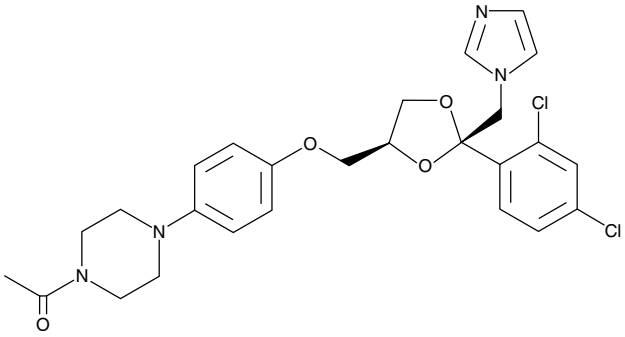
Product Information

Ketoconazole

Item No. 15212

CAS Registry No.: 65277-42-1
Formal Name: 1-[4-[4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]-ethanone
Synonyms: Nizoral, R 41400
MF: $C_{26}H_{28}Cl_2N_4O_4$
FW: 531.4
Purity: ≥98%
Stability: ≥2 years at -20°C
Supplied as: A crystalline solid
UV/Vis.: λ_{max}: 244, 297 nm



Laboratory Procedures

For long term storage, we suggest that ketoconazole be stored as supplied at -20°C. It should be stable for at least two years.

Ketoconazole is supplied as a crystalline solid. A stock solution may be made by dissolving the ketoconazole in the solvent of choice. Ketoconazole is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of ketoconazole in these solvents is approximately 1, 2, and 5 mg/ml, respectively.

Ketoconazole is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, ketoconazole should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Ketoconazole has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Ketoconazole is an orally active broad spectrum antifungal agent that blocks ergosterol biosynthesis by inhibiting the fungal cytochrome P450 (CYP) isoform CYP51, also known as lanosterol 14α-demethylase.[1-2] It potently inhibits the mammalian analog CYP51A1 (IC_{50} = 63.5 nM), as well as a variety of other CYP isoforms.[2-6]

References

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2. Dilmaghanian, S., Gerber, J.G., Filler, D.G. , *et al.* Enantioselectivity of inhibition of cytochrome P450 3A4 (CYP3A4) by ketoconazole: Testosterone and methadone as substrates. *Chirality* **16(2)**, 79-85 (2004).
3. Walker, K.A.M., Kertesz, D.J., Rotstein, D.M., *et al.* Selective inhibition of mammalian lanosterol 14α-demethylase: A possible strategy for cholesterol lowering. *J. Med. Chem.* **36(15)**, 2235-2237 (1993).
4. Njar, V.C.O., Kato, K., Nnane, I.P., *et al.* Novel 17-azolyl steroids, potent inhibitors of human cytochrome 17α-hydroxylase-$C_{17,20}$-lyase ($P450_{17\alpha}$): Potential agents for the treatment of prostate cancer. *J. Med. Chem.* **41(6)**, 902-912 (1998).
5. McNulty, J., Nair, J.J., Wurgun, N., *et al.* Discovery of a novel class of aldol-derived 1,2,3-triazoles: Potent and selective inhibitors of human cytochrome P450 19A1 (aromatase). *Bioorg. Med. Chem. Lett.* **22(1)**, 718-722 (2012).
6. Rotstein, D.M., Kertesz, D.J., Walker, K.A., *et al.* Stereoisomers of ketoconazole: Preparation and biological activity. *J. Med. Chem.* **35(15)**, 2818-2825 (1992).

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