

**Searching for potential drugs against SARS-CoV-2 through virtual screening on
several molecular targets**

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Supplementary material

Table S1. Docking results for the drugs with SC2 proteins.

Ligand	SC2M^{pro}		SC2PL^{pro}		SC2Spyke	
	MolDock score (Kcal/mol)	E_H-bond (Kcal/mol)	MolDock score (Kcal/mol)	E_H-bond (Kcal/mol)	MolDock score (Kcal/mol)	E_H-bond (Kcal/mol)
Amphotericin B	-106.17	-10.04	-122.09	-10.086	-134.96	-8.27
Cobicistat	-166.09	-15.20	-133.15	-1.73	-125.13	-0.91
Deferoxamine	-104.52	-13.58	-67.79	-8.05	-78.36	-10.67
Elbasvir	-180.26	-10.42	-198.99	-3.29	-165.40	-6.35
Itraconazole	-143.89	-6.74	-134.61	-0.96	-120.66	-5.27
Nystatin	-97.68	-8.88	-101.01	-2.06	-138.25	-13.38
Remdesivir	-146.95	-8.89	-106.00	-7.09	-99.58	-8.04
Ritonavir	-159.39	-8.60	-92.95	-4.82	-110.34	-1.35
Reference ligand	-140.35	-8.31	-135.45	-7.96	-864.59	-33.63

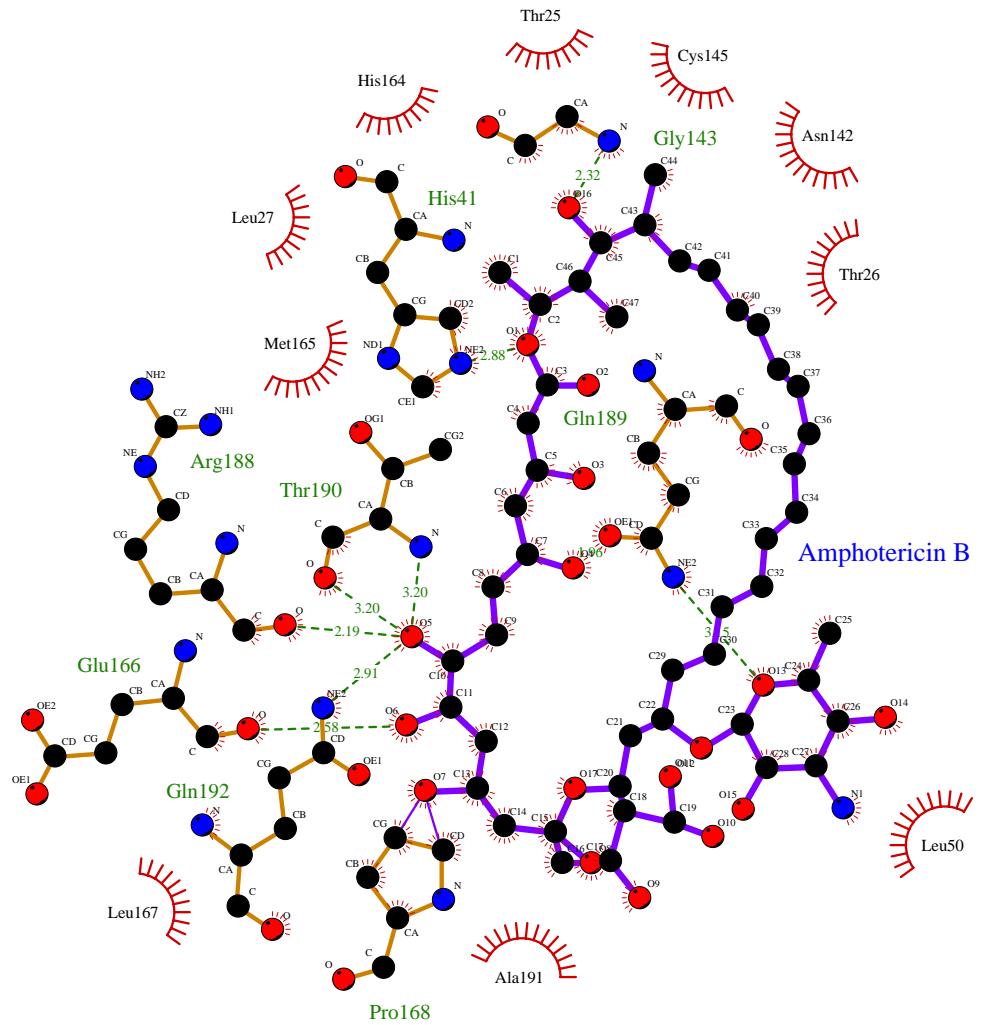


Figure S1. 2D representation of the interactions of the best pose of amphotericin B with $SC2M^{pro}$.

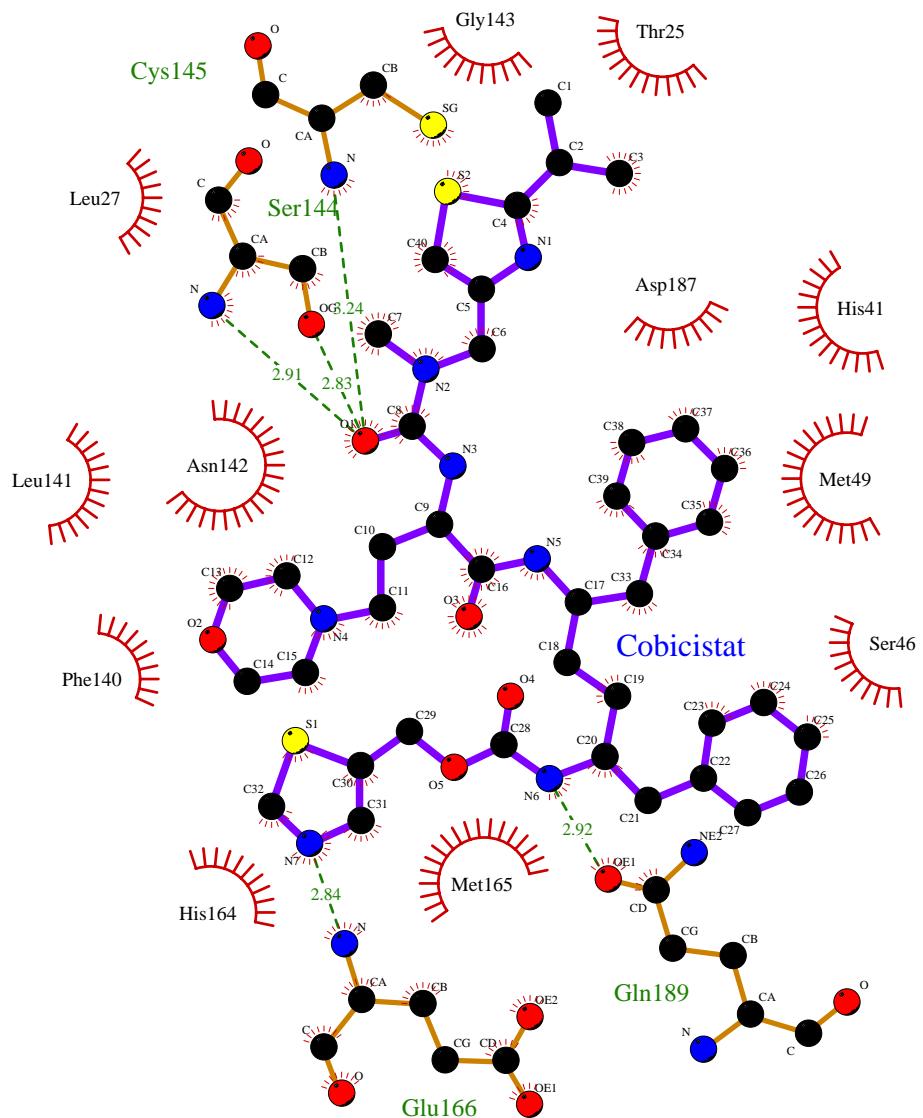


Figure S2. 2D representation of the interactions of the best pose of cobicistat with *SC2M^{pro}*.

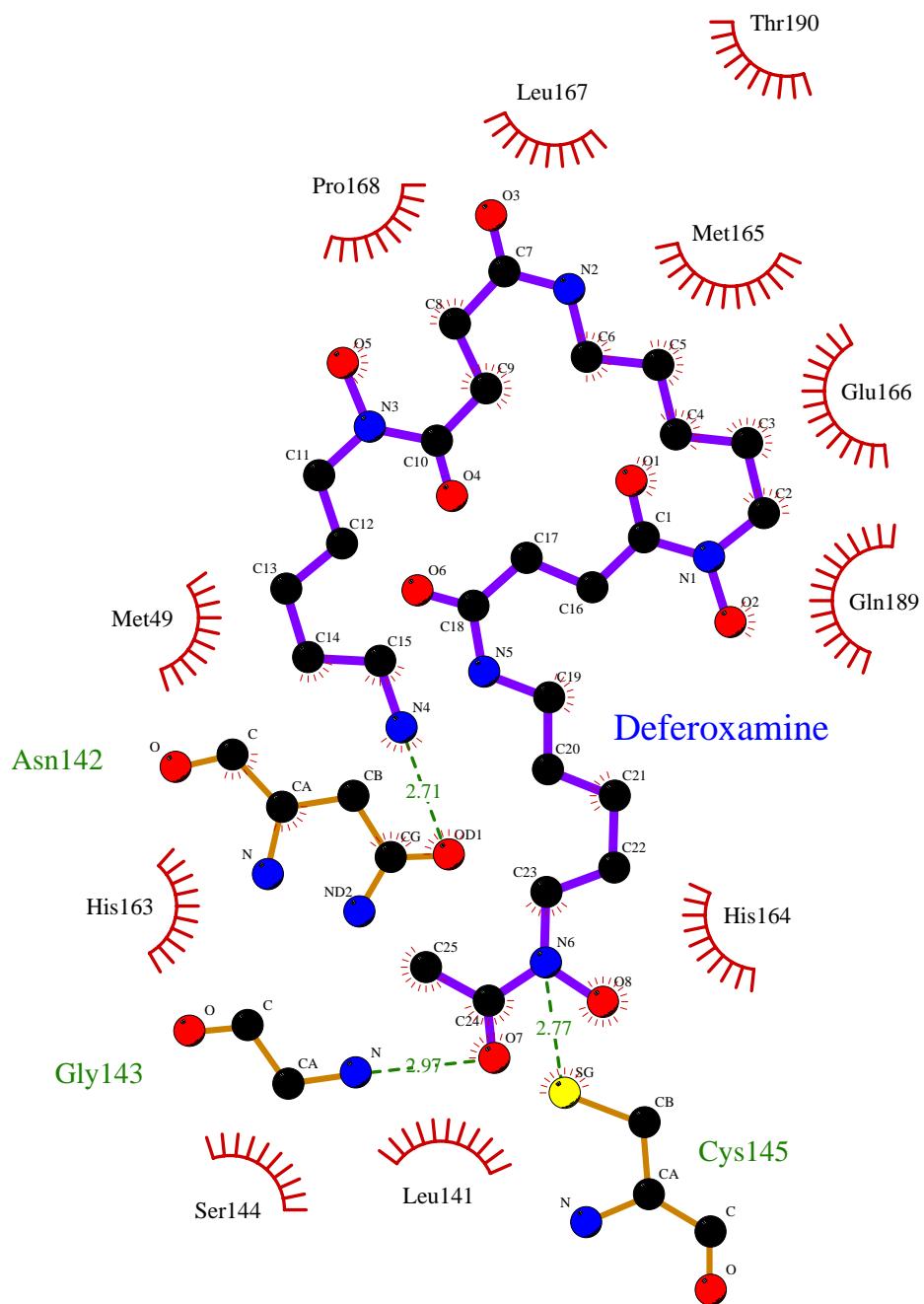


Figure S3. 2D representation of the interactions of the best pose of deferoxamine with $SC2M^{pro}$.

