

B4R pLDDT=88.03

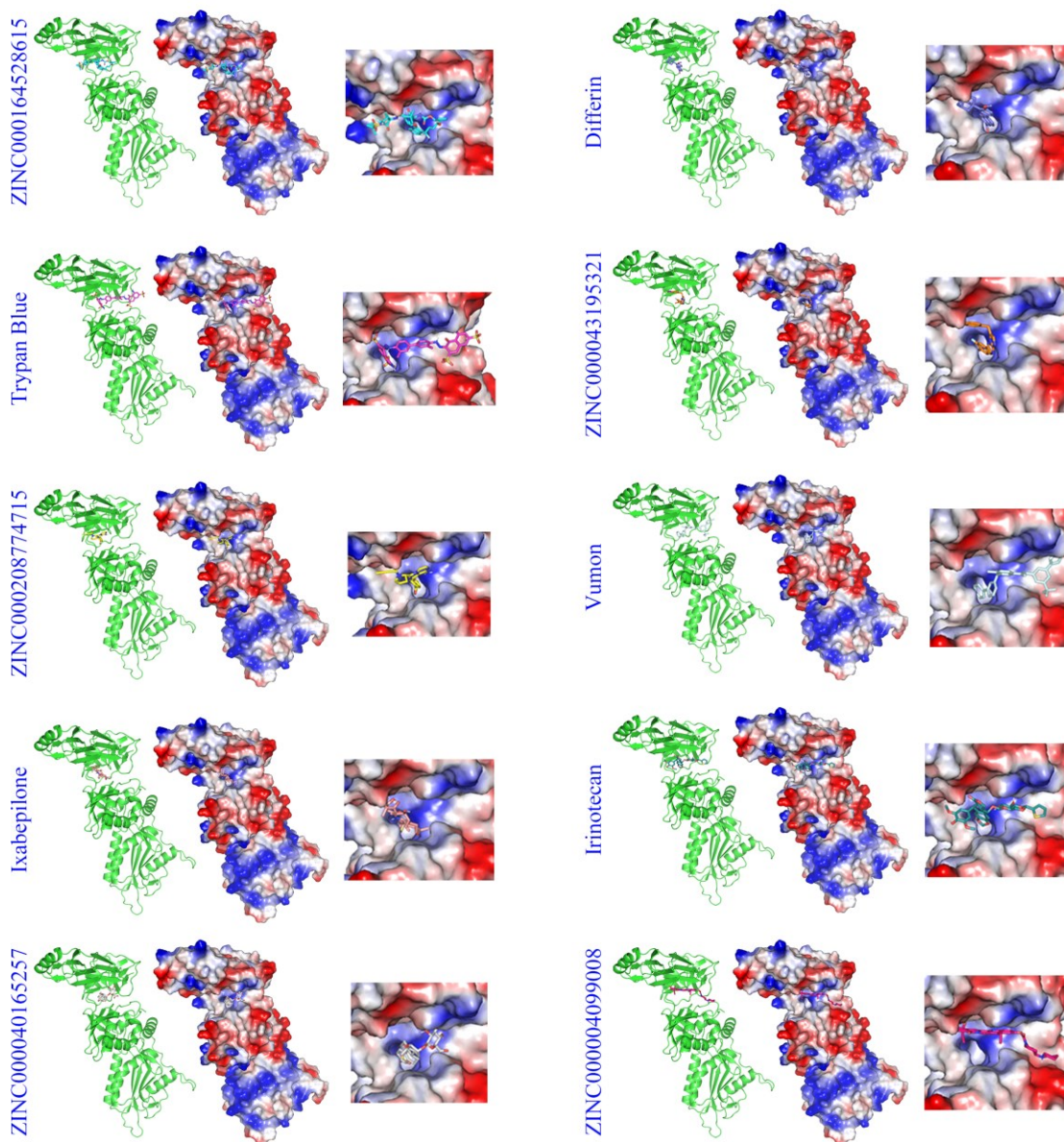


Figure S1. The top ten best docking drugs targeting B4R, including ZINC164528615, Trypan Blue, ZINC208774715, Ixabepilone, ZINC40165257, Differin, Vumon, Irinotecan, and Bisotrizole.

