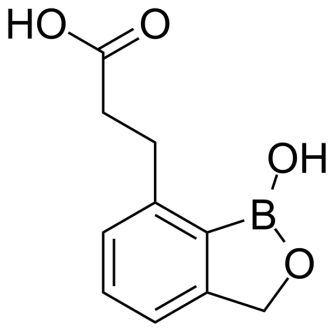
AN3661

Cat. No.:	HY-128204
CAS No.:	1268335-33-6
Molecular Formula:	$C_{10}H_{11}BO_4$
Molecular Weight:	206
Target:	Parasite
Pathway:	Anti-infection
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 (1213.59 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	4.8544 mL	24.2718 mL	48.5437 mL
	5 mM	0.9709 mL	4.8544 mL	9.7087 mL
	10 mM	0.4854 mL	2.4272 mL	4.8544 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 (10.10 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (10.10 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (10.10 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

AN3661, a potent antimalarial lead compound, targets a Plasmodium falciparum cleavage and polyadenylation specificity factor homologue subunit 3 (PfCPSF3). AN3661 inhibits Plasmodium falciparum laboratory-adapted strains (mean IC_{50}=32 nM), Ugandan field isolates (mean ex vivo IC_{50}=64 nM), and murine P. berghei and P. falciparum infections[1].

In Vitro

AN3661 is active at nanomolar (IC_{50}=20-56 nM) concentrations against P. falciparum laboratory strains known to be sensitive (3D7) or resistant (W2, Dd2, K1, HB3, FCR3 and TM90C2B), and AN3661 is similarly active in ex vivo studies of fresh Ugandan field isolates (mean ex vivo IC_{50}=64 nM). AN3661 shows minimal cytotoxicity against mammalian cell lines, with the CC_{50}

	60.5 μM against Jurkat cells, and all other CC_{50} values greater than the highest concentrations tested (25 μM or above)[1]. AN3661 inhibits the stability of P. falciparum transcripts[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	AN3661 (50-200 mg.kg; p.o.; daily for 4 days) inhibits murine P. berghei infections with ED_{90} (4 days) 0.34 mg/kg[1]. AN3661 is administered orally for 4 days, beginning on the third day of infection, the ED_{90} 4 days after initiation of treatment is 0.57 mg/kg[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	P. berghei-infected mice (malaria model)[1]
Dosage:	50, 100, 200 mg/kg
Administration:	Orally; daily for 4 days
Result:	Rapidly controlled parasitemias, with an ED_{90} of 0.34 mg/kg. Daily dosages of 50 mg/kg and 100 mg/kg extended survival, and mice treated with 200 mg/kg per day demonstrated long-term cures.

CUSTOMER VALIDATION

- RNA. 2021 Jul 6;rna.078764.121.

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REFERENCES

[1]. Sonoiki E, et al. A potent antimalarial benzoxaborole targets a Plasmodium falciparum cleavage and polyadenylation specificity factor homologue. Nat Commun. 2017;8:14574. Published 2017 Mar 6.

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