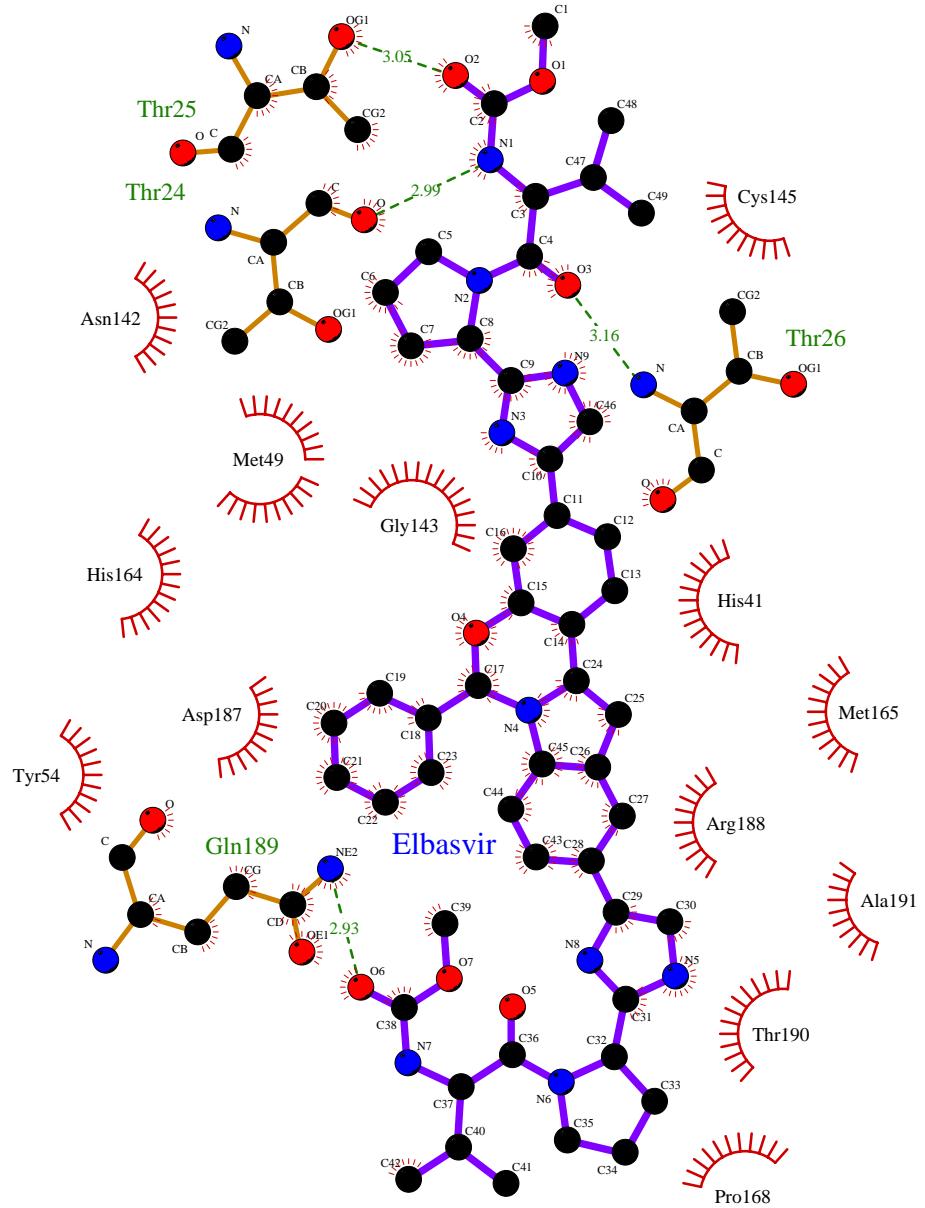


Figure S4. 2D representation of the interactions of the best pose of elbasvir with $SC2M^{pro}$.

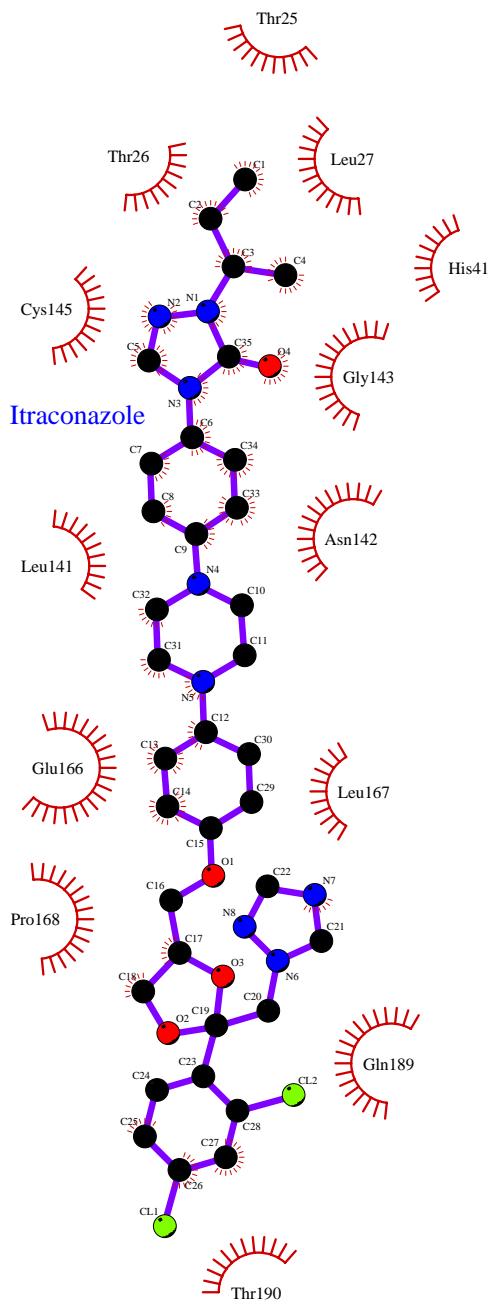


Figure S5. 2D representation of the interactions of the best pose of itraconazole with *SC2M^{pro}*.

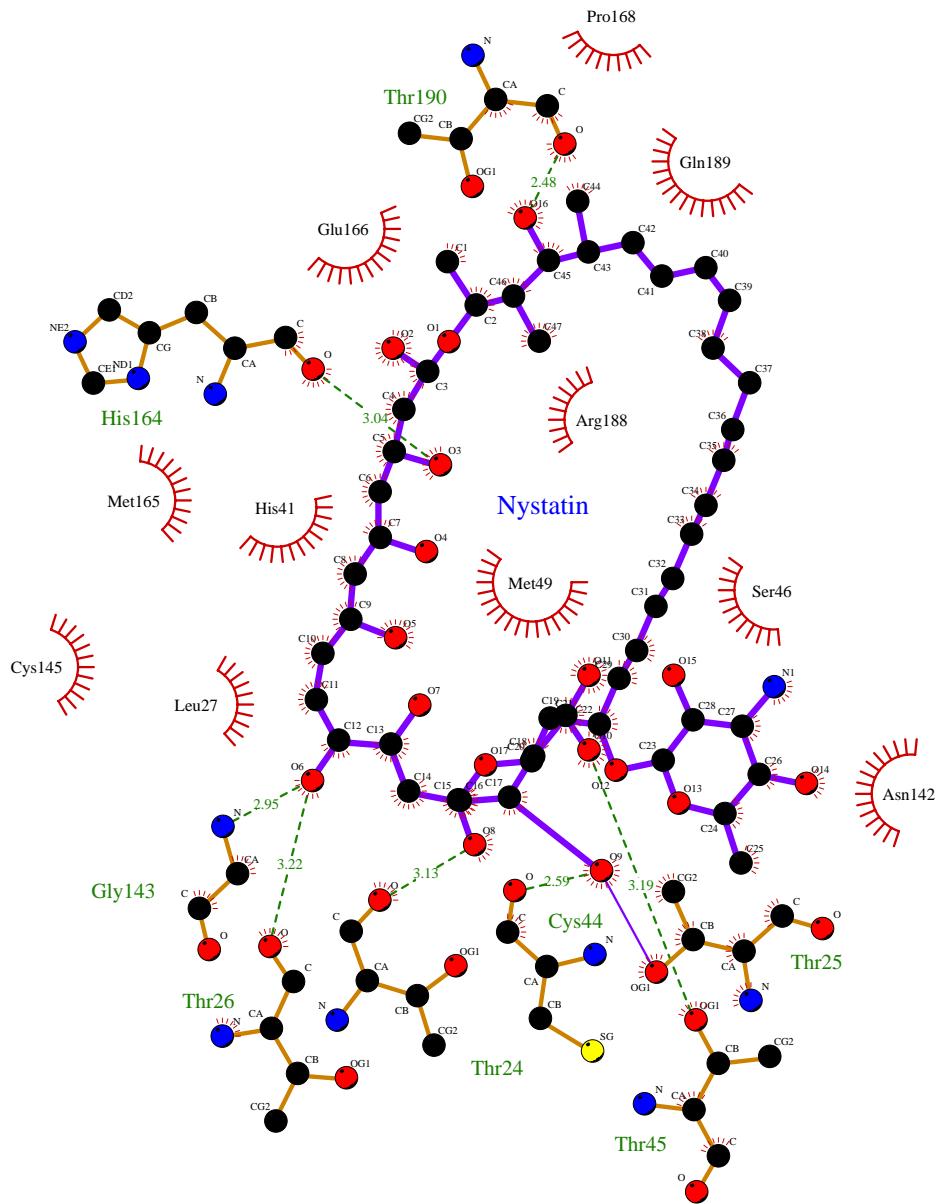


Figure S6. 2D representation of the interactions of the best pose of nystatin with $SC2M^{pro}$.

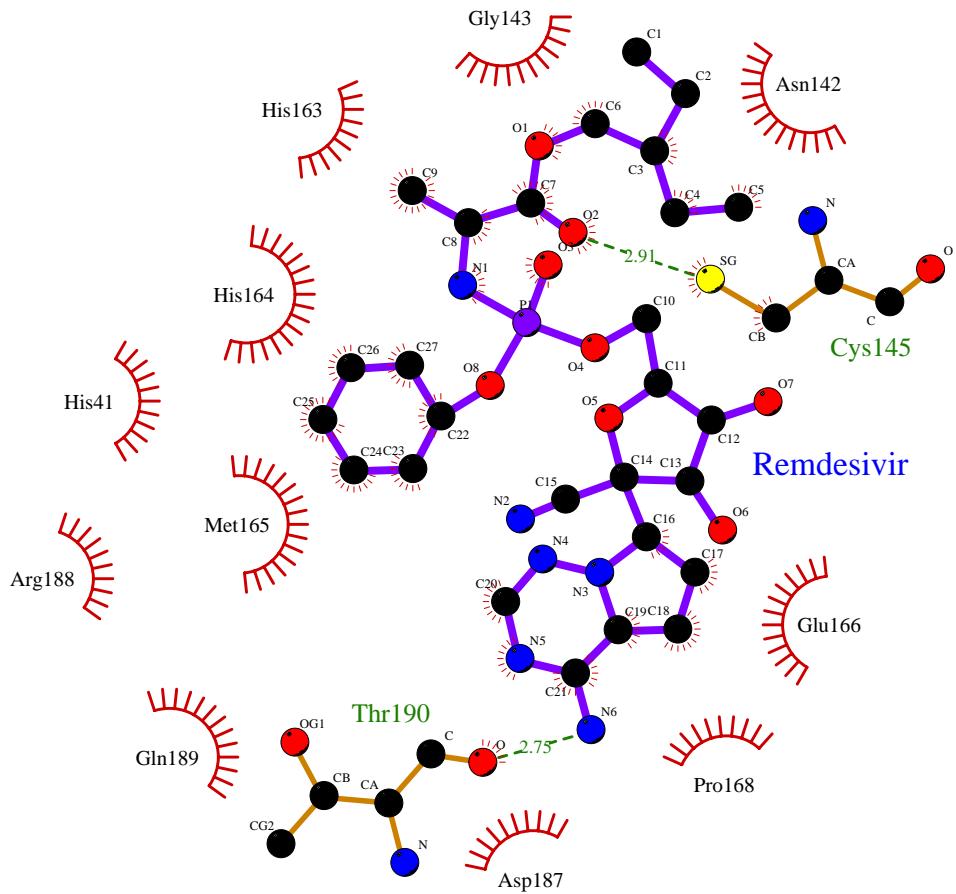


Figure S7. 2D representation of the interactions of the best pose of remdesivir with $SC2M^{pro}$.

