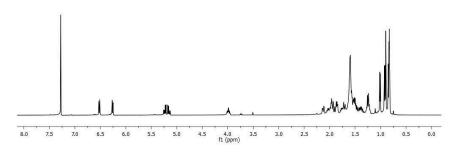
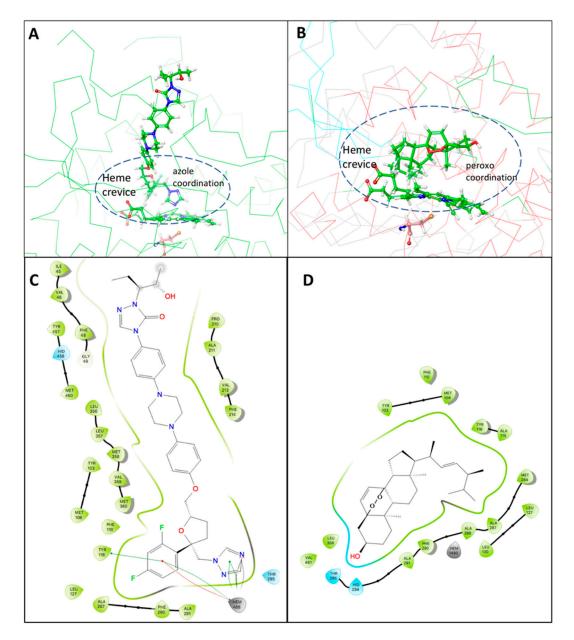


B)



SI-1. Proton NMR spectrum for ergosterol peroxide (5α , 8α -epidioxy-22E-ergosta-6,22-dien-3 β -ol). In image A amplified spectrum and B compete signal spectrum.



SI-2 Comparison of posaconazole and ergosterol peroxide binding modes to CYP51 P450 of T. cruzi proteins: A) co-crystallized posaconazole complexed with CYP51 P450 (PDB code: 3K1O); B) ergosterol peroxide complexed with CYP51 P450 of T. cruzi. The binding site between both ligands is the same (next to the heme group, in its crevice); C) ligand interaction diagram of the whole interaction zone between posaconazole and CPY51 P450; D) ligand interaction diagram of the proposed interaction zone between ergosterol peroxide and CYP51 P450.