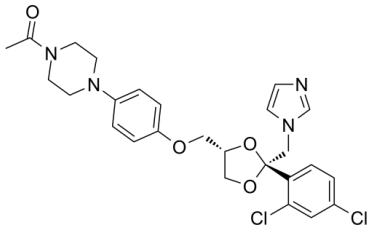
Data Sheet

Product Name:	Ketoconazole
Cat. No.:	CS-1845
CAS No.:	65277-42-1
Molecular Formula:	$C_{26}H_{28}Cl_2N_4O_4$
Molecular Weight:	531.43
Target:	Cytochrome P450; Fungal; Ras
Pathway:	Anti-infection; GPCR/G Protein; Metabolic Enzyme/Protease
Solubility:	DMSO : 25 mg/mL (47.04 mM; Need ultrasonic)



relative stereochemistry

BIOLOGICAL ACTIVITY:

Ketoconazole (R-41400) is an imidazole anti-fungal agent, a CYP3A4 and CYP24A1 inhibitor. IC50 & Target: CYP3A4, CYP24A1. **In Vitro:** Ketoconazole (R-41400), an imidazole anti-fungal agent, has often produced features of androgen deficiency including decreased libido, gynecomastia, impotence, oligospermia, and decreased testosterone levels, in men being treated for chronic mycotic infections[1]. Ketoconazole (R-41400) also is a cytochrome P450 inhibitor[2]. Ketoconazole (R-41400), on the antischistosomal potential of these quinolines against Schistosoma mansoni infection by evaluating parasitological, histopathological, and biochemical parameters. Mice were classified into 7 groups: uninfected untreated (I), infected untreated (II), infected treated orally with PZQ (1,000 mg/kg) (III), QN (400 mg/kg) (IV), KTZ (10 mg/kg)+QN as group IV (V), HF (400 mg/kg) (VI), and KTZ (as group V)+HF (as group VI) (VII). KTZ plus QN or HF produced more inhibition ($P<0.05$) in hepatic CYP450 (85.7% and 83.8%) and CYT b5 (75.5% and 73.5%) activities, respectively, than in groups treated with QN or HF alone. This was accompanied with more reduction in female (89.0% and 79.3%), total worms (81.4% and 70.3%), and eggs burden (hepatic; 83.8%, 66.0% and intestinal; 68%, 64.5%), respectively, and encountering the granulomatous reaction to parasite eggs trapped in the liver[3]. CYP24A1 inhibitor enhances antiproliferative effects, increases systemic calcitriol exposure, and promotes the activation of caspase-independent apoptosis pathway. Ketoconazole is also a potent exosome biogenesis and/or secretion inhibitor[4].

References:

[1]. Seif El-Din SH, et al. Effect of ketoconazole, a cytochrome P450 inhibitor, on the efficacy of quinine and halofantrine against Schistosoma mansoni in mice. Korean J Parasitol. 2013 Apr;51(2):165-75.

[2]. Eil C. Ketoconazole binds to the human androgen receptor. Horm Metab Res. 1992 Aug;24(8):367-70.

[3]. Muindi JR et al. CYP24A1 inhibition enhances the antitumor activity of calcitriol. Endocrinology. 2010 Sep;151(9):4301-12.

[4]. Amrita Datta, et al. High-throughput screening identified selective inhibitors of exosome biogenesis and secretion: A drug repurposing strategy for advanced cancer. Sci Rep. 2018 May 25;8(1):8161.

CAIndexNames:

Ethanone, 1-[4-[4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]-, rel-

SMILES:

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

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