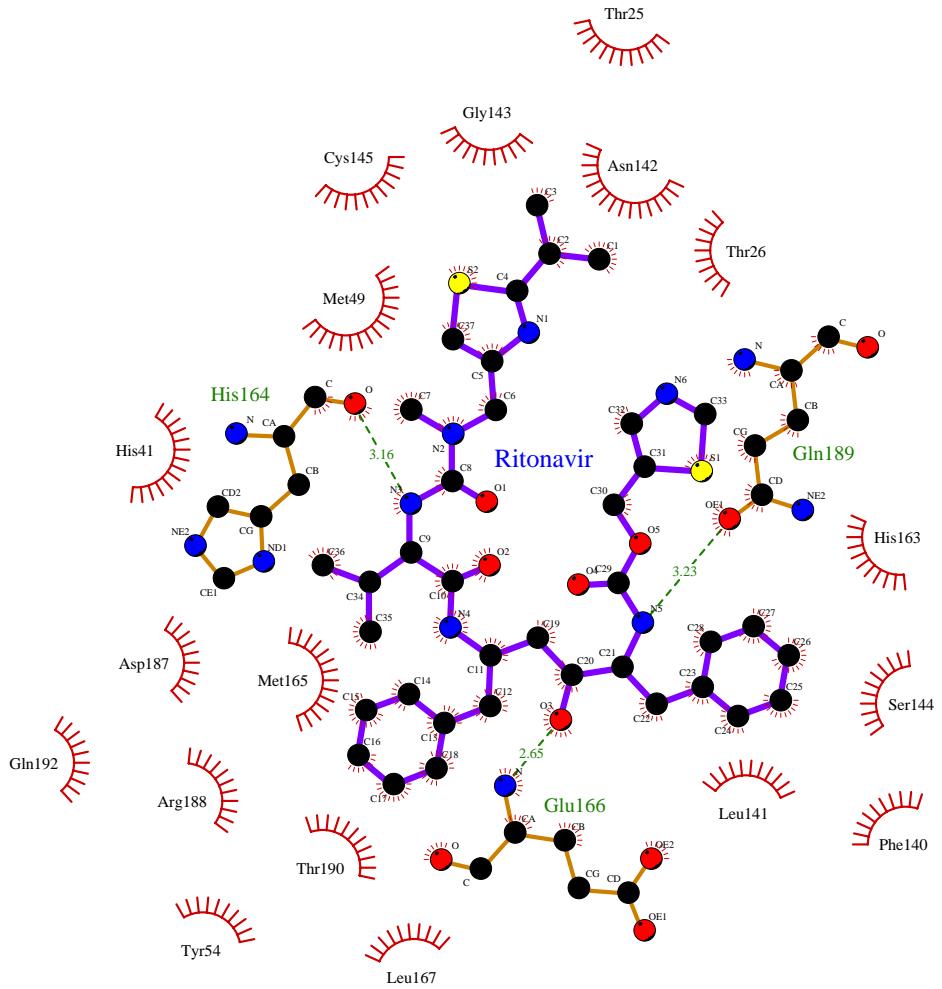


Figure S8. 2D representation of the interactions of the best pose of ritonavir with *SC2M^{PRO}*.

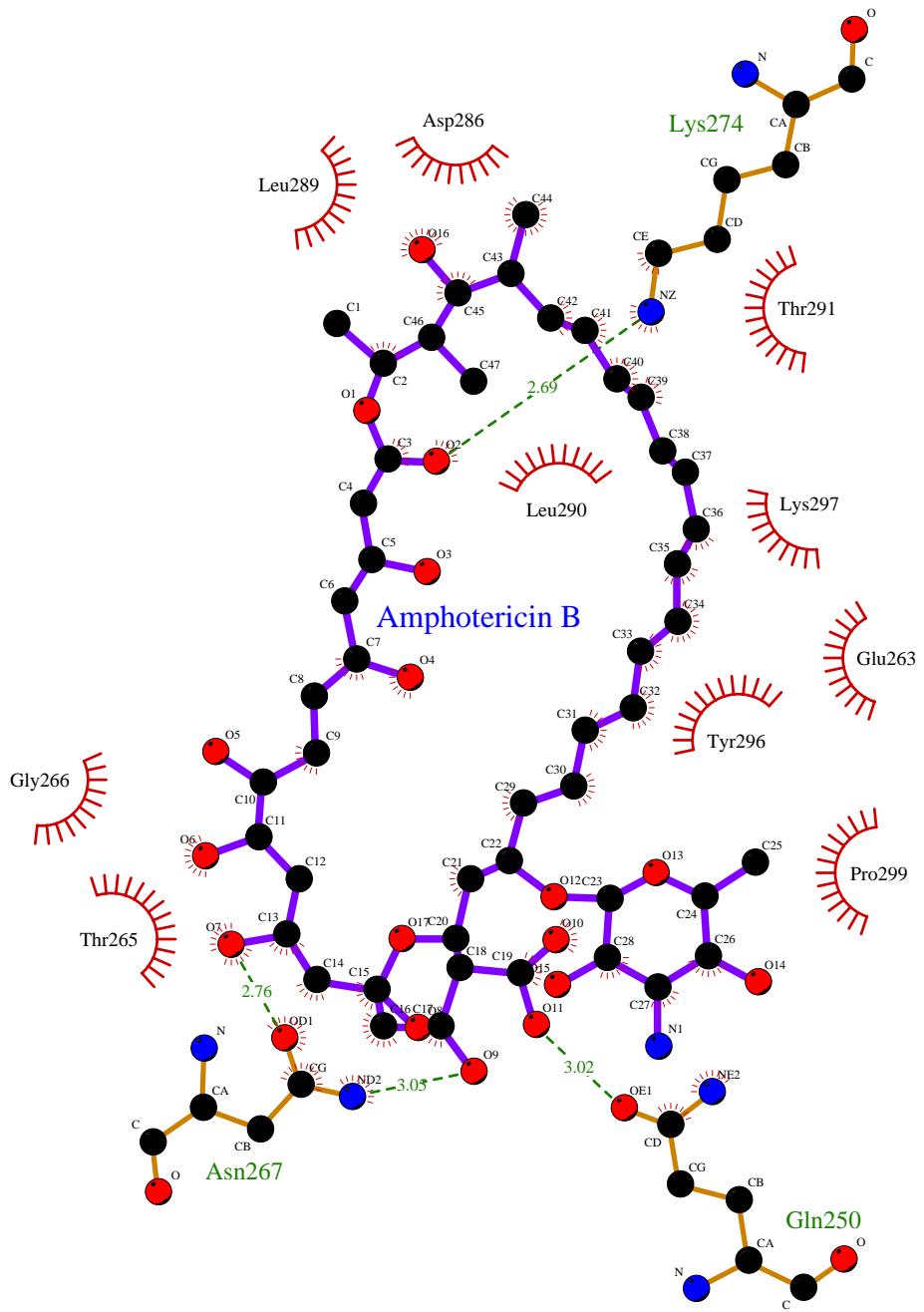


Figure S9. 2D representation of the interactions of the best pose of amphotericin B with $SC2PL^{pro}$.

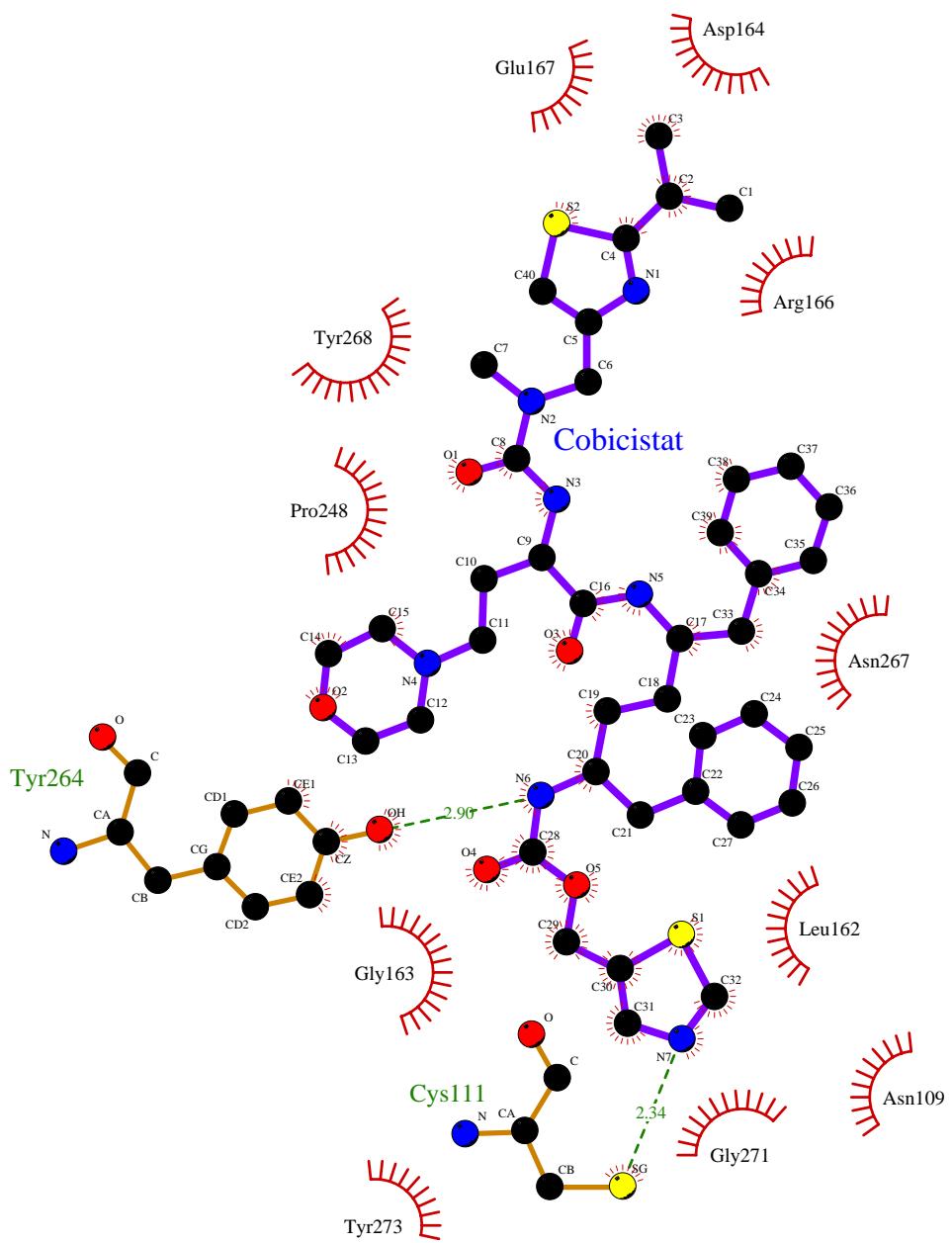


Figure S10. 2D representation of the interactions of the best pose of cobicistat with *SC2PL*^{pro}.

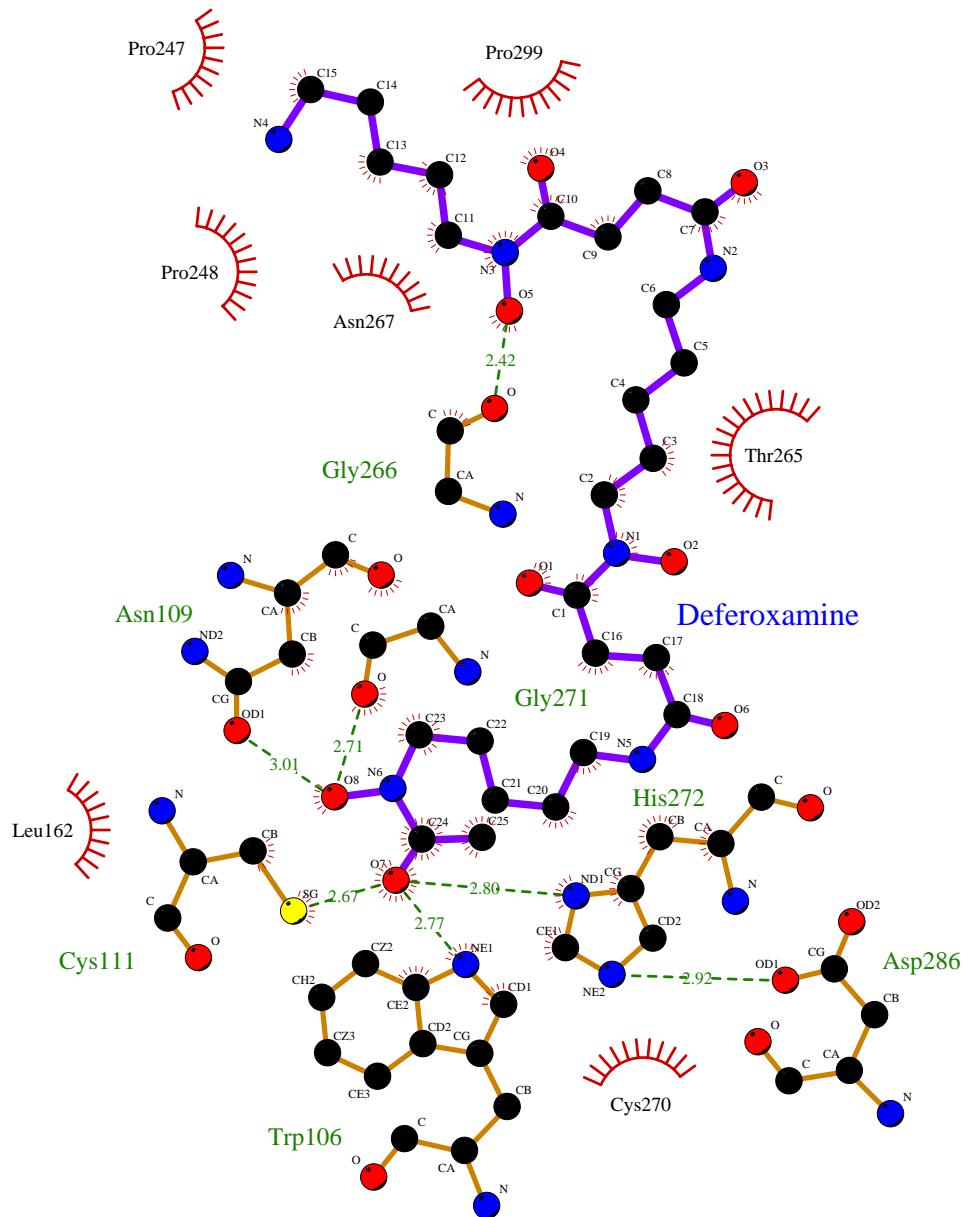


Figure S11. 2D representation of the interactions of the best pose of deferoxamine with $SC2PL^{pro}$.

