ML385

Cat. No.: HY-100523

CAS No.: 846557-71-9

Molecular Formula: $C_{29}H_{25}N_3O_4S$

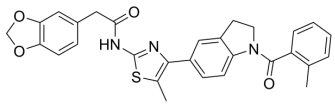
Molecular Weight: 512

Target: Keap1-Nrf2; Ferroptosis

Pathway: NF-κB; Apoptosis

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (48.83 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9531 mL	9.7656 mL	19.5312 mL
	5 mM	0.3906 mL	1.9531 mL	3.9062 mL
	10 mM	0.1953 mL	0.9766 mL	1.9531 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 50% PEG300 >> 50% saline
   Solubility: 10 mg/mL (19.53 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 0.5% CMC-Na/saline water
   Solubility: 9.01 mg/mL (17.60 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 15% Solutol HS 15 >> 10% Cremophor EL >> 35% PEG 400 >> 40% water
   Solubility: 5 mg/mL (9.77 mM); Suspended solution; Need ultrasonic
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.88 mM); Clear solution
5. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.06 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML385 is a specific nuclear factor erythroid 2-related factor 2 (NRF2) inhibitor with an IC_{50} of 1.9 μM.

IC_{50} & Target	IC50: 1.9 μM (NRF2)[1]
In Vitro	ML385 interacts with NRF2 and affects the DNA binding activity of the NRF2-MAFG protein complex. The addition of ML385 decreases anisotropy in a dose-dependent manner, with an IC_{50} of 1.9 μM. A dose-dependent reduction in the NRF2 transcriptional activity is observed and the maximum inhibitory concentration is 5 μM by ML385. Treatment with ML385 leads to a significant reduction in NRF2 and downstream target gene expression selectively in KEAP1 mutant H460 cells. ML385 selectively affects the colony forming ability or growth of lung cancer cells with gain of NRF2 function[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ML385 in combination with carboplatin leads to a significant reduction in tumor cell proliferation, demonstrated by fewer Ki-67 positive cells. Tumor samples treated with ML385 show a significant reduction in NRF2 protein level and its downstream target genes[1]. ML385 (intraperitoneal injection; 30 mg/kg; 7 days) weakens the therapeutic effects of MSC-Exo on inflammation-induced astrocytic activation in mice, and reduces reactive astrogliosis, NF-κB deactivation[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	8-week-old C57B/6 male mice[3]
Dosage:	30 mg/kg; 7 days
Administration:	Intraperitoneal injection
Result:	Reversed inhibition of MSC-Exo on hippocampal astrocytic activation in vivo.

CUSTOMER VALIDATION

- Nature. 2022 Oct;610(7931):366-372.
- Cancer Cell. 2021 May 10;39(5):678-693.e11.
- Cell Metab. 2023 Oct 3;35(10):1688-1703.e10.
- Nat Commun. 2018 Oct 24;9(1):4429.
- Adv Sci (Weinh). 2024 Feb 2:e2307143.

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REFERENCES

[1]. Singh A, et al. Small Molecule Inhibitor of NRF2 Selectively Intervenes Therapeutic Resistance in KEAP1-Deficient NSCLC Tumors. ACS Chem Biol. 2016 Nov 18;11(11):3214-3225.

[2]. Xinnong Liu, et al. Isoliquiritigenin ameliorates acute pancreatitis in mice via inhibition of oxidative stress and modulation of the Nrf2/HO-1 pathway. Oxid Med Cell Longev. 20 March 2018.

[3]. Xian P, et al. Mesenchymal stem cell-derived exosomes as a nanotherapeutic agent for amelioration of inflammation-induced astrocyte alterations in mice.Theranostics. 2019 Aug 14;9(20):5956-5975.

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

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