

Virtual screening and molecular dynamics simulation study of influenza polymerase PB2 inhibitors

Supporting information

Verification of docking method

Figure S1 Comparison between the highest ranked pose of VX-787 and the original pose in the crystal structure. The original pose was presented as green stick, the predicted highest ranking pose was presented as blue stick.

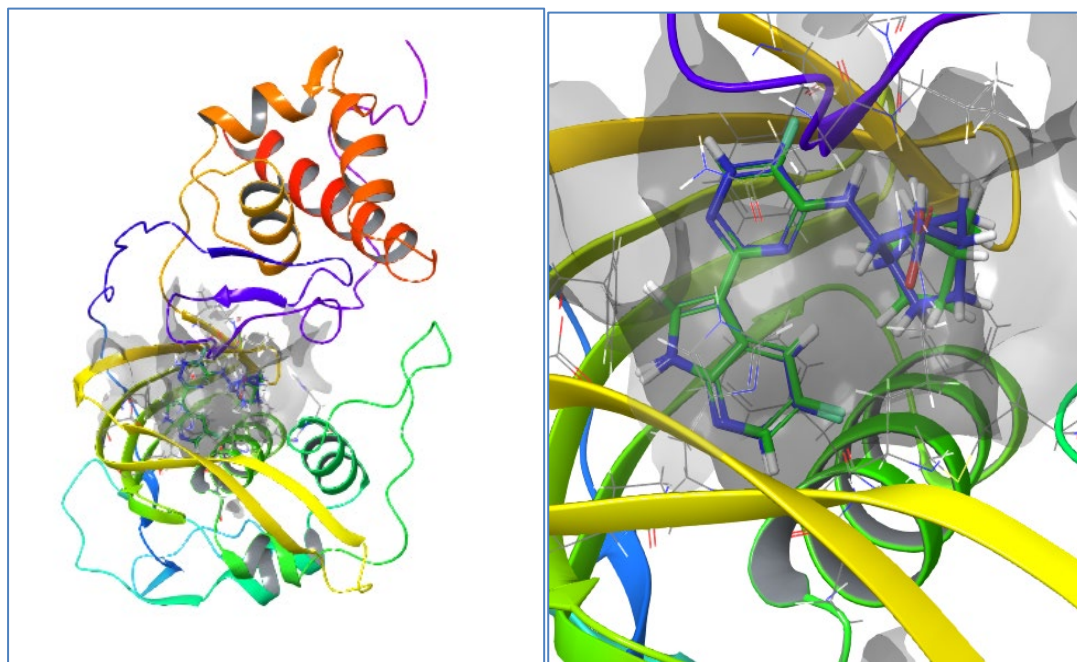
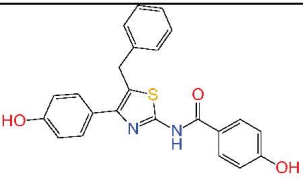
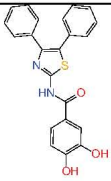
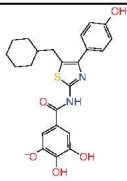
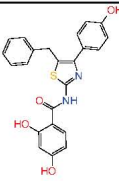
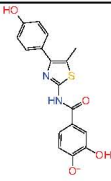
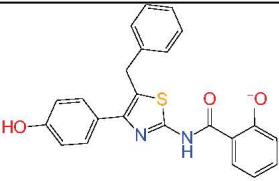
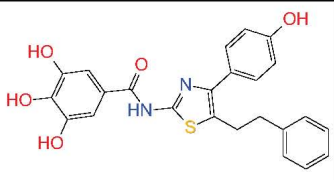
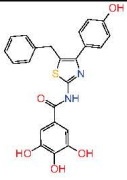
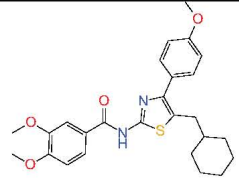
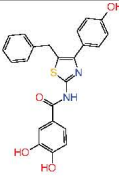
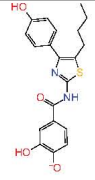
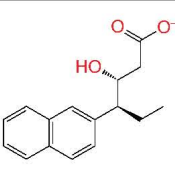
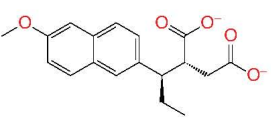
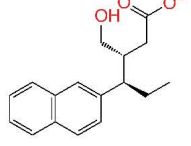
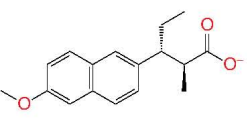
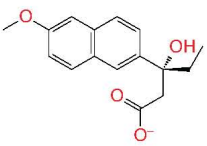
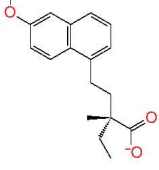
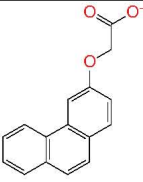
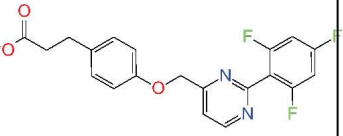
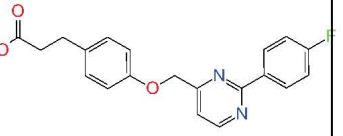
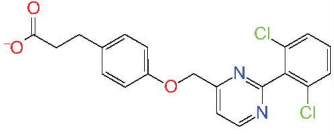
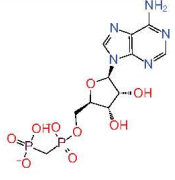
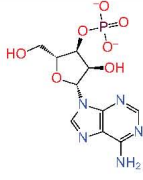
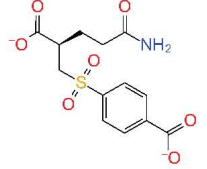
