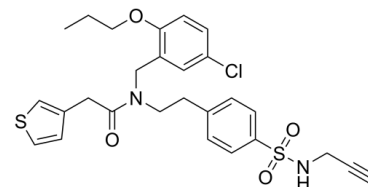


Data Sheet

Product Name:	YQ128
Cat. No.:	CS-0106043
CAS No.:	2454246-18-3
Molecular Formula:	C ₂₇ H ₂₉ ClN ₂ O ₄ S ₂
Molecular Weight:	545.11
Target:	Interleukin Related; NOD-like Receptor (NLR)
Pathway:	Immunology/Inflammation
Solubility:	DMSO : 250 mg/mL (458.62 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

YQ128 is a potent and selective second-generation **NLRP3 (NOD-like receptor P3) inflammasome** inhibitor with an **IC₅₀** of 0.30 μ M. YQ128 significantly and selectively suppresses the production of **IL-1 β** , but not TNF- α , and it can cross the BBB to reach the CNS. YQ128 has anti-inflammatory activity^[1]. **In Vitro:** YQ128 (0.3-100 μ M; 30 mins) dose dependently suppressed the release of IL-1 β from peritoneal macrophages upon LPS/ATP challenge with an IC₅₀ of 1.59 μ M^[1].

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

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 ($V_{d_{ss}}$) 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-1 β production in a NLRP3- dependent manner in C57BL/6 mice^[1].

References:

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

CAIndexNames:

3-Thiopheneacetamide, N-[(5-chloro-2-propoxyphenyl)methyl]-N-[2-[4-[(2-propyn-1-ylamino)sulfonyl]phenyl]ethyl]-

SMILES:

O=S(C1=CC=C(CCN(CC2=C(C=CC(Cl)=C2)OCCC)C(CC3=CSC=C3)=O)C=C1)(NCC#C)=O

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

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