

Simultaneous Binding Mechanism of Multiple Substrates for Multidrug Resistance Transporter P-glycoprotein

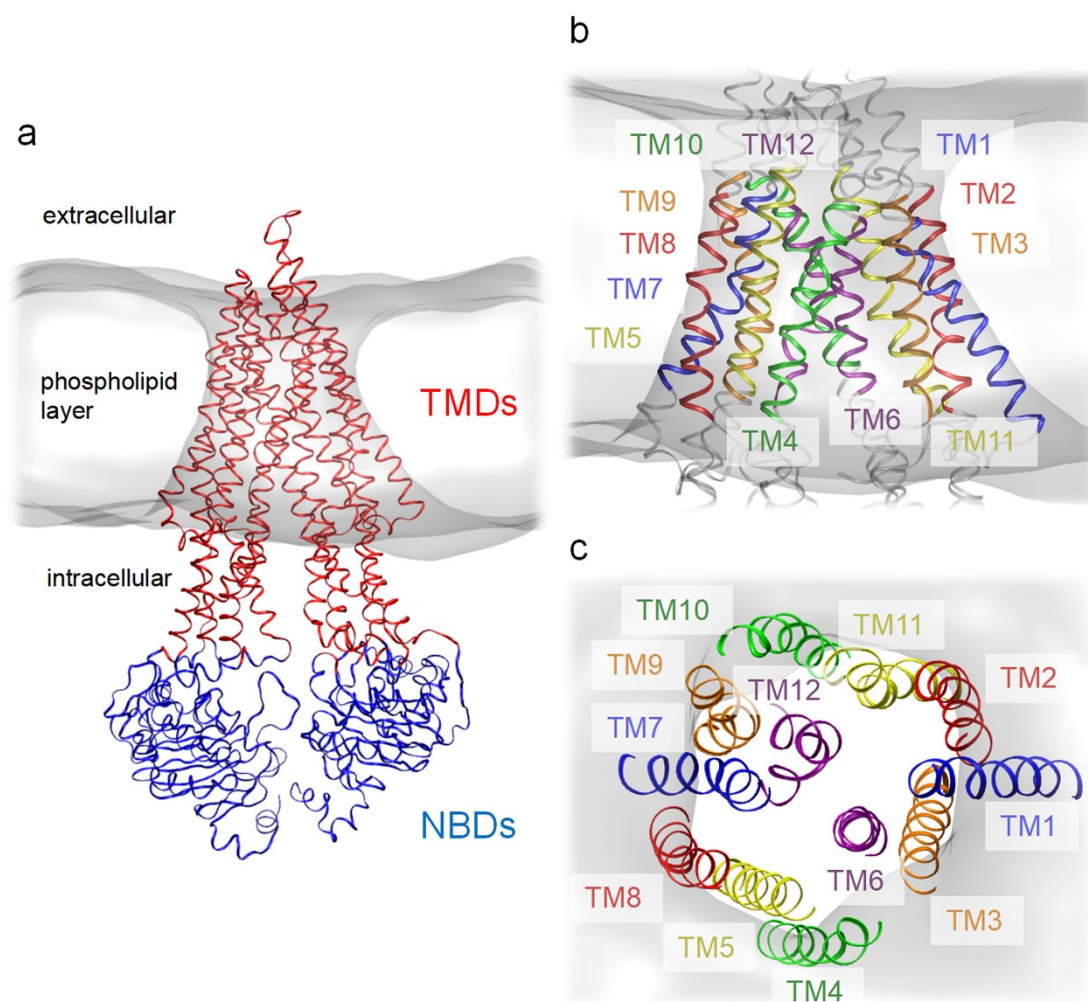


Figure S1. (a) Structure of P-glycoprotein. (b,c) Structure of transmembrane segments in P-gp. (b: Front view; c: Top view)