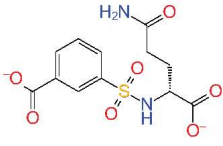
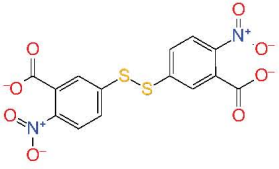
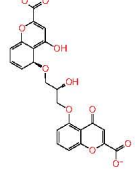
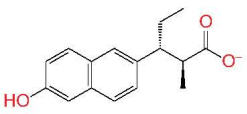
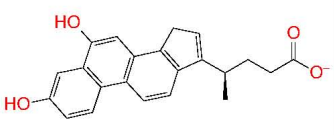
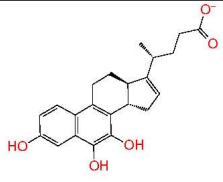
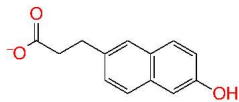
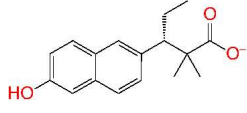
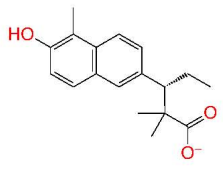
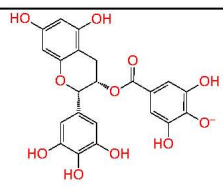
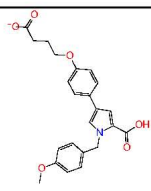
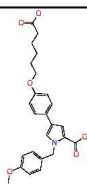
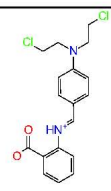
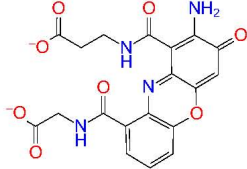
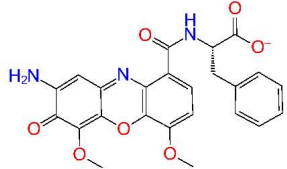
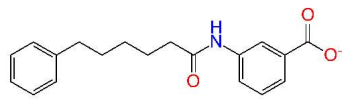
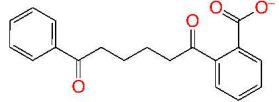
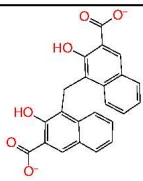
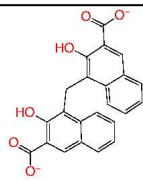
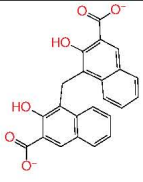
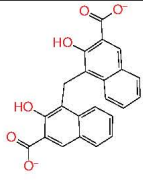
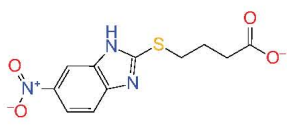
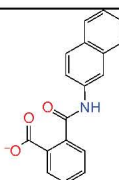
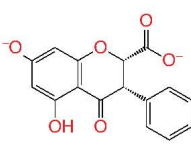
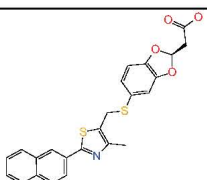
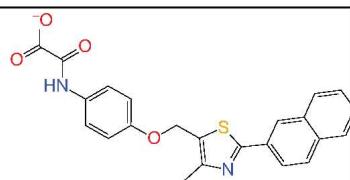
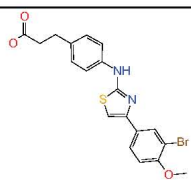
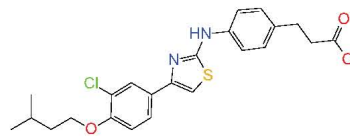
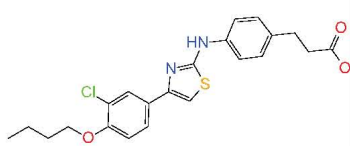
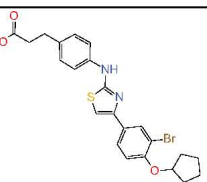
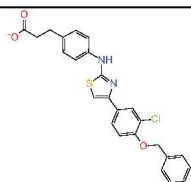
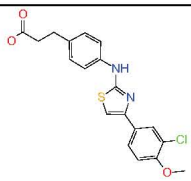
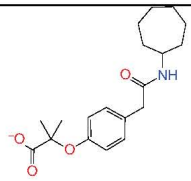
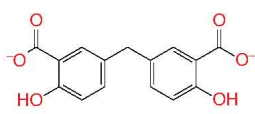


