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Supporting information for article:

Structural insights into the effects of glycerol on ligand binding to cytochrome P450

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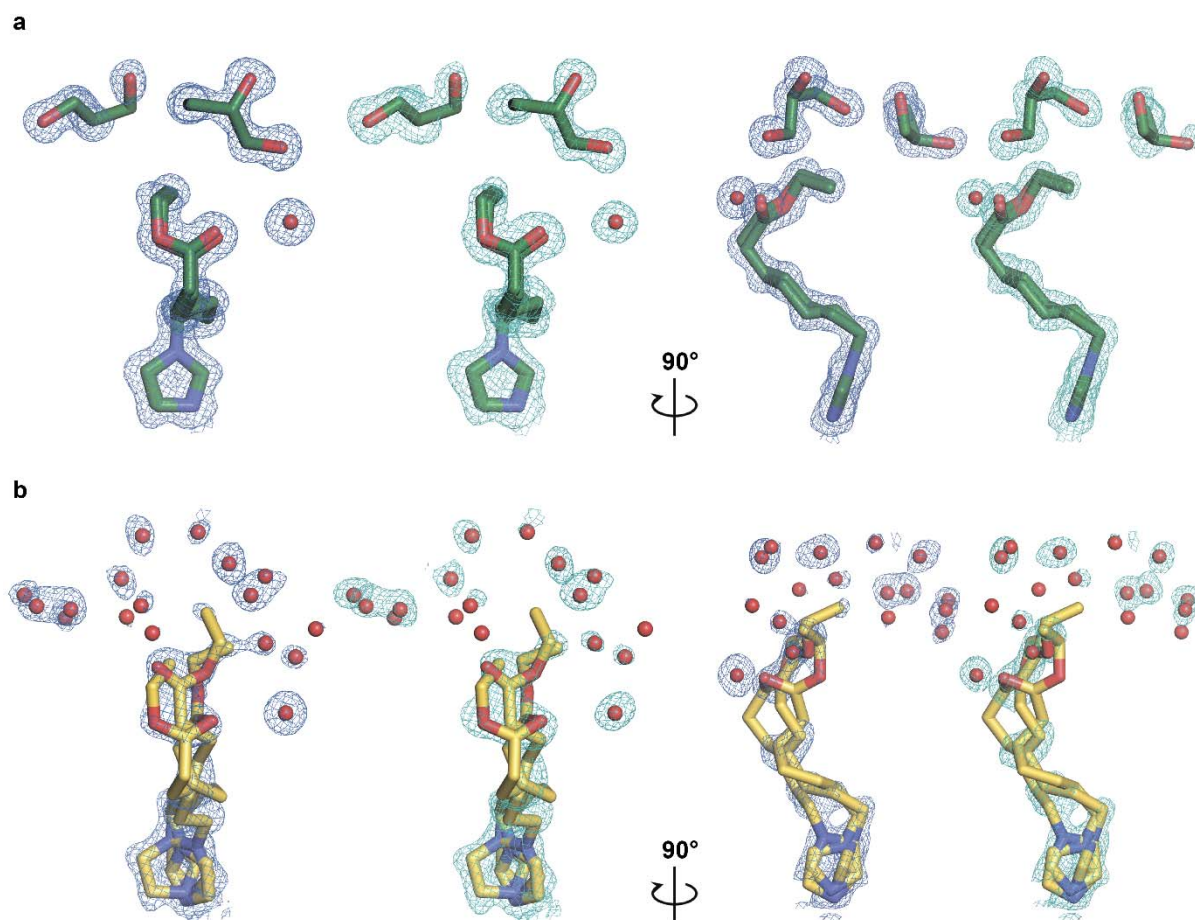
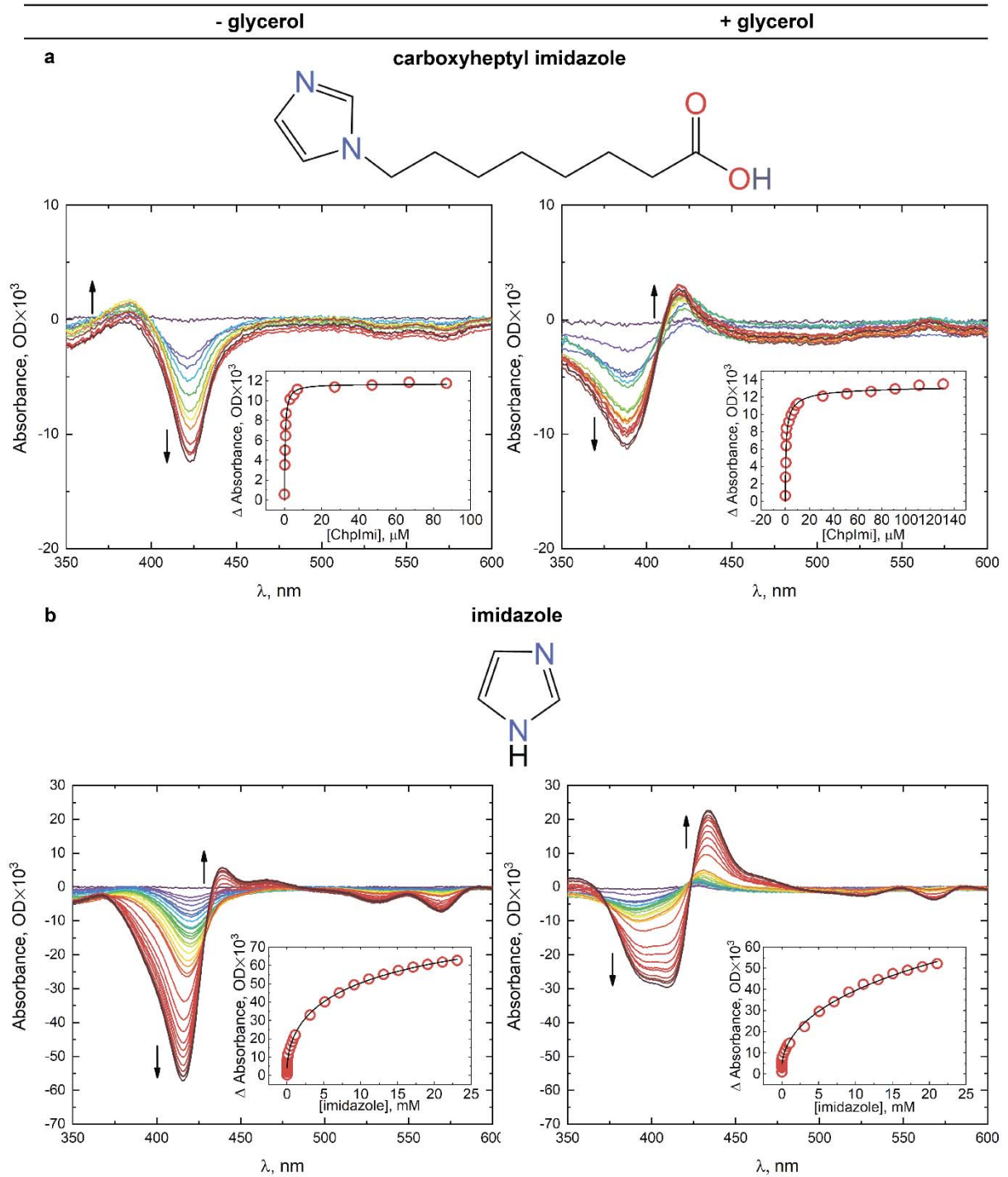
