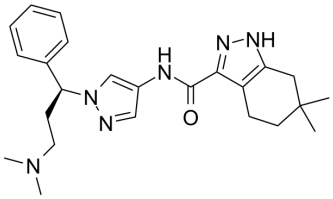
GNE-9822

Cat. No.:	HY-12410
CAS No.:	1557232-32-2
Molecular Formula:	$C_{24}H_{32}N_6O$
Molecular Weight:	420.55
Target:	Itk
Pathway:	Protein Tyrosine Kinase/RTK
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 : 62.5 mg/mL (148.61 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3778 mL	11.8892 mL	23.7784 mL
	5 mM	0.4756 mL	2.3778 mL	4.7557 mL
	10 mM	0.2378 mL	1.1889 mL	2.3778 mL

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

BIOLOGICAL ACTIVITY

Description

GNE-9822 is a potent, orally active and selective ITK inhibitor with a K_i value of 0.7 nM, and an EC_{50} value of 354.5 nM. GNE-9822 has good ADME properties. GNE-9822 can be used in research of asthma[1][2].

IC_{50} & Target

EC50: 354.5 nM (ITK)[2]

In Vitro

GNE-9822 (compound 28) inhibits the phosphorylation of PLCγ with an IC_{50} value of 55 nM[1].

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

In Vivo

GNE-9822 (compound 28; po and iv; 1 and 5 mg/kg) has good bioavailability and halflives observed in mouse and rats[1].

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Animal Model:	BALB/c mouse and Sprague-Dawley rats[1]
Dosage:	1 and 5 mg/kg

Administration:	po (5 mg/kg) and iv (1 mg/kg)

Result:

species	route	dose volume (mL/kg)	dose (mg/kg)	C_{max} (μM)	AUC (μM·h)	Cl (mL/min/kg)	$T_{1/2}$ (h)	V_{ss} (L/kg)	%F
mouse (BALB/c)	IV	1.0	1.0		1.5	40	2.9	10	
mouse (BALB/c)	PO	5.0	50	3.8	2.7				36

Animal Model:	BALB/c mouse and Sprague-Dawley rats[1]
Dosage:	1 and 5 mg/kg
Administration:	po (5 mg/kg) and iv (1 mg/kg)

Result:

species	route	dose volume (mL/kg)	dose (mg/kg)	C_{max} (μM)	AUC (μM·h)	Cl (mL/min/kg)	$T_{1/2}$ (h)	V_{ss} (L/kg)	%F
rat (Sprague-Dawley	IV	1.0	1.0		0.6	70	3.0	14	
rat (Sprague-Dawley	PO	2.0	5.0	0.2	1.1				40

REFERENCES

[1]. Burch JD, et, al. Property- and structure-guided discovery of a tetrahydroindazole series of interleukin-2 inducible T-cell kinase inhibitors. J Med Chem. 2014 Jul 10;57(13):5714-27.

[2]. Zhou D, et al. Discovery of Potent and Highly Selective Interleukin-2-Inducible T-Cell Kinase Degraders with In Vivo Activity. J Med Chem. 2023 Apr 13;66(7):4979-4998.

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