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

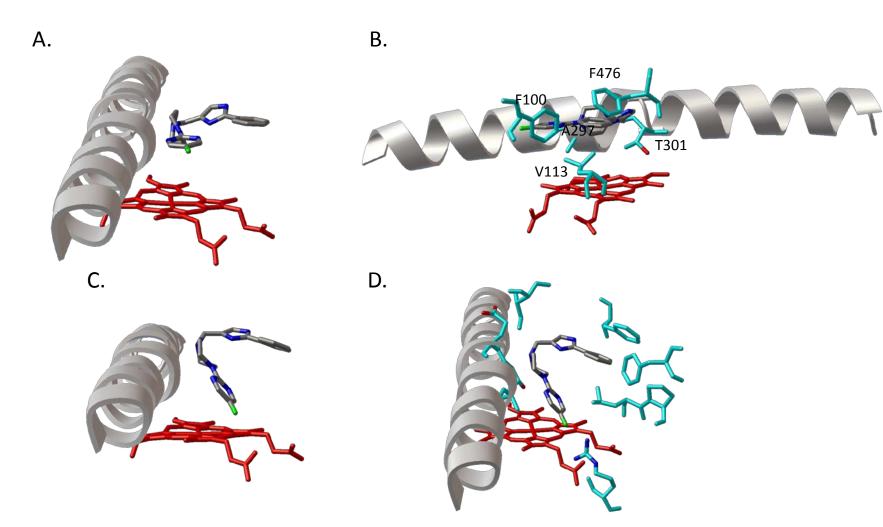


Figure S7. Molecular modeling of SCH 66712 bound to CYP2C9. Helix I is also shown. (A) SCH 66712 in horizontal binding orientation with heme and Helix I. (B) SCH 66712 in horizontal binding orientation with heme and active site residues of CYP2C9. (C) SCH 66712 with flourine pointing to heme and Helix I. (D) SCH 66712 with flourine pointing to heme heme and active site residues of CYP2C9.