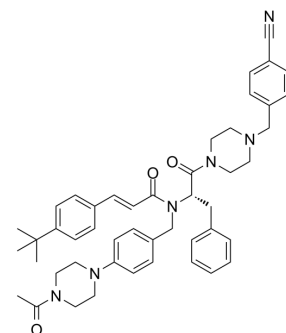


ACT-451840

Cat. No.:	HY-111817		
CAS No.:	1984890-99-4		
Molecular Formula:	C ₄₇ H ₅₄ N ₆ O ₃		
Molecular Weight:	750.97		
Target:	Parasite		
Pathway:	Anti-infection		
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 : 41.67 mg/mL (55.49 mM); ultrasonic and warming and heat to 60°C)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	1.3316 mL	6.6581 mL	13.3161 mL
	5 mM	0.2663 mL	1.3316 mL	2.6632 mL
	10 mM	0.1332 mL	0.6658 mL	1.3316 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.08 mg/mL (2.77 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: 2.08 mg/mL (2.77 mM); Suspended solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.08 mg/mL (2.77 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ACT-451840 is an orally active, potent and low-toxicity compound, showing activity against sensitive and resistant plasmodium falciparum strains. ACT-451840 targets all asexual blood stages of the parasite, has a rapid onset of action. ACT-451840 behaves in a way similar to artemisinin derivatives, with very rapid onset of action and elimination of parasite. ACT-451840 can be used for the research of malarial^{[1][2][3]}.

In Vitro

ACT-451840 shows a 50 % inhibition concentration of 0.4 nM against the drug-sensitive P. falciparum NF54 strain. The IC₅₀ value of ACT-451840 against the murine malaria parasite P. berghei is 13.5 nM in in vitro ex vivo assays.

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ACT-451840 (10 and 60 mg/kg) starts to show significant antimalarial effects (parasite reduction) in vivo at 20 mg/kg. ACT-451840 exhibits curative activity at 300 mg/kg and significant antimalarial effects already at 100 mg/kg. ACT-451840 shows excellent reduction at 30 mg/kg, resulting in 99.80 % activity ^[2] . ACT-451840 shows efficacy in the Plasmodium berghei mouse model ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

- [1]. Bruderer S, et al. First-in-humans study of the safety, tolerability, and pharmacokinetics of ACT-451840, a new chemical entity with antimalarial activity. Antimicrob Agents Chemother. 2015;59(2):935-942.
- [2]. Boss C, et al. Discovery and Characterization of ACT-451840: an Antimalarial Drug with a Novel Mechanism of Action. ChemMedChem. 2016;11(18):1995-2014.
- [3]. Le Bihan A, et al. Characterization of Novel Antimalarial Compound ACT-451840: Preclinical Assessment of Activity and Dose-Efficacy Modeling. PLoS Med. 2016;13(10):e1002138. Published 2016 Oct 4.
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Caution: Product has not been fully validated for medical applications. For research use only.

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