

SUPPLEMENTAL DATA

Figure S1. Correlation of $\text{Ln}K_{\text{eq}}$ with pressure for CYP2B1 WT and the three cys variants.

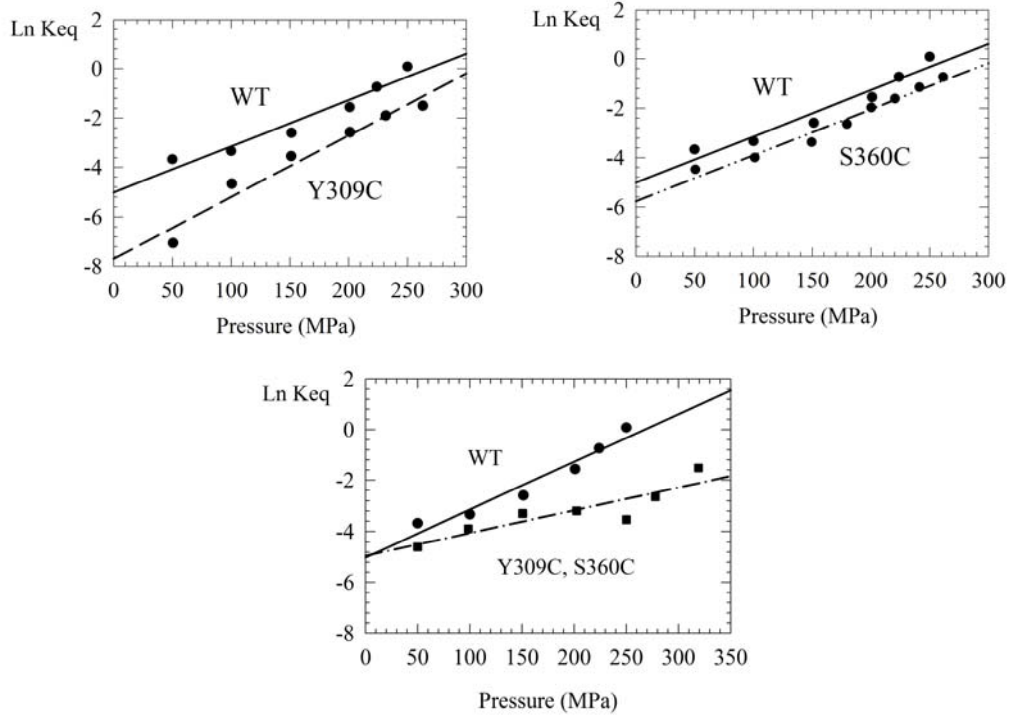


Figure S2. Time dependence of the $C\alpha$ RMSD of CYP2B1 WT (solid line) and the Y309C/S360C variant (dashed line) obtained from a 2 ns MD simulations at 300K. The initial coordinate was used as reference to calculate the RMSD.

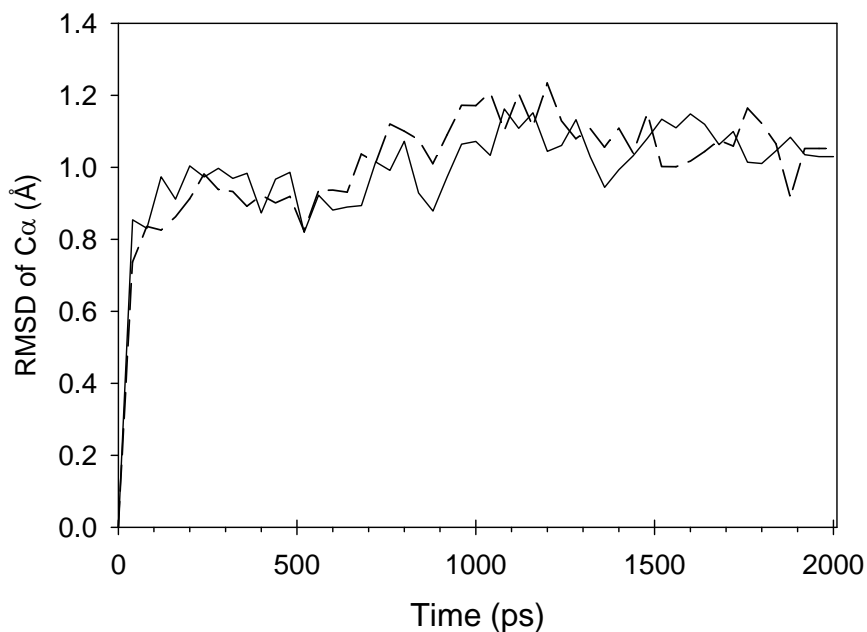


Figure S3. RMSD values of CYP2B1 WT and Y309CS360C (YS) obtained from 2 ns MD simulations at 300K. The initial coordinate was used as reference to calculate the RMSD. The horizontal bars represent the plastic regions identified by Zhao et al. (6)