Figure S2. The Structure, ID, XP glidescore, clusters and predicted absorption level and solubility level of compounds retained by VSW.

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 title: Str1586 XP GScore: 8.759 ADMET Absorption Level: 1 ADMET Solubility Level: 2 Cluster: 1	 title: Str1606 XP GScore: 8.902 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 1	 title: Str1587 XP GScore: 8.914 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 1
 title: Str1614 XP GScore: 9.321 ADMET Absorption Level: 2 ADMET Solubility Level: 2 Cluster: 1	 title: Str1589 XP GScore: 9.641 ADMET Absorption Level: 2 ADMET Solubility Level: 2 Cluster: 1	 title: Str1597 XP GScore: 7.052 ADMET Absorption Level: 2 ADMET Solubility Level: 1 Cluster: 1
 title: Str1569 XP GScore: 10.8 ADMET Absorption Level: 1 ADMET Solubility Level: 2 Cluster: 1	 title: Str1616 XP GScore: 9.854 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 1	 title: Str8061 XP GScore: 8.276 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2
 title: Str7418 XP GScore: 8.078 ADMET Absorption Level: 0 ADMET Solubility Level: 4 Cluster: 2	 title: Str5903 XP GScore: 8.762 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2	 title: Str1056 XP GScore: 7.84 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2

 title: Str5757 XP GScore: 7.226 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2	 title: Str1054 XP GScore: 7.539 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 2	 title: Str7337 XP GScore: 7.503 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2
 title: Str2169 XP GScore: 7.279 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 3	 title: Str2165 XP GScore: 7.636 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 3	 title: Str2157 XP GScore: 7.195 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 3
 title: Str2163 XP GScore: 7.38 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 3	 title: Str921 XP GScore: 8.241 ADMET Absorption Level: 3 ADMET Solubility Level: 4 Cluster: 4	 title: Str922 XP GScore: 8.39 ADMET Absorption Level: 3 ADMET Solubility Level: 4 Cluster: 4
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 title: Str4660 XP GScore: 7.437 ADMET Absorption Level: 3 ADMET Solubility Level: 5 Cluster: 7	 title: Str924 XP GScore: 8.951 ADMET Absorption Level: 3 ADMET Solubility Level: 4 Cluster: 8	 title: Str5748 XP GScore: 8.365 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 9

