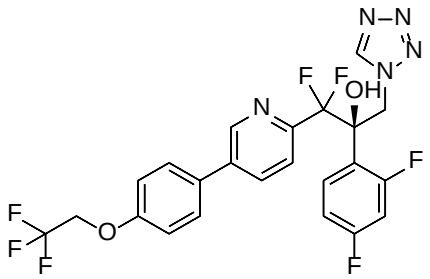
Product data sheet

MedKoo Cat#: 319588 Name: Oteseconazole CAS: 1340593-59-0 Chemical Formula: $C_{23}H_{16}F_7N_5O_2$ Exact Mass: 527.1192 Molecular Weight: 527.4028	
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:
Oteseconazole, also known as VT-1161, is a tetrazole antifungal agent potentially for the treatment of candidal vaginal infection. VT-1161 Protects Immunosuppressed Mice from Rhizopus arrhizus var. arrhizus Infection. VT-1161 dosed once daily or once weekly exhibits potent efficacy in treatment of dermatophytosis in a guinea pig model.

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	250.0	474.02

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.90 mL	9.48 mL	18.96 mL
5 mM	0.38 mL	1.90 mL	3.79 mL
10 mM	0.19 mL	0.95 mL	1.90 mL
50 mM	0.04 mL	0.19 mL	0.38 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. Break TJ, Desai JV, Natarajan M, Ferre EMN, Henderson C, Zelazny AM, Siebenlist U, Hoekstra WJ, Schotzinger RJ, Garvey EP, Lionakis MS. VT-1161 protects mice against oropharyngeal candidiasis caused by fluconazole-susceptible and -resistant Candida albicans. J Antimicrob Chemother. 2018 Jan 1;73(1):151-155. doi: 10.1093/jac/dkx352. PMID: 29040636; PMCID: PMC5890729.
2. Warrilow AG, Hull CM, Parker JE, Garvey EP, Hoekstra WJ, Moore WR, Schotzinger RJ, Kelly DE, Kelly SL. The clinical candidate VT-1161 is a highly potent inhibitor of Candida albicans CYP51 but fails to bind the human enzyme. Antimicrob Agents Chemother. 2014 Dec;58(12):7121-7. doi: 10.1128/AAC.03707-14. Epub 2014 Sep 15. PMID: 25224009; PMCID: PMC4249504.

In vivo study

1. Gebremariam T, Alkhazraji S, Lin L, Wiederhold NP, Garvey EP, Hoekstra WJ, Schotzinger RJ, Patterson TF, Filler SG, Ibrahim AS. Prophylactic Treatment with VT-1161 Protects Immunosuppressed Mice from Rhizopus arrhizus var. arrhizus Infection. Antimicrob Agents Chemother. 2017 Aug 24;61(9):e00390-17. doi: 10.1128/AAC.00390-17. PMID: 28652241; PMCID: PMC5571349.
2. Garvey EP, Hoekstra WJ, Moore WR, Schotzinger RJ, Long L, Ghannoum MA. VT-1161 dosed once daily or once weekly exhibits potent efficacy in treatment of dermatophytosis in a guinea pig model. Antimicrob Agents Chemother. 2015 Apr;59(4):1992-7. doi: 10.1128/AAC.04902-14. Epub 2015 Jan 20. PMID: 25605358; PMCID: PMC4356789.

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7. Bioactivity

Biological target:

Oteseconazole (VT-1161) is an orally active anti-fungal agent, potently binds to and inhibits Candida albicans CYP51 (K_d, <39 nM).

In vitro activity

VT-1161 produced a type II binding spectrum with Candida albicans CYP51, characteristic of heme iron coordination. In reconstitution assays, VT-1161 inhibited Candida albicans CYP51 activity in a tight-binding fashion with a potency similar to that of the pharmaceutical azoles but failed to inhibit the human enzyme at the highest concentration tested (50 μM). In addition, VT-1161 (MIC = 0.002 μg ml(-1)) had a more pronounced fungal sterol disruption profile (increased levels of methylated sterols and decreased levels of ergosterol) than the known CYP51 inhibitor voriconazole (MIC = 0.004 μg ml(-1)).

Reference: Antimicrob Agents Chemother. 2014 Dec;58(12):7121-7. https://pubmed.ncbi.nlm.nih.gov/25224009/

In vivo activity

In pharmacokinetic studies supporting testing in a guinea pig model of dermatophytosis, VT-1161 plasma concentrations following single oral doses were dose proportional and persisted at or above the MIC values for at least 48 h, indicating potential in vivo efficacy with once-daily and possibly once-weekly dosing. Subsequently, in a guinea pig dermatophytosis model utilizing Trichophyton mentagrophytes and at oral doses of 5, 10, or 25 mg/kg of body weight once daily or 70 mg/kg once weekly, VT-1161 was statistically superior to untreated controls in fungal burden reduction ($P < 0.001$) and improvement in clinical scores ($P < 0.001$).

Reference: Antimicrob Agents Chemother. 2015 Apr;59(4):1992-7. https://pubmed.ncbi.nlm.nih.gov/25605358/