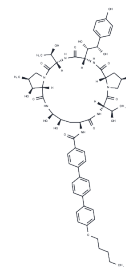


Anidulafungin

Chemical Properties

| | |
|-------------------|--|
| CAS No. : | 166663-25-8 |
| Formula: | C ₅₈ H ₇₃ N ₇ O ₁₇ |
| Molecular Weight: | 1140.24 |
| Appearance: | no data available |
| Storage: | store at low temperature Powder: -20°C for 3 years In solvent: -80°C for 1 year |



Biological Description

| | |
|---------------|--|
| Description | Anidulafungin (Ecalta) (LY303366) is an echinocandin derivative used as an antifungal drug. It inhibits glucan synthase activity. |
| Targets(IC50) | Antibiotic,Antifungal |
| In vitro | Anidulafungin (LY-303366) demonstrates potent in vitro antifungal activity, with minimum inhibitory concentrations (MICs) of ≤ 0.32 $\mu\text{g/mL}$ against all isolates of <i>Candida albicans</i> (n=99), <i>Candida glabrata</i> (n=18), and <i>Candida tropicalis</i> (n=10). It exhibits significant efficacy against <i>Aspergillus</i> species with a minimum effective concentration (MEC) of 0.02 $\mu\text{g/mL}$ for 90% inhibition (n=20). However, its activity is reduced against <i>Candida parapsilosis</i> (MIC ₉₀ , 5.12 $\mu\text{g/mL}$) (n=10), and it is ineffective against <i>C. neoformans</i> (MIC ₉₀ >10.24 $\mu\text{g/mL}$) (n=15) and <i>B. dermatitidis</i> (MIC ₉₀ , 16 $\mu\text{g/mL}$) (n=29). Compared to fluconazole, anidulafungin retains low MICs (0.08 to 1.28 $\mu\text{g/mL}$) against fluconazole-resistant <i>Candida</i> strains, demonstrating a broad range of action. Strains showing resistance to CD101 exhibit a corresponding increase in MIC for anidulafungin and/or caspofungin, highlighting cross-resistance. This strong antifungal activity, notably against <i>Candida</i> species and <i>Aspergillus</i> , contrasts with its limited effects against <i>C. neoformans</i> and <i>B. dermatitidis</i> , for which ketoconazole and amphotericin B show superior efficacy. |
| Kinase Assay | FITC-S1P quantification/Caliper assay: A 384-well format of the SphK enzyme assay based on separation of FITC-S1P from unreacted FITC-sphingosine substrate using a microfluidic capillary electrophoresis mobility-shift system is developed. Briefly, 3 nM SphK1-His6 is incubated with 1 μM FITC-sphingosine, 20 μM ATP and 10 μM compound (a final concentration of DMSO of 2 %) in a buffer containing 100 mM Hepes (pH 7.4), 1 mM MgCl ₂ , 0.01% Triton X-100, 10% glycerol, 100 μM sodium orthovanadate and 1 mM DTT for 1 h in a 384-well Matrical MP-101-1-PP plate. Reaction mixtures (10 μL) are quenched by the addition of 20 μL of 30 mM EDTA and 0.15% Coating Reagent-3 in 100 mM Hepes, and a small aliquot of each reaction (a few nanolitres) is analysed in the Caliper LabChip 3000 instrument under -1.5 psi (psi=6.9 kPa) pressure, a downstream voltage of -1900 V and a sip time of 0.2 s. Phosphorylated fluorescent product and unphosphorylated fluorescent substrate appeared as distinctive peaks and are quantified using the Caliper data. |
| Cell Research | Anidulafungin is dissolved in DMSO and stored, and then diluted[2]. Stocks of CD101 (formerly SP 3025, bialafungin, AF-025) are prepared fresh in 100% DMSO prior to use. The |

comparator antifungals Anidulafungin (ANF), Caspofungin (CSF), and Amphotericin B (AMB) are also prepared in 100% DMSO. MIC assays are performed via broth microdilution in accordance with CLSI guidelines, with the exception that test compounds are made up at a 50× final assay concentration and 100 µL assay mixture volumes are used (2 µL added to 98 µL of broth containing cells at 0.5×10³ to 2.5×10³ CFU/mL). All MIC assays are run at least three times, and a representative data set is shown. Quality control (QC) is assessed throughout the study via comparison of MIC values derived for WT *C. krusei* strain ATCC 6258 for AMB, CSF, and ANF with previously reported CLSI 24-h broth microdilution QC ranges[2].

Solubility Information

| | |
|------------|---|
| Solubility | H ₂ O: < 1 mg/mL (insoluble or slightly soluble), DMSO: 93 mg/mL (81.56 mM), Sonication is recommended. Ethanol: < 1 mg/mL (insoluble or slightly soluble), (< 1 mg/mL refers to the product slightly soluble or insoluble) |
|------------|---|

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|-----------|-----------|-----------|
| 1 mM | 0.877 mL | 4.385 mL | 8.7701 mL |
| 5 mM | 0.1754 mL | 0.877 mL | 1.754 mL |
| 10 mM | 0.0877 mL | 0.4385 mL | 0.877 mL |
| 50 mM | 0.0175 mL | 0.0877 mL | 0.1754 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

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- Locke JB, et al. Characterization of In Vitro Resistance Development to the Novel Echinocandin CD101 in *Candida* Species. *Antimicrob Agents Chemother.* 2016 Sep 23;60(10):6100-7.
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