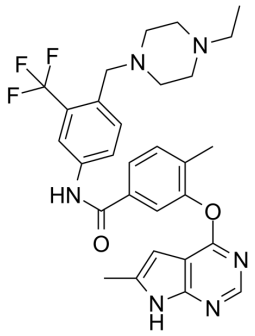
TAK1/MAP4K2 inhibitor 1

Cat. No.:	HY-77251
CAS No.:	1315330-11-0
Molecular Formula:	$C_{29}H_{31}F_3N_6O_2$
Molecular Weight:	552.59
Target:	MAP4K; MAP3K
Pathway:	MAPK/ERK Pathway
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 : 50 mg/mL (90.48 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8097 mL	9.0483 mL	18.0966 mL
5 mM	0.3619 mL	1.8097 mL	3.6193 mL
10 mM	0.1810 mL	0.9048 mL	1.8097 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: ≥ 2.75 mg/mL (4.98 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.75 mg/mL (4.98 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TAK1/MAP4K2 inhibitor 1 is a potent dual TGFβ-activated kinase 1 (TAK1) and mitogen-activated protein kinase kinase kinase kinase 2 (MAP4K2) inhibitor, with IC_{50}s of 41.1 nM and 18.2 nM, respectively.

IC_{50} & Target

TAK1	MAP4K2
41.1 nM (IC_{50})	18.2 nM (IC_{50})

In Vivo

TAK1/MAP4K2 inhibitor 1 has moderate terminal elimination half-life ($t_{1/2}$=2.94 h for mice (1 mg/kg, iv))[1].

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

CUSTOMER VALIDATION

- Korean J Physiol Pharmacol. 2022 Nov 1;26(6):469-478.

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REFERENCES

[1]. Tan L, et al. Discovery of type II inhibitors of TGFβ-activated kinase 1 (TAK1) and mitogen-activated protein kinase kinase kinase kinase 2 (MAP4K2). J Med Chem. 2015 Jan 8;58(1):183-96.

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