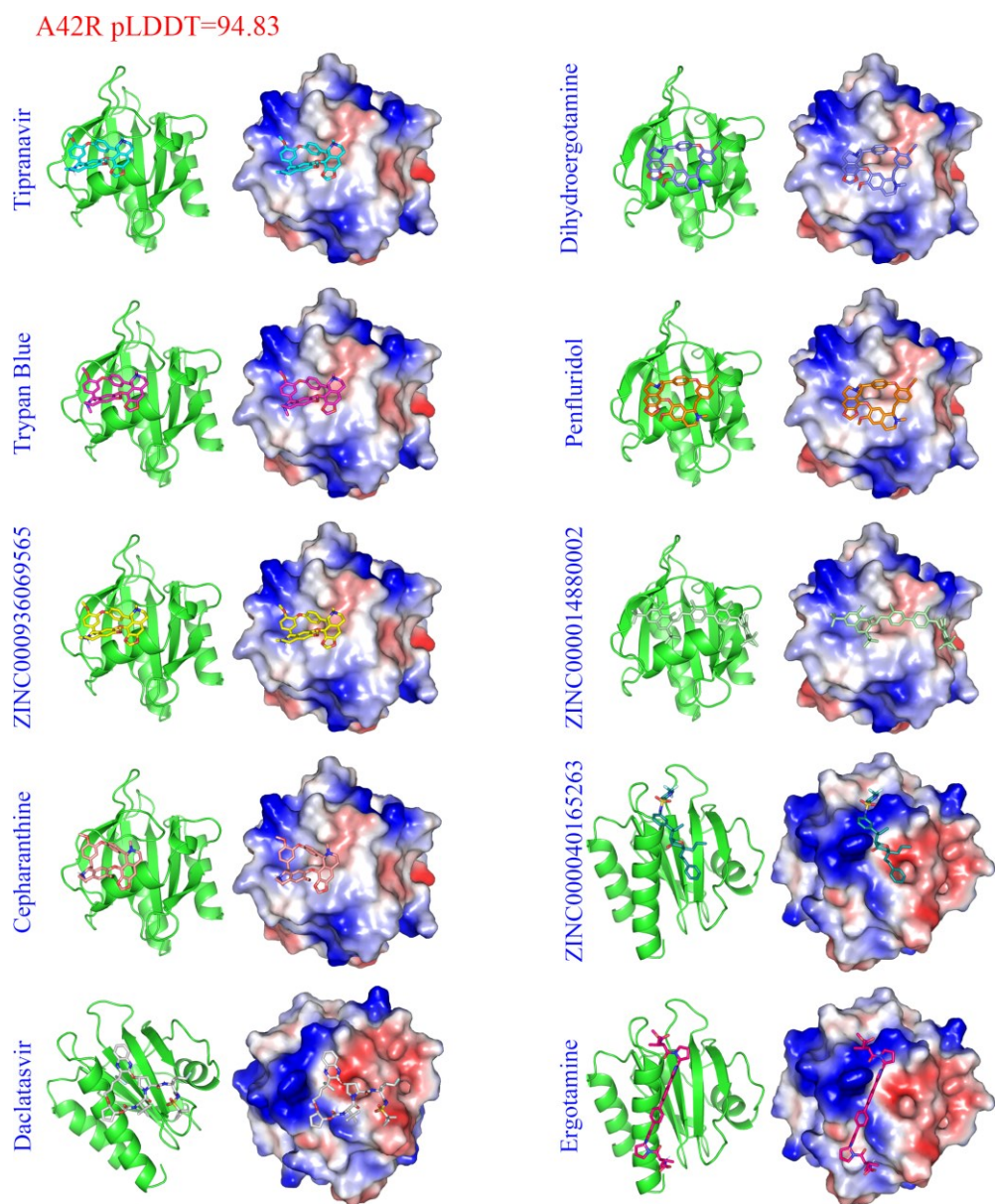


Figure S2. The top ten best docking drugs targeting A42R, including tipranavir, trypan blue, zinc936069565, cepharanthine, daclatasvir, dihydroergotamine, penfluridol, dihydroergotamine, zinc40165263, and ergotamine