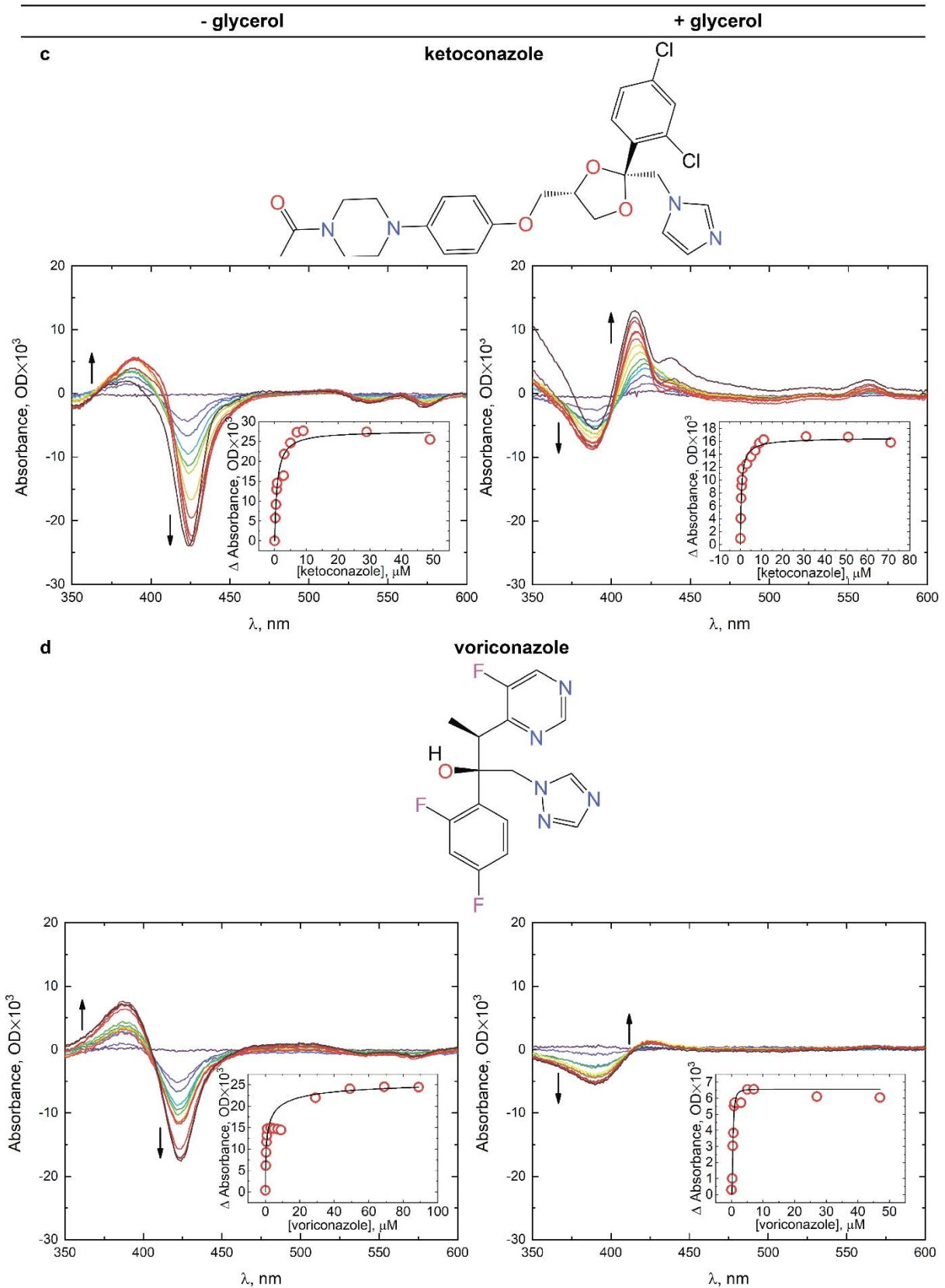


Figure S1 Electron density at the active site of CYP124-CHimi complex. **a**, Two views of CHImi, bounded glycerol molecules, and a water molecule in the Cryo structure (PDB ID: 6T0K). 2mFo-DFc (colored blue) and simulated annealing omit 2mFo-DFc (colored cyan) electron density maps are contoured at 1.0 σ level. **b**, Two views of CHImi and water molecules, filling the glycerol binding site, in the NoCryo structure (PDB ID: 7ZB9). 2mFo-DFc and simulated annealing omit 2mFo-DFc electron density maps are contoured at 1.0 σ level.