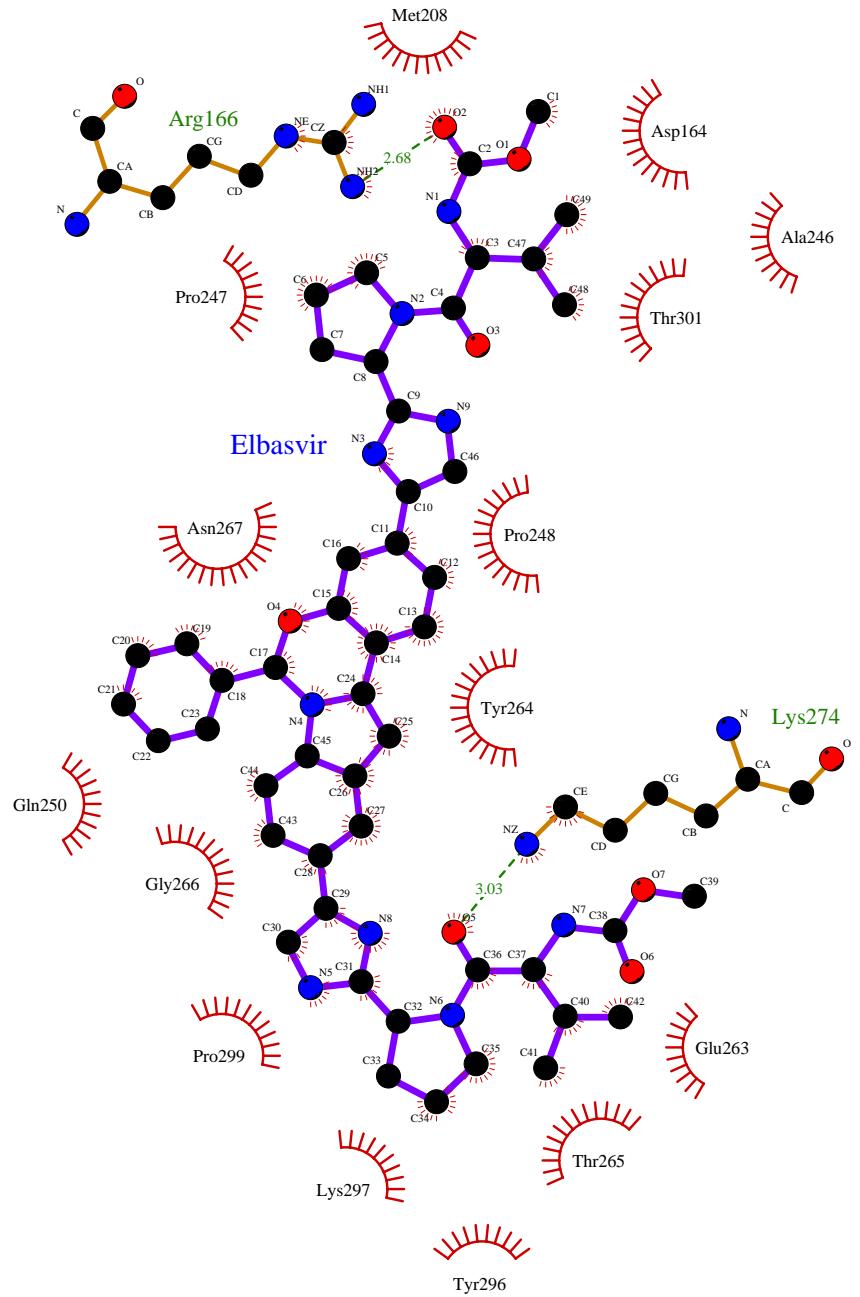


Figure S12. 2D representation of the interactions of the best pose of elbasvir with $SC2PL^{pro}$.

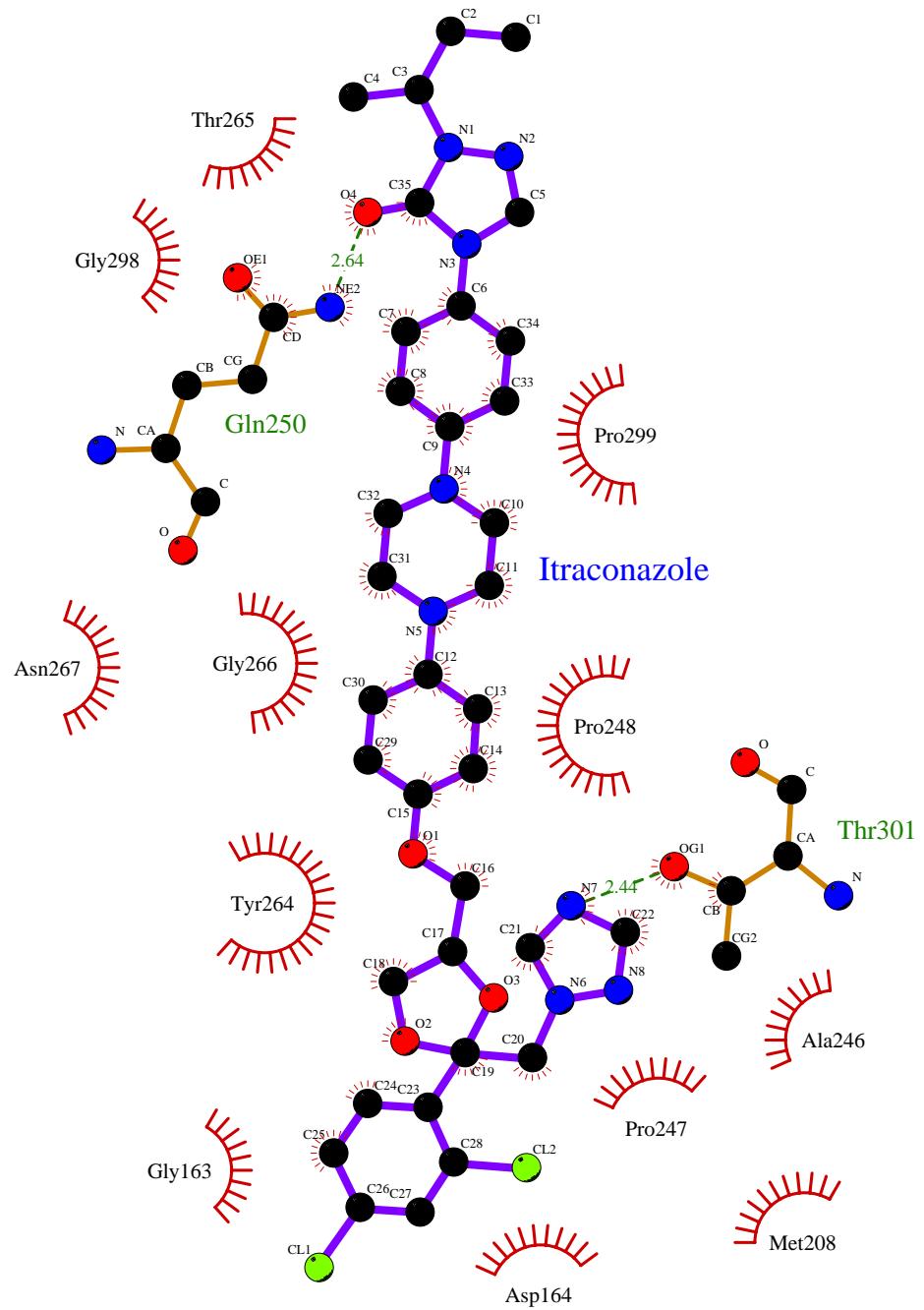


Figure S13. 2D representation of the interactions of the best pose of itraconazole with $SC2PL^{pro}$.

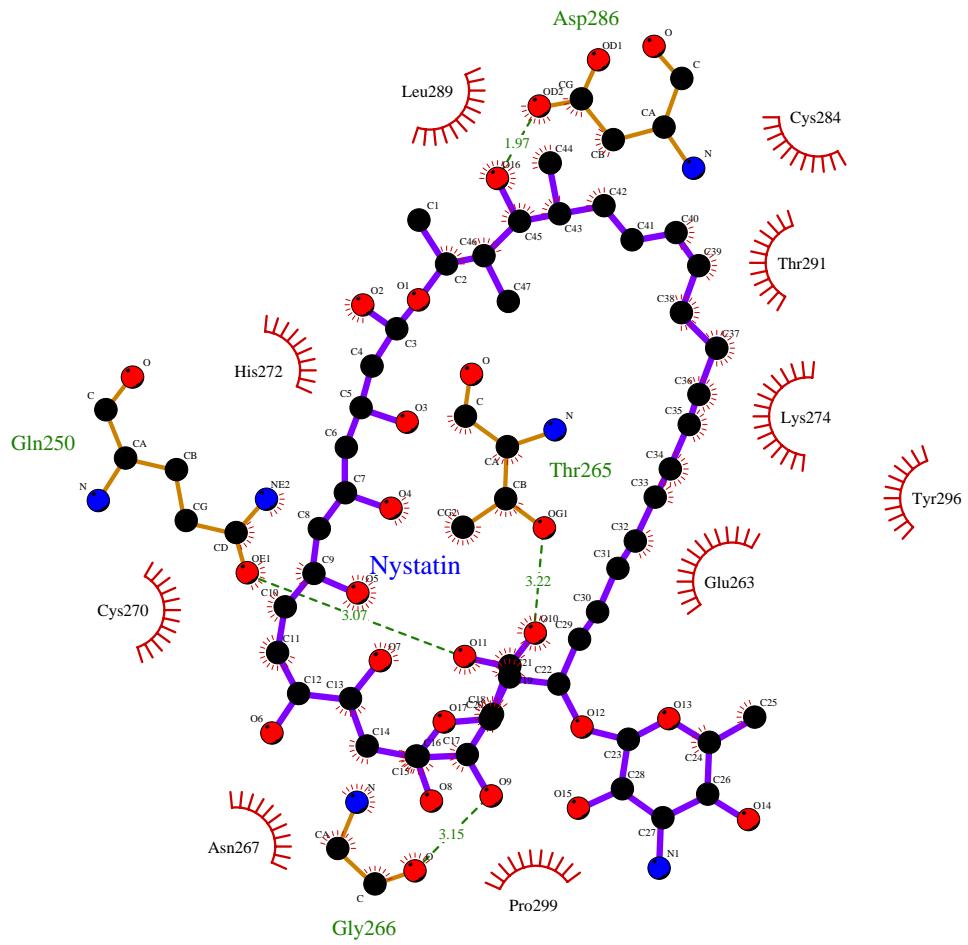


Figure S14. 2D representation of the interactions of the best pose of nystatin with SC2PL^{pro}.

