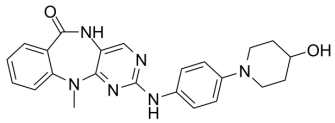
XMD16-5

Cat. No.:	HY-101243
CAS No.:	1345098-78-3
Molecular Formula:	$C_{23}H_{24}N_6O_2$
Molecular Weight:	416.48
Target:	Tyrosinase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (240.11 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4011 mL	12.0054 mL	24.0108 mL
	5 mM	0.4802 mL	2.4011 mL	4.8022 mL
	10 mM	0.2401 mL	1.2005 mL	2.4011 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 (6.00 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.00 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	XMD16-5 is a potent TNK2 inhibitor with IC_{50} values of 16 and 77 nM for the D163E and R806Q mutations, respectively.
IC_{50} & Target	IC50: 16 nM (TNK2, D163E mutation), 77 nM (TNK2, R806Q mutation)[1]
In Vitro	XMD16-5 potently inhibits the growth of the TNK2 mutant expressing cell lines while having little or no effect on the control cells out to the highest tested concentrations (1,000 nM). XMD16-5 has IC_{50}s of 16 nM and 77 nM for the D163E and R806Q mutations. The effects of XMD16-5 on TNK2 cell lines are largely due to on-target effects on TNK2. Auto-phosphorylation of overexpressed TNK2 mutants could be blocked with TNK2 inhibitor XMD16-5[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	Kinase targets are tested with biochemical enzymatic kinase assays using the SelectScreen Kinase Profiling Service to determine IC_{50} values. The compounds (XMD16-5) are assayed at 10 concentrations (3-fold serial dilutions starting from 1 μM) at an ATP concentration equal to the ATP Km[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Cell Assay [1]	Cells are treated with the following inhibitors for 72 hours: dasatinib, AIM-100, XMD8-87 and XMD16-5. Cell viability is measured using a methanethiosulfonate (MTS)-based assay and absorbance (490 nm) is read at 1 and 3 hours after adding reagent[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Maxson JE, et al. Identification and Characterization of Tyrosine Kinase Nonreceptor 2 Mutations in Leukemia through Integration of Kinase Inhibitor Screening and Genomic Analysis.

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