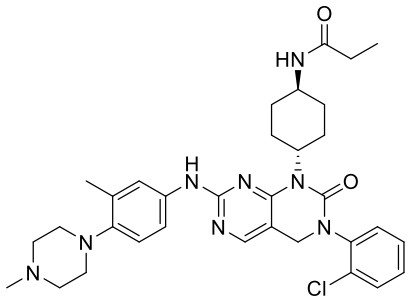
Product data sheet

MedKoo Cat#: 407933 Name: JND3229 CAS: 2260886-64-2 Chemical Formula: $C_{33}H_{41}ClN_8O_2$ Exact Mass: 616.3041 Molecular Weight: 617.195	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
JND3229 is a New EGFRC797S Mutant Inhibitor with In Vivo Monodrug Efficacy (IC50 = 5.8 nM). JND3229 potently inhibited EGFRC797S mutated kinase and strongly suppressed the proliferation of BaF3 cells harboring the EGFRL858R/T790M/C797S and EGFR19D/T790M/C797S mutations with IC50 values of 0.51 and 0.32 μM, respectively.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	56.25	91.14
Ethanol	100.0	162.02

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.62 mL	8.10 mL	16.20 mL
5 mM	0.32 mL	1.62 mL	3.24 mL
10 mM	0.16 mL	0.81 mL	1.62 mL
50 mM	0.03 mL	0.16 mL	0.32 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Lu X, Zhang T, Zhu SJ, Xun Q, Tong L, Hu X, Li Y, Chan S, Su Y, Sun Y, Chen Y, Ding J, Yun CH, Xie H, Ding K. Discovery of JND3229 as a New EGFRC797S Mutant Inhibitor with In Vivo Monodrug Efficacy. ACS Med Chem Lett. 2018 Oct 8;9(11):1123-1127. doi: 10.1021/acsmedchemlett.8b00373. PMID: 30429956; PMCID: PMC6231186.

In vivo study

1. Lu X, Zhang T, Zhu SJ, Xun Q, Tong L, Hu X, Li Y, Chan S, Su Y, Sun Y, Chen Y, Ding J, Yun CH, Xie H, Ding K. Discovery of JND3229 as a New EGFRC797S Mutant Inhibitor with In Vivo Monodrug Efficacy. ACS Med Chem Lett. 2018 Oct 8;9(11):1123-1127. doi: 10.1021/acsmedchemlett.8b00373. PMID: 30429956; PMCID: PMC6231186.

7. Bioactivity
Biological target:

JND3229 is a reversible $EGFR^{C797S}$ inhibitor with IC50 values of 5.8, 6.8 and 30.5 nM for $EGFR^{L858R/T790M/C797S}$, $EGFR^{WT}$ and $EGFR^{L858R/T790M,}$ respectively.

In vitro activity

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The strong kinase inhibition of JND3229 was further validated by investigating its potential suppression on activity of EGFR signals in BaF3 cells stably transfected with $EGFR^{L858R/T790M/C797S}$ and $EGFR^{19D/T790M/C797S}$ (Figure 3). It was shown that JND3229 potently inhibited the phosphorylation of $EGFR^{L858R/T790M/C797S}$ and $EGFR^{19D/T790M/C797S}$ in a dose-dependent manner. Consistent with its nonselective inhibition against $EGFR^{WT}$, JND3229 also obviously suppressed the proliferation of A431 cancer cells overexpressing $EGFR^{WT}$ with an IC_{50} value of 0.27 μM.

Reference: ACS Med Chem Lett. 2018 Oct 8;9(11):1123-1127. https://pubmed.ncbi.nlm.nih.gov/30429956/

In vivo activity

The in vivo anticancer efficacy of JND3229 was also examined using a xenograft mouse model. The data showed that administration of JND3229 caused an obvious suppression of tumor growth with a tumor growth inhibition (TGI) value of 42.2% (Figure 5A), which was more potent than that of EAI045/cetuximab combination (TGI = 22.3%, Figure 5B).

Reference: ACS Med Chem Lett. 2018 Oct 8;9(11):1123-1127. https://pubmed.ncbi.nlm.nih.gov/30429956/