RPO132 pLDDT=92.80

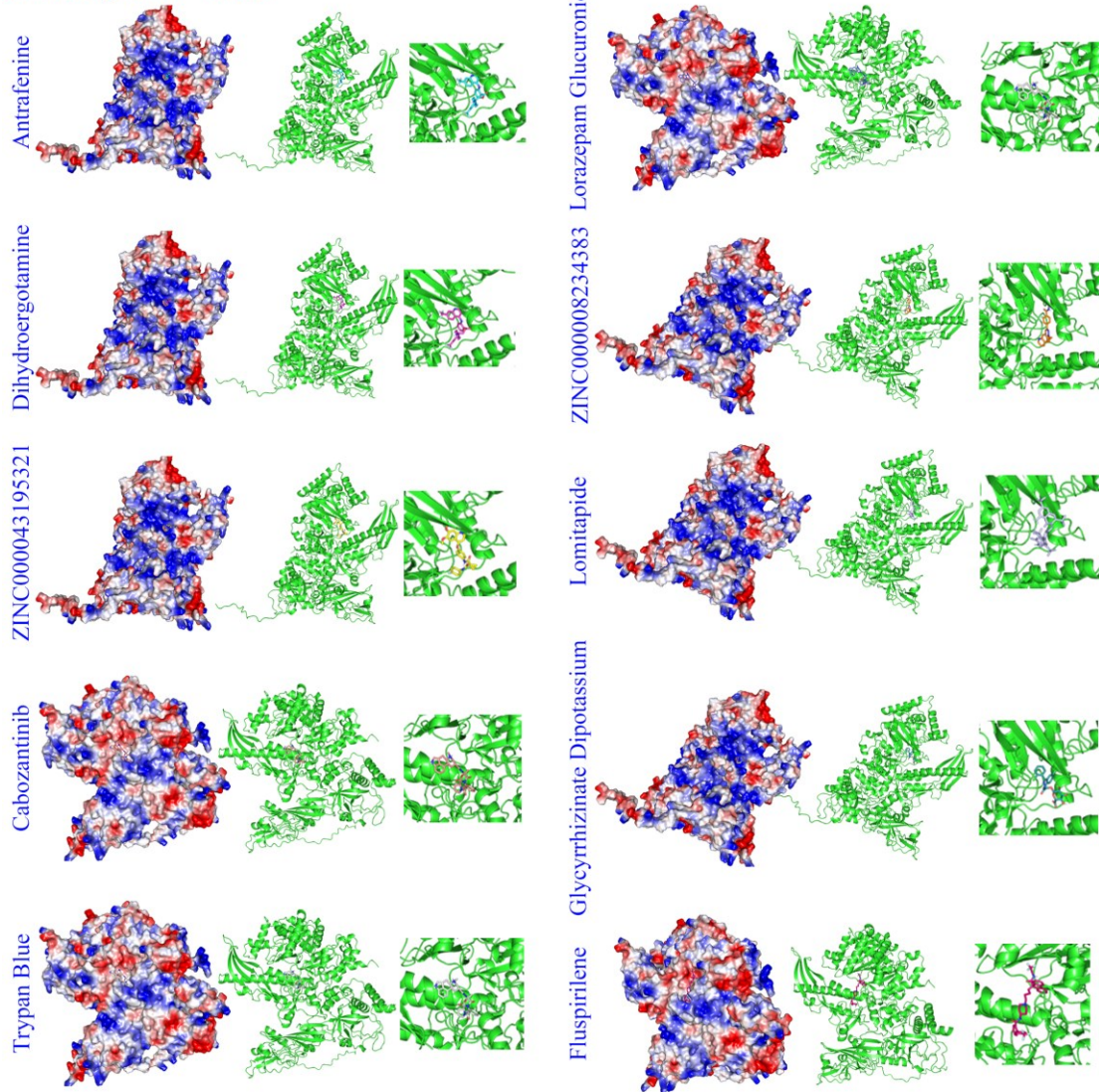


Figure S3. The top ten best docking drugs targeting PRO132, including antrafenine, dihydroergotamine, zinc43195321, cabozantinib, trypan blue, lorazepam glucuronide, zinc8234383, lomitapide, glycyrrhizinate dipotassium, and fluspirilene.

