# **Product data sheet**



MedKoo Cat#: 314268		HO NH2	
Name: Caspofungin acetate		, OH O HO	
CAS#: 179463-17-3 (acetate)		N <sup>10</sup>	
Chemical Formula: C56H96N10O19			
Molecular Weight: 1213.42			2 C
Product supplied as:	Powder	N O OHO NH	он
Purity (by HPLC):	$\geq$ 98%		) )
Shipping conditions	Ambient temperature		Ĺ
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.	HN	`ОН
	In solvent: -80°C 3 months; -20°C 2 weeks.		
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### 1. Product description:

Caspofungin acetate is a lipopeptide antifungal drug. It is a member of a new class of antifungals termed the echinocandins. It works by inhibiting the enzyme  $(1 \rightarrow 3)$ -  $\beta$ -D-glucan synthase and thereby disturbing the integrity of the fungal cell wall. Caspofungin acetate for injection was originally approved by FDA in USA, and the EMEA in Europe, in 2001.

# 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	69.0	56.86
H2O	100.0	82.41

#### 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	0.82 mL	4.12 mL	8.24 mL
5 mM	0.16 mL	0.82 mL	1.65 mL
10 mM	0.08 mL	0.41 mL	0.82 mL
50 mM	0.02 mL	0.08 mL	0.16 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. Bowman JC, Hicks PS, Kurtz MB, Rosen H, Schmatz DM, Liberator PA, Douglas CM. The antifungal echinocandin caspofungin acetate kills growing cells of Aspergillus fumigatus in vitro. Antimicrob Agents Chemother. 2002 Sep;46(9):3001-12. doi: 10.1128/AAC.46.9.3001-3012.2002. PMID: 12183260; PMCID: PMC127409.

2. Bachmann SP, VandeWalle K, Ramage G, Patterson TF, Wickes BL, Graybill JR, López-Ribot JL. In vitro activity of caspofungin against Candida albicans biofilms. Antimicrob Agents Chemother. 2002 Nov;46(11):3591-6. doi: 10.1128/AAC.46.11.3591-3596.2002. PMID: 12384370; PMCID: PMC128731.

#### In vivo study

1. Ibrahim AS, Bowman JC, Avanessian V, Brown K, Spellberg B, Edwards JE Jr, Douglas CM. Caspofungin inhibits Rhizopus oryzae 1,3-beta-D-glucan synthase, lowers burden in brain measured by quantitative PCR, and improves survival at a low but not a high dose during murine disseminated zygomycosis. Antimicrob Agents Chemother. 2005 Feb;49(2):721-7. doi: 10.1128/AAC.49.2.721-727.2005. PMID: 15673756; PMCID: PMC547300.

2. Demirci M, Tünger Ö, Çetin ÇB, Senol Ş. Comparison of the effectiveness of caspofungin and liposomal amphotericin-B for the treatment of C. tropicalis-induced peritonitis in mice. Infez Med. 2019 Jun 1;27(2):155-158. PMID: 31205038.

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# 7. Bioactivity

# Biological target:

Caspofungin Acetate (MK-0991 Acetate) is an antifungal drug that noncompetitively inhibits 1,3-β-D glucan synthase activity.

#### In vitro activity

A sharp reduction of the metabolic activity of cells within the biofilm as assessed by the XTT reduction assay was demonstrated when preformed C. albicans 3153A biofilms were exposed to caspofungin (Fig.1). By this method, the 48-h MIC50 of caspofungin for sessile C. albicans 3153A cells within biofilms was  $0.0625 \ \mu$  g/ml. Although complete sterility of biofilms was not achieved by treatment with caspofungin, the experiments showed a >97% reduction in the metabolic activity of sessile cells with caspofungin concentrations as low as  $0.125 \ \mu$ g/ml. Caspofungin was also active against biofilms formed by all the C. albicans clinical isolates tested (n = 18), with MIC50s for sessile cells ranging between  $0.0625 \ \mu$ g/ml, compared to fluconazole MIC50s for sessile cells within the XTT assays, only residual metabolic activity was detected in cells within the caspofungin-treated biofilms, which showed a diffuse green fluorescence pattern characteristic of dead cells (Fig.3B). In confirmation of the SEM results, CLSM demonstrated that caspofungin treatment resulted in biofilms that were less hyphal and also showed minor distortions of the overall biofilm architecture. As shown in Fig.4, coating with caspofungin resulted in significant (up to 60%) reduction of the metabolic activity of adherent cells compared to that of cells in untreated (control) wells. Together these findings indicate that caspofungin displays potent activity against C. albicans biofilms in vitro and merits further investigation for the treatment of biofilm-associated infections.

Reference: Antimicrob Agents Chemother. 2002 Nov; 46(11): 3591–3596. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC128731/

#### In vivo activity

The inhibition of R. oryzae GS by CAS (caspofungin acetate ) and the discovery of an FKS homolog demonstrate that the drug target is present in this organism. CAS might be effective against R. oryzae in vivo, despite the high MIC, especially given the known constraints of MIC testing with molds (13, 29). The in vivo efficacy of CAS was tested in diabetic ketoacidotic mice infected with R. oryzae. Intravenous treatment with AMB (0.5 mg/kg b.i.d.) or CAS (0.5, 2.5, or 5 mg/kg b.i.d.) was initiated 24 h after the mice were infected with  $5 \times 102$  or  $5 \times 103$  spores of R. oryzae. At 0.5 mg/kg b.i.d., CAS, but not AMB, improved the survival of mice infected with  $5 \times 102$  spores of R. oryzae compared to that of the infected untreated mice (P = 0.049) (Fig.2a). Eighty percent of the diabetic mice treated with CAS at 0.5 mg/kg/day were alive 10 days after infection, whereas 30% of the infected untreated mice were alive at that time. Surprisingly, higher doses of CAS (2.5 or 5 mg/kg b.i.d.) did not improve the rate of survival. These results indicate that CAS has significant but limited activity against R. oryzae in vivo and demonstrates an inverse dose-response effect.

Reference: Antimicrob Agents Chemother. 2005 Feb; 49(2): 721-727. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC547300/

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.