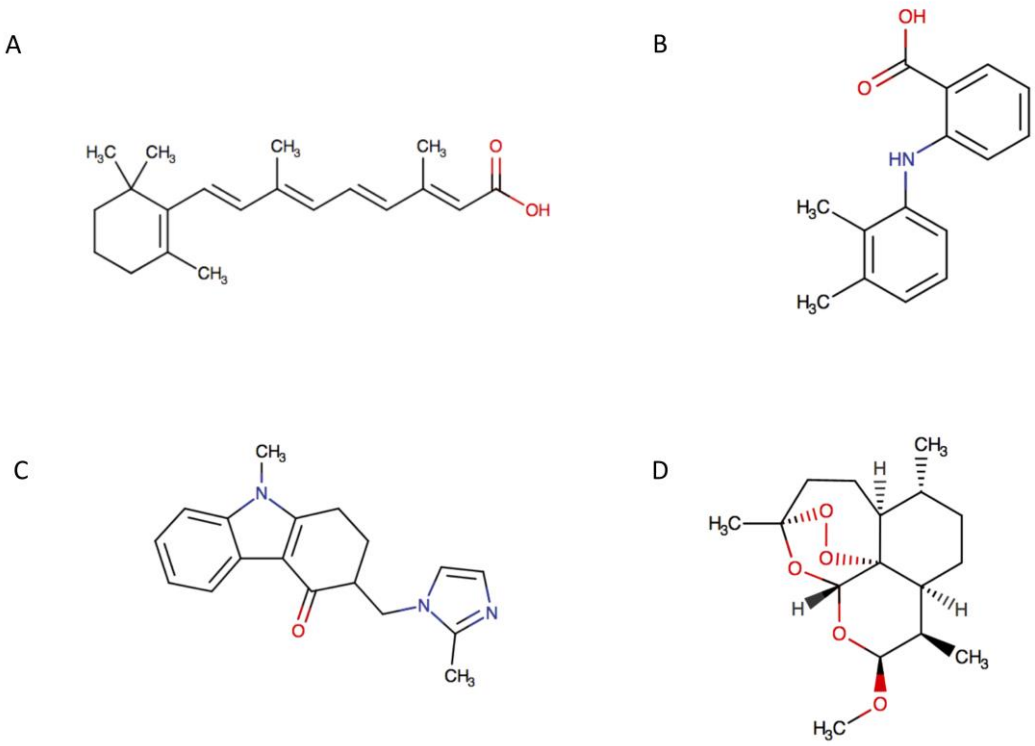
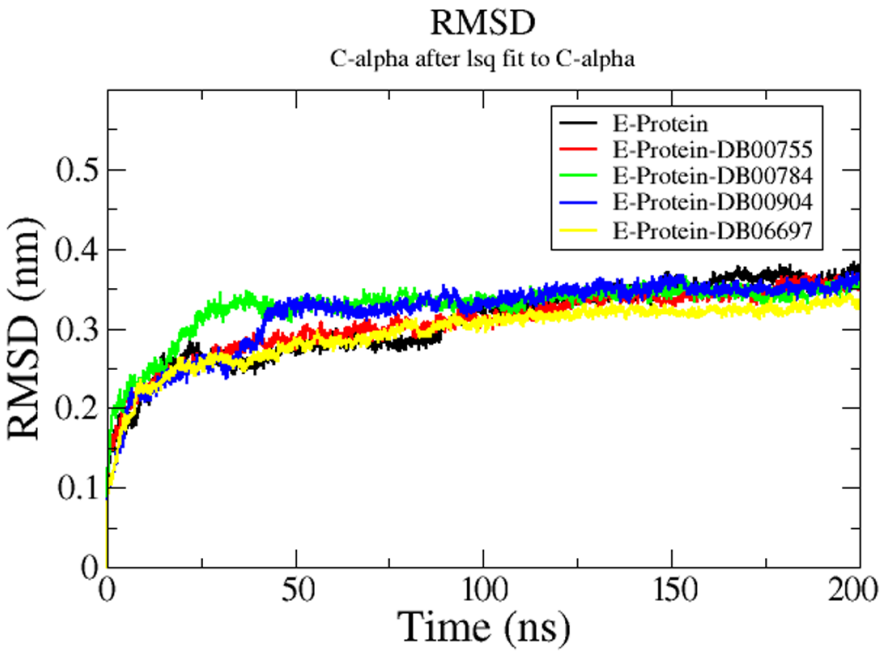
Supplementary Information:



Supplementary Figure S1: 2D chemical structure of (A) Tretinoin, (B) Mefenamic acid, (C) Ondansetron and (D) Artemether.



Supplementary Figure S2: RMSD analysis of SARS-CoV-2 E apo form and drug complexes during simulation (representative run).

Supplementary Table 1: Selected list of FDA-approved drugs.

S.No.	Drug ID
1	DB00377
2	DB00755
3	DB00972
4	DB00985
5	DB01619
6	DB00751
7	DB09274
8	DB00904
9	DB06697
10	DB00784
11	DB00670
12	DB09216
13	DB00934
14	DB00266
15	DB00216

Supplementary Table 2: Binding energy values of Tretinoin (2LBD) and Mefenamic acid (5IKR) bound to their respective targets.

PDB ID	Binding Energy (kJ/mol)	Electrostatic Energy (kJ/mol)	Polar Solvation Energy (kJ/mol)	Van der waal's Energy (kJ/mol)	SASA Energy (kJ/mol)
2LBD	**-85.8 +/- 13.26**	**-131.6 +/- 29.0**	**250.9 +/- 20.2**	**-185.7 +/- 13.9**	**-19.3 +/- 0.8**
5IKR	**-178.2 +/- 12.6**	**-236.8 +/- 13.2**	**250.5 +/- 11.5**	**-177.4 +/- 11.5**	**-14.5 +/- 0.6**

Supplementary Table 3: Binding energy values of the four ligands in complex with SARS CoV-2 E protein (triplicate runs).

DRUG ID	Binding Energy (kJ/mol)	Electrostatic Energy (kJ/mol)	Polar Solvation Energy (kJ/mol)	Van der waal's Energy (kJ/mol)	SASA Energy (kJ/mol)
DB00755	-400.7 +/- 11.7	-478.5 +/- 11.4	262.1 +/- 7.9	-166.4 +/- 13.1	-17.7 +/- 0.9
	-391.6 +/- 10.7	-430.9 +/- 13.6	268.6 +/- 11.5	-193.2.4 +/- 11.7	-18.9 +/- 0.8
DB00784	-379.5 +/-10.5	-426.1 +/-	245.1 +/-6.5	-183.4 +/-10.7	-15.1 +/-0.7
	-372.1 +/-13.9	-432.3 +/-11.4	257.1 +/-7.9	-182.8 +/-12.1	14.8 +/-0.6
DB00904	-222.4 +/-9.2	0.3 +/-0.8	22.3 +/-1.9	-227.8 +/-9.5	-17.2 +/-0.8
	-220.2 +/-8.4	-0.9 +/-0.9	21.1 +/-2.6	-223.5 +/-8.9	-16.9 0.9
DB06697	-172.1 +/-11.2	-2.0 +/-3.0	36.6 +/-5.7	-191.7 +/-9.8	-14.9 +/-0.7
	-166.6 +/-7.3	-0.7 +/-1.0	27.3 +/-4.0	-177.7 +/-7.8	-15.5 0.8