Screening Libraries

Product Data Sheet



Hexaconazole

Cat. No.: HY-A0278 CAS No.: 79983-71-4 Molecular Formula: $C_{14}H_{17}Cl_2N_3O$

Molecular Weight: 314.21

Target: Fungal; Reactive Oxygen Species

Pathway: Anti-infection; Immunology/Inflammation; Metabolic Enzyme/Protease; NF-κΒ

-20°C 3 years Storage: Powder

4°C 2 years -80°C 2 years

In solvent

-20°C 1 year

SOLVENT & SOLUBILITY

In Vitro

DMSO: $\geq 100 \text{ mg/mL} (318.26 \text{ mM})$

H₂O: < 0.1 mg/mL (insoluble)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.1826 mL	15.9129 mL	31.8258 mL
	5 mM	0.6365 mL	3.1826 mL	6.3652 mL
	10 mM	0.3183 mL	1.5913 mL	3.1826 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (7.96 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (7.96 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (7.96 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Hexaconazole is a systemic fungicide used for the control of many fungi particularly Ascomycetes and Basidiomycetes. In vitro: Among the enzymatic antioxidants, superoxide dismutase and peroxidase are significantly up-regulated by hexaconazole. [1] Hexaconazole and its enantiomers cause the down-regulation of tryptophan levels and the up-regulation of kynurenine (KYN) levels, suggesting a role for hexaconazole in the activation of the KYN pathway and providing information for the mechanism of its toxicity.[2]

REFERENCES

[1]. Dubey P et al. Comparative analyses of genotoxicity, oxidative stress and antioxidative defence system under exposure of methyl parathion and hexaconazole in barley (Hordeum vulgare L.) Environ Sci Pollut Res Int. 2015 Dec;22(24):19848-59.

[2]. Wang Y et al. Monitoring tryptophan metabolism after exposure to hexaconazole and the enantioselective metabolism ofhexaconazole in rat hepatocytes in vitro. J Hazard Mater. 2015 Sep 15;295:9-16.

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

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Page 2 of 2 www.MedChemExpress.com