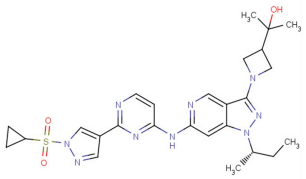
Data Sheet (Cat.No.T11159)

TargetMol
A DRUG SCREENING EXPERT

EGFR-IN-2

Chemical Properties



CAS No.:	1643497-70-4
Formula:	C26H33N9O3S
Molecular Weight:	551.66
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	EGFR-IN-2 is a non-covalent, mutation-selective and irreversible second-generation EGFR inhibitor.
Targets(IC_{50})	EGFR: None
In vitro	EGFR-IN-2 demonstrats strong antiproliferative effect on the T790M mutant carrying H1975 cell line (IC50=0.361 μM) and the single activating mutant PC9 cell line (IC50=0.151 μM). Furthermore, EGFR-IN-2 also shows good selectivity against other kinases when evaluated in a 225-kinase panel (12/225 kinases inhibited at >70% when tested at 0.1 μM, 61-fold over the TMLR Ki and 63-fold over the TMdel Ki).In addition, EGFR-IN-2 inhibits EGFR autophosphorylation with IC50s of 0.027 μM, 0.009 μM ,0.033 μM , and 0.218 μM in double mutant TMLR cell line H1975, double mutant TMdel cell line PC9-ER, activating mutant del<sub<746-750 cell line PC9, and wild type cell line H292.
In vivo	To examine its inhibitory effect on pEGFR levels in vivo, EGFR-IN-2 is studied in a mouse H1975 (TMLR) xenograft model. After a single oral dose of 21 at 50 mg/kg, free plasma concentrations of EGFR-IN-2 at or exceeding the in vitro p-EGFR IC50 of 0.027 μM are sustained over 8 h. When administered at 100 mg/kg, the coverage of p-EGFR IC50 is extended to the last measured time point of 16 h postdose. Corresponding knockdown of p-EGFR and the downstream effectors pERK1/2 and AKT levels are observed at those time points, suggesting target engagement in vivo.

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.813 mL	9.064 mL	18.127 mL
5 mM	0.363 mL	1.813 mL	3.625 mL
10 mM	0.181 mL	0.906 mL	1.813 mL
50 mM	0.036 mL	0.181 mL	0.363 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.

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