little transdermal absorption.

Reference: J Med Chem. 2020 Jan 9;63(1):418-424. <https://pubmed.ncbi.nlm.nih.gov/31702924/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.