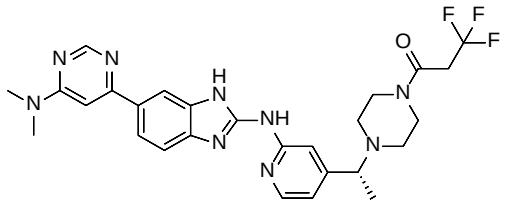
Product data sheet

MedKoo Cat#: 408059 Name: BAY-985 CAS#: 2409479-29-2 (R-isomer) Chemical Formula: $C_{27}H_{30}F_3N_9O$ Exact Mass: 553.2525 Molecular Weight: 553.59	
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:
BAY-985 is a dual inhibitor of TANK-binding kinase 1 (TBK1) and IκB kinase ε (IKKε; IC50 = 2 nM for both). It is selective for TBK1 and IKKε over FLT3, RSK4, DRAK1, and ULK1 (IC50s = 123, 276, 311, and 7,390 nM, respectively). BAY-985 inhibits phosphorylation of interferon regulatory factor 3 (IRF3) in MDA-MB-231 cells expressing mouse IRF3 (IC50 = 74 nM). It inhibits the proliferation of SK-MEL-2 cells in vitro (IC50 = 900 nM) and reduces tumor weight in an SK-MEL-2 mouse xenograft model when administered at a dose of 200 mg/kg.

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	30.0	54.19
DMF:PBS (pH 7.2) (1:2)	0.30	0.54
DMSO	75.0	135.48

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.81 mL	9.03 mL	18.06 mL
5 mM	0.36 mL	1.81 mL	3.61 mL
10 mM	0.18 mL	0.90 mL	1.81 mL
50 mM	0.04 mL	0.18 mL	0.36 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. Lefranc J, Schulze VK, Hillig RC, Briem H, Prinz F, Mengel A, Heinrich T, Balint J, Rengachari S, Irlbacher H, Stöckigt D, Bömer U, Bader B, Gradl SN, Nising CF, von Nussbaum F, Mumberg D, Panne D, Wengner AM. Discovery of BAY-985, a Highly Selective TBK1/IKKε Inhibitor. J Med Chem. 2020 Jan 23;63(2):601-612. doi: 10.1021/acs.jmedchem.9b01460. Epub 2020 Jan 10. PMID: 31859507.

In vivo study

1. Lefranc J, Schulze VK, Hillig RC, Briem H, Prinz F, Mengel A, Heinrich T, Balint J, Rengachari S, Irlbacher H, Stöckigt D, Bömer U, Bader B, Gradl SN, Nising CF, von Nussbaum F, Mumberg D, Panne D, Wengner AM. Discovery of BAY-985, a Highly Selective TBK1/IKKε Inhibitor. J Med Chem. 2020 Jan 23;63(2):601-612. doi: 10.1021/acs.jmedchem.9b01460. Epub 2020 Jan 10. PMID: 31859507.

7. Bioactivity

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Biological target: BAY-985 is a dual inhibitor of TBK1 and IKKε with IC50s of 2/30 and 2 nM for TBK1 (low/high ATP) and IKKε, respectively.

In vitro activity

BAY-985 inhibited the cellular phosphorylation of interferon regulatory factor 3 and displayed antiproliferative efficacy in the melanoma cell line SK-MEL-2.

Reference: J Med Chem. 2020 Jan 23;63(2):601-612. https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.9b01460

In vivo activity

BAY-985 showed only weak antitumor activity in the SK-MEL-2 human melanoma xenograft model.

Reference: J Med Chem. 2020 Jan 23;63(2):601-612. https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.9b01460

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.