VITF3L pLDDT=90.84

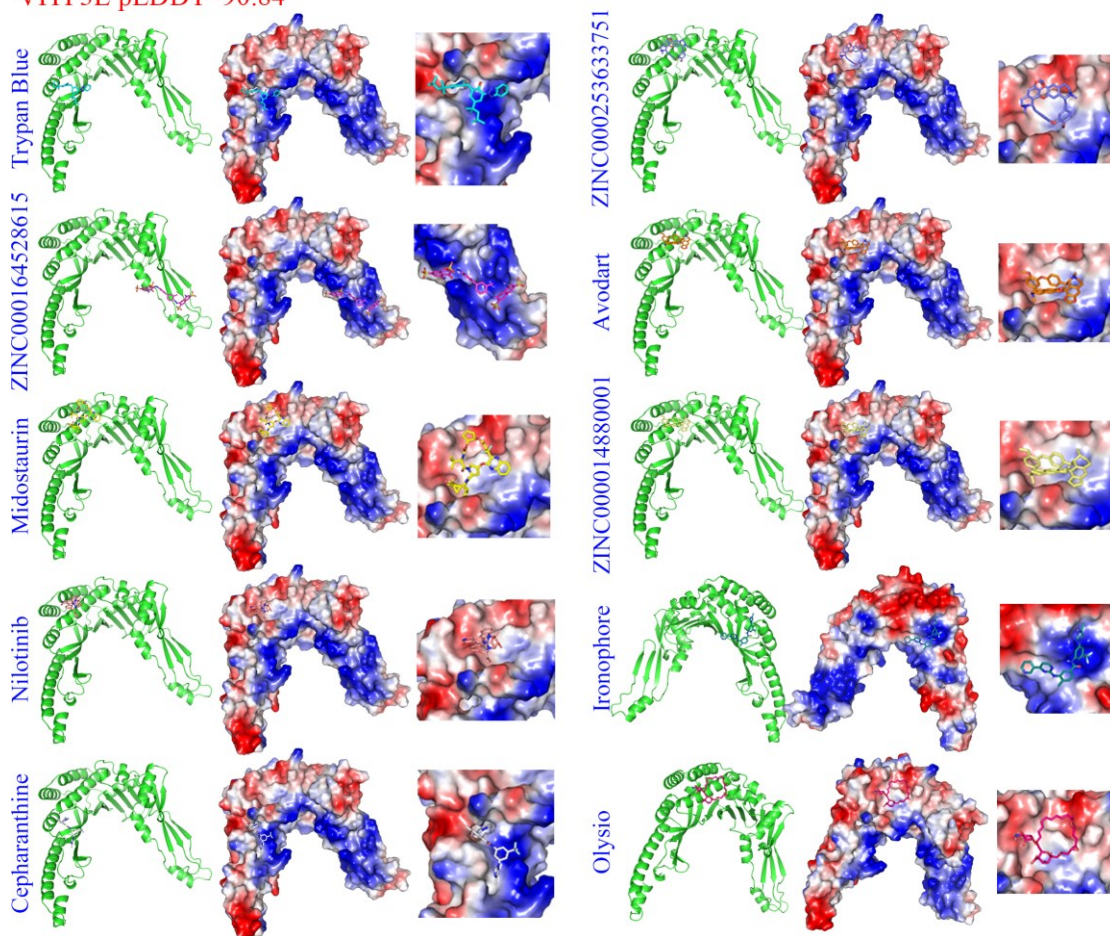


Figure S4. The top ten best docking drugs targeting PRO132, including trypan blue, zinc164528615, midostaurin, nilotinib, cepharanthine, zinc253633751, avodart, zinc14880001, ironophore, and olysis.

E8L pLDDT=89.86

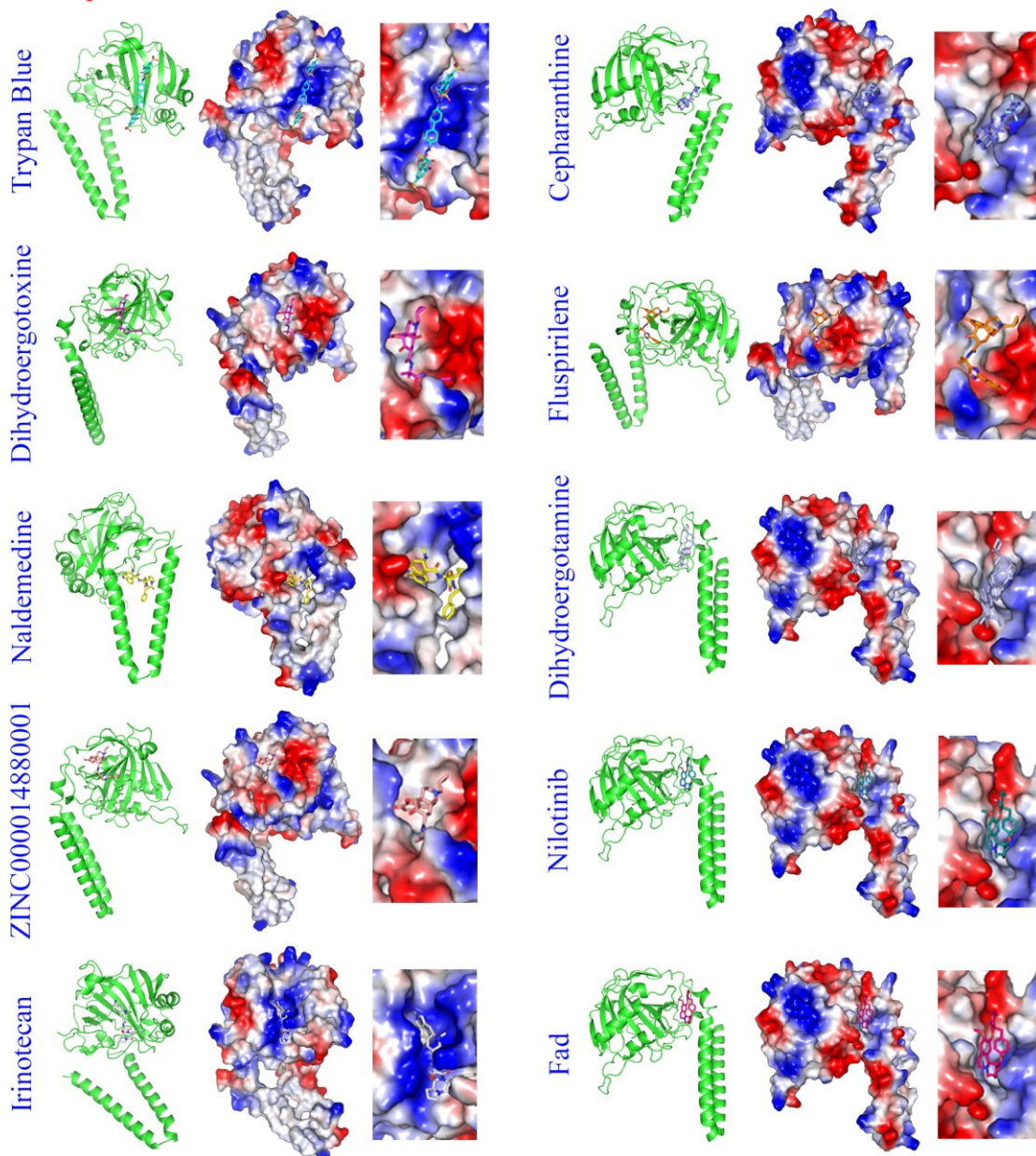


Figure S5. The top ten best docking drugs targeting E8L, including trypan blue, dihydroergotoxine, naldemedine, zinc14880001, irinotecan, cepharanthine, fluspirilene, dihydroergotamine, nilotinib, and fad.

