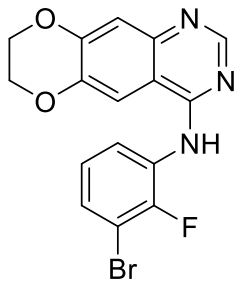
Product data sheet

MedKoo Cat#: 462076 Name: JCN037 CAS: 2305154-31-6 Chemical Formula: $C_{16}H_{11}BrFN_3O_2$ Exact Mass: 375.0019 Molecular Weight: 376.1854	
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:
JCN037 is a potent brain-penetrant EGFR tyrosine kinase inhibitor against malignant brain tumors. JCN037 displayed potent activity against EGFR amplified/mutant patient-derived cell cultures, significant BBB penetration (2:1 brain-to-plasma ratio), and superior efficacy in an EGFR-driven orthotopic glioblastoma xenograft model.

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	250.0	664.57

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.66 mL	13.29 mL	26.58 mL
5 mM	0.53 mL	2.66 mL	5.32 mL
10 mM	0.27 mL	1.33 mL	2.66 mL
50 mM	0.05 mL	0.27 mL	0.53 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. Tsang JE, Urner LM, Kim G, Chow K, Baufeld L, Faull K, Cloughesy TF, Clark PM, Jung ME, Nathanson DA. Development of a Potent Brain-Penetrant EGFR Tyrosine Kinase Inhibitor against Malignant Brain Tumors. ACS Med Chem Lett. 2020 May 1;11(10):1799-1809. doi: 10.1021/acsmedchemlett.9b00599. PMID: 33062157; PMCID: PMC7549123.

In vivo study

1. Tsang JE, Urner LM, Kim G, Chow K, Baufeld L, Faull K, Cloughesy TF, Clark PM, Jung ME, Nathanson DA. Development of a Potent Brain-Penetrant EGFR Tyrosine Kinase Inhibitor against Malignant Brain Tumors. ACS Med Chem Lett. 2020 May 1;11(10):1799-1809. doi: 10.1021/acsmedchemlett.9b00599. PMID: 33062157; PMCID: PMC7549123.

7. Bioactivity
Biological target:

JCN037 (JGK037) is non-covalent and BBB-penetrant EGFR tyrosine kinase inhibitor, with IC_{50} values of 2.49 nM, 3.95 nM, 4.48 nM for EGFR, p-wtEGFR and pEGFRvIII, respectively.

In vitro activity

Product data sheet

Together, these results indicate that 5 (JCN037) can potently inhibit the signaling and growth of EGFRvIII mutant and EGFR amplified primary GBM cells at levels on par with or better than that of both erlotinib and lapatinib.

Reference: ACS Med Chem Lett. 2020 May 1;11(10):1799-1809. https://pubmed.ncbi.nlm.nih.gov/33062157/

In vivo activity

Conversely, tumors from 5 (JCN037)-treated mice showed a significant decrease in EGFRvIII activity that was associated with reduced RAS-MAPK and PI3K-AKT-mTOR signaling (Figure 2B and C). These data support the hypothesis that the heightened BBB penetration of 5 would result in a greater capacity to inhibit EGFR signaling in an orthotopic GBM xenograft model.

Reference: ACS Med Chem Lett. 2020 May 1;11(10):1799-1809. https://pubmed.ncbi.nlm.nih.gov/33062157/