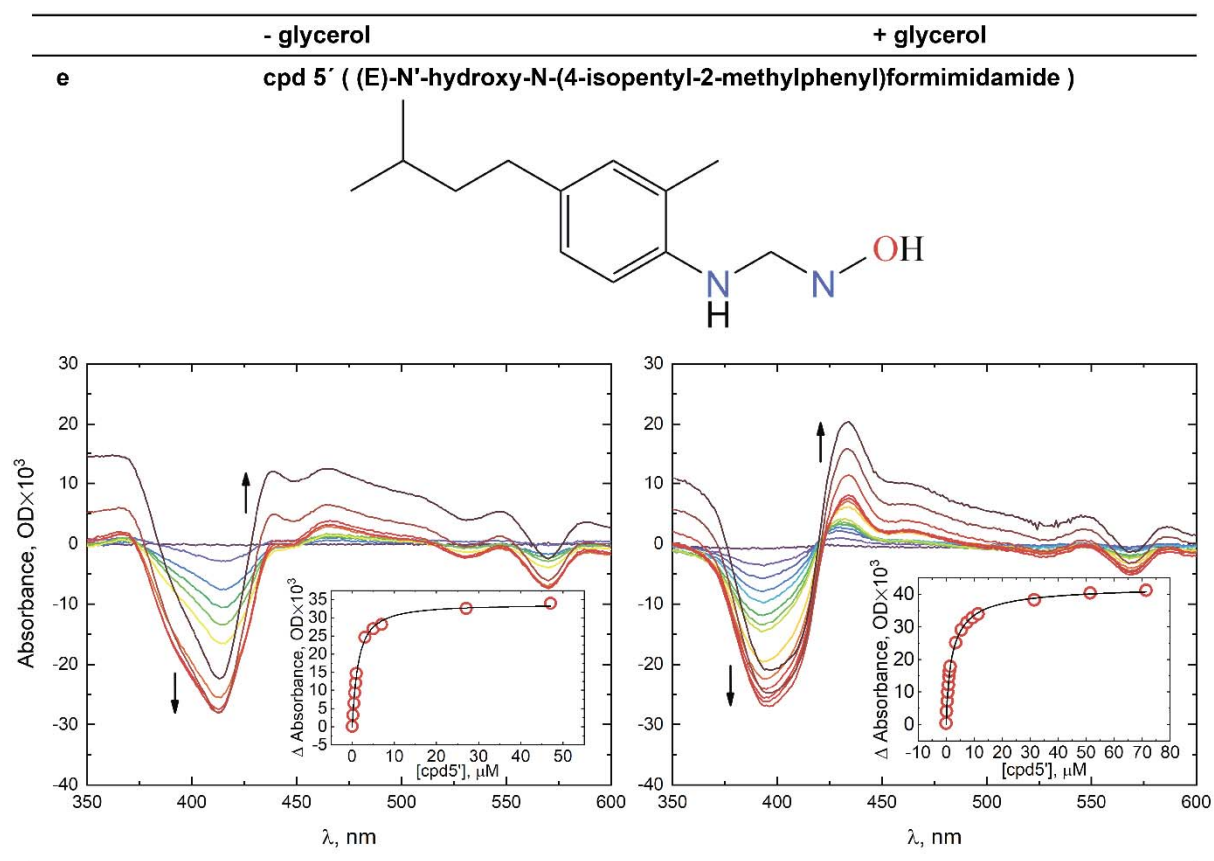


Figure S2 Effect of glycerol on binding of various ligands to CYP124. **a-e**, Difference spectra of CYP124 are shown upon titration with carbethoxyheptyl imidazole, imidazole, ketoconazole, voriconazole, and cpd 5', correspondingly, in two buffers: 50 mM KPi pH=7.4 (left) and 50 mM KPi pH=7.4 with 20% (w/v) glycerol (right).