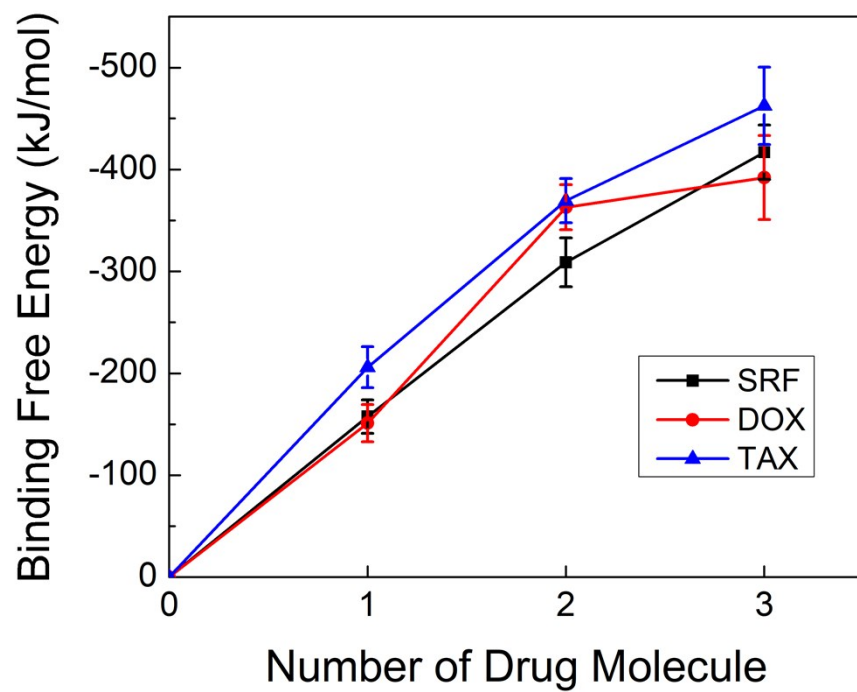


Figure S2. Relationship between binding free energy of P-gp with multiple drugs and the number of drug molecules

