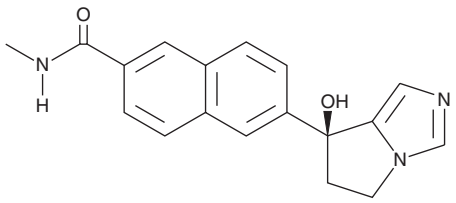
PRODUCT INFORMATION

Orteronel

Item No. 24191

CAS Registry No.:	566939-85-3
Formal Name:	6-[(7S)-6,7-dihydro-7-hydroxy-5H-pyrrolo[1,2-c]imidazol-7-yl]-N-methyl-2-naphthalenecarboxamide
Synonym:	TAK-700
MF:	$C_{18}H_{17}N_3O_2$
FW:	307.3
Purity:	≥98%
UV/Vis.:	λ_{max}: 237, 280 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

Orteronel is supplied as a crystalline solid. A stock solution may be made by dissolving the orteronel in the solvent of choice. Orteronel is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of orteronel in ethanol is approximately 0.2 mg/ml and approximately 10 mg/ml in DMSO and DMF.

Description

Orteronel is a non-steroidal inhibitor of the 17,20-lyase activity of the cytochrome P450 (CYP) isoform CYP17A1 (IC_{50}s = 48 and 19 nM for the rat and human enzyme, respectively), which is the CYP17A1 activity that converts progestogens into androgens.[1] Orteronel is selective for the 17,20-lyase activity of CYP17A1 over its 11-hydroxylase activity and CYP3A4 (IC_{50}s = >1,000 and >10,000 nM, respectively). It decreases adrenocorticotropic hormone-induced production of DHEA, androstenedione, cortisol, and aldosterone in monkey adrenal cells (IC_{50}s = 110, 130, 310, and 4,400 nmol/L, respectively) and inhibits DHEA production in NCI-H295R human adrenocortical tumor cells.[2] A single oral dose of orteronel (0.3-10 mg/kg) dose-dependently decreases DHEA, cortisol, and testosterone levels in the plasma of intact cynomolgus monkeys for at least 10 hours, and chronic dosing of 15 mg/kg twice daily suppresses levels for up to seven days of treatment. It also decreases DHEA and testosterone plasma levels in castrated monkeys, indicating an effect on extra-gonadal production of testosterone.

References

1. Kaku, T., Hitaka, T., Ojida, A., *et al.* Discovery of orteronel (TAK-700), a naphthylmethylimidazole derivative, as a highly selective 17,20-lyase inhibitor with potential utility in the treatment of prostate cancer. *Bioorg. Med. Chem.* **19(21)**, 6383-6399 (2011).
2. Yamaoka, M., Hara, T., Hitaka, T., *et al.* Orteronel (TAK-700), a novel non-steroidal 17,20-lyase inhibitor: Effects on steroid synthesis in human and monkey adrenal cells and serum steroid levels in cynomolgus monkeys. *J. Steroid. Biochem. Mol. Biol.* **129(3-5)**, 115-128 (2012).

WARNING
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA
This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent *via* email to your institution.

WARRANTY AND LIMITATION OF REMEDY
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