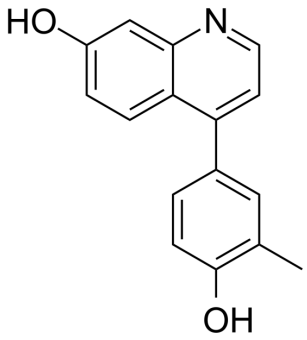
CU-CPT9b



Cat. No.: HY-112051

CAS No.: 2162962-69-6

Molecular Formula: $C_{16}H_{13}NO_2$

Molecular Weight: 251.28

Target: Toll-like Receptor (TLR)

Pathway: Immunology/Inflammation

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO : 83.33 mg/mL (331.62 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.9796 mL	19.8981 mL	39.7962 mL
	5 mM	0.7959 mL	3.9796 mL	7.9592 mL
	10 mM	0.3980 mL	1.9898 mL	3.9796 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 (8.28 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (8.28 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (8.28 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CU-CPT9b is a specific TLR8 antagonist, with an IC_{50} of 0.7 nM. CU-CPT9b shows high binding affinity towards TLR8 with a K_d of 21 nM[1].

IC_{50} & Target

TLR8 0.7 nM (IC_{50})	TLR8 21 nM (Kd)

In Vitro

CU-CPT9b is a specific TLR8 antagonist, with an IC_{50} of 0.7±0.2 nM. ITC experiments have confirmed the strong binding of

CU-CPT9b with a K_d of 21 nM. It is shown that CU-CPT-9b binds to the inactive TLR8 dimer in a similar way to CU-CPT8m. CU-CPT9b utilizes hydrogen bonds with G351 and V520*, which are conserved among TLR8/antagonist structures. Additionally, CU-CPT9b forms water-mediated contacts with S516* and Q519*, which are not observed in TLR8/CU-CPT8m structure, suggesting that the enhanced potency of CU-CPT9b derives from the new interactions with these polar residues. The orientation of Y567* also changes to facilitate van der Waals interactions with CU-CPT9b as compared to TLR8/CU-CPT8m[1].

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

CUSTOMER VALIDATION

- BMC Med. 2021 Oct 15;19(1):247.

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REFERENCES

[1]. Zhang S, et al. Small-molecule inhibition of TLR8 through stabilization of its resting state. Nat Chem Biol. 2018 Jan;14(1):58-64.

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