

Product Data Sheet

Product Name: MSI-1436 (Trodesquamine)

Cat. No.: GC32396

Chemical Properties

Cas. No. 186139-09-3

SMILES NCCCCCCCCNCCCN[C@@H]1C[C@@](C[C@@H](O)[C@]2([H])[C@]3([H])CC[C@@]4(C)[C@@]2([H])CC[C@@]4([C@H](C)CC[C@@H](OS(=O)(O)=O)C(C)C)[H])([H])[C@]3(C)CC1

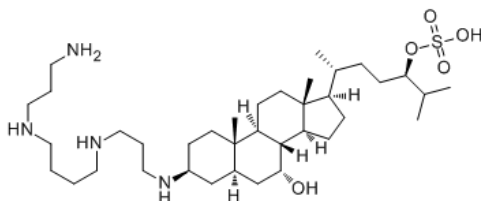
Formula $C_{37}H_{72}N_4O_5S$ M.Wt 685.06

Solubility Soluble in DMSO Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Cell experiment [1]:

Cell lines

MPC83 cells

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

Preparation Method	MPC83 cells were cultured in RPMI-1640 medium, supplemented with 10% fetal bovine serum (FBS) and 1% penicillin/streptomycin at 37°C in an incubator with 5% CO ₂ . Cells were seeded in a 96-well plate at a density of 1×10^5 cells/well for 24h, and incubated with Caerulin (10μM) for 12h. Cells were treated with MSI-1436 (1μM), after 48h, the cell proliferation ability was tested, and ELISA was used to detect IL-18 and IL-1β in the supernatant of cells.
Reaction Conditions	1μM; 48h
Applications	MSI-1436 treatment inhibited Caerulin-induced cell death and reduced the levels of IL-18 and IL-1β in MPC83 cells.
Animal experiment [2]:	
Animal models	C57BL/6J mice
Preparation Method	C57BL/6J mice (22-25g) were anesthetized using 2% isoflurane and 100% oxygen at a flow rate of 2.5L/min. The left coronary artery was ligated with a 7-0 suture at about 2mm below the left auricle to induce a permanent occlusion. Ischemia was confirmed by segment elevation using an electrocardiogram system and decreased coloration of the heart muscle. After closure of the chest and resumption of spontaneous respiration, mice were returned to their cages and provided with standard chow and water. Twenty-four hours after surgery, transthoracic echocardiography was performed. Mice with compromised heart function were then administered by i.p. injection vehicle or MSI-1436 (0.125mg/kg). Injections were repeated every 3 days to maintain plasma drug concentrations. Mouse hearts were extracted for analysis.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

Dosage form	0.125mg/kg; every 3 days; 4 weeks; i.p.
Applications	MSI-1436 treatment improved heart function, reduced infarct size, reduced ventricular wall thinning, and increased cardiomyocyte proliferation in mice.
References: [1] Wang J, Huang Y, Zhang J, et al. Inhibition of PTP1B Through NADH Dehydrogenase Activity Reduces Acute Pancreatic Acinar Cell Pyroptosis by Inhibiting the ROS/TXNIP/NLRP3 Pathway[J]. Digestive diseases and sciences, 2026, 71(3): 991-1002. [2] Smith A M, Maguire-Nguyen K K, Rando T A, et al. The protein tyrosine phosphatase 1B inhibitor MSI-1436 stimulates regeneration of heart and multiple other tissues[J]. NPJ Regenerative medicine, 2017, 2(1): 4.	

Background

MSI-1436 (Trodesquamine) is a non-competitive protein-tyrosine phosphatase 1B (PTP1B) inhibitor that can cross the blood-brain barrier, with an IC_{50} value of $1\mu M$ ^[1]. MSI-1436 binds to the major binding site of the C-terminal helix $\alpha 9$, inducing conformational changes in the PTP1B protein and rendering PTP1B inactive, while simultaneously antagonizing the HER2 signaling pathway to block xenograft tumorigenesis^[2]. MSI-1436 has been widely used in neurology research to inhibit the aggregation of α -synuclein and to cause the transformation of A β 42 oligomers into fibrillar forms^[3].

In vitro, MSI-1436 ($1\mu M$) treatment for 48 hours alleviated the Caerulein ($10\mu M$)-induced necrosis of MPC83 cells and reduced the levels of IL-1 β and IL-18^[4]. $2\mu M$ of MSI-1436 treatment for 24 hours inhibited endoplasmic reticulum stress and apoptosis triggered by Tunicamycin in HepG2 cells, and maintained mitochondrial membrane potential^[5]. Treatment with $1\mu M$ MSI-1436 for 24 hours reduced the expression of pro-inflammatory cytokines in peripheral blood mononuclear cells (PBMCs) derived from equine metabolic syndrome (EMS), and increased the levels of IL-10 and IL-4^[6].

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

In vivo, MSI-1436 administration via a single intraperitoneal injection at a dose of 10mg/kg reduced the body weight and decreased fat accumulation in the atherosclerosis mouse model over a period of 4 weeks^[7]. After inducing myocardial infarction in adult mice, intraperitoneal injection of MSI-1436 (0.125mg/kg) was administered once every three days for 4 weeks, which increased the survival rate of mice and improved cardiac function^[8].

References:

- [1] Maccari R, Ottanà R. Can allosteric be a key strategy for targeting PTP1B in drug discovery? A lesson from trodusquemine[J]. International Journal of Molecular Sciences, 2023, 24(11): 9621.
- [2] Krishnan N, Koveal D, Miller D H, et al. Targeting the disordered C terminus of PTP1B with an allosteric inhibitor[J]. Nature chemical biology, 2014, 10(7): 558-566.
- [3] Limbocker R, Errico S, Barbut D, et al. Squalamine and trodusquemine: two natural products for neurodegenerative diseases, from physical chemistry to the clinic[J]. Natural Product Reports, 2022, 39(4): 742-753.
- [4] Wang J, Huang Y, Zhang J, et al. Inhibition of PTP1B Through NADH Dehydrogenase Activity Reduces Acute Pancreatic Acinar Cell Pyroptosis by Inhibiting the ROS/TXNIP/NLRP3 Pathway[J]. Digestive diseases and sciences, 2026, 71(3): 991-1002.
- [5] Bourebaba L, Komakula S S B, Weiss C, et al. The PTP1B selective inhibitor MSI-1436 mitigates Tunicamycin-induced ER stress in human hepatocarcinoma cell line through XBP1 splicing modulation[J]. PLoS One, 2023, 18(1): e0278566.
- [6] Bourebaba L, Serwotka-Suszczak A, Bourebaba N, et al. The PTP1B inhibitor trodusquemine (MSI-1436) improves glucose uptake in equine metabolic syndrome affected liver through anti-inflammatory and antifibrotic activity[J]. International Journal of Inflammation, 2023, 2023(1): 3803056.
- [7] Thompson D, Morrice N, Grant L, et al. Pharmacological inhibition of protein tyrosine phosphatase 1B protects against atherosclerotic plaque formation in the LDLR^{-/-} mouse model of atherosclerosis[J]. Clinical Science, 2017, 131(20): 2489-2501.
- [8] Smith A M, Maguire-Nguyen K K, Rando T A, et al. The protein tyrosine phosphatase 1B inhibitor

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

MSI-1436 stimulates regeneration of heart and multiple other tissues[J]. NPJ Regenerative medicine, 2017, 2(1): 4.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA