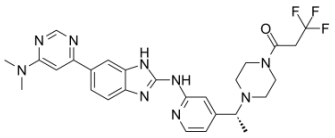
BAY-985

Cat. No.:	HY-133117
CAS No.:	2409479-29-2
Molecular Formula:	$C_{27}H_{30}F_3N_9O$
Molecular Weight:	553.58
Target:	IKK
Pathway:	NF-κB

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (90.32 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8064 mL	9.0321 mL	18.0642 mL
	5 mM	0.3613 mL	1.8064 mL	3.6128 mL
	10 mM	0.1806 mL	0.9032 mL	1.8064 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.76 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.76 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.76 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-985 is a highly potent, orally active and selective ATP-competitive dual inhibitor of TBK1 and IKKε with IC_{50}s of 2/30 and 2 nM for TBK1 (low/high ATP) and IKKε, respectively. Antitumor efficacy[1].

IC_{50} & Target	TBK1	TBK1	IKKε
	2 nM (IC_{50}, low ATP)	30 nM (IC_{50}, high ATP)	2 nM (IC_{50})

In Vitro

BAY-985 inhibits FLT3, RSK4, DRAK1, and ULK1 with IC_{50}s of 123, 276, 311, and 7930 nM, respectively[1].

BAY-985 inhibits the cellular phosphorylation of interferon regulatory factor 3 (IRF3) with an IC_{50} of 74 nM[1].
BAY-985 is active in cellular mechanistic assay and shows anti-proliferative activity in a few cancer cell lines with IC_{50}s of 900 and 7260 nM for SK-MEL2 (NRAS and TP53 mutated) and ACHN (CDKN2A mutated) cells, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	ACHN and SK-MEL-2 cell lines
Concentration:	
Incubation Time:	96 hours
Result:	Inhibited proliferation in SK-MEL2 and ACHN cells with IC_{50}s of 900 and 7260 nM, respectively.

In Vivo

BAY-985 (200 mg/kg; p.o.; b.i.d.; 111 days) results in weak antitumor efficacy[1].
BAY-985 shows high clearance (CL_b= 4.0 L/h/kg, ca. 95% hepatic extraction), large volume of distribution at steady state (V_{ss} =2.9 L/kg) and a short terminal half-life ($t_{1/2}$=0.79 h)[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female NMRI nude mice bearing SK-MEL-2 human melanoma xenograft model[1]
Dosage:	200 mg/kg
Administration:	Applied p.o.; twice daily (b.i.d.) continuously 111 days
Result:	Treatment resulted in weak antitumor efficacy with a $T/C_{tumor\ weight}$ ratio of 0.6. The treatment was well tolerated, with a maximum body weight loss of less than 10%.

REFERENCES

[1]. Lefranc J, et al. Discovery of BAY-985, a Highly Selective TBK1/IKKε Inhibitor. J Med Chem. 2020 Jan 10.

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