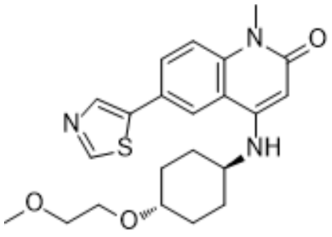
CD38 inhibitor 1

Cat. No.:	HY-123999
CAS No.:	1700637-55-3
Molecular Formula:	$C_{22}H_{27}N_3O_3S$
Molecular Weight:	413.53
Target:	CD38
Pathway:	Immunology/Inflammation
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 (60.46 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4182 mL	12.0910 mL	24.1820 mL
	5 mM	0.4836 mL	2.4182 mL	4.8364 mL
	10 mM	0.2418 mL	1.2091 mL	2.4182 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 (24.18 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: corn oil
   Solubility: 10 mg/mL (24.18 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.05 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (6.05 mM); Suspended solution; Need ultrasonic
5. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.05 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	CD38 inhibitor 1 (compound 78c) is a potent CD38 inhibitor with IC_{50}s of 7.3 nM and 1.9 nM for hCD38 and mouse CD38[1].
IC_{50} & Target	IC50: 7.3 nM (hCD38), 1.9 nM (mouse CD38)[1]

	Ki: 0.3 nM (WT hCD38)[1]
In Vivo	CD38 inhibitor (30 mg/kg; oral administration; 2 and 6 hours) significantly elevates NAD levels in liver and muscle[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Diet induced obese (DIO) C57Bl6 mice[1]
Dosage:	30 mg/kg
Administration:	Orally once
Result:	NAD levels were significantly increased at both the 2 and 6 h time points in liver and muscle.

CUSTOMER VALIDATION

- Signal Transduct Target Ther. 2023 Sep 18;8(1):353.
- Cell Metab. 2021 Jan 5;33(1):110-127.e5.
- Brain Behav Immun. 2023 Oct 2:115:64-79.
- Cell Death Dis. 2020 Jan 6;11(1):15.
- Cell Rep. 2022 Dec 13;41(11):111803.

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REFERENCES

[1]. Tarragó MG, Chini CCS, Kanamori KS, et al. A Potent and Specific CD38 Inhibitor Ameliorates Age-Related Metabolic Dysfunction by Reversing Tissue NAD+ Decline. Cell Metab. 2018;27(5):1081-1095.e10.

[2]. Haffner CD, et al. Discovery, Synthesis, and Biological Evaluation of Thiazoloquin(az)olin(on)es as Potent CD38 Inhibitors. J Med Chem. 2015 Apr 23;58(8):3548-71.

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