Pharmacoinformatics-based identification of anti-bacterial Catalase-peroxidase enzyme inhibitors

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Supplementary materials data

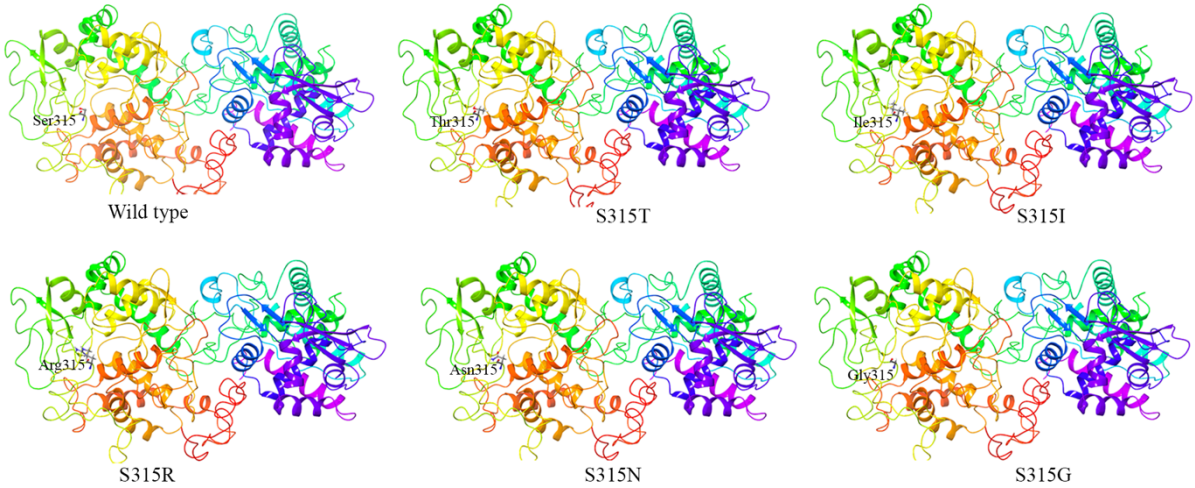

Figure S1. Mutant and wild type katG enzyme.

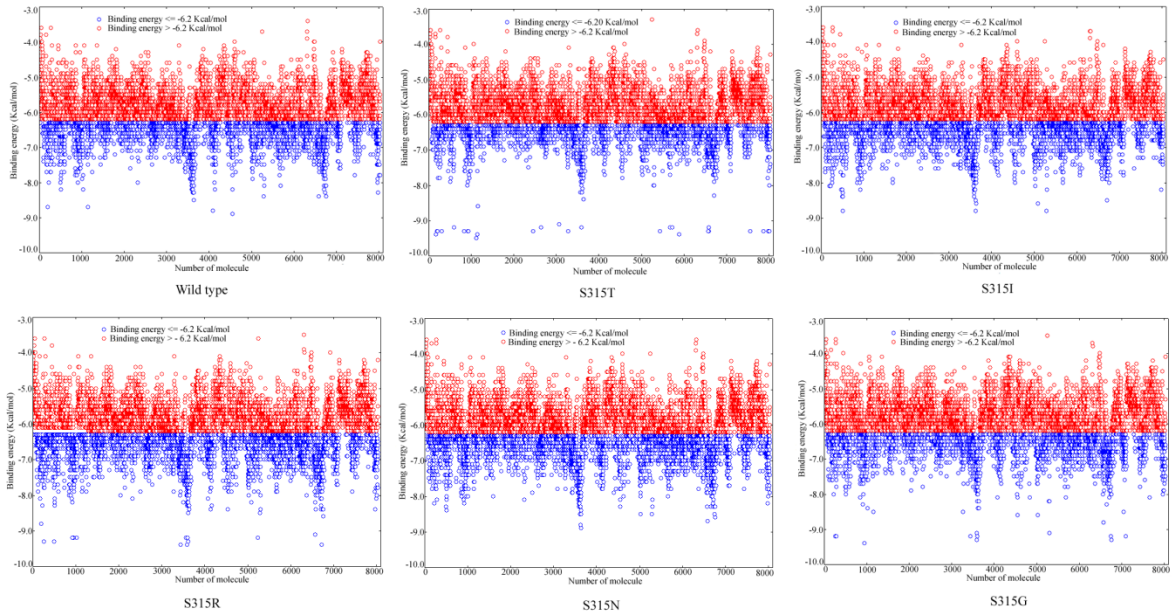

Figure S2: Distribution of the binding affinity scores obtained for 8044 compounds docked with five different mutant katG and wild type katG protein.

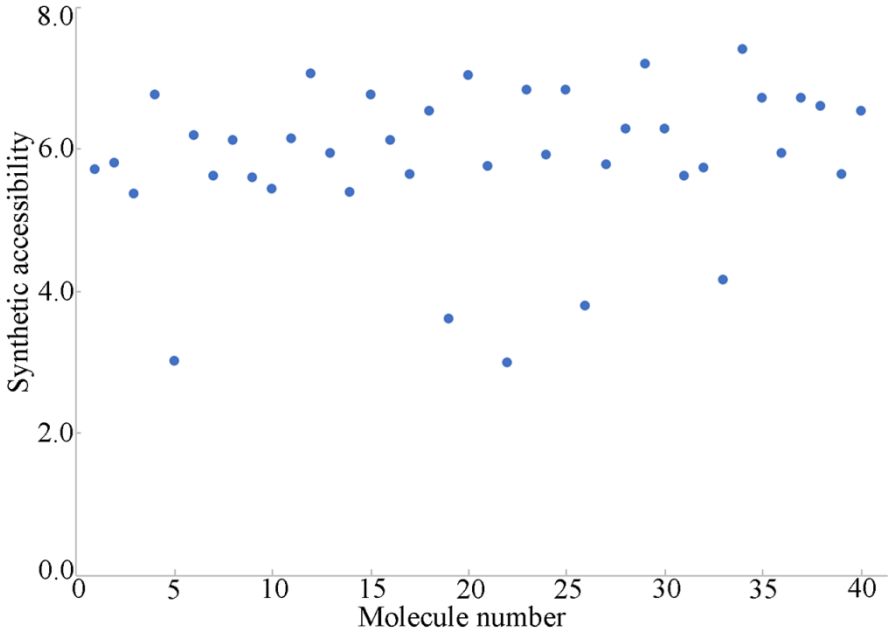

Figure S3. Synthetic accessibility values for 40 molecules shown good ADME and pharmacokinetics profile.

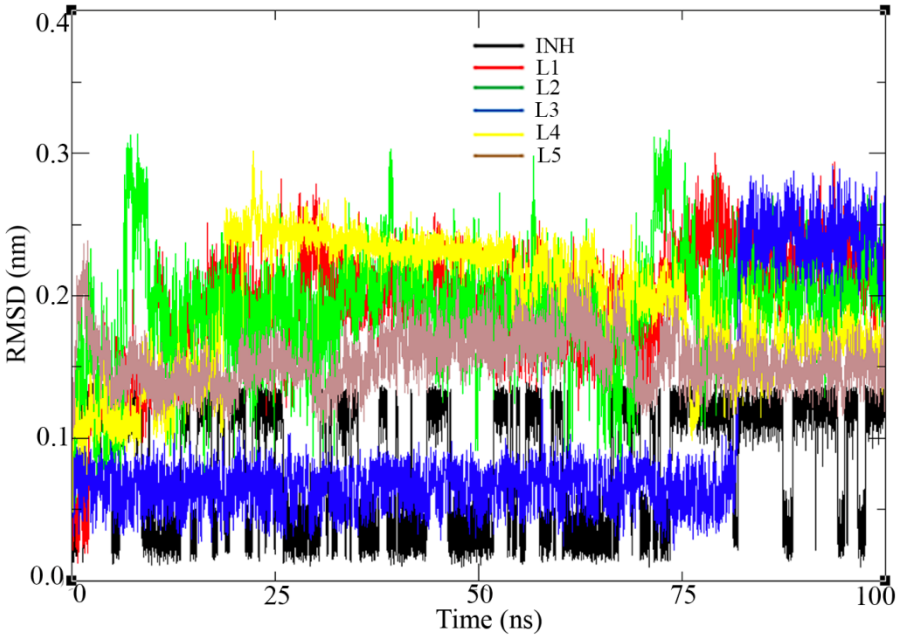

Figure S4. RMSD plot of ligands vs. time of five screened katG inhibitors and INH.