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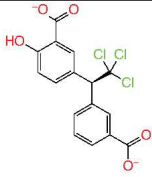
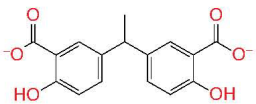
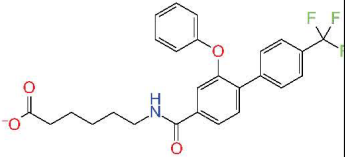
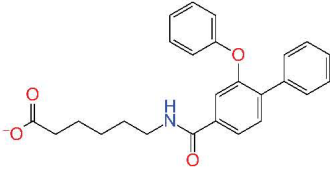
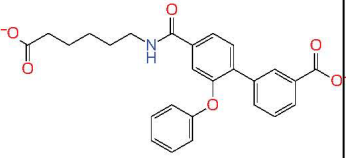
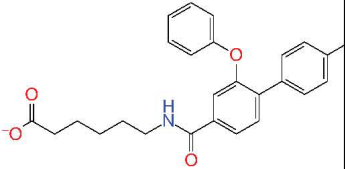
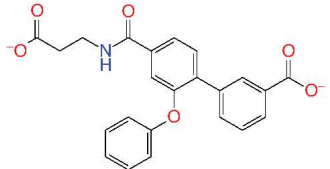
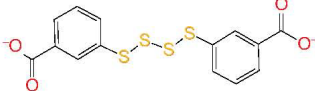
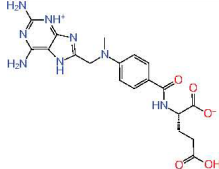
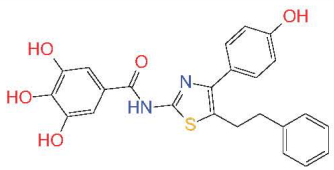
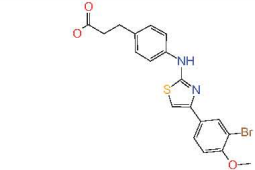
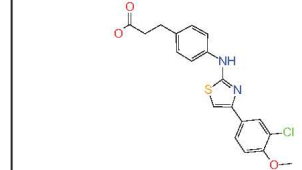
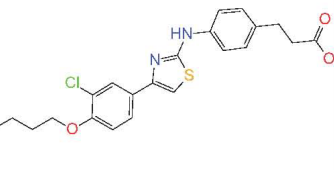
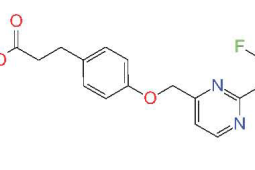
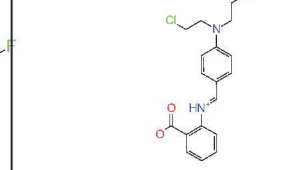
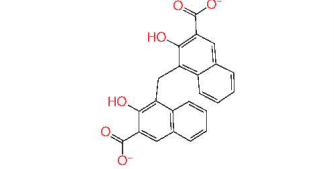
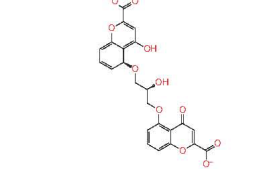
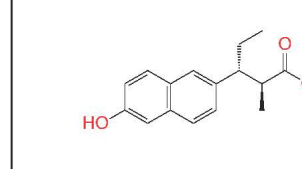
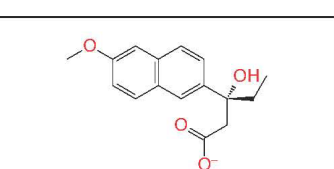
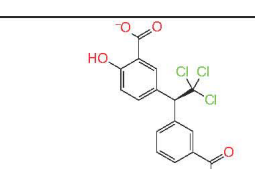
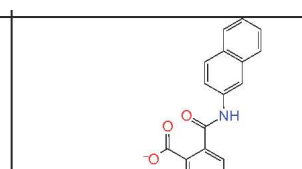
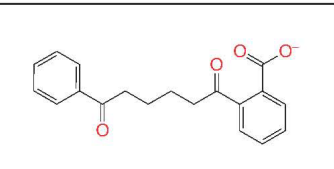
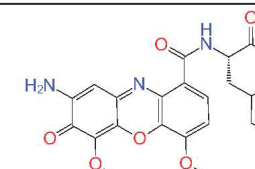
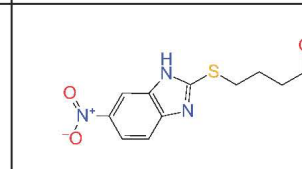
 title: Str5776 XP GScore: 8.569 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 22	 title: Str5760 XP GScore: 9.728 ADMET Absorption Level: 0 ADMET Solubility Level: 4 Cluster: 22	 title: Str613 XP GScore: 8.004 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 23
 title: Str611 XP GScore: 9.486 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 23	 title: Str618 XP GScore: 9.752 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 23	 title: Str612 XP GScore: 8.966 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 23
 title: Str627 XP GScore: 8.894 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 23	 title: Str6666 XP GScore: 7.19 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 24	 title: Str6860 XP GScore: 7.583 ADMET Absorption Level: 3 ADMET Solubility Level: 3 Cluster: 25

