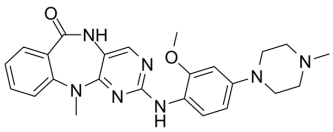
XMD8-87

Cat. No.:	HY-15811
CAS No.:	1234480-46-6
Molecular Formula:	$C_{24}H_{27}N_7O_2$
Molecular Weight:	445.52
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 : ≥ 26 mg/mL (58.36 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2446 mL	11.2228 mL	22.4457 mL
	5 mM	0.4489 mL	2.2446 mL	4.4891 mL
	10 mM	0.2245 mL	1.1223 mL	2.2446 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 (4.67 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.67 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

XMD8-87 is a potent TNK2 inhibitor with IC_{50} values of 38 and 113 nM for the D163E and R806Q mutations, respectively.

IC_{50} & Target

IC50: 38 nM (TNK2, D163E mutation), 113 nM (TNK2, R806Q mutation)[1]

In Vitro

XMD8-87 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). XMD8-87 has IC_{50}s of 38 nM and 113 nM for the D163E and R806Q mutations. The effects of XMD8-87 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 XMD8-87[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 (XMD8-87) 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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