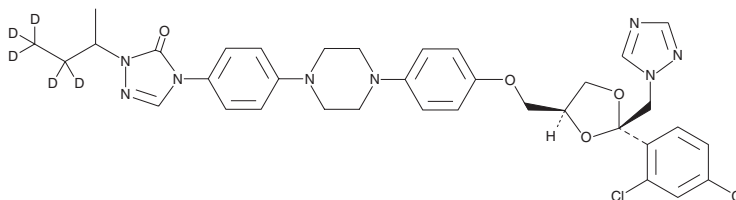


# PRODUCT INFORMATION



## Itraconazole-d<sub>5</sub> Item No. 25219

**CAS Registry No.:** 1217510-38-7  
**Formal Name:** 4-(4-(4-(((2R,4S)-2-((1H-1,2,4-triazol-1-yl)methyl)-2-(2,4-dichlorophenyl)-1,3-dioxolan-4-yl)methoxy)phenyl)piperazin-1-yl)phenyl)-2-(butan-2-yl-3,3,4,4,4-d<sub>5</sub>)-2,4-dihydro-3H-1,2,4-triazol-3-one  
**MF:** C<sub>35</sub>H<sub>33</sub>Cl<sub>2</sub>D<sub>5</sub>N<sub>8</sub>O<sub>4</sub>  
**FW:** 710.7  
**Chemical Purity:** ≥98% (Itraconazole)  
**Deuterium Incorporation:** ≥99% deuterated forms (d<sub>1</sub>-d<sub>5</sub>); ≤1% d<sub>0</sub>  
**Supplied as:** A solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

Itraconazole-d<sub>5</sub> is intended for use as an internal standard for the quantification of itraconazole (Item No. 13288) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Itraconazole-d<sub>5</sub> is supplied as a solid. A stock solution may be made by dissolving the itraconazole-d<sub>5</sub> in the solvent of choice, which should be purged with an inert gas. Itraconazole-d<sub>5</sub> is slightly soluble in chloroform and methanol.

### Description

Itraconazole is an antifungal agent and inhibitor of hedgehog signaling (IC<sub>50</sub> = 800 nM).<sup>1,2</sup> It binds to 14- $\alpha$  sterol demethylase/CYP51 isoform B (AF51B; K<sub>d</sub> = 31 nM for *A. fumigatus* enzyme expressed in *E. coli*) and inhibits ergosterol biosynthesis in *C. neoformans* (IC<sub>50</sub> = 6 nM after a 16-hour incubation).<sup>1,3</sup> It inhibits the growth of *C. neoformans* by 50% when used at a concentration of 3.2 nM. Itraconazole inhibits hedgehog signaling, reducing accumulation of Smoothed induced by sonic hedgehog (Shh) in primary cilia of NIHT-3T3 cells.<sup>2</sup> It suppresses growth of medulloblastomas in a *Ptch*<sup>+/+</sup>-*p53*<sup>-/-</sup> mouse allograft model when administered at a dose of 100 mg/kg twice daily. Itraconazole (1.25-100  $\mu$ M) also reduces viral titers of several enteroviruses, including human rhinovirus 17, in infected cells, effects that can be reversed by overexpression of OSBP, the gene encoding oxysterol-binding protein (OSBP).<sup>4</sup>

### References

1. Vanden Bossche, H., Marichal, P., Le Jeune, L., et al. *Antimicrob. Agents Chemother.* **37**(10), 2101-2105 (1993).
2. Kim, J., Tang, J.Y., Gong, R., et al. *Cancer Cell* **17**(4), 388-399 (2010).
3. Warrilow, A.G., Melo, N., Martel, C.M., et al. *Antimicrob. Agents Chemother.* **54**(10), 4225-4234 (2010).
4. Strating, J.R.P.M., van der Linden, L., Albulescu, L., et al. *Cell Rep.* **10**(4), 600-615 (2015).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

**PHONE:** [800] 364-9897  
[734] 971-3335

**FAX:** [734] 971-3640

CUSTSERV@CAYMANCHEM.COM  
WWW.CAYMANCHEM.COM