Figure S3. The structure, ID, XP glidescore, clusters, and predicted absorption levels and solubility levels of compounds selected for biological evaluation.

 title: Str1614 XP GScore: 9.321 ADMET Absorption Level: 2 ADMET Solubility Level: 2 Cluster: 1	 title: Str1902 XP GScore: 8.191 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 20	 title: Str1912 XP GScore: 7.818 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 20
 title: Str1916 XP GScore: 8.115 ADMET Absorption Level: 0 ADMET Solubility Level: 2 Cluster: 20	 title: Str2165 XP GScore: 7.636 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 3	 title: Str3839 XP GScore: 7.327 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 12
 title: Str3952 XP GScore: 8.874 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 15	 title: Str4660 XP GScore: 7.437 ADMET Absorption Level: 3 ADMET Solubility Level: 5 Cluster: 7	 title: Str5748 XP GScore: 8.365 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 9
 title: Str5757 XP GScore: 7.226 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 2	 title: Str5776 XP GScore: 8.569 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 22	 title: Str6038 XP GScore: 7.494 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 17
 title: Str6318 XP GScore: 7.389 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 14	 title: Str7374 XP GScore: 8.511 ADMET Absorption Level: 2 ADMET Solubility Level: 3 Cluster: 13	 title: Str7642 XP GScore: 7.046 ADMET Absorption Level: 0 ADMET Solubility Level: 3 Cluster: 16

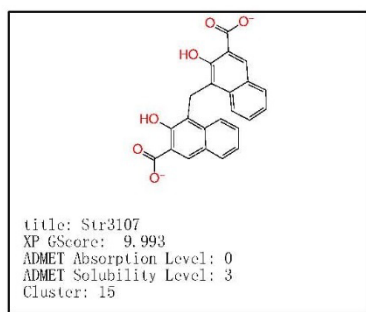
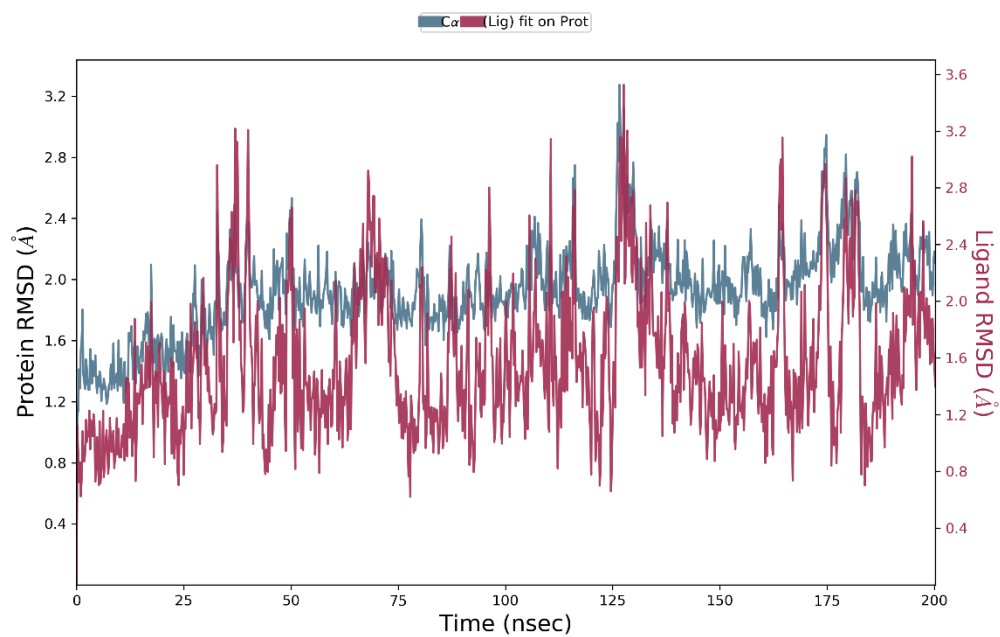
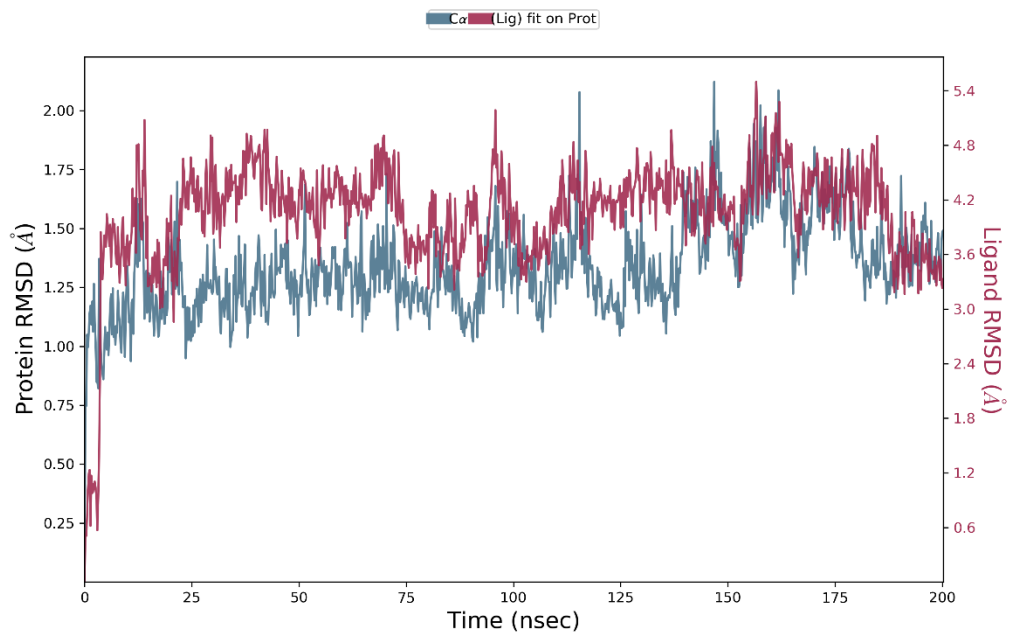