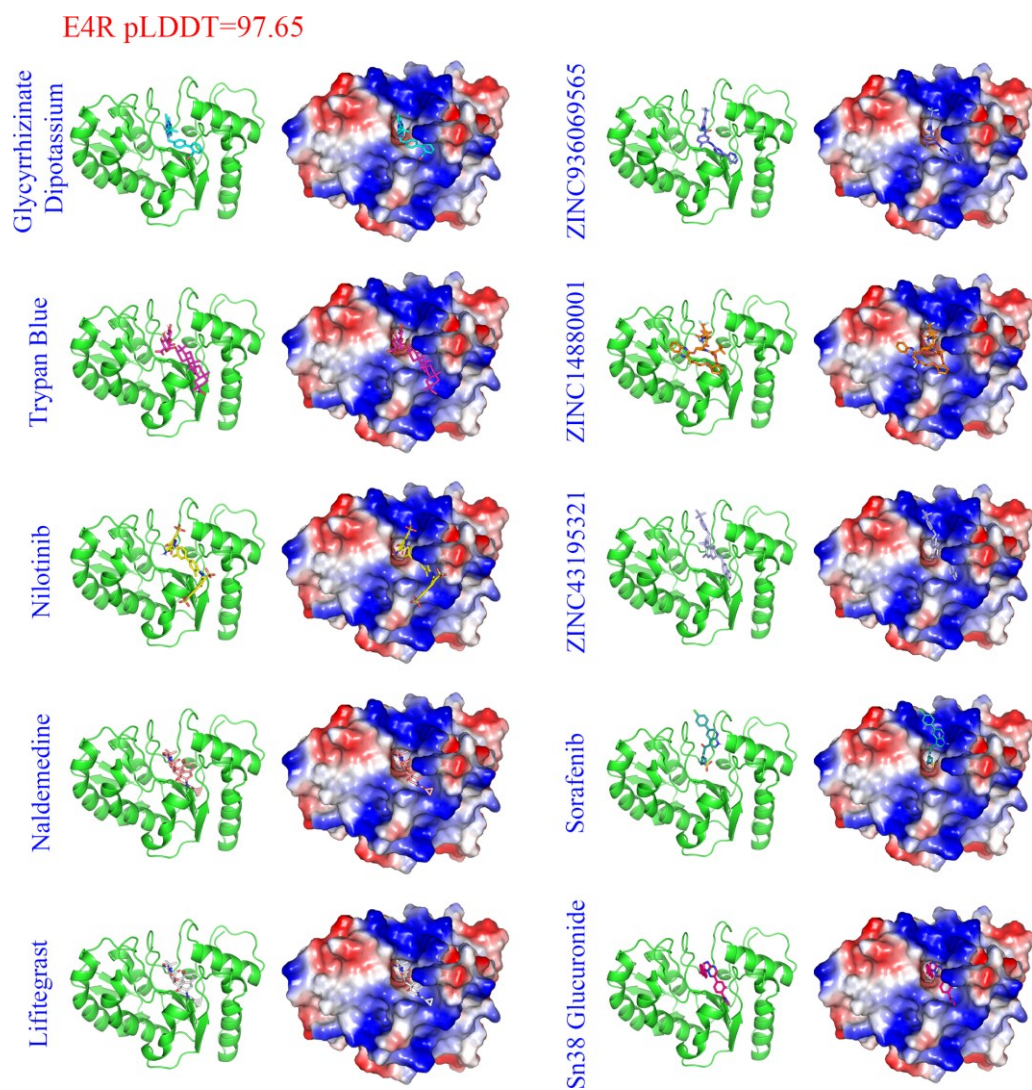


Figure S6. The top ten best docking drugs targeting E8L, including glycyrrhizinate dipotassium, trypan blue, nilotinib, naldemedine, lifitegrast, zinc936069565, zinc14880001, zinc43195321, sorafenib, and sn38 glucuronide.

