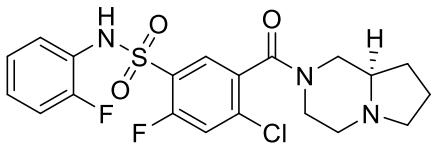
Product data sheet

MedKoo Cat#: 522460 Name: ABT-639 CAS#: 1235560-28-7 Chemical Formula: $C_{20}H_{20}ClF_2N_3O_3S$ Exact Mass: 455.0882 Molecular Weight: 455.9	
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:

ABT-639 is a potent and selective T-type calcium channel blocker. ABT-639 effectively reduces nociceptive and neuropathic pain in rats. ABT-639 produces robust antinociceptive activity in experimental pain models at doses that do not significantly alter psychomotor or hemodynamic function in the rat. ABT-639 was significantly less active at other Ca^{2+} channels (e.g. Ca(v)1.2 and Ca(v)2.2) (IC_{50} > 30 μM). ABT-639 has high oral bioavailability (%F = 73), low protein binding (88.9%) and a low brain:plasma ratio (0.05:1) in rodents.

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	9.71	21.30
DMF	14.0	30.71
DMF:PBS (pH 7.2) (1:20)	0.04	0.09
Ethanol	0.5	1.10

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.19 mL	10.97 mL	21.93 mL
5 mM	0.44 mL	2.19 mL	4.39 mL
10 mM	0.22 mL	1.10 mL	2.19 mL
50 mM	0.04 mL	0.22 mL	0.44 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

1. Wang MX, Liu X, Li JM, Liu L, Lu W, Chen GC. Inhibition of CACNA1H can alleviate endoplasmic reticulum stress and reduce myocardial cell apoptosis caused by myocardial infarction. Eur Rev Med Pharmacol Sci. 2020 Dec;24(24):12887-12895. doi: 10.26355/eurrev_202012_24192. PMID: 33378039.
2. Hu J, Wu Q, Wang Z, Hong J, Chen R, Li B, Hu Z, Hu X, Zhang M. Inhibition of CACNA1H attenuates doxorubicin-induced acute cardiotoxicity by affecting endoplasmic reticulum stress. Biomed Pharmacother. 2019 Dec;120:109475. doi: 10.1016/j.biopha.2019.109475. Epub 2019 Sep 30. PMID: 31580970.

In vivo study

Product data sheet

1. Zhang Q, Xia Z, Joshi S, Scott VE, Jarvis MF. Optimization of ADME Properties for Sulfonamides Leading to the Discovery of a T-Type Calcium Channel Blocker, ABT-639. ACS Med Chem Lett. 2015 Apr 28;6(6):641-4. doi: 10.1021/acsmedchemlett.5b00023. PMID: 26101566; PMCID: PMC4468402.
2. Jarvis MF, Scott VE, McGaraughty S, Chu KL, Xu J, Niforatos W, Milicic I, Joshi S, Zhang Q, Xia Z. A peripherally acting, selective T-type calcium channel blocker, ABT-639, effectively reduces nociceptive and neuropathic pain in rats. Biochem Pharmacol. 2014 Jun 15;89(4):536-44. doi: 10.1016/j.bcp.2014.03.015. Epub 2014 Apr 12. PMID: 24726441.

7. Bioactivity

Biological target:

ABT-639 is a novel, peripherally acting, selective T-type Ca^{2+} channel blocker.

In vitro activity

At the same time, in order to verify whether the CACNA1H inhibitor ABT-639 has an inhibitory effect on H9c2 cells, this study used TUNEL staining (Figure 3A and 3B). The results showed that H9c2 cells had dramatically increased apoptosis after I/H treatment, and the apoptosis rate was markedly higher than the control group. After ABT-639 treated with H9c2 cells, it was found that the apoptosis rate was dramatically reduced. In addition, the results of immunofluorescence staining also found that ABT-639 can effectively inhibit the increase of CHOP into the nucleus induced by I/H treatment (Figure 3C and 3D).

Reference: Eur Rev Med Pharmacol Sci. 2020 Dec;24(24):12887-12895. https://pubmed.ncbi.nlm.nih.gov/33378039/

In vivo activity

ABT-639 dose-dependently attenuates nociception in a capsaicin-induced secondary mechanical hyperalgesia model (Cap-SMH) (Figure 3). The antinociceptive activity of ABT-639 in this model is consistent with its dose-dependent antinociceptive activity in multiple models of neuropathic pain. Additionally, ABT-639 did not produce any decrement in balance or motor performance in the rat Edge test (ED_{50} > 300 mg/kg, or rat plasma 114 μg/mL, p.o.).

Reference: ACS Med Chem Lett. 2015 Jun 11; 6(6): 641–644. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4468402/

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.