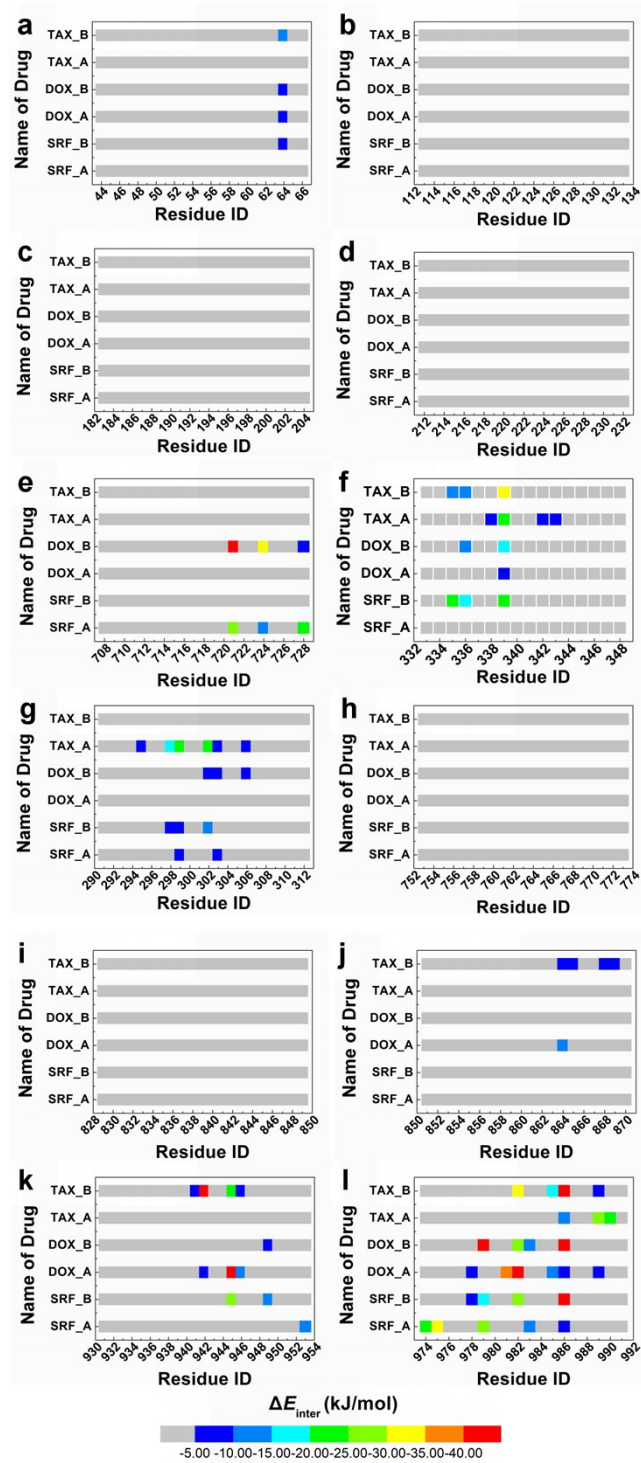


Figure S3. Binding Energy of drug molecules binding with P-gp residues in 2-drug systems

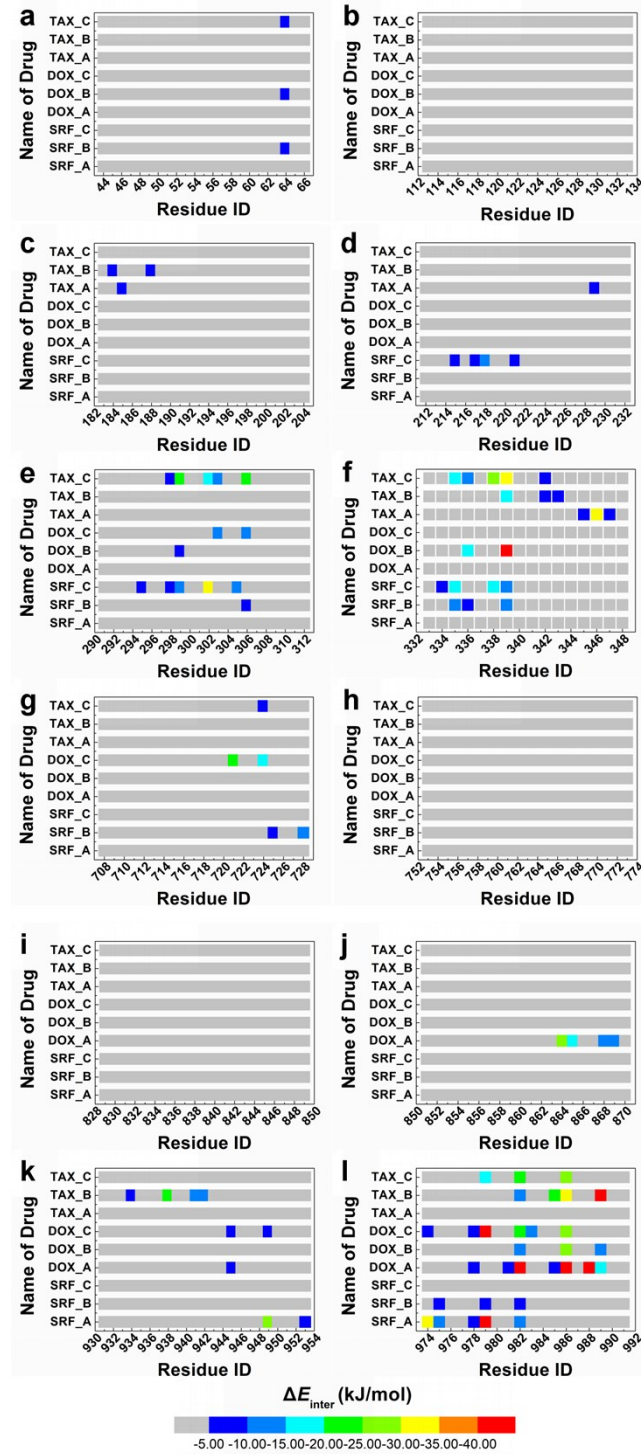


Figure S4. Binding Energy of drug molecules binding with P-gp residues in 3-drug systems