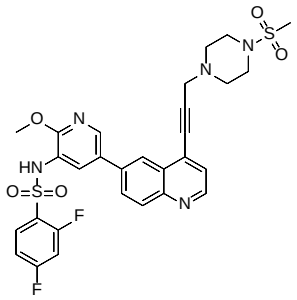
Product data sheet

MedKoo Cat#: 564415 Name: NSC781406 CAS: 1676893-24-5 Chemical Formula: $C_{29}H_{27}F_2N_5O_5S_2$ Exact Mass: 627.1422 Molecular Weight: 627.6818	
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:
NSC781406 is a highly potent PI3K/mTOR dual inhibitor, exhibiting potent tumor growth inhibition in the hepatocellular carcinoma BEL-7404 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
DMF	10.0	15.93
DMSO	85.0	135.42
DMSO:PBS (pH 7.2) (1:4)	0.2	0.32

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.59 mL	7.97 mL	15.93 mL
5 mM	0.32 mL	1.59 mL	3.19 mL
10 mM	0.16 mL	0.80 mL	1.59 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. Guo Y, Zhu H, Weng M, Zhang H, Wang C, Sun L. CC-223, NSC781406, and BGT226 Exerts a Cytotoxic Effect Against Pancreatic Cancer Cells via mTOR Signaling. Front Pharmacol. 2020 Nov 11;11:580407. doi: 10.3389/fphar.2020.580407. PMID: 33343350; PMCID: PMC7741184.

In vivo study

1. Chen Y, Zhang L, Yang C, Han J, Wang C, Zheng C, Zhou Y, Lv J, Song Y, Zhu J. Discovery of benzenesulfonamide derivatives as potent PI3K/mTOR dual inhibitors with in vivo efficacies against hepatocellular carcinoma. Bioorg Med Chem. 2016 Mar 1;24(5):957-66. doi: 10.1016/j.bmc.2016.01.008. Epub 2016 Jan 6. PMID: 26819001.

7. Bioactivity
Biological target:

NSC781406 is a highly potent PI3K and mTOR inhibitor with an IC_{50} of 2 nM for PI3Kα.

In vitro activity

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Consistently, the proliferation ability of SW1990, Patu8988, BxPC-3, and CFPAC-1 cells reduced within 24 h after treatment with CC-223, NSC781406, and BGT226 inhibitors (Figures 2E,H). Colony formation assay confirmed that CC-223, NSC781406, and BGT226 inhibitors constrained the proliferation and clone formation of PANC-1 cells (Figures 3A,B).

Reference: Front Pharmacol. 2020 Nov 11;11:580407. https://pubmed.ncbi.nlm.nih.gov/33343350/

In vivo activity

Compound 7k (NSC781406) was identified as a highly potent dual inhibitor, which exhibited potent tumor growth inhibition in the hepatocellular carcinoma BEL-7404 xenograft model. Compound 7k may be a potential therapeutic drug candidate for HCC.

Reference: Bioorg Med Chem. 2016 Mar 1;24(5):957-66. https://pubmed.ncbi.nlm.nih.gov/26819001/