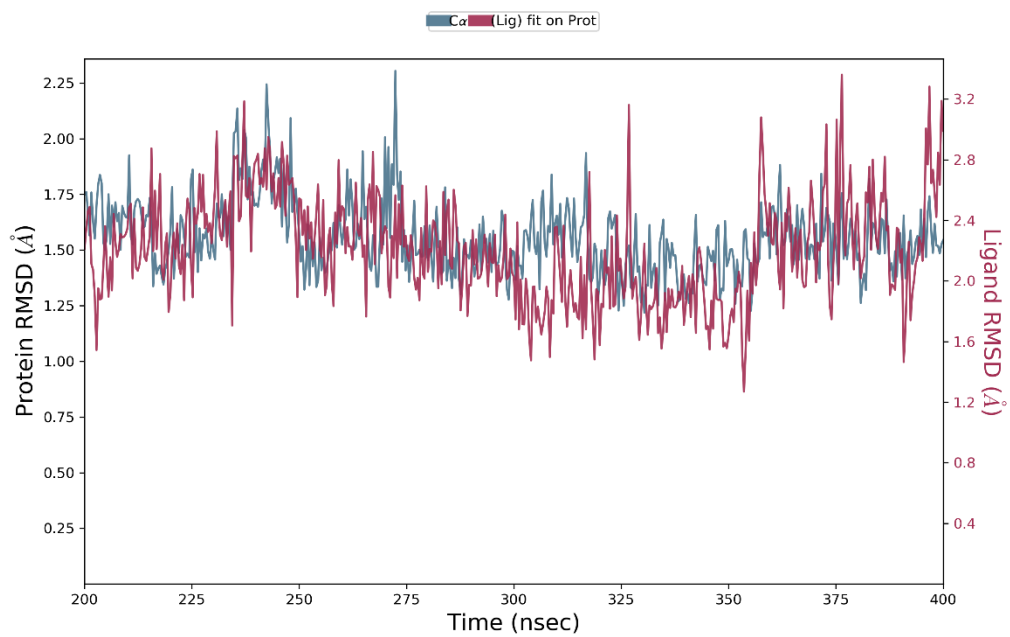
Figure S4. The RMSD of PB2 protein $\text{C}\alpha$ atoms and Lig fit Prot of Ligand in MD simulations.



