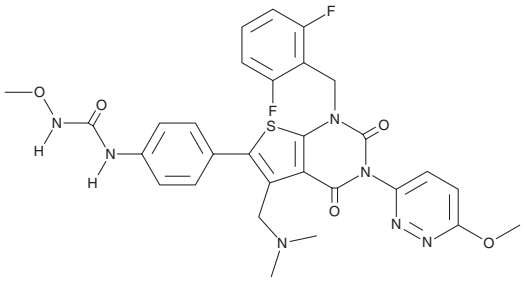
PRODUCT INFORMATION

TAK-385

Item No. 29512

CAS Registry No.:	737789-87-6
Formal Name:	N-[4-[1-[(2,6-difluorophenyl) methyl]-5-[(dimethylamino) methyl]-1,2,3,4-tetrahydro-3-(6-methoxy-3-pyridazinyl)-2,4-dioxothieno[2,3-d]pyrimidin-6-yl] phenyl]-N'-methoxy-urea
Synonym:	Relugolix
MF:	$C_{29}H_{27}F_2N_7O_5S$
FW:	623.6
Purity:	≥98%
UV/Vis.:	λ_{max}: 291 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

TAK-385 is supplied as a crystalline solid. A stock solution may be made by dissolving the TAK-385 in the solvent of choice, which should be purged with an inert gas. TAK-385 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of TAK-385 in these solvents is approximately 1, 20, and 25 mg/ml, respectively.

DMF is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, DMF should first be dissolved in PBS and then diluted with the aqueous buffer of choice. DMF has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

TAK-385 is an orally bioavailable gonadotropin-releasing hormone receptor (GnRHR) antagonist (IC_{50s} = 0.33 and 0.32 nM for the human and monkey receptors, respectively).[1] It is selective for these receptors over the rat GnRHR receptor (IC_{50} = 9,800 nM), as well as a panel of 134 enzymes and receptors at 10 µM. TAK-385 is 95-fold more potent at inhibiting GnRH-induced arachidonic acid (Item Nos. 90010 | 90010.1 | 10006607) release in CHO cells expressing human GnRHR compared with those expressing monkey GnRHR. It decreases testis, ventral prostate, ovary, and uterus weight in human *GNRHR* knock-in mice when administered at doses ranging from 3 to 200 mg/kg per day for 28 days.[2] TAK-385 (1 and 3 mg/kg) also decreases plasma luteinizing hormone levels in castrated cynomolgus monkeys.[1]

References

1. Miwa, K., Hitaka, T., Imada, T., *et al. J. Med. Chem.* **54(14)**, 4998-5012 (2011).
2. Nakata, D., Masaki, T., Tanaka, A., *et al. Eur. J. Pharmacol.* **723**, 167-174 (2014).

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