

Product Data Sheet

Product Name: Ketoconazole-d3

Cat. No.: GC40109

Chemical Properties

Cas. No. 1217766-70-5

SMILES O=C(C([2H])([2H])([2H])N1CCN(C2=CC=C(OC[C@@H]3O[C@](C4=CC=C(Cl)C=C4Cl)(CN5C=CN=C5)OC3)C=C2)CC1

Formula C₂₆H₂₅Cl₂D₃N₄O₄

M.Wt 534.5

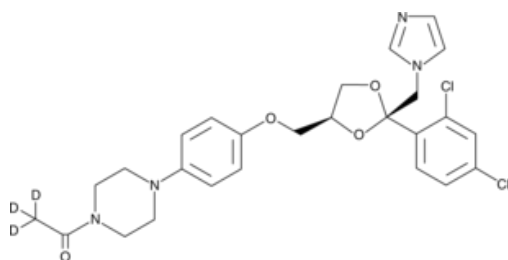
Solubility Chloroform: slightly soluble, Methanol: slightly soluble

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

Ketoconazole-d3 is intended for use as an internal standard for the quantification of ketoconazole by GC- or LC-MS. Ketoconazole is a broad-spectrum triazole antifungal agent that has activity against *C. albicans*, *C. krusei*, *C. tropicalis*, *C. glabrata*, *C. parapsilosis*, *C. neoformans*, and *A. fumigatus* strains (IC₅₀s = 0.031-8 µg/ml). It inhibits the fungal cytochrome P450 (CYP) isoform CYP51, also known as lanosterol 14α-demethylase, which arrests ergosterol biosynthesis at the fungal membrane. Ketoconazole also inhibits human CYP3A4 (IC₅₀ = 0.54 µM). Formulations containing ketoconazole have been used in the treatment of fungal infections.

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

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