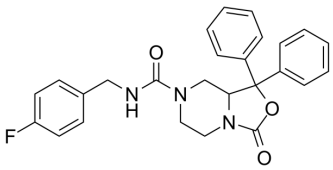
SHA 68

Cat. No.:	HY-108625
CAS No.:	847553-89-3
Molecular Formula:	$C_{26}H_{24}FN_3O_3$
Molecular Weight:	445.49
Target:	Neuropeptide Y Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
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 : 250 mg/mL (561.18 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2447 mL	11.2236 mL	22.4472 mL
	5 mM	0.4489 mL	2.2447 mL	4.4894 mL
	10 mM	0.2245 mL	1.1224 mL	2.2447 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% corn oil
   Solubility: ≥ 2.08 mg/mL (4.67 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SHA 68 is a potent and selective non-peptide neuropeptide S receptor (NPSR) antagonist with IC_{50}s of 22.0 and 23.8 nM for NPSR Asn^{107} and NPSR Ile^{107}, respectively. SHA 68 has limited the blood-brain barrier (BBB) penetration and the activity in neuralgia[1][2].

IC_{50} & Target

IC50: 22 nM (Asn^{107}) and 23.8 nM (Ile^{107})[1]

In Vivo

SHA 68 (i.p.; 5 and 50 mg/kg) reduces NPS-induced horizontal activity and vertical rearing and climbing[1].
SHA 68 (i.v.; 1 mg/kg) has a $T_{1/2}$ of 0.74 hours, a CL of 4.29 mL/min/kg, and a V_{ss} of 2.53 L/kg[1].
SHA 68 (i.p.; 2.5 mg/kg) has a $T_{1/2}$ of 0.43 hours, a CL of 4.56 mL/min/kg[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male C57BL/6 mice age 8-12 weeks[1]
Dosage:	5 and 50 mg/kg
Administration:	i.p.
Result:	Reduced NPS-induced horizontal activity and vertical rearing and climbing.

Animal Model:	Male C57BL/6 mice age 8-12 weeks[1]
Dosage:	1 mg/kg (Pharmacokinetic Analysis)
Administration:	i.p.
Result:	Had a $T_{1/2}$ of 0.74 hours, a CL of 4.29 mL/min/kg, and a V_{ss} of 2.53 L/kg.

CUSTOMER VALIDATION

- Peptides. 12 August 2022, 170860.

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REFERENCES

[1]. Okamura N, et al. Synthesis and pharmacological in vitro and in vivo profile of 3-oxo-1,1-diphenyl-tetrahydro-oxazolo[3,4-a]pyrazine-7-carboxylic acid 4-fluoro-benzylamide (SHA 68), a selective antagonist of the neuropeptide S receptor.J Pharmacol Exp The

[2]. Ensho T, et al. Neuropeptide S increases motor activity and thermogenesis in the rat through sympathetic activation.Neuropeptides. 2017 Oct;65:21-27.

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