

Antifungal agent 124

Chemical Properties

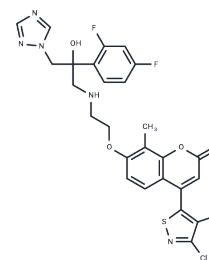
CAS No. :

Formula: C₂₆H₂₁Cl₂F₂N₅O₄S

Molecular Weight: 608.444

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	Antifungal agent 257 (Compound 7e) is a broad-spectrum antifungal agent with an EC ₅₀ value of 4.15 μM against <i>F. graminearum</i> .
Targets(IC ₅₀)	Antifungal
In vitro	Antifungal agent 257 is an inhibitor of <i>Fusarium graminearum</i> 14-α-demethylase, with an IC ₅₀ value of 0.59 μM, showing significantly greater inhibitory activity than fluconazole phosphate [1]. Throughout most of the simulation process, Antifungal agent 257 interacts with <i>Fusarium graminearum</i> through hydrogen bonding [1]. The ΔG Total for Antifungal agent 257 with 14-α-demethylase is -55.45 kcal/mol, considerably lower than that of fluconazole, which is -18.05 kcal/mol, indicating higher activity against the enzyme [1]. Antifungal agent 257 interacts with the enzyme at residues Tyr105, Phe113, Val118, Ile359, Ile362, His447-Leu126, Met284, Thr287, Leu228, Ala291, Cys449, and Ile450 [1]. It exhibits minimal to no toxicity to mammals [1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.6435 mL	8.2177 mL	16.4355 mL
5 mM	0.3287 mL	1.6435 mL	3.2871 mL
10 mM	0.1644 mL	0.8218 mL	1.6435 mL
50 mM	0.0329 mL	0.1644 mL	0.3287 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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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