Elagolix sodium

Cat. No.: HY-14369

CAS No.: 832720-36-2

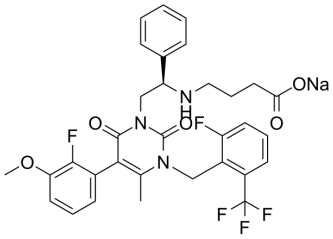
Molecular Formula: $C_{32}H_{29}F_5N_3NaO_5$

Molecular Weight: 653.57

Target: GnRH Receptor

Pathway: GPCR/G Protein

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

H_2O : ≥ 50 mg/mL (76.50 mM)
DMSO : 50 mg/mL (76.50 mM; Need ultrasonic)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	1.5301 mL	7.6503 mL	15.3006 mL
5 mM	0.3060 mL	1.5301 mL	3.0601 mL
10 mM	0.1530 mL	0.7650 mL	1.5301 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (76.50 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (3.83 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (3.83 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.83 mM); Clear solution

BIOLOGICAL ACTIVITY

Description Elagolix sodium is a human GnRH receptor (GnRHR) antagonist with an IC_{50} and K_i of 0.25 and 3.7 nM, respectively.

IC_{50} & Target
IC50: 0.25 nM (GnRHR)[1]
Ki: 3.7 nM (GnRHR)[2]

In Vitro	Elagolix sodium is a human GnRH receptor (GnRHR) antagonist with an IC_{50} of 0.25 nM in Kinase assay. Elagolix sodium has advanced to phase 3 trials for the treatment of endometriosis and uterine fibroids. Elagolix sodium also shows NFAT inhibition with an IC_{50} of 5.4 nM and effectively blocks Ca^{2+} flux with an IC_{50} of 0.86 nM[1]. Kinase assay also demonstrates that Elagolix sodium is a human GnRH receptor (GnRHR) antagonist with a K_i value of 3.7 nM[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [2]	The affinity of Elagolix sodium for hGnRH-R is determined by a competitive displacement of the radioligand GnRH from membranes prepared from HEK293 cells stably transfected with the full-length human GnRH receptor[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Cell Assay [2]	RBL-1 cells stably expressing the human cloned GnRH receptor are seeded into 96 well plates at a density of 15 000 cells per well in inositol-free DMEM containing 10% dialyzed FBS, 10 mM HEPES, 2 mM L-glutamine, 1 mM sodium pyruvate, 0.1 mM nonessential amino acids, and 50 μg/mL penicillin/streptomycin and are labeled for 48 h with 0.2 μCi myo-2-[^{3}H]inositol. The cells are washed once in PBS and pretreated with assay buffer for 15 to 60 min at 37°C. The cells are then stimulated with GnRH (6 nM) in the presence or absence of Elagolix sodium and incubated for 60 min at 37°C[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Kim SM, et al. Discovery of an Orally Bioavailable Gonadotropin-Releasing Hormone Receptor Antagonist. J Med Chem. 2016 Oct 13;59(19):9150-9172. Epub 2016 Sep 27.

[2]. Chen C, et al. Discovery of sodium R-(+)-4-{2-[5-(2-fluoro-3-methoxyphenyl)-3-(2-fluoro-6-[trifluoromethyl]benzyl)-4-methyl-2,6-dioxo-3,6-dihydro-2H-pyrimidin-1-yl]-1-phenylethylamino}butyrate (elagolix), a potent and orally available nonpeptide antagonis

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