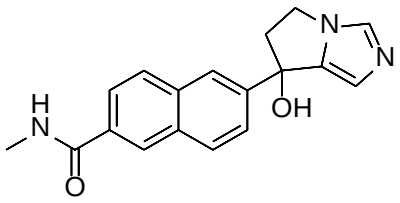
Product data sheet

MedKoo Cat#: 206784 Name: Orteronel (racemic) CAS#: 426219-18-3 (racemic) Chemical Formula: $C_{18}H_{17}N_3O_2$ Exact Mass: 307.1321 Molecular Weight: 307.35	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Orteronel (racemic) is a mixture of S-Orteronel and R-Orteronel isomers. Orteronel, aslo known as TAK-700, is an orally bioavailable non-steroidal androgen synthesis inhibitor of steroid 17alpha-monooxygenase (17,20 lyase) with potential antiandrogen activity. TAK-700 binds to and inhibits the steroid 17alpha-monooxygenase in both the testes and adrenal glands, thereby inhibiting androgen production. This may decrease androgen-dependent growth signaling and may inhibit cell proliferation of androgen-dependent tumor cells.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	50.0	162.7

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.25 mL	16.27 mL	32.54 mL
5 mM	0.65 mL	3.25 mL	6.51 mL
10 mM	0.33 mL	1.63 mL	3.25 mL
50 mM	0.07 mL	0.33 mL	0.65 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Yamaoka M, Hara T, Hitaka T, Kaku T, Takeuchi T, Takahashi J, Asahi S, Miki H, Tasaka A, Kusaka M. 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. 2012 Apr;129(3-5):115-28. doi: 10.1016/j.jsbmb.2012.01.001. Epub 2012 Jan 12. PMID: 22249003.

In vivo study

1. Yamaoka M, Hara T, Hitaka T, Kaku T, Takeuchi T, Takahashi J, Asahi S, Miki H, Tasaka A, Kusaka M. 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. 2012 Apr;129(3-5):115-28. doi: 10.1016/j.jsbmb.2012.01.001. Epub 2012 Jan 12. PMID: 22249003.

7. Bioactivity
Biological target: Orteronel (TAK-700) is a highly selective inhibitor of human 17,20-lyase (CYP17) with IC50 of 38 nM.

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In vitro activity

Orteronel potently suppressed androgen production in monkey adrenal cells but only weakly suppressed corticosterone and aldosterone production; the IC50 value of orteronel for cortisol was ~3-fold higher than that for DHEA. In terms of human CYP17A1 and human adrenal tumor cells, orteronel inhibited 17,20-lyase activity 5.4 times more potently than 17-hydroxylase activity in cell-free enzyme assays and DHEA production 27 times more potently than cortisol production in human adrenal tumor cells, suggesting greater specificity of inhibition between 17,20-lyase and 17-hydroxylase activities in humans vs monkeys.

Reference: J Steroid Biochem Mol Biol. 2012 Apr;129(3-5):115-28.
https://www.sciencedirect.com/science/article/abs/pii/S0960076012000118?via%3Dihub

In vivo activity

After a single oral dose of orteronel, serum levels of DHEA, cortisol, and testosterone were rapidly suppressed in intact cynomolgus monkeys. In castrated monkeys treated twice daily with orteronel, suppression of DHEA and testosterone persisted throughout the treatment period. Overall, orteronel reduced serum androgen levels in vivo in monkeys.

Reference: J Steroid Biochem Mol Biol. 2012 Apr;129(3-5):115-28.
https://www.sciencedirect.com/science/article/abs/pii/S0960076012000118?via%3Dihub

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.