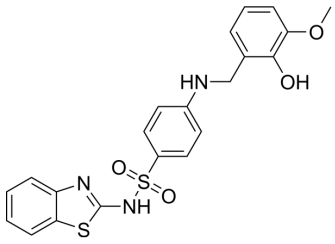
ML355

Cat. No.:	HY-12341
CAS No.:	1532593-30-8
Molecular Formula:	$C_{21}H_{19}N_3O_4S_2$
Molecular Weight:	441.52
Target:	Lipoxygenase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 1 year -20°C 6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 42 mg/mL (95.13 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2649 mL	11.3245 mL	22.6490 mL
5 mM	0.4530 mL	2.2649 mL	4.5298 mL
10 mM	0.2265 mL	1.1325 mL	2.2649 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution
4. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML355 is a potent and selective inhibitor of 12-Lipoxygenase (12-LOX) with an IC_{50} of 0.34 μM, shows excellent selectivity over related lipoxygenases and cyclooxygenases, and possesses favorable ADME properties.

IC_{50} & Target

12-LOX

	0.34 μM (IC_{50})
In Vitro	ML355 inhibits PAR-4 induced aggregation and calcium mobilization in human platelets and reduce 12-HETE in β-cells[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ML355 (1.88-30 mg/kg; i.g.; 2 times per day for two days) strongly inhibits the thrombus formation in mice at higher dose compared to WT controls[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	C57BL/6 mice[3]
Dosage:	1.88, 3.75, 7.5, 15, 30 mg/kg
Administration:	Oral gavage; 2 times per day for two days
Result:	The thrombus formation in mice was strongly inhibited by higher doses of ML355.

CUSTOMER VALIDATION

- Nat Med. 2018 Jan;24(1):73-83.
- Cell Metab. 2021 Sep 16;S1550-4131(21)00377-6.
- Cell Commun Signal. 2020 May 4;18(1):70.

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REFERENCES

[1]. Luci DK, et al. Synthesis and structure-activity relationship studies of 4-((2-hydroxy-3-methoxybenzyl)amino)benzenesulfonamide derivatives as potent and selective inhibitors of 12-lipoxygenase. J Med Chem. 2014 Jan 23;57(2):495-506.

[2]. Zhang XJ, et al. An ALOX12-12-HETE-GPR31 signaling axis is a key mediator of hepatic ischemia-reperfusion injury. Nat Med. 2018 Jan;24(1):73-83.

[3]. Adili R, et al. First Selective 12-LOX Inhibitor, ML355, Impairs Thrombus Formation and Vessel Occlusion In Vivo With Minimal Effects on Hemostasis. Arterioscler Thromb Vasc Biol. 2017 Oct;37(10):1828-1839.

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