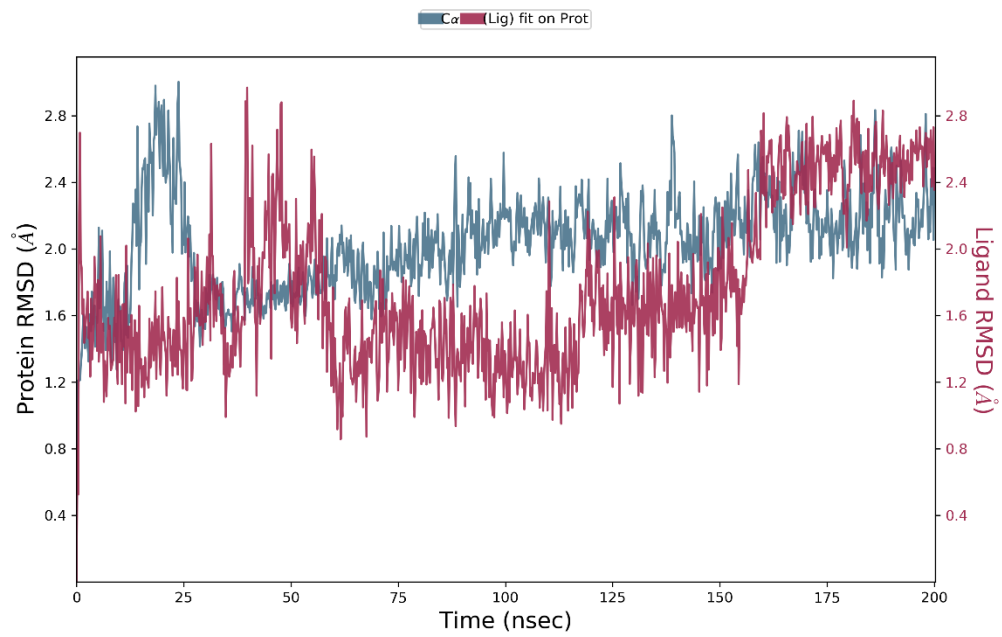
VX-787



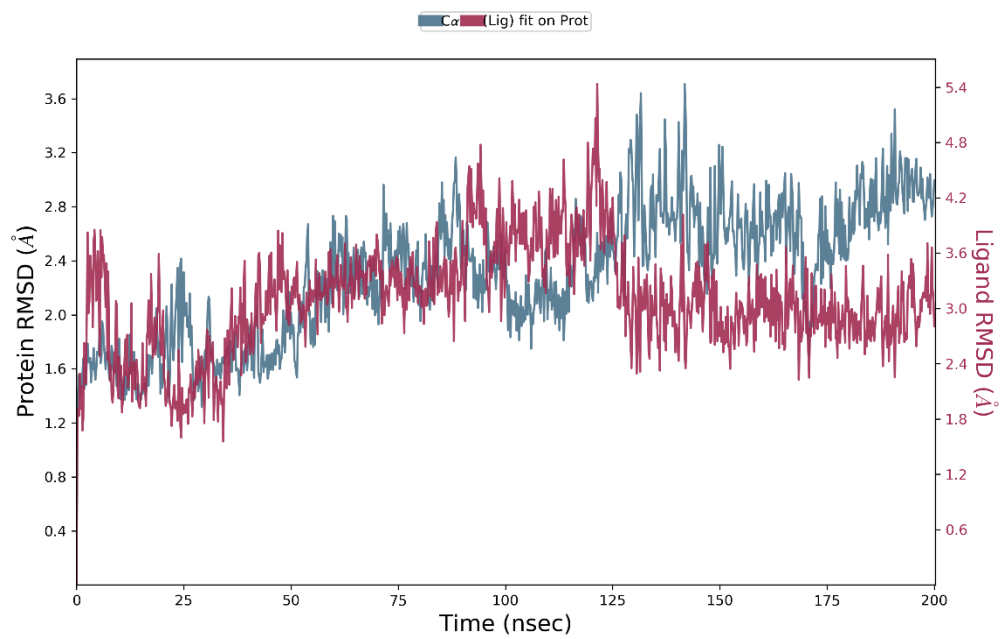
STR1614



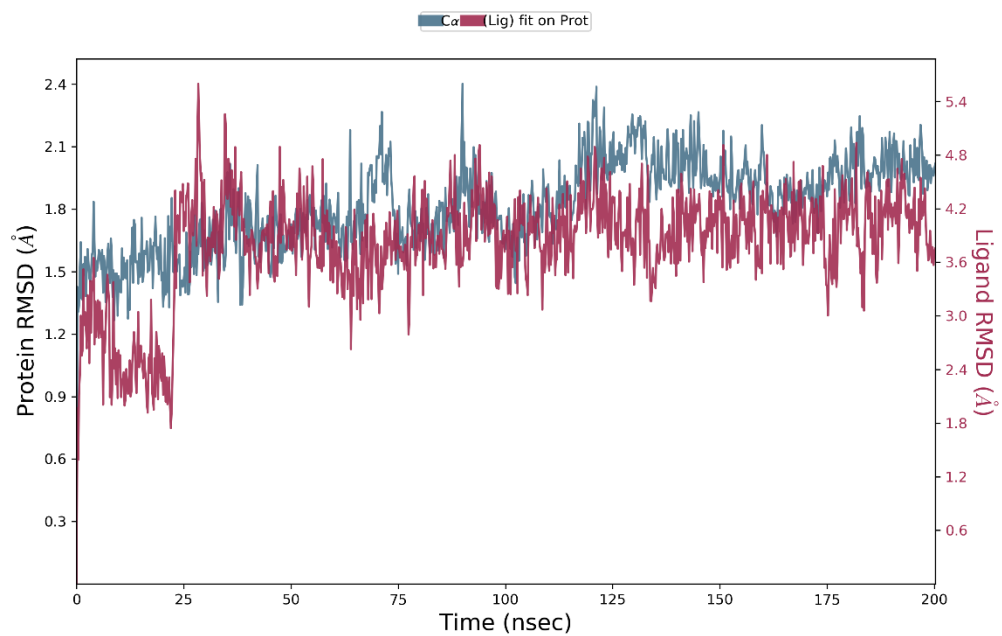