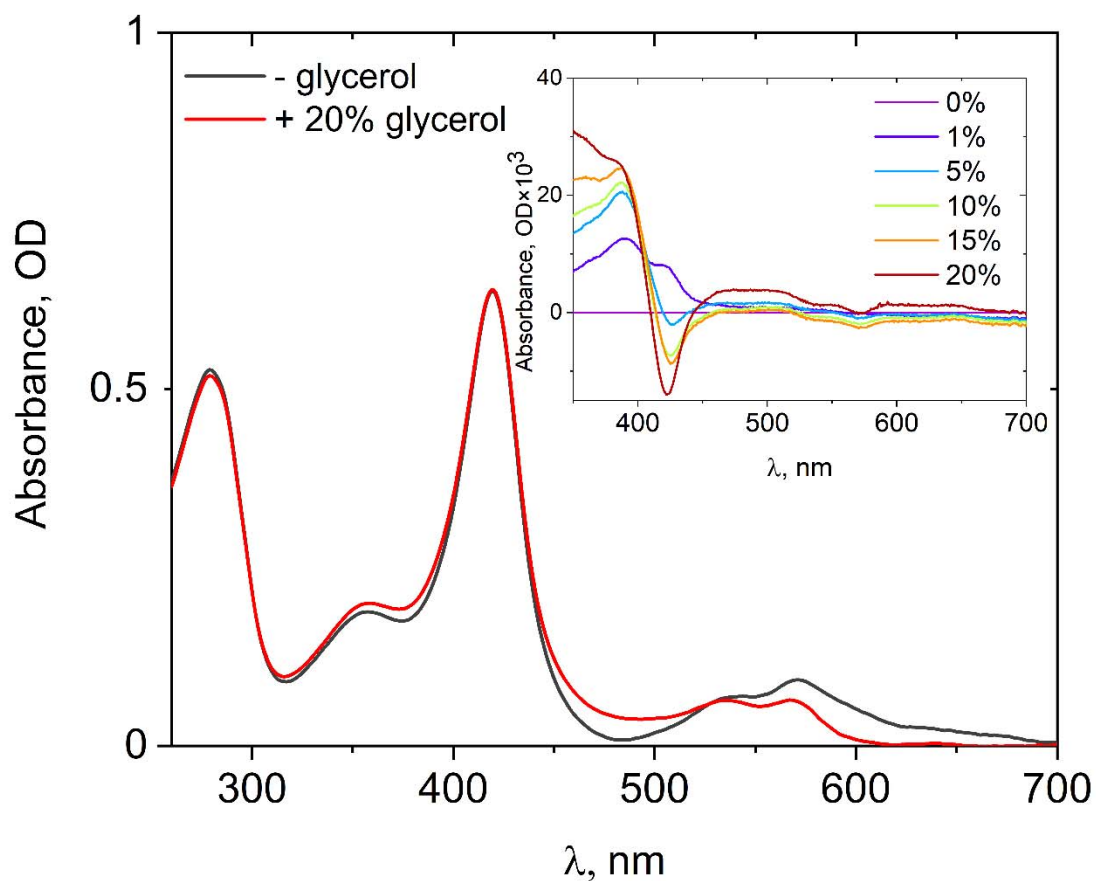


Figure S3 Spectrophotometric titration of CYP124 with glycerol. Absolute spectra in the absence of glycerol (gray line) and in the presence of 20% (w/v) glycerol (red line). Inserted picture - difference spectrum of CYP124 glycerol titration.