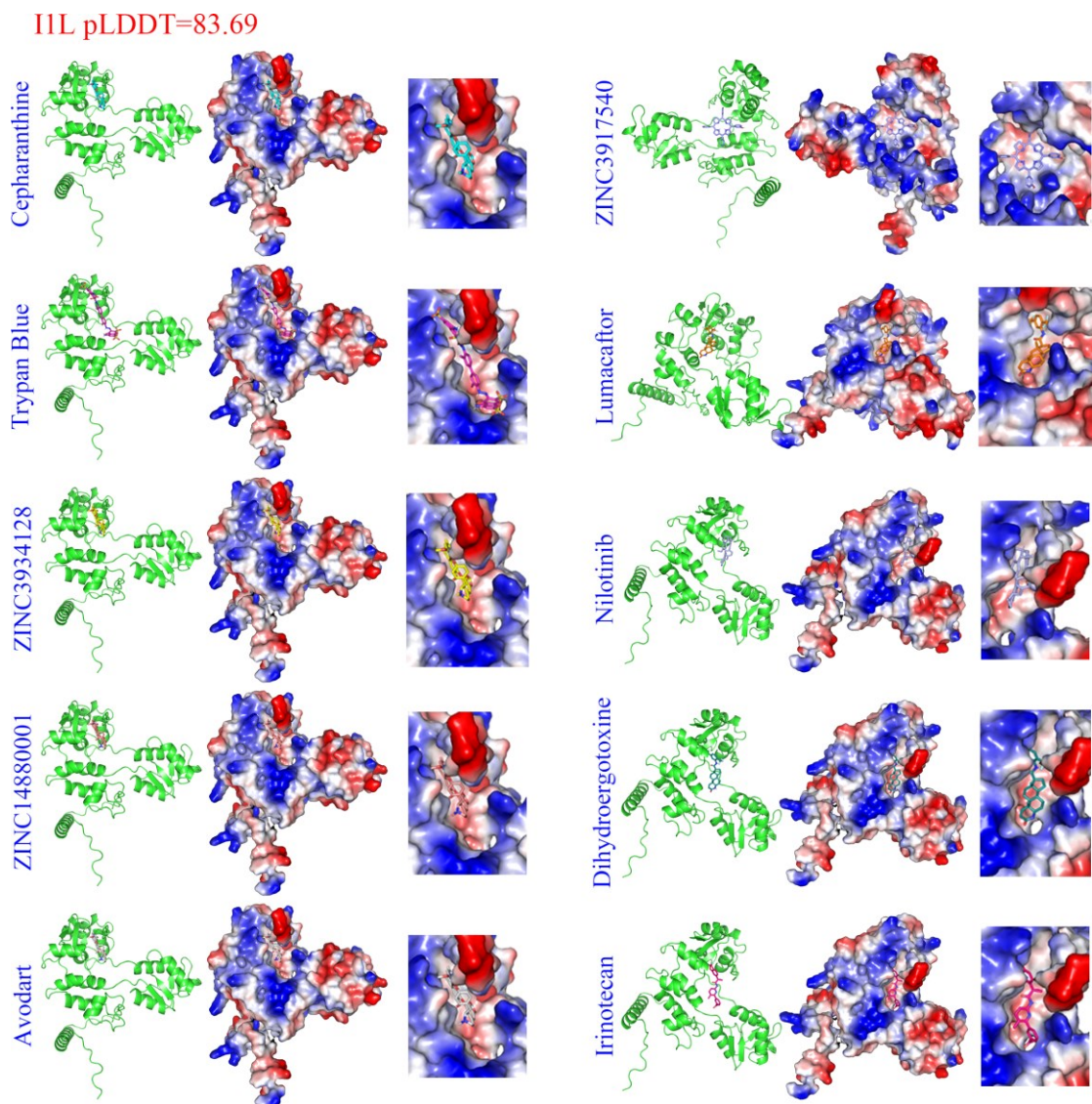


Figure S7. The top ten best docking drugs targeting I1L, including cepharanthine, trypan blue, zinc3934128, zinc14880001, avodart, zinc3917540, lumacaftor, nilotinib, dihydroergotoxine, and irinotecan.

