Figure S5. Key residues (E216, D301, F120, F483, S304 and Q244) located in the active site of each CYP2D6 most prevalent conformation compared to the x-ray structures (ligands are left out for clarity). The active site is shown for the most prevalent conformation in cyan, and the x-ray structure in white (A-C: 3QM4, D-I: 4WNU). (A-C) Prinomastat (inhibitor) with wild-type (wt) (A), CYP2D6*17 (V17) (B) and CYP2D6*53 (V53) (C), (D-F) Quinidine (inhibitor) with wild-type (wt) (D), CYP2D6*17 (V17) (E) and CYP2D6*53 (V53) (F), (G-I) wild-type together with substrates: bufuralol (G), tamoxifen (H), and veliparib (I).