

## **Product** Data Sheet

## Itraconazole-d<sub>9</sub>

 Cat. No.:
 HY-17514S2

 CAS No.:
 1309272-50-1

 Molecular Formula:
  $C_{35}H_{29}D_9Cl_2N_8O_4$ 

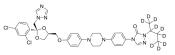
Molecular Weight: 714.69

Target: Fungal; Hedgehog; Bacterial; Autophagy; Cytochrome P450; Antibiotic

Pathway: Anti-infection; Stem Cell/Wnt; Autophagy; Metabolic Enzyme/Protease

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.



## **BIOLOGICAL ACTIVITY**

Description Itraconazole-d<sub>9</sub> is the deuterium labeled Itraconazole[1]. Itraconazole (R51211) is a triazole antifungal agent and a potent and orally active Hedgehog (Hh) signaling pathway antagonist with an IC50 of ~800 nM. Itraconazole potently inhibits

lanosterol  $14\alpha$ -demethylase (cytochrome P450 enzyme), thereby inhibits the oxidative conversion of lanosterol to ergosterol. Itraconazole has anticancer and antiangiogenic effects. Itraconazole is a oxysterol-binding protein (OSBP)

inhibitor[2][3][4][5].

In Vitro Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as

tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to

affect the pharmacokinetic and metabolic profiles of  $drugs^{[1]}$ .

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## **REFERENCES**

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

[2]. Kim, J., et al., Itraconazole, a commonly used antifungal that inhibits Hedgehog pathway activity and cancer growth. Cancer Cell, 2010. 17(4): p. 388-99.

[3]. Chong, C.R., et al., Inhibition of angiogenesis by the antifungal drug itraconazole. ACS Chem Biol, 2007. 2(4): p. 263-70.

[4]. Pace JR, et al. Repurposing the Clinically Efficacious Antifungal Agent Itraconazole as an Anticancer Chemotherapeutic. J Med Chem. 2016 Apr 28;59(8):3635-49.

[5]. Albulescu L, et al. Uncovering oxysterol-binding protein (OSBP) as a target of the anti-enteroviral compound TTP-8307. Antiviral Res. 2017;140:37-44.

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

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Inhibitors

Proteins