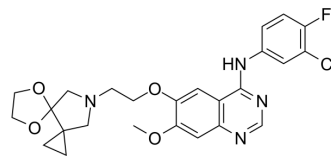


Simotinib

Cat. No.:	HY-101820		
CAS No.:	944258-89-3		
Molecular Formula:	C ₂₅ H ₂₆ ClFN ₄ O ₄		
Molecular Weight:	500.95		
Target:	EGFR		
Pathway:	JAK/STAT Signaling; 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 : 125 mg/mL (249.53 mM; ultrasonic and adjust pH to 3 with HCl)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	1.9962 mL	9.9810 mL	19.9621 mL
		5 mM	0.3992 mL	1.9962 mL	3.9924 mL
10 mM		0.1996 mL	0.9981 mL	1.9962 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (4.15 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.08 mg/mL (4.15 mM); Suspended solution; Need ultrasonic Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.15 mM); Clear solution 				

BIOLOGICAL ACTIVITY

Description	Simotinib is a selective, specific, and orally bioavailable EGFR tyrosine kinase inhibitor, with an IC ₅₀ of 19.9 nM. Antineoplastic activities ^[1] .
IC₅₀ & Target	EGFR 19.9 nM (IC ₅₀)
In Vitro	Simotinib inhibits in a dose-dependent manner EGFR and the growth of human A431 tumor cells with high expression of

EGFR, with no significant activity on other investigated kinases^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Simotinib has been shown to exert its antitumor activity by inhibiting EGFR phosphorylation in nude xenograft model^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Hu XS, et al. Safety, tolerability, and pharmacokinetics of simotinib, a novel specific EGFR tyrosine kinase inhibitor, in patients with advanced non-small cell lung cancer: results of a phase Ib trial. *Cancer Manag Res.* 2019;11:4449-4459. Published 2019

Caution: Product has not been fully validated for medical applications. For research use only.

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