

Antifungal Azoles: Structural Insights into Undesired Tight Binding to Cholesterol-Metabolizing

CYP46A1

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Molecular Pharmacology

Supplemental Table 1

Crystallographic statistics

CYP46A1 complex	Posaconazole
PDB code	4J14
Space group	I4 ₁ 22
Unit cell dimensions (Å)	121.6 121.6 143.4
Molecules per asymmetric unit	1
Solvent content	50.9%
Data	
Total observations > 0 σ_F	134,563
Unique reflections > 0 σ_F	18,956
Redundancy	7.1
Completeness	100.0%
Resolution range (last shell) (Å)	92.78 – 2.50 (2.65 – 2.50)
<I/ σ_I > all data (last shell)	5.8 (1.4)
Rmerge all data (last shell)	0.110 (0.535)
Refinement	
R-factor	0.213
Rfree	0.263
Reflections used	17,968
Test set	977 (5.2%)
RMSD from ideality	
Bond lengths (Å)	0.014
Bond angles (deg.)	1.38
Ramachandran plot	
Favored regions	96.3%
Allowed regions	100.0%
Model	Residues / Avg. B (Å ²)
Protein	436 (31.0)
Heme	1 (15.0)
X2N (posaconazole)	1 (56.4)
H ₂ O molecules	82 (29.9)