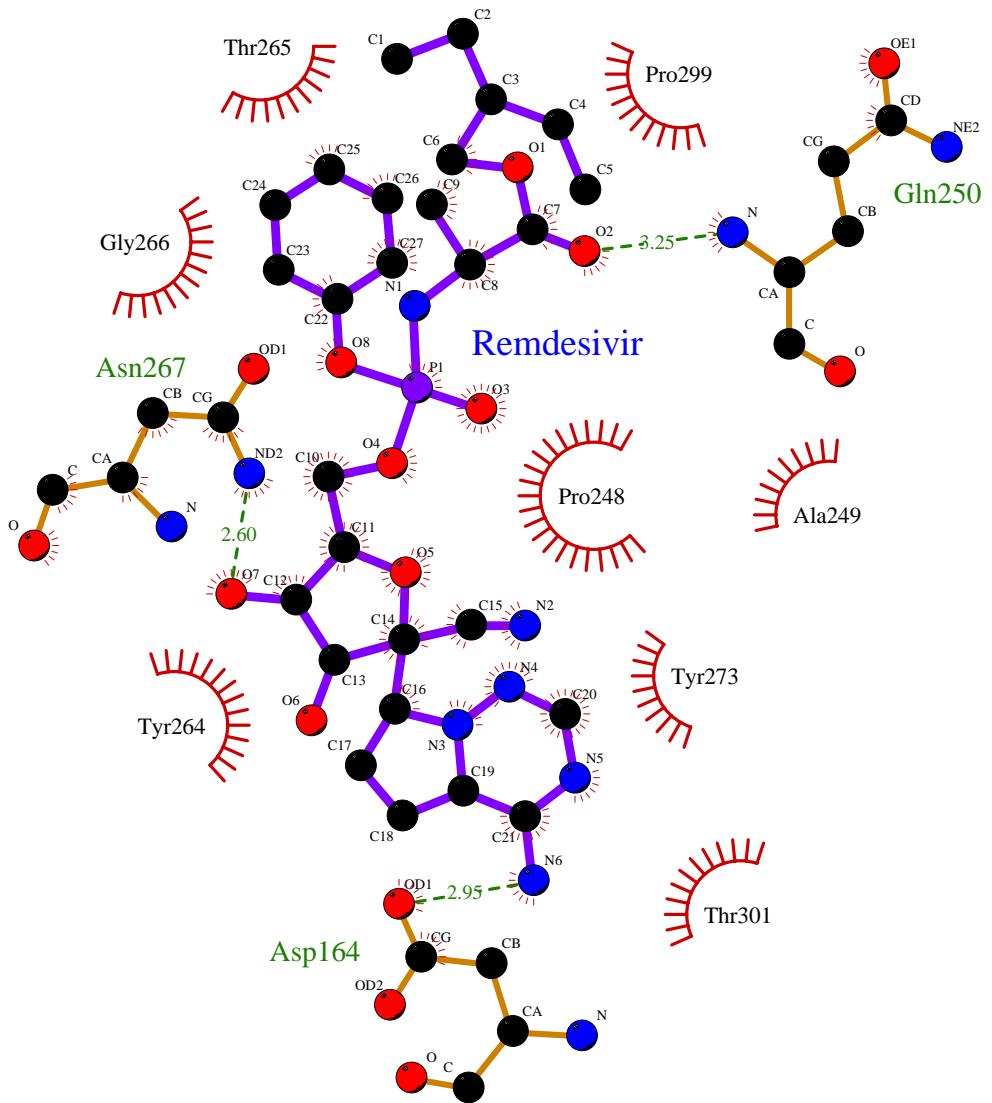


Figure S15. 2D representation of the interactions of the best pose of remdesivir with $SC2PL^{pro}$.

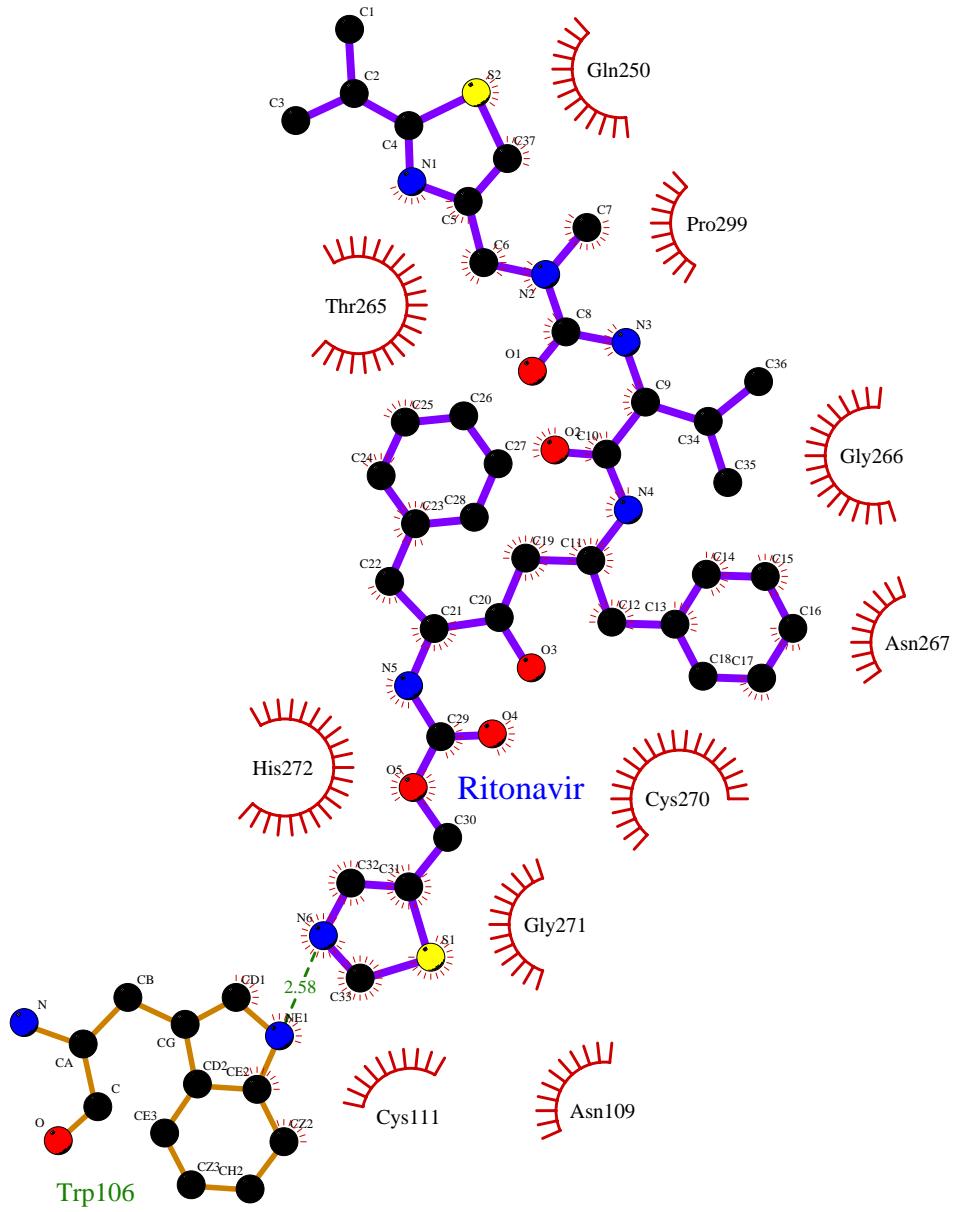


Figure S16. 2D representation of the interactions of the best pose of ritonavir with SC2PL^{pro}.

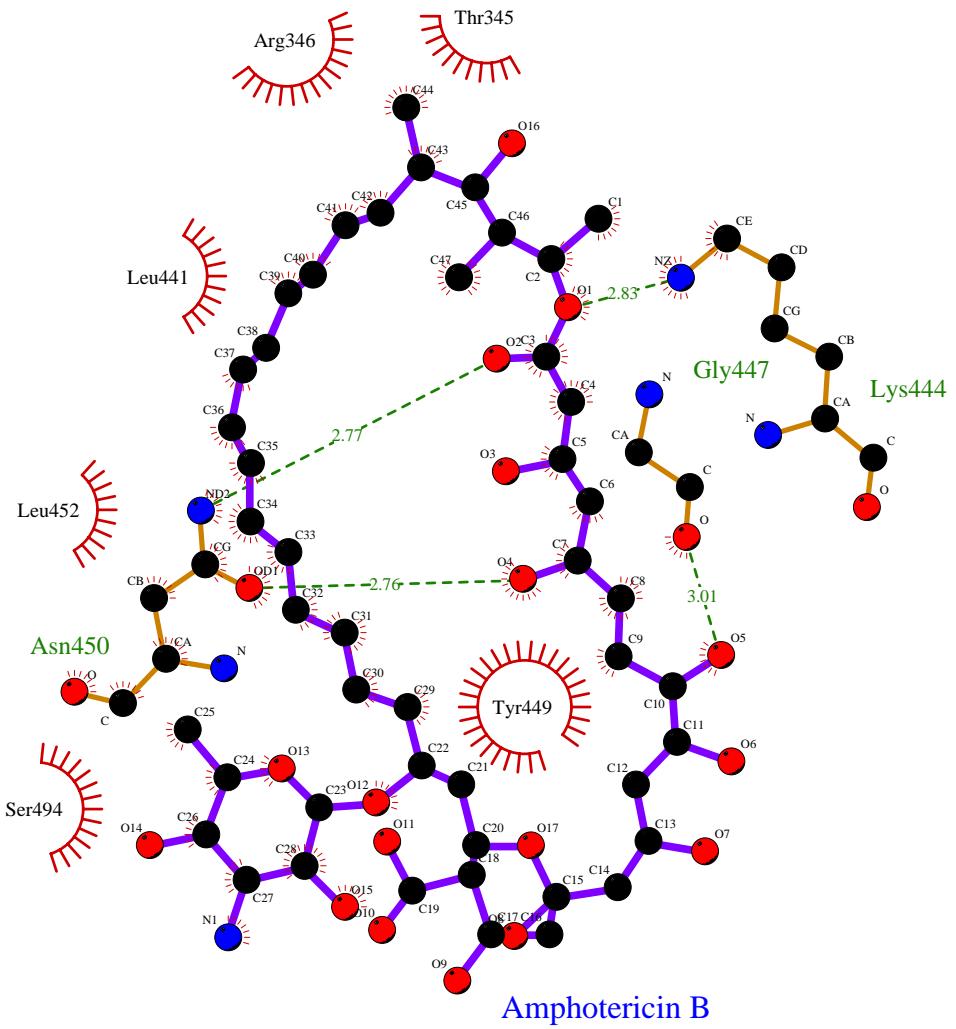


Figure S17. 2D representation of the interactions of the best pose of amphotericin B with SC2Spyke.

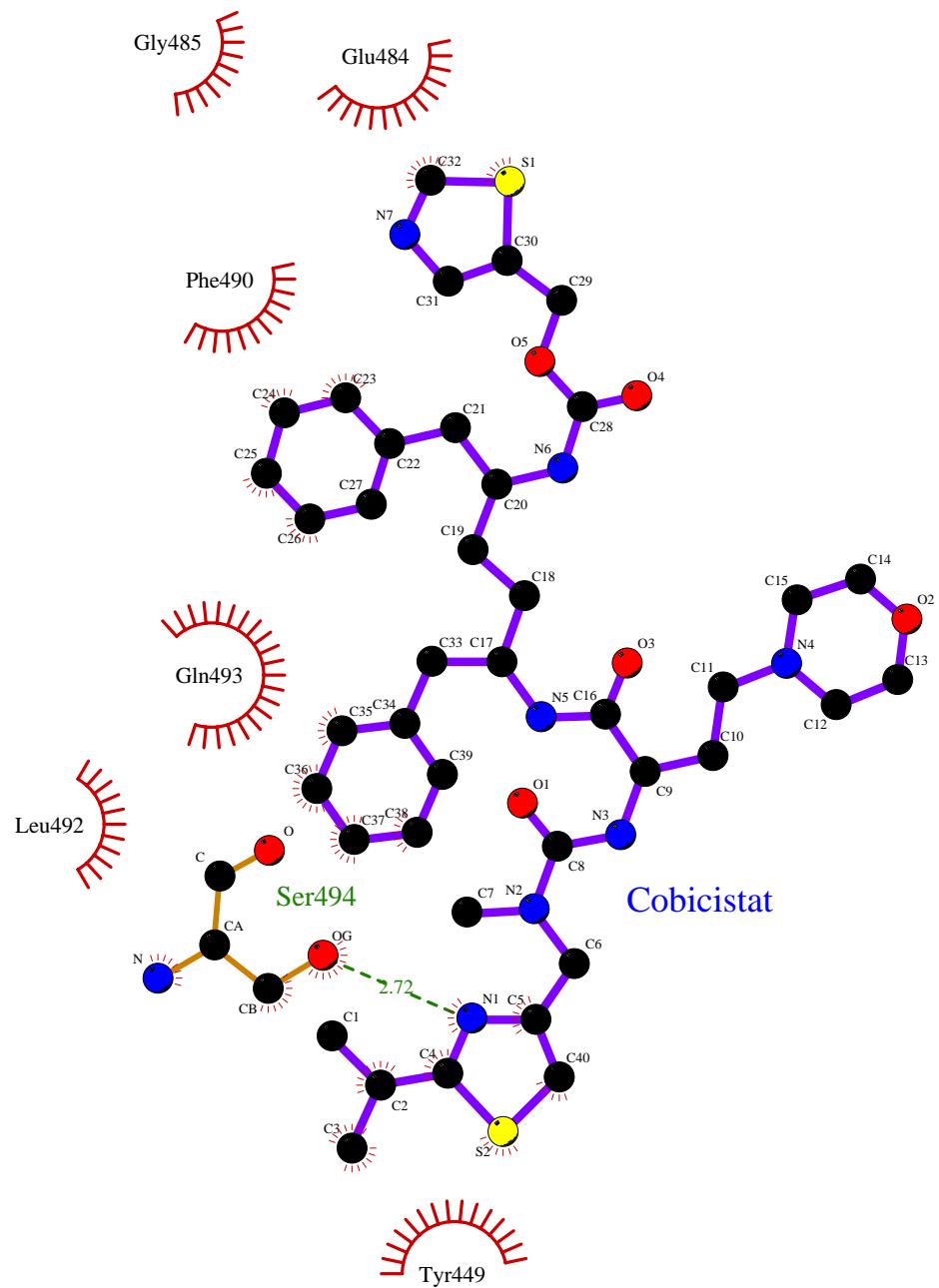


Figure S18. 2D representation of the interactions of the best pose of cobicistat with SC2Spyke.

