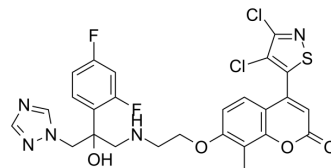


## Antifungal agent 124

Cat. No.:	HY-170359
Molecular Formula:	C <sub>26</sub> H <sub>21</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>5</sub> O <sub>4</sub> S
Molecular Weight:	608.44
Target:	Fungal
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



### BIOLOGICAL ACTIVITY

<b>Description</b>	Antifungal agent 257 is broad spectrum antifungal. Antifungal agent 257 inhibits <i>F. graminearum</i> with an EC <sub>50</sub> value of 4.15 μM <sup>[1]</sup> .
<b>In Vitro</b>	<p>Antifungal agent 257 (Compound 7e) binds with <i>F.graminearum</i> 14-α demethylase , forming the hydrogen bond and hydrophobic interaction which favors the fungicidal activity.<sup>[1]</sup></p> <p>Antifungal agent 257 against <i>A. solani</i>, <i>Botrytis cinerea</i>, <i>C. arachidicola</i>, <i>F. graminearum</i>, <i>S. sclerotiorum</i> at 50 μg/mL with EC<sub>50</sub>s of 4.02μg/mL, 6.03μg/mL, 4.15μg/mL and 3.81 μg/mL respectively, showing a broad fungicidal spectrum<sup>[1]</sup>.</p> <p>Antifungal agent 257 inhibits <i>F. graminearum</i>14-α-demethylase with an IC<sub>50</sub> value of 0.59 μM, showing a higher inhibitory activity than Flutriafof (HY-W019852)<sup>[1]</sup>.</p> <p>Antifungal agent 257 can form hydrogen-bond interactions with <i>F. graminearum</i> 14-α demethylase for most of the time during the simulation<sup>[1]</sup>.</p> <p>The ΔG<sub>Total</sub> value of <i>F. graminearum</i> 14-α demethylase with Antifungal agent 257 (-55.45 kcal/mol) is significantly lower than that of the flutriafof (-18.05 kcal/mol), implying that Antifungal agent 257 against the <i>F. graminearum</i> 14-α demethylase is more active than flutriafof<sup>[1]</sup>.</p> <p>Antifungal agent 257 interacts with in <i>F. graminearum</i> 14-α demethylase at Tyr105, Phe113, Val118, Ile359, Ile362, His447, Leu126, Met284, Thr287, Leu228, Ala291, Cys449, and Ile450 residues<sup>[1]</sup>.</p> <p>Antifungal agent 257 has minimal or no toxicity to mammals<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

### REFERENCES

[1]. Lv Y, Li K, et al. Z. Design, Synthesis, and Assessment of Fungicidal Activity of Active Substructure 1,2,4-Triazole Containing Coumarin. *J Agric Food Chem*. 2024 Dec 11;72(49):27075-27083. doi: 10.1021/acs.jafc.4c07227. Epub 2024 Nov 26.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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