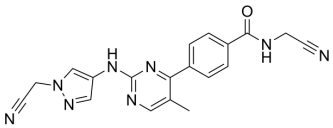
JAK-IN-21

Cat. No.:	HY-148060
CAS No.:	2445499-20-5
Molecular Formula:	$C_{19}H_{16}N_8O$
Molecular Weight:	372.38
Target:	JAK
Pathway:	Epigenetics; JAK/STAT Signaling; Protein Tyrosine Kinase/RTK; Stem Cell/Wnt
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 : 125 mg/mL (335.68 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.6854 mL	13.4271 mL	26.8543 mL
5 mM	0.5371 mL	2.6854 mL	5.3709 mL
10 mM	0.2685 mL	1.3427 mL	2.6854 mL

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

BIOLOGICAL ACTIVITY

Description

JAK-IN-21 (Example 4) is a selective and potent JAK inhibitor with IC_{50}s of 1.73, 2.04, 109 and 62.9 nM against JAK1, JAK2, J2V617F and TYK2, respectively[1].

IC_{50} & Target

JAK1	JAK2	Tyk2	JAK2-V617F
1.73 nM (IC_{50})	2.04 nM (IC_{50})	62.9 nM (IC_{50})	109 nM (IC_{50})

In Vitro

JAK-IN-21 (Example 4) doses not inhibit CYPs and shows good liver microsome stability[1].

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

In Vivo

JAK-IN-21 (Example 4) shows low bioavailability (F=1.9%)[1].

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

Animal Model:	SD rats[1]

Dosage:	10 mg/kg
Administration:	Oral gavage (Pharmacokinetic Study)
Result:	Rat Colon Pharmacokinetic Study[1]

Compound	Plasma C_{max} (ng/mL)	Plasma AUC (h*ng/mL)	$t_{1/2}$ (h)	Colon AUC (h*ng/g)	Colon + Feces AUC (h*ng/g)
JAK-IN-21	68.8	96	1.6	6,623	545,501

Animal Model:	SD rats[1]
Dosage:	1 mg/kg or 2 mg/kg
Administration:	Intravenous injection (1 mg/kg) or oral gavage (2 mg/kg) (Pharmacokinetic Study)
Result:	Pharmacokinetic Parameters in Sprague-Dawley Rats by Intravenous Administration and Oral Administration[1]

Compound	Dose (mg/kg)	AUC (h*ng/mL)	$T_{1/2}$ (h)	Cl (mL/min/kg)	Vd (L/kg)	C_{max} (ng/mL)	F (%)
JAK-IN-21 (iv)	1	854.8	0.22	19.4	0.37		
JAK-IN-21 (ig)	2	29.8	0.38			40.4	1.9

REFERENCES

[1]. Zhaokui WAN, et al. Benzamides of pyrazolyl-amino-pyrimidinyl derivatives, and compositions and methods thereof. Patent WO2020119819.

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