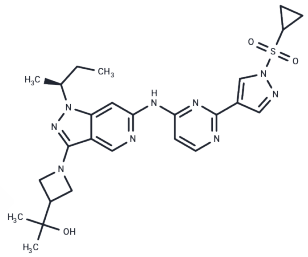
Data Sheet (Cat.No.T11159)

TargetMol

EGFR-IN-2

Chemical Properties



CAS No. : 1643497-70-4

Formula: C26H33N9O3S

Molecular Weight: 551.66

Storage: Store at low temperature,Keep away from moisture
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	EGFR-IN-2 is a non-covalent, orally available and mutation-selective EGFR inhibitor for the treatment of non-small cell lung cancer (NSCLC), with high selectivity for resistant single and double mutant T790M with IC50 = 27 nm to 33 nM, and low inhibitory activity for wild-type H292 (IC50 = 218 nM).
Targets(IC50)	EGFR
In vitro	EGFR-IN-2 (Compound 21) demonstrated excellent inhibitory activity in various EGFR-mutant NSCLC cell lines. Inhibition of EGFR autophosphorylation was evaluated in H1975 (T790M/L858R), PC9-ER (T790M/del746-750), and PC9 (del746-750) cell lines, with IC_{50} values of 0.027 μM, 0.008 μM, and 0.033 μM respectively. In a kinase panel of 225 kinases, only 12 were inhibited >70% at 0.1 μM, demonstrating high target specificity. EGFR-IN-2 exhibited low clearance in human liver microsomes and hepatocytes (3.8 and 2.7 mL/min/kg, respectively), and good predicted oral bioavailability [1].
In vivo	In a H1975 xenograft mouse model, EGFR-IN-2 was evaluated for in vivo target engagement and pharmacokinetics. After oral administration at 50 mg/kg, free plasma concentrations remained above the in vitro IC_{50} (0.027 μM) for up to 8 hours; at 100 mg/kg, this duration extended to 16 hours. Corresponding suppression of phosphorylated EGFR, ERK1/2, and AKT confirmed effective target inhibition in vivo. The EGFR-IN-2 exhibited moderate plasma clearance in mice (104 mL/min/kg) with 19% oral bioavailability, and in dogs, clearance was 13 mL/min/kg with 30% bioavailability[1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.8127 mL	9.0636 mL	18.1271 mL
5 mM	0.3625 mL	1.8127 mL	3.6254 mL
10 mM	0.1813 mL	0.9064 mL	1.8127 mL
50 mM	0.0363 mL	0.1813 mL	0.3625 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

Chan BK, et al. Discovery of a Noncovalent, Mutant-Selective Epidermal Growth Factor Receptor Inhibitor. J Med Chem. 2016 Oct 13;59(19):9080-9093.