D10L pLDDT=96.36

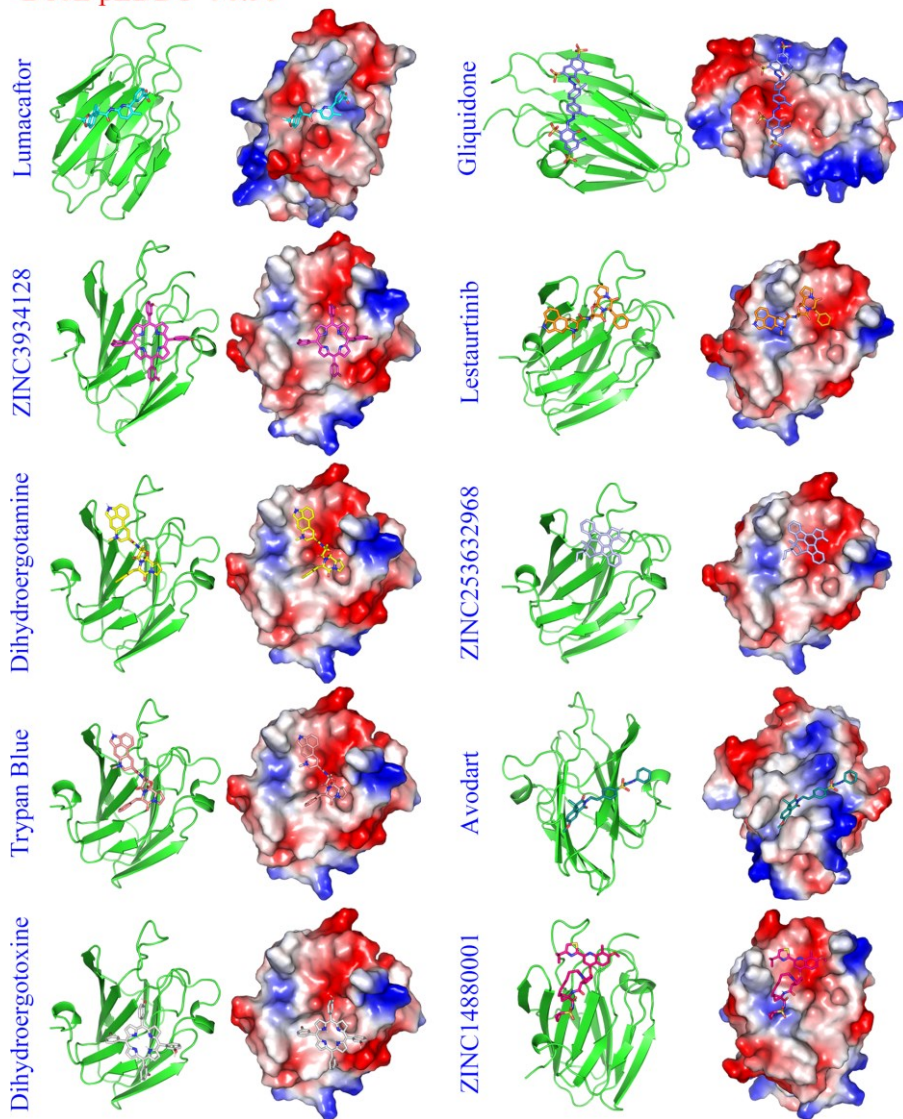


Figure S8. The top ten best docking drugs targeting D10L, including lumacaftor, zinc3934128, dihydroergotamine, trypan blue, dihydroergotoxine, gliquidone, lestaurtinib, zinc253632968, avodart, and zinc14880001.



