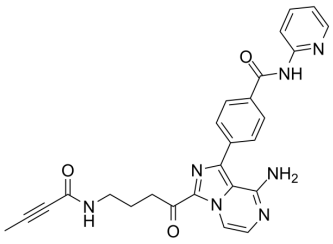
ACP-5862

Cat. No.:	HY-135334
CAS No.:	2230757-47-6
Molecular Formula:	$C_{26}H_{23}N_7O_3$
Molecular Weight:	481.51
Target:	Drug Metabolite; Btk; Cytochrome P450
Pathway:	Metabolic Enzyme/Protease; Protein Tyrosine Kinase/RTK
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 (519.20 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0768 mL	10.3840 mL	20.7680 mL
	5 mM	0.4154 mL	2.0768 mL	4.1536 mL
	10 mM	0.2077 mL	1.0384 mL	2.0768 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 (4.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ACP-5862 is a major active, circulating, pyrrolidine ring-opened metabolite of Acalabrutinib with an IC_{50} of 5.0 nM for Bruton tyrosine kinase (BTK). ACP‑5862 is a weak time‑dependent inactivator of CYP3A4 and CYP2C8. Acalabrutinib is an orally active, irreversible, and highly selective BTK inhibitor, with an IC_{50} of 3 nM and EC_{50} of 8 nM[1][2].

IC_{50} & Target		
	CYP2C8	CYP3A4

In Vivo

Following a single oral dose of 100 mg Acalabrutinib, the half‑life of ACP‑5862 is 6.9 hours and the mean exposure is approximately twofold to threefold higher than that of Acalabrutinib[2].

ACP-5862 (M27) is the major single metabolite in the systemic circulation and accountes for 57.4% and 42.1% of the AUC_{0-t} total radioactivity in male and female rat plasma, respectively. ACP-5862, the major human metabolite, is a relatively minor component in the systemic circulation and accountes for 6.1% and 8.1% of the AUC_{0-t} total radioactivity in male and female dog plasma, respectively[1].

ACP-5862 (1 or 10 μM) has reversible protein binding of 98.6%, 99.8%, 94.3%, 98.6% in mouse, rat, dog, and human plasma[1].

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

CUSTOMER VALIDATION

- Biochem Biophys Res Commun. 2021 Jan 1;534:995-1002.

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REFERENCES

[1]. Herman SE, et al. The Bruton's tyrosine kinase (BTK) inhibitor acalabrutinib demonstrates potent on-target effects and efficacy in two mouse models of chronic lymphocytic leukemia. Clin Cancer Res. 2016 Nov 30

[2]. Diansong Zhou, et al. Evaluation of the Drug-Drug Interaction Potential of Acalabrutinib and Its Active Metabolite, ACP-5862, Using a Physiologically-Based Pharmacokinetic Modeling Approach. CPT Pharmacometrics Syst Pharmacol. 2019 Jul;8(7):489-499.

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