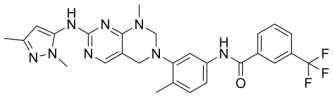
XMU-MP-3

Cat. No.:	HY-136531
CAS No.:	2031152-08-4
Molecular Formula:	$C_{27}H_{27}F_3N_8O$
Molecular Weight:	536.55
Target:	Btk; Apoptosis
Pathway:	Protein Tyrosine Kinase/RTK; Apoptosis
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 : 100 mg/mL (186.38 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8638 mL	9.3188 mL	18.6376 mL
	5 mM	0.3728 mL	1.8638 mL	3.7275 mL
	10 mM	0.1864 mL	0.9319 mL	1.8638 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: ≥ 2.5 mg/mL (4.66 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

XMU-MP-3 is a potent non-covalent BTK inhibitor with IC_{50}s of 10.7 nM and 17.0 nM for BTK WT and BTK C481S mutation in the presence of 10 μM ATP, respectively. XMU-MP-3 also induces apoptosis[1].

IC_{50} & Target

IC50: 10.7 nM (BTK WT), 17.0 nM (BTK C481S), Apoptosis[1]

In Vitro

XMU-MP-3 (0.001-10000 nM; 48 hours) inhibits BTK-transformed Ba/F3 cell proliferation with an IC_{50} of 11.4 nM[1].
XMU-MP-3 (1-10000 nM) inhibits the proliferation of JeKo-1, Ramos and NALM-6 with IC_{50} values of 326.6 nM, 685.6 nM and 1065 nM, respectively[1].
XMU-MP-3 (0.001-10000 nM) maintains inhibitory potency with an IC_{50} of 182.3 nM against BTK(C481S)-Ba/F3 cells[1].
XMU-MP-3 (5000 nM) induces apoptosis in BTK (C481S) Ba/F3 cells[1].

XMU-MP-3 (10-1000 nM; 4 hours) inhibits both the auto- and trans-phosphorylation of BTK at the site of Y223 and Y551 in a dose-dependent manner in BTK-transformed Ba/F3 cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	BTK-transformed and parental Ba/F3 cells
Concentration:	0.001, 0.01, 0.1, 1, 10, 100, 1000, 10000 nM
Incubation Time:	48 hours
Result:	Inhibited BTK-transformed Ba/F3 cell proliferation with an IC_{50} of 11.4 nM, while it showed negligible anti-proliferative effects on parental wild-type Ba/F3 cells (IC_{50} >10000 nM).

Western Blot Analysis[1]

Cell Line:	BTK-transformed Ba/F3 cells
Concentration:	10, 50, 100, 500, 1000 nM
Incubation Time:	4 hours
Result:	The phosphorylation levels of BTK Y223 and Y551 were reduced significantly at concentrations as low as 100 nM, and completely suppressed at the concentration of 1000 nM.

In Vivo

XMU-MP-3 (25 and 50 mg/kg) substantially suppresses tumor growth in mouse xenograft models[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Nu/nu BALB/c mice (4-6 weeks of age) bearing BTK-transformed Ba/F3 and Ramos xenograft models[1]
Dosage:	25 and 50 mg/kg
Administration:	Treated by tail vein injection; the injection volume was 0.1 mL per 10 g; daily for 14 days
Result:	Significantly reduced the tumor size without affecting animal weights.

REFERENCES

[1]. Fu Gui, et al. A Non-Covalent Inhibitor XMU-MP-3 Overrides Ibrutinib-Resistant Btk C481S Mutation in B-cell Malignancies. Br J Pharmacol. 2019 Dec;176(23):4491-4509.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA