

Electronic Supplementary Information

Consensus screening for a challenging target: the quest for P-glycoprotein inhibitors

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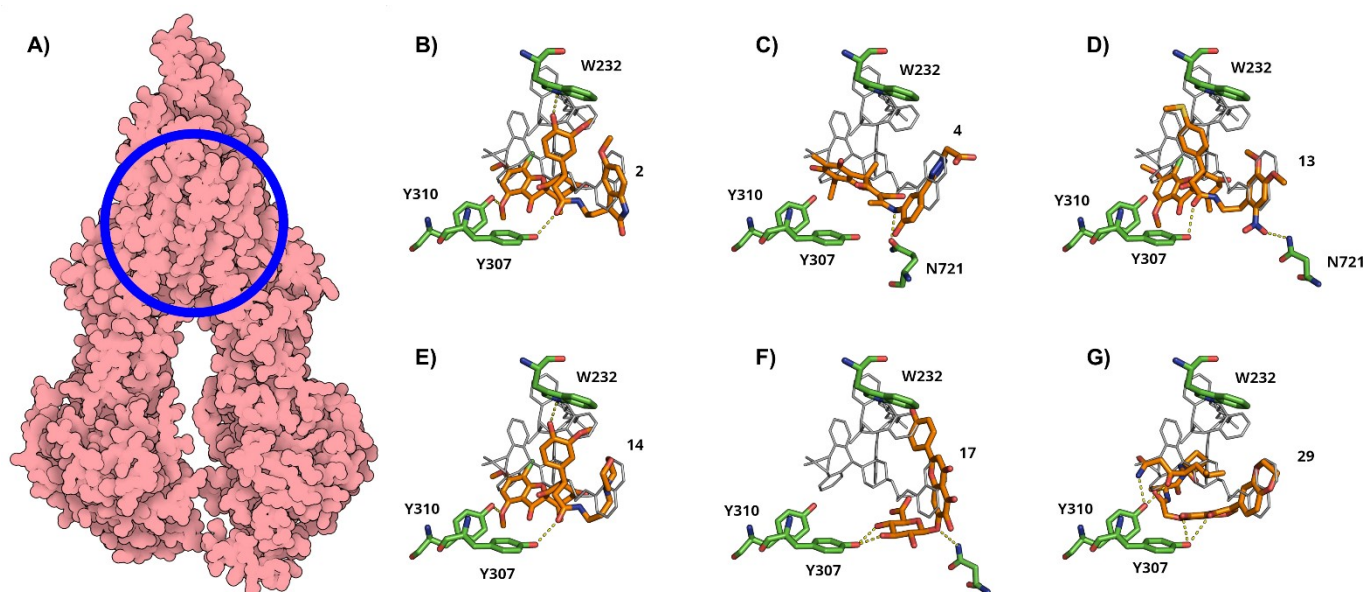


Fig. S1. P-gp binding site (A) and best docked pose of compounds 2 (B), 4 (C), 13 (D), 14 (E), 17 (F), and 29 (G) in the binding site of P-gp. Compounds are shown as orange sticks, while Trp232, Tyr307, Tyr310, and Asn721 are shown as green sticks. Hydrogen bonds are shown as yellow dashed lines. For comparison, the experimental binding pose of the two copies of zosuquidar is also shown in grey.