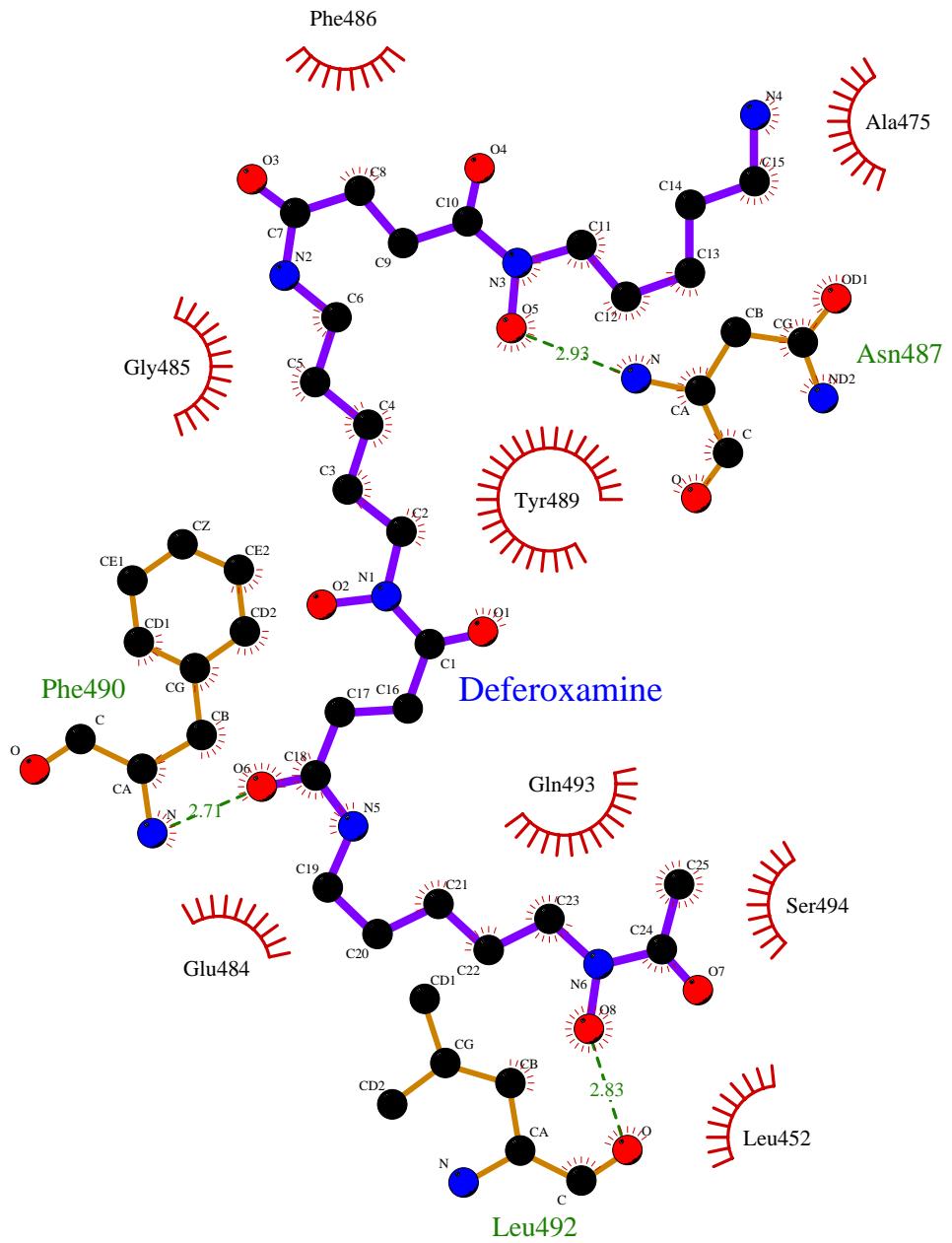


Figure S19. 2D representation of the interactions of the best pose of deferoxamine with SC2Spyke.

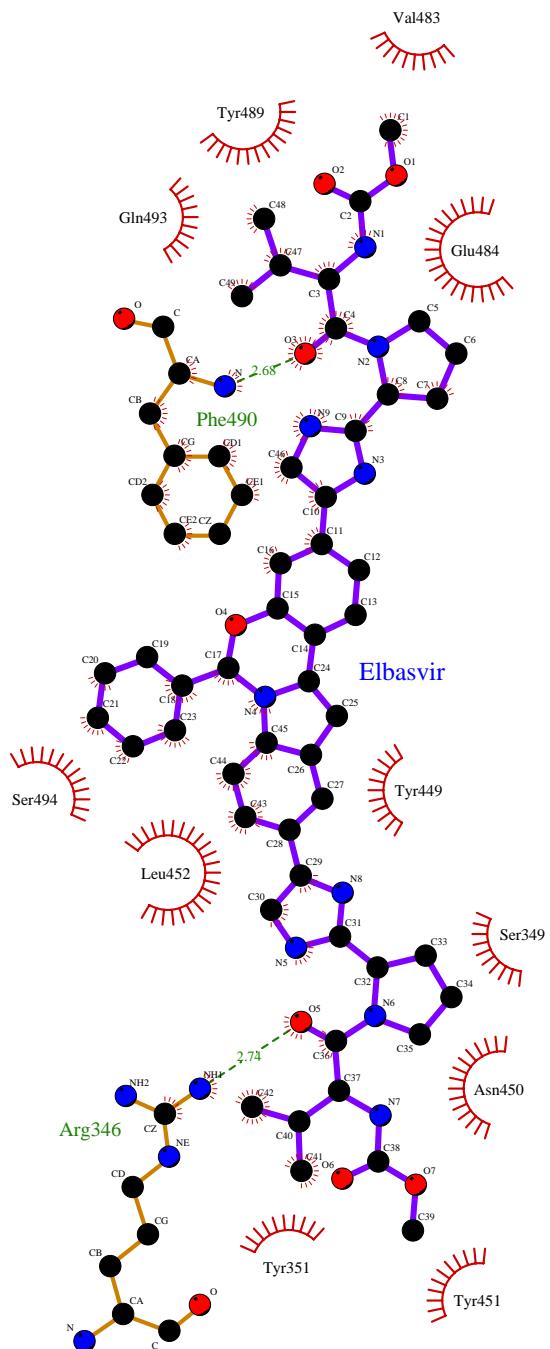


Figure S20. 2D representation of the interactions of the best pose of elbasvir with SC2Spyke.

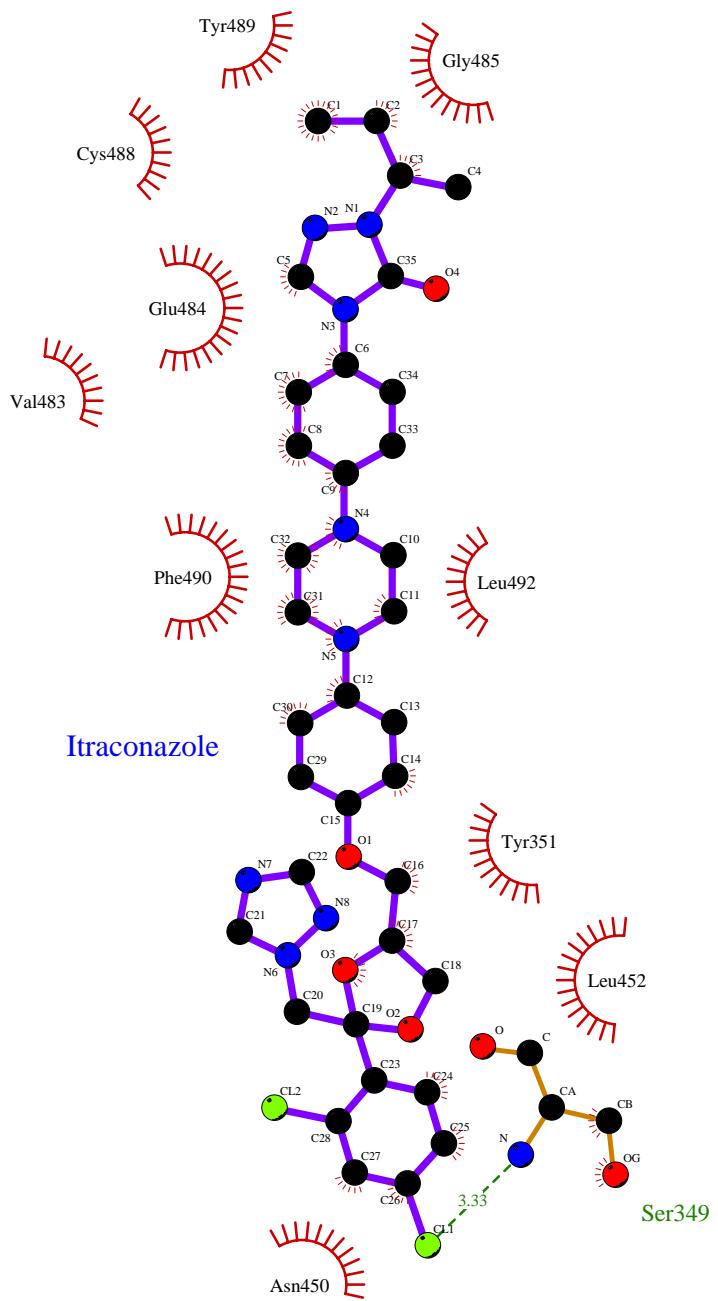


Figure S21. 2D representation of the interactions of the best pose of itraconazole with SC2Spyke.