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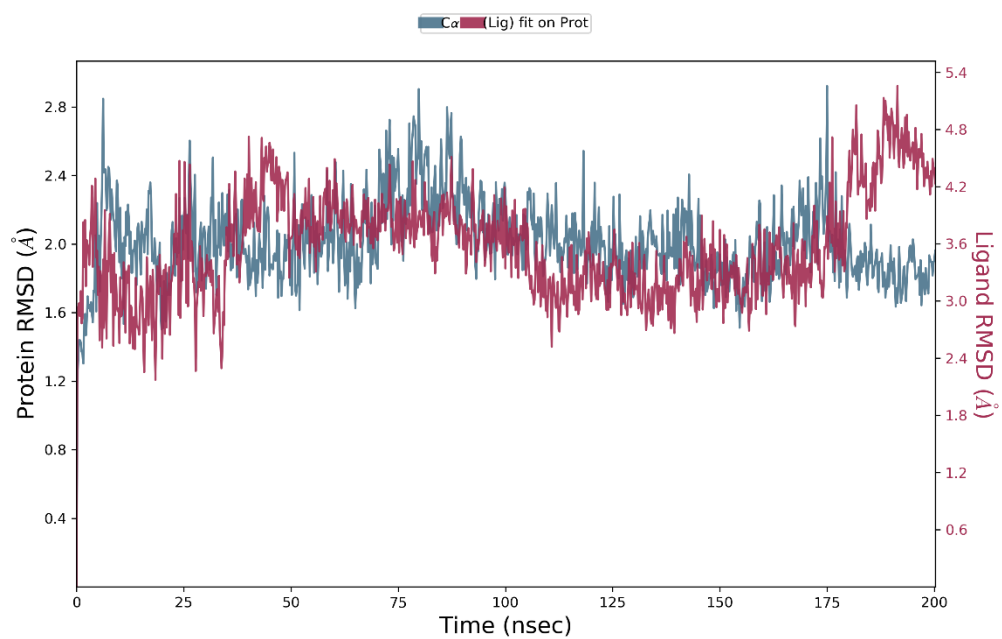
STR3107



STR5776



Str6318



STR7374