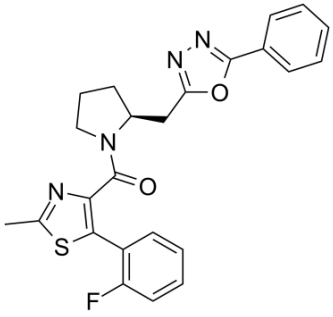
SB-674042

Cat. No.:	HY-10898
CAS No.:	483313-22-0
Molecular Formula:	$C_{24}H_{21}FN_4O_2S$
Molecular Weight:	448.51
Target:	Orexin Receptor (OX Receptor)
Pathway:	GPCR/G Protein; Neuronal Signaling
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (55.74 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2296 mL	11.1480 mL	22.2960 mL
5 mM	0.4459 mL	2.2296 mL	4.4592 mL
10 mM	0.2230 mL	1.1148 mL	2.2296 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: ≥ 1.43 mg/mL (3.19 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.43 mg/mL (3.19 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.43 mg/mL (3.19 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SB-674042 is a potent and selective non-peptide orexin OX1 receptor antagonist (Kd = 3.76 nM); exhibits 100-fold selectivity for OX1 over OX2 receptors.IC50 value: 3.76 nM (Kd)Target: OX1 receptorSB-674042 has no effect at serotonergic, dopaminergic, adrenergic or purinergic receptors. Inhibits orexin 1-induced Ca2+ mobilization in CHO-DG44 cells stably transfected with the OX1 receptor.

REFERENCES

[1]. Heifetz, Alexander; Morris, G. Benjamin; Biggin, Philip C. et al. Study of Human Orexin-1 and -2 G-Protein-Coupled Receptors with Novel and Published Antagonists by Modeling, Molecular Dynamics Simulations, and Site-Directed Mutagenesis. Biochemistry (2012), 51(15), 3178-3197.

[2]. Malherbe, Pari; Roche, Olivier; Marcuz, Anne et al. Mapping the binding pocket of dual antagonist Almorexant to human orexin 1 and orexin 2 receptors: comparison with the selective OX1 antagonist SB-674042 and the selective OX2 antagonist N-ethyl-2-[(6-methoxy-pyridin-3-yl)-(toluene-2-sulfonyl)-amino]-N-pyridin-3-ylmethyl-acetamide (EMPA). Molecular Pharmacology (2010), 78(1), 81-93.

[3]. Malherbe, Pari; Borroni, Edilio; Pinard, Emmanuel et al. Biochemical and electrophysiological characterization of almorexant, a dual orexin 1 receptor (OX1)/orexin 2 receptor (OX2) antagonist: comparison with selective OX1 and OX2 antagonists. Molecular Pharmacology (2009), 76(3), 618-631.

[4]. Ellis, James; Pediani, John D.; Canals, Meritxell et al. Orexin-1 Receptor-Cannabinoid CB1 Receptor Heterodimerization Results in Both Ligand-dependent and -independent Coordinated Alterations of Receptor Localization and Function. Journal of Biological Chemistry (2006), 281(50), 38812-38824.

[5]. Langmead, Christopher J.; Jerman, Jeffrey C.; Brough, Stephen J. et al. Characterisation of the binding of [3H]-SB-674042, a novel nonpeptide antagonist, to the human orexin-1 receptor. British Journal of Pharmacology (2004), 141(2), 340-346.

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