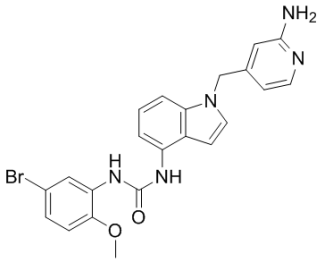
JI-101

Cat. No.:	HY-16265
CAS No.:	900573-88-8
Molecular Formula:	$C_{22}H_{20}BrN_5O_2$
Molecular Weight:	466.33
Target:	Ephrin Receptor; PDGFR; VEGFR
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 : ≥ 100 mg/mL (214.44 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	2.1444 mL	10.7220 mL	21.4440 mL
	5 mM	0.4289 mL	2.1444 mL	4.2888 mL
	10 mM	0.2144 mL	1.0722 mL	2.1444 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: ≥ 2.5 mg/mL (5.36 mM); Clear solution
2. Add each solvent one by one: **10% DMSO >> 90% (20% SBE-β-CD in saline)**
   Solubility: ≥ 2.5 mg/mL (5.36 mM); Clear solution
3. Add each solvent one by one: **10% DMSO >> 90% corn oil**
   Solubility: ≥ 2.5 mg/mL (5.36 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	JI-101 is an orally available multi-kinase inhibitor of **VEGFR2□PDGFRβ** and **EphB4** with potent anti-cancer activity.	
IC_{50} & Target	VEGFR2	PDGFRβ
In Vitro	JI-101 is found to be stable in all preclinical and human liver microsomes. The % metabolized is ranged between 3.03-	

	3.95 across the tested species liver microsomes. The % metabolized is relatively higher in mice liver microsomes followed by dog, human and rat liver microsomes[1].
In Vivo	JI-101excreted through bile along with its mono- and di-hydroxy metabolites. Following oral administration, JI-101 is rapidly absorbed, reaching C_{max} within 2 h. The $t_{1/2}$ of JI-101 with intravenous and oral route is found to be 1.75±0.79 and 2.66±0.13 h, respectively. The Cl and Vd by intravenous route for JI-101 are found to be 13.0±2.62 mL/min/kg and 2.11±1.42 L/kg, respectively. The tissue distribution of JI-101 is extensive with rapid and preferred uptake into lung tissue. Overall, the oral bioavailability of JI-101 is 55% and the primary route of elimination for JI-101 is feces[1].

PROTOCOL

Animal Administration [1]	Rats: Pharmacokinetics and bioavailability assessment of JI-101 are evaluated in a preliminary parallel-group study in male S.D. rats. Four rats (195–210 g) per route receive JI-101 at a dose of 3 and 30 mg/kg for i. v. (via tail vein) and oral dose (by gavage), respectively. Serial blood samples (100 μL) are collected from retro-orbital plexus at pre-dose, 0.12 (i. v. only) 0.25, 0.5, 1, 2, 4, 8, 10 (oral only) and 24 h. Blood samples are collected in tubes containing K_2 EDTA as the anticoagulant and centrifuged for 5 min maintained at 4 °C for plasma separation and stored frozen at −80±10 °C until analysis[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Gurav SD, et al. Pharmacokinetics, tissue distribution and identification of putative metabolites of JI-101 - a novel triple kinase inhibitor in rats. Arzneimittelforschung. 2012 Jan;62(1):27-34.

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