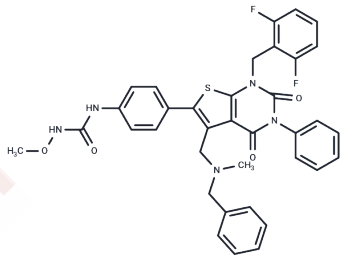
Data Sheet (Cat.No.T3538)

TargetMol

Sufugolix

Chemical Properties



CAS No. : 308831-61-0

Formula: C36H31F2N5O4S

Molecular Weight: 667.72

Storage: Powder: -20°C for 3 years
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Sufugolix (TAK-013) is a potent and orally available luteinizing hormone-releasing hormone (LHRH) receptor antagonist.
Targets(IC50)	GNRH Receptor,LHRH
In vitro	Sufugolix exhibits more than 3- and 2000-fold selectivity for the human receptor over the monkey and rat receptors, respectively. It effectively antagonizes LHRH function on CHO cells expressing the human (IC50=0.1 nM) and monkey (IC50=0.6 nM) receptors. High-temperature molecular dynamics calculation during the conformational analysis of sufugolix reveals that the cis conformer of the methoxyurea is more populated than the trans conformer[1].
In vivo	Oral administration of sufugolix at a 30 mg/kg dose causes almost complete suppression of plasma LH levels in castrated male cynomolgus monkeys for more than 24 hours. Sufugolix exhibits sufficient lipophilicity for enhanced membrane permeability and improved oral absorption in monkeys. Maximum plasma concentrations are 0.34 μM (6 hours post-administration) and 0.18 μM (4 hours post-administration) at 30 and 10 mg/kg doses, respectively[1].
Kinase Assay	The receptor-expressing CHO cells are seeded into 24-well plates at a density of 4×104 cells/well and cultured for 1 day. The cells are then incubated with [5,6,8,9,11,12,14,15-3H]arachidonic acid (11 kBq/well) for 1 day and ished with DMEM supplemented with 20 mM HEPES and 0.2% BSA. The cells are then preincubated with the compounds (Sufugolix) at 37 °C for 60 min and the reaction is started by addition of LHRH (1 nM). After incubation at37 °C for 40 min, radioactivity in the medium is measured with a liquid scintillation counter[1].

Solubility Information

Solubility	DMSO: 25 mg/mL (37.44 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.4976 mL	7.4882 mL	14.9763 mL
5 mM	0.2995 mL	1.4976 mL	2.9953 mL
10 mM	0.1498 mL	0.7488 mL	1.4976 mL
50 mM	0.030 mL	0.1498 mL	0.2995 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Sasaki S, et al. Discovery of a thieno[2,3-d]pyrimidine-2,4-dione bearing a p-methoxyureidophenyl moiety at the 6-position: a highly potent and orally bioavailable non-peptide antagonist for the human luteinizing hormone-releasing hormone receptor. J Med Chem. 2003 Jan 2;46(1):113-24.