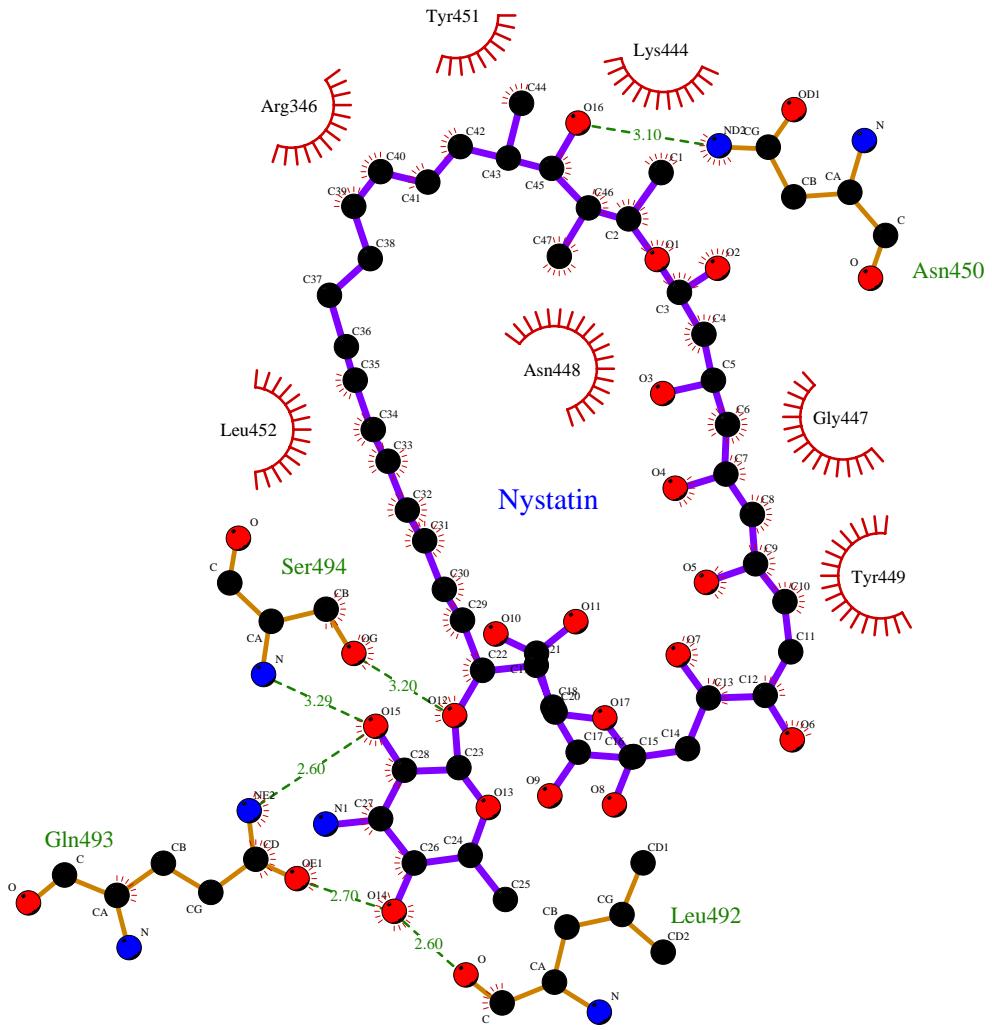


Figure S22. 2D representation of the interactions of the best pose of nystatin with SC2Spyke.

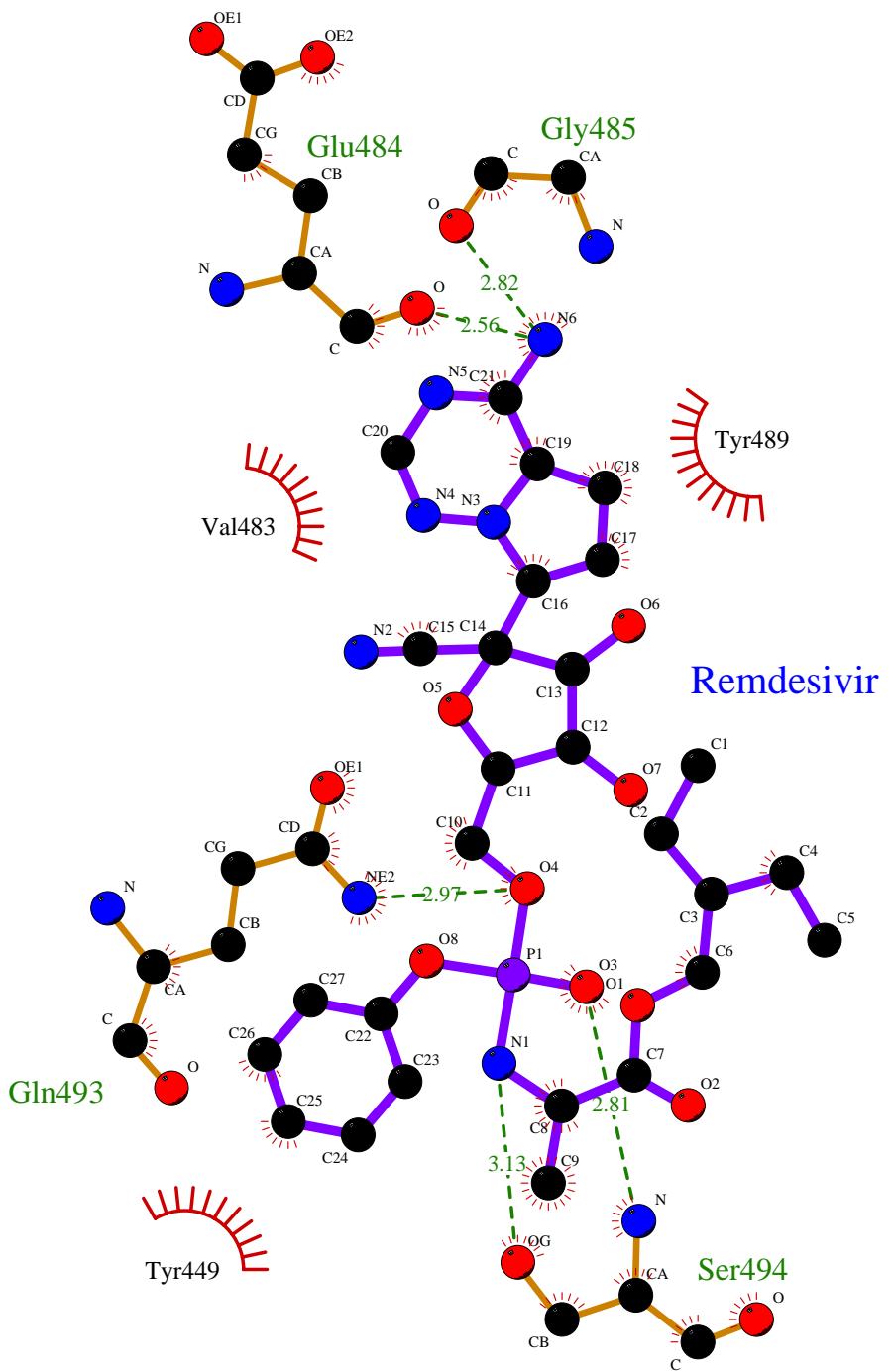


Figure S23. 2D representation of the interactions of the best pose of remdesivir with SC2Spyke.

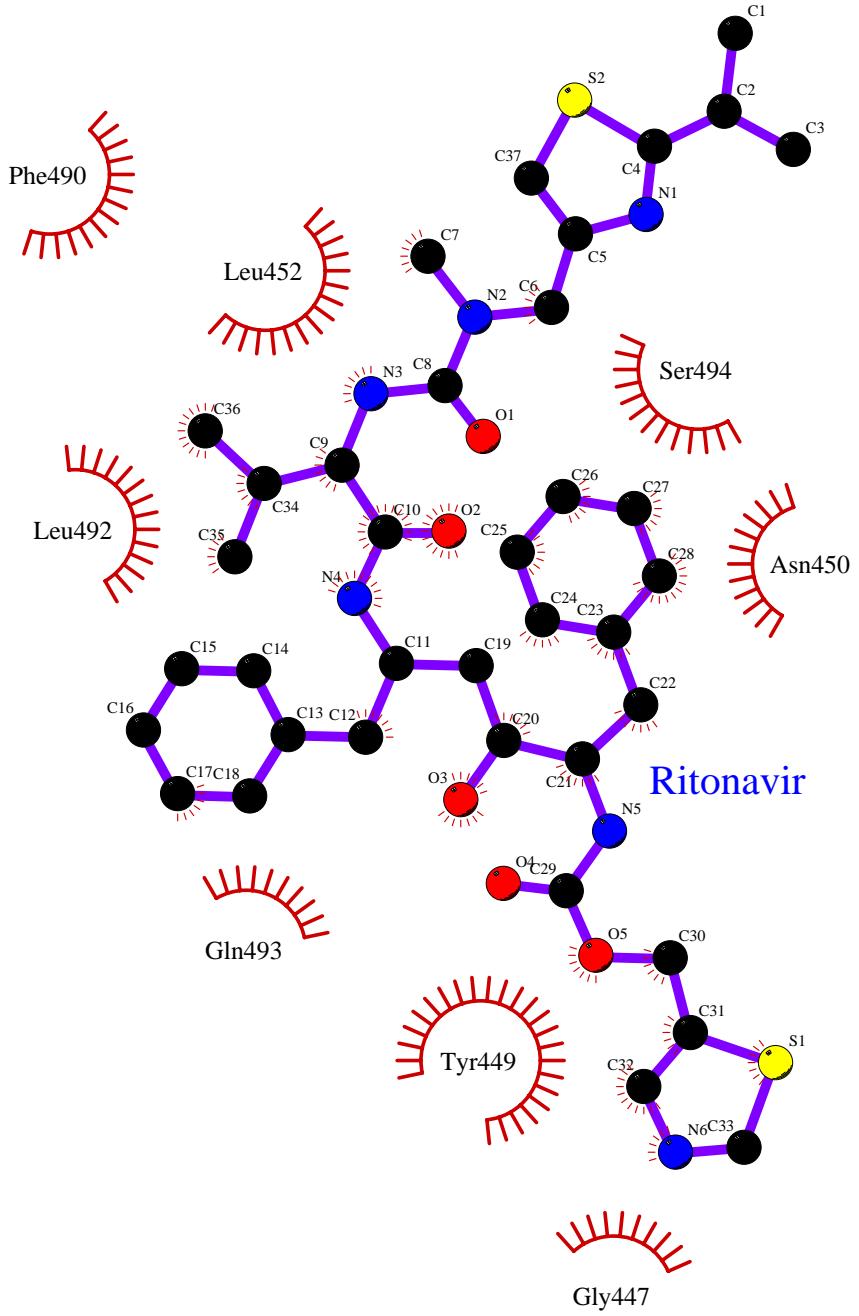


Figure S24. 2D representation of the interactions of the best pose of ritonavir with SC2Spyke.

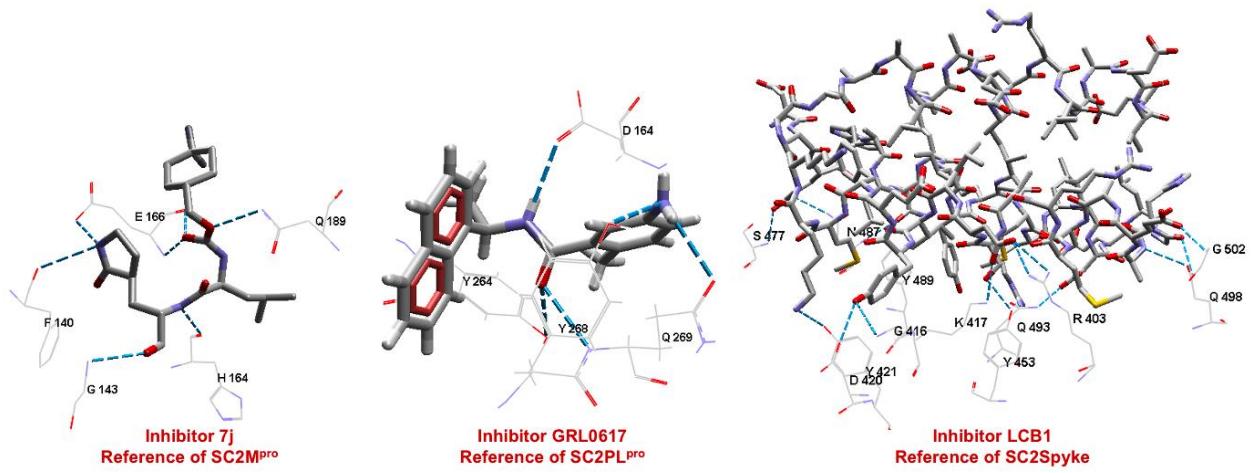


Figure S25. Interactions of the reference ligands inside SC2M^{pro}, SC2PL^{pro} and SC2Spyke.

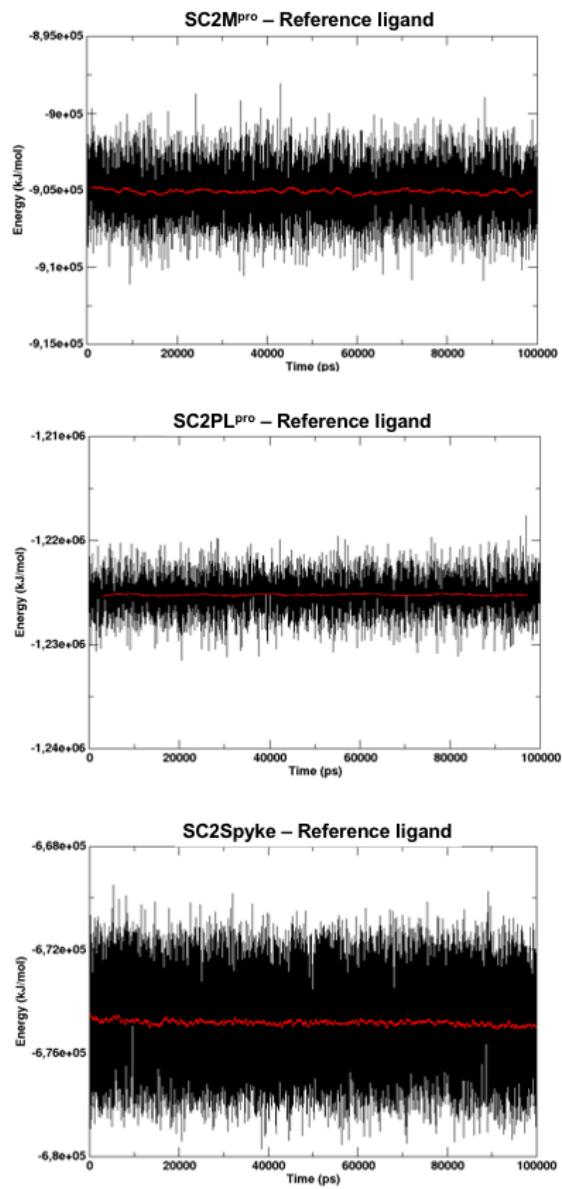


Figure S26. Total energy for the systems target/reference ligand.

