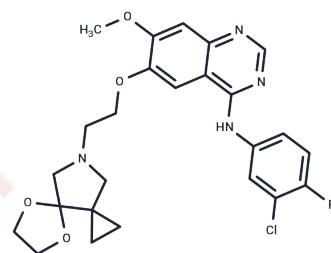


Simotinib

Chemical Properties

CAS No. :	944258-89-3
Formula:	C ₂₅ H ₂₆ ClFN ₄ O ₄
Molecular Weight:	500.95
Storage:	Store at low temperature Powder: -20°C for 3 years In solvent: -80°C for 1 year <i>Actual storage temperature shall be subject to the COA.</i>



Biological Description

Description	Simotinib (AL-6802) is a selective and orally bioactive EGFR tyrosine kinase inhibitor (IC ₅₀ : 19.9 nM) with anti-tumour activity for the study of non-small cell lung cancer.
Targets(IC ₅₀)	EGFR
In vitro	In vitro studies have shown that sunitinib inhibits the growth of EGFR and EGFR-overexpressing human A431 tumor cells in a dose-dependent manner, with no significant activity against other kinases examined in the study[1].
In vivo	Multiple doses of sunitinib reduced rat body weight by decreasing food intake, similar to human patients, indicating adverse effects of sunitinib on the gastrointestinal tract[2].

Solubility Information

Solubility	DMSO: 10 mg/mL (19.96 mM), when pH is adjusted to 3 with HCl. Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (2 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9962 mL	9.981 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
50 mM	0.0399 mL	0.1996 mL	0.3992 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.

Zhu Q, et al. Drug interaction studies reveal that simotinib upregulates intestinal absorption by increasing the paracellular permeability of intestinal epithelial cells. *Drug Metab Pharmacokinet.* 2014;29(4):317-24.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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