Title: Substituted Imidazole of 5-Fluoro-2-[4-[(2-phenyl-1H-imidazol-5-yl)methyl]-1-piperazinyl]pyrimidine Inactivates Cytochrome P450 2D6 by Protein Adduction Authors: Nagy, Mocny, Diffenderfer, Hsi, Butler, Arthur, Fletke, Palamanda, Nomeir, Furge Journal: Drug Metabolism and Disposition

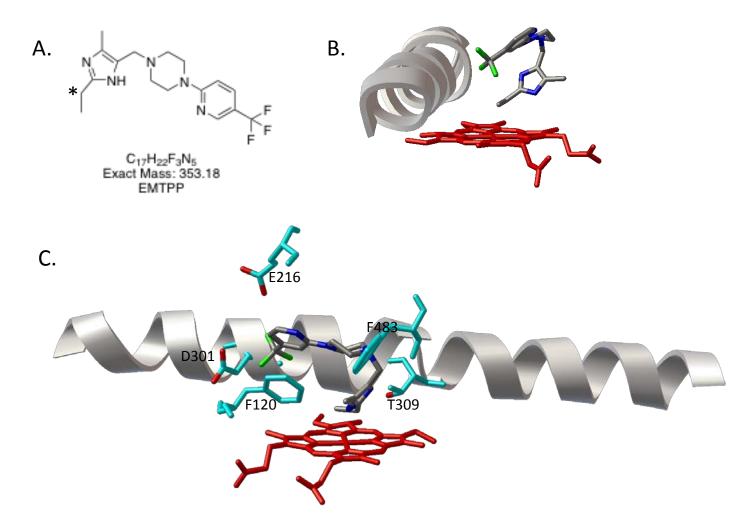


Figure S8. Molecular modeling of EMTPP bound to CYP2D6. (A) Structure of EMTPP with the location of metabolism site as identified by Hutzler et al. (*32*) indicated with an asterisk. (B) Molecular model of CYP2D6 with EMTPP. Heme is shown in red. (C) Active site residues Phe120, Phe483, Glu216, Asp301, and Thr 309 are indicated in turquoise. The carbon of EMTPP that is the site of oxidation is 4.1 Å from Thr309.