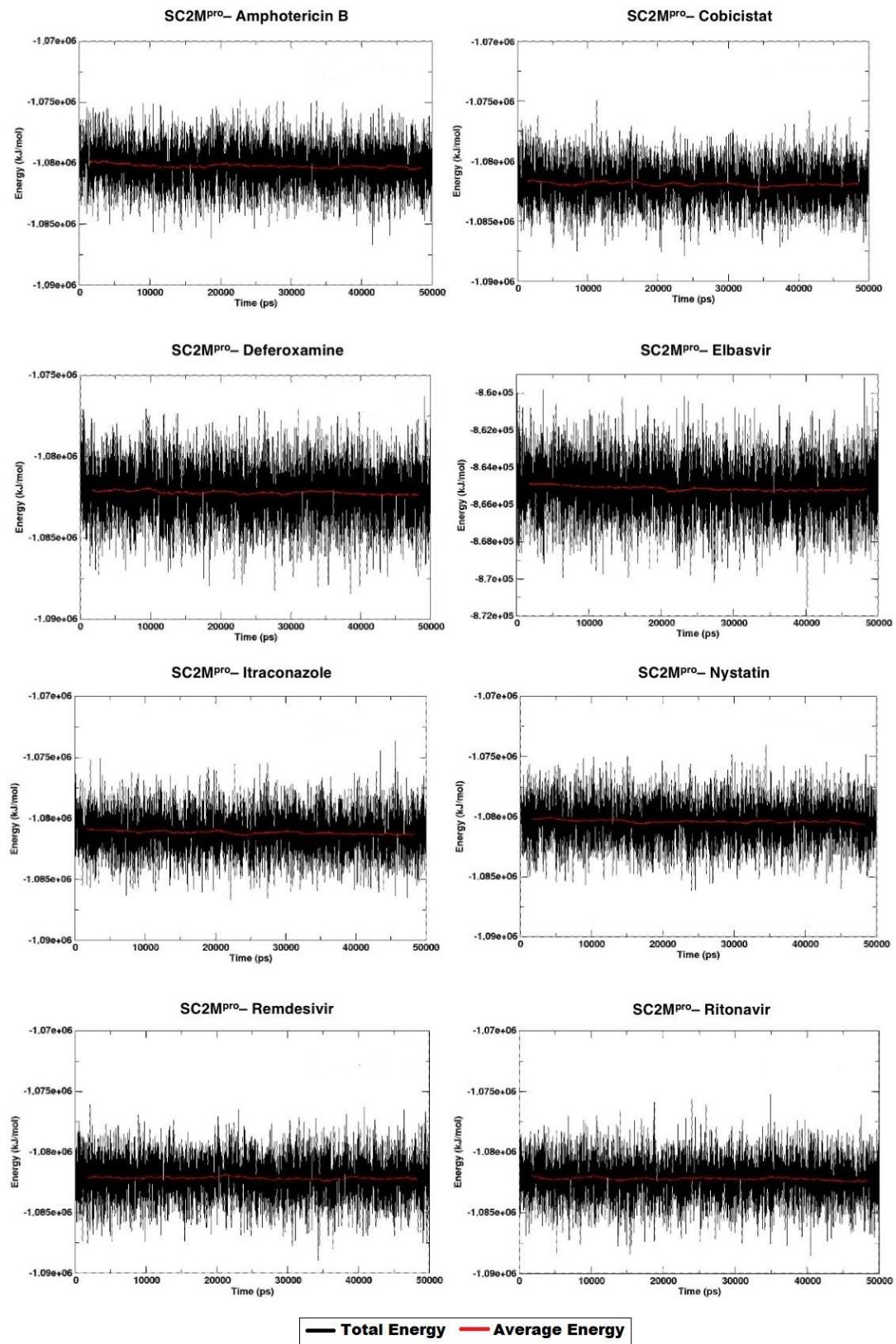


Figure S27. Total energy for the systems SC2M^{pro}/drug.

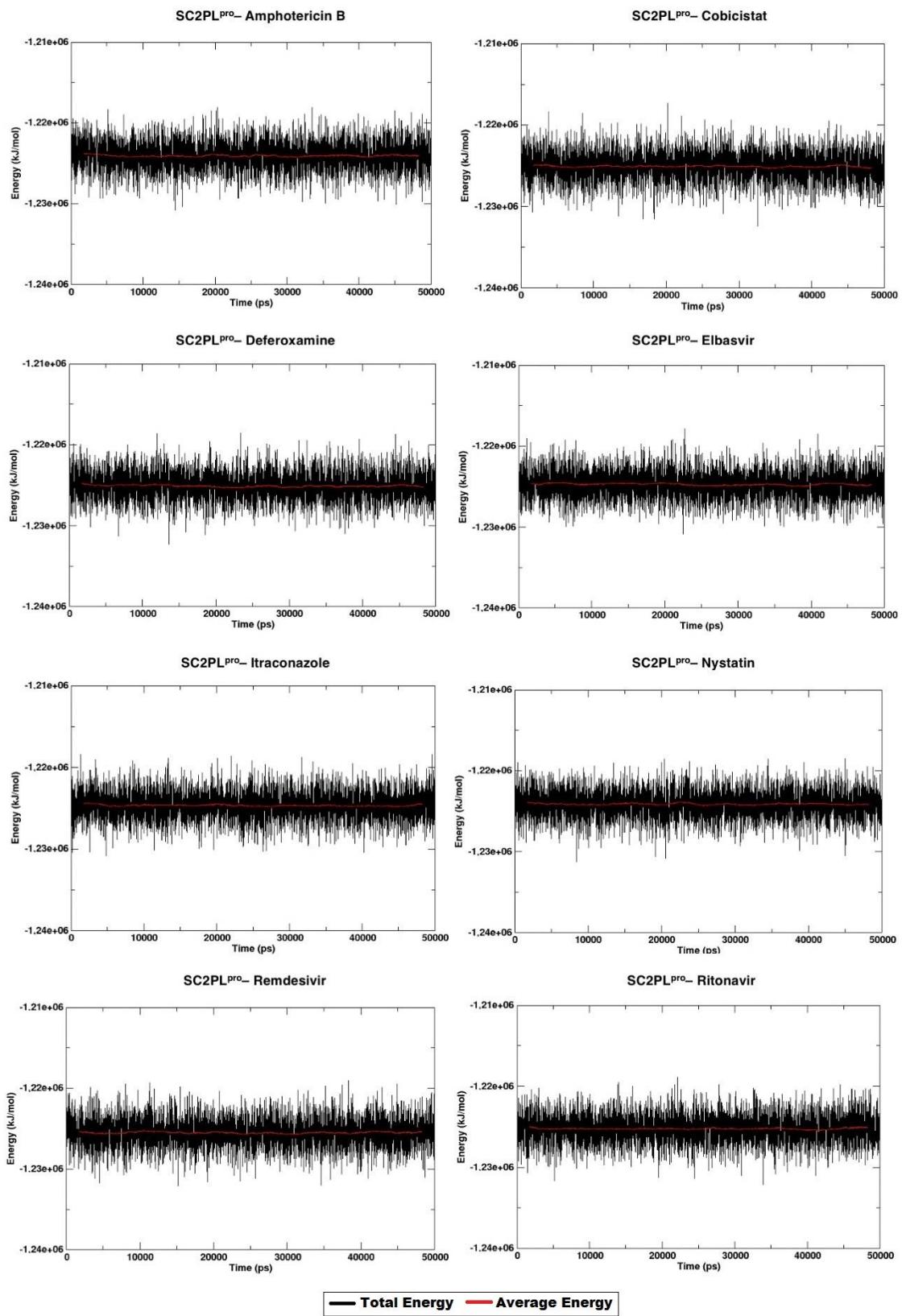


Figure S28. Total energy for the systems $SC2PL^{pro}$ /drug.

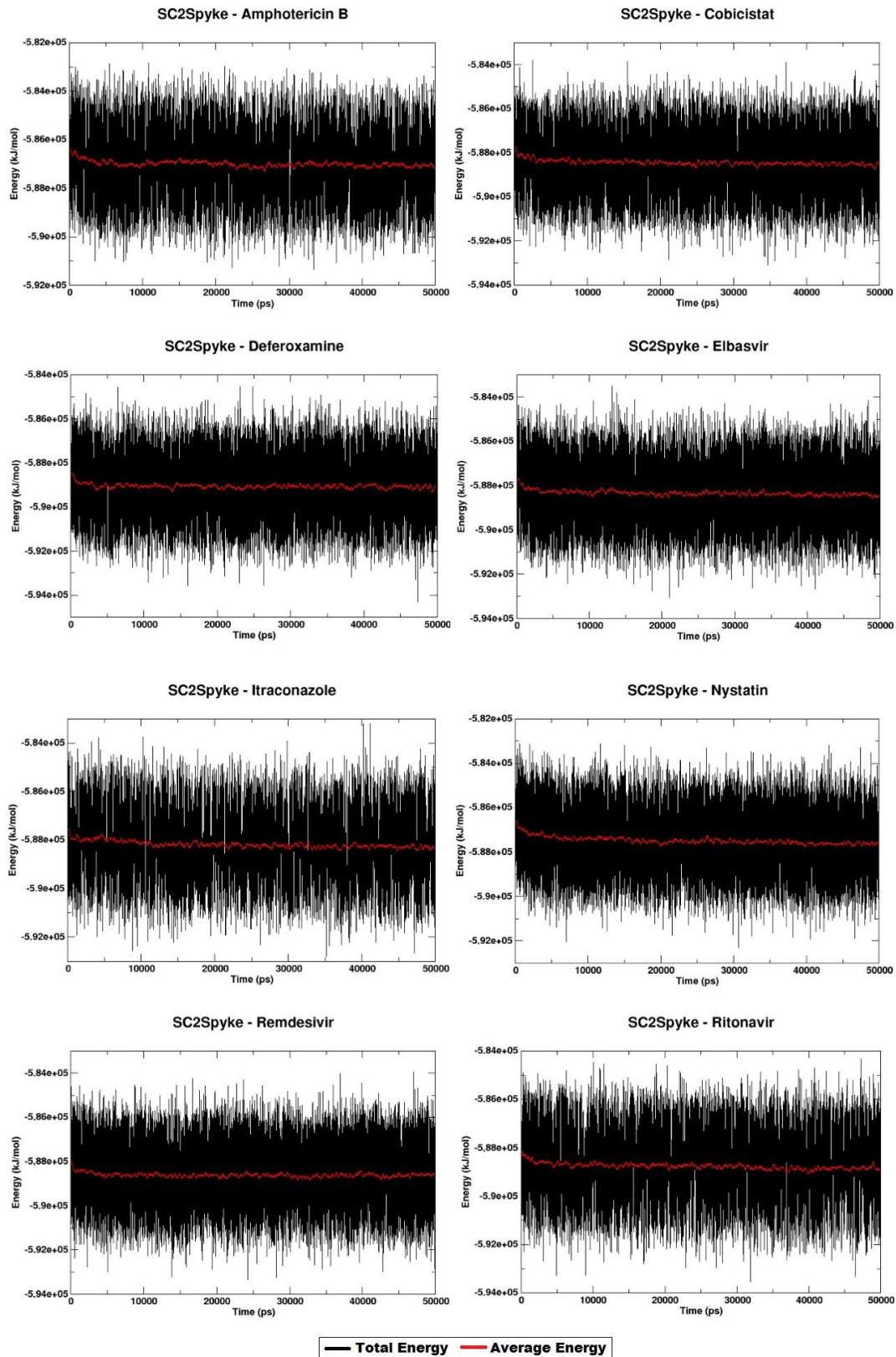


Figure S29. Total energy for the systems SC2Spyke/drug.