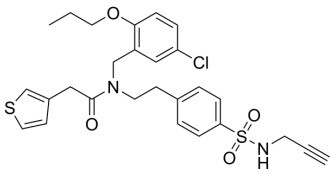
YQ128

Cat. No.:	HY-130252
CAS No.:	2454246-18-3
Molecular Formula:	$C_{27}H_{29}ClN_2O_4S_2$
Molecular Weight:	545.11
Target:	NOD-like Receptor (NLR); Interleukin Related
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 : 250 mg/mL (458.62 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8345 mL	9.1725 mL	18.3449 mL
5 mM	0.3669 mL	1.8345 mL	3.6690 mL
10 mM	0.1834 mL	0.9172 mL	1.8345 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: ≥ 2.08 mg/mL (3.82 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.82 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

YQ128 is a potent and selective second-generation NLRP3 (NOD-like receptor P3) inflammasome inhibitor with an IC_{50} of 0.30 μM. YQ128 significantly and selectively suppresses the production of IL-1β, but not TNF-α, and it can cross the BBB to reach the CNS. YQ128 has anti-inflammatory activity[1]. YQ128 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

NLRP3 0.30 μM (IC_{50})	IL-1β

In Vitro

YQ128 (0.3-100 μM; 30 mins) dose dependently suppressed the release of IL-1β from peritoneal macrophages upon LPS/ATP challenge with an IC_{50} of 1.59 μM[1].

YQ128 (20 μM; 2 hours) shows no significant toxic effects on hCMEC/D3 cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	Mouse peritoneal macrophages
Concentration:	0.3, 1.0, 3.0, 10, 30, 100 μM
Incubation Time:	30 mins
Result:	Suppressed the release of IL-1β from peritoneal macrophages upon LPS/ATP challenge with an IC_{50} of 1.59 μM.

In Vivo

YQ128 (iv; 20 mg/kg) has an intermediate terminal plasma half-life ($t_{1/2}$) of 6.6 hours after iv administration[1].

YQ128 (oral; 20 mg/kg) shows delayed gastrointestinal absorption with a t_{max} and c_{max} of 12 h and 73 ng/mL, respectively. Oral bioavailability (F_{oral}) is estimated as 10%[1].

YQ128 exhibits extensive extravascular distribution with a large steady-state volume of distribution (Vd_{ss}) of 8.5 L/kg and rapid total clearance (CL_{tot}) of 41 mL/min/kg[1].

YQ128 (10 mg/kg) has been shown to trigger IL-1β production in a NLRP3- dependent manner in C57BL/6 mice[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Sprague-Dawley rats (200-250 g)[1]
Dosage:	20 mg/kg (Pharmacokinetic Analysis)
Administration:	Iv
Result:	Had an intermediate terminal plasma half-life ($t_{1/2}$) of 6.6 hours after iv administration.

CUSTOMER VALIDATION

- Cell Chem Biol. 2023 Oct 12:S2451-9456(23)00335-5.

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REFERENCES

[1]. Jiang Y, et al. Discovery of Second-Generation NLRP3 Inflammasome Inhibitors: Design, Synthesis, and Biological Characterization. J Med Chem. 2019 Oct 31.

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