P28 pLDDT=91.07

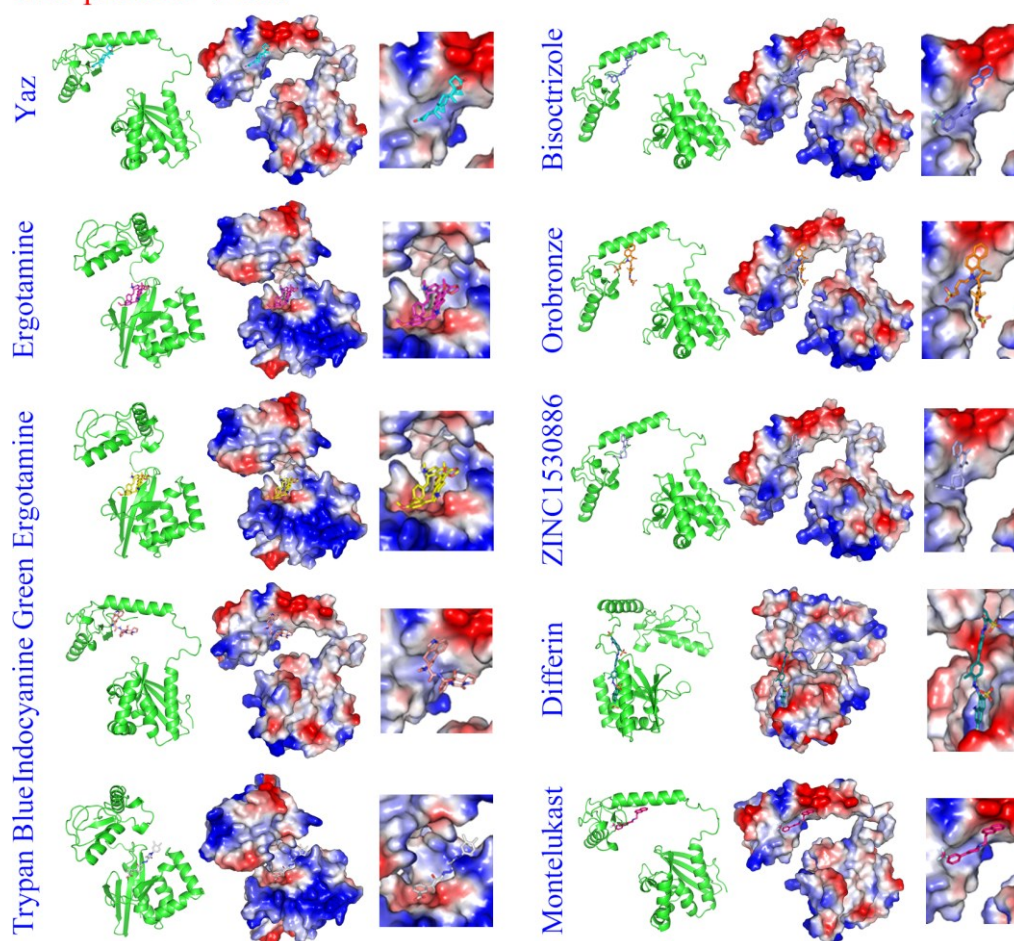


Figure S9. The top ten best docking drugs targeting P28, including yaz, ergotamine, xaliproden, indocyanine green, trypan blue, bisotrizole, orobronze, zinc1530886, differin, and montelukast.

G9R pLDDT=89.38

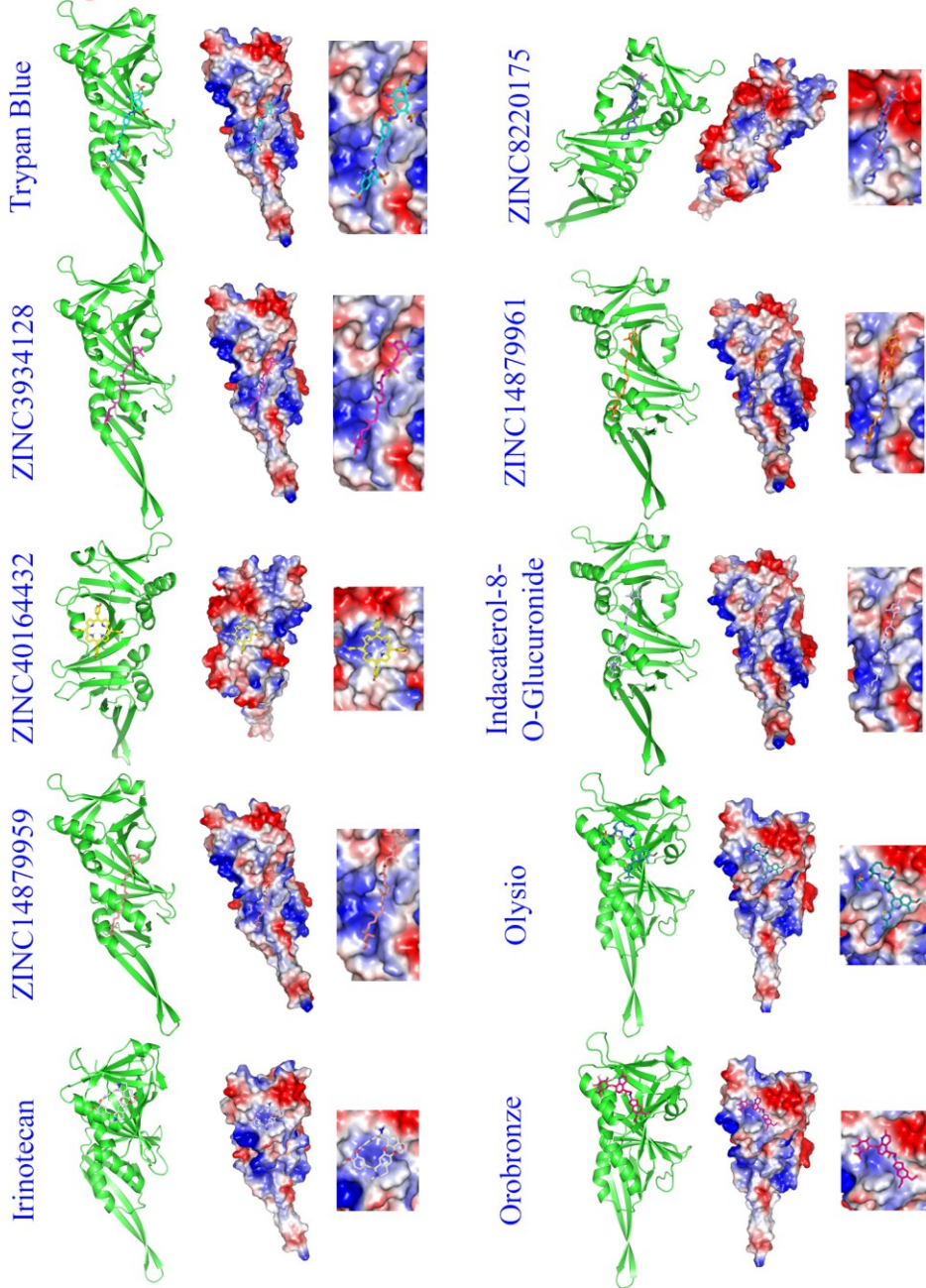


Figure S10. The top ten best docking drugs targeting G9R, including trypan blue, zinc3934128, zinc40164432, zinc14879959, irinotecan, zinc8220175, zinc14879961, indacaterol-8-o-glucuronide, olysis, and orobronze.