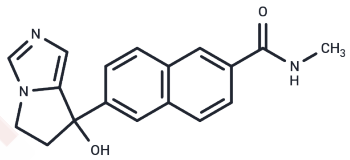
Data Sheet (Cat.No.T6050)

TAK-700

Chemical Properties



CAS No. : 426219-18-3

Formula: C18H17N3O2

Molecular Weight: 307.35

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	TAK-700 (Orteronel) (Orteronel) is a potent and highly selective human 17, 20-lyase inhibitor with IC50 of 38 nM, exhibits >1000-fold selectivity over other CYPs (e.g. 11-hydroxylase and CYP3A4). Phase 3.
Targets(IC50)	Cytochromes P450
In vitro	In vitro, TAK-700 shows the potent inhibitory activity against rat and human steroid 17,20-lyase with IC50 of 54 nM and 38 nM, respectively. While other CYP isoforms including 11-hydroxylase and CYP3A4 are not significantly affected by TAK-700. [1] In microsomes expressing human CYP isoforms, TAK-700 exhibit greater inhibitory effects on 17,20-lyase with IC50 of 19 nM compared to the other CYP isoforms. [1] TAK-700 shows the inhibitory activity against monkey 17,20-lyase and 17-hydroxylase with IC50 of 27 nM and 38 nM, respectively. [2] In monkey adrenal cells, TAK-700 inhibits the ACTH stimulated production of DHEA and androstenedione with IC50 of 110 nM and 130 nM, respectively. Moreover, TAK-700 also potently inhibits DHEA production in human adrenocortical tumor line H295R cells with IC50 of 37 nM. [2]
In vivo	In cynomolgus monkeys, oral treatment of TAK-700 at a dose of 1 mg/kg markedly reduces serum testosterone and dehydroepiandrosterone (DHEA) levels. [1] Oral treatment of TAK-700 at a dose of 1 mg/kg results in favorable pharmacokinetic parameters with Tmax, Cmax, t1/2 and AUC0-24 hours of 1.7 hours, 0.147 μg/mL, 3.8 hours and 0.727 μg h/mL, respectively. [2]

Solubility Information

Solubility	DMSO: 57 mg/mL (185.46 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 8 mg/mL (26.03 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.2536 mL	16.2681 mL	32.5362 mL
5 mM	0.6507 mL	3.2536 mL	6.5072 mL
10 mM	0.3254 mL	1.6268 mL	3.2536 mL
50 mM	0.0651 mL	0.3254 mL	0.6507 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.

Reference

Kaku T, et al. Bioorg Med Chem. 2011, 19(21), 6383-6399.
Yamaoka M, et al. J Steroid Biochem Mol Biol. 2012, 129(3-5), 115-128.

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