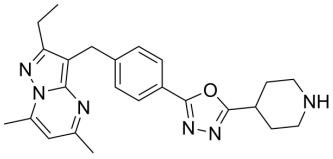
NE 52-QQ57

Cat. No.:	HY-101784
CAS No.:	1401728-56-0
Molecular Formula:	$C_{24}H_{28}N_6O$
Molecular Weight:	416.52
Target:	GPR4
Pathway:	GPCR/G Protein

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 : 20 mg/mL (48.02 mM; ultrasonic and warming and adjust pH to 5 with HCl and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.4008 mL	12.0042 mL	24.0085 mL
5 mM	0.4802 mL	2.4008 mL	4.8017 mL
10 mM	0.2401 mL	1.2004 mL	2.4008 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 mg/mL (4.80 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2 mg/mL (4.80 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2 mg/mL (4.80 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NE 52-QQ57 is a selective, and orally available GPR4 antagonist with an IC_{50} of 70 nM. NE 52-QQ57 has anti-inflammatory activity[1].

IC_{50} & Target

IC50: 70 nM (GPR4)[1].

In Vitro

NE 52-QQ57 effectively blocks GPR4-mediated cAMP accumulation (IC_{50} 26.8 nM in HEK293 cells)[2].

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

In Vivo

NE 52-QQ57 (Compound 13) shows a significant anti-inflammatory effect in the rat antigen induced arthritis model after oral administration at 30 mg/kg bid for 20 days[1].NE 52-QQ57 (30 mg/kg bid po for 4 days) also prevents angiogenesis in the mouse chamber model as well as pain as demonstrated in the rat complete Freund's adjuvant model[1].

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

Animal Model:	Female FVB mice (8-10 weeks)[1]
Dosage:	30 mg/kg
Administration:	Oral, 4 days, bid
Result:	Treatment at 30 mg/kg p.o. bid starting on day 0, the day of the chamber implantation, showed a statistically significant reduction (46.8±10.6%) of tissue growth by day 4. The blood levels of 13 on day 4 at 2 and 16 h after compound application in this model were 9.03±2.87 and 0.09±0.06 μM[1].

Animal Model:	Male Wistar Han rats[1]
Dosage:	3, 10, and 30 mg/kg
Administration:	Oral, 20 days, bid
Result:	Displayed not only higher exposures in the rat AIA but also lower plasma protein binding in rat (95%)[1].

CUSTOMER VALIDATION

- Cell Death Dis. 2022 Feb 14;13(2):152.
- Preprints. 2021, 2021040223.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Velcicky J, et al. Development of Selective, Orally Active GPR4 Antagonists with Modulatory Effects on Nociception, Inflammation, and Angiogenesis. J Med Chem. 2017 May 11;60(9):3672-3683.

[2]. Hosford PS, et al. CNS distribution, signalling properties and central effects of G-protein coupled receptor 4. Neuropharmacology. 2018 Aug;138:381-392.

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