

## **Product** Data Sheet

## Elagolix-<sup>13</sup>C,d<sub>3</sub> sodium

**Cat. No.:** HY-14369S

Molecular Formula:  $C_{31}^{13}CH_{26}D_3F_5N_3NaO_5$ 

Molecular Weight: 657.58

Target: GnRH Receptor; Isotope-Labeled Compounds

Pathway: GPCR/G Protein; Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

## **BIOLOGICAL ACTIVITY**

Description	Elagolix- $^{13}$ C,d $_3$ (sodium) is the $^{13}$ C- and deuterium labeled Elagolix sodium. Elagolix sodium is a human GnRH receptor (GnRHR) antagonist with an IC50 and Ki of 0.25 and 3.7 nM, respectively.
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs <sup>[56]</sup> .  MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## **REFERENCES**

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-223.

[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 antagonist of the human gonadotropin-releasing hormone receptor. J Med Chem. 2008 Dec 11;51(23):7478-85.

[3]. 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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