Supplementary information

Site mapping and small molecule blind docking reveal a possible target site on the SARS-CoV-2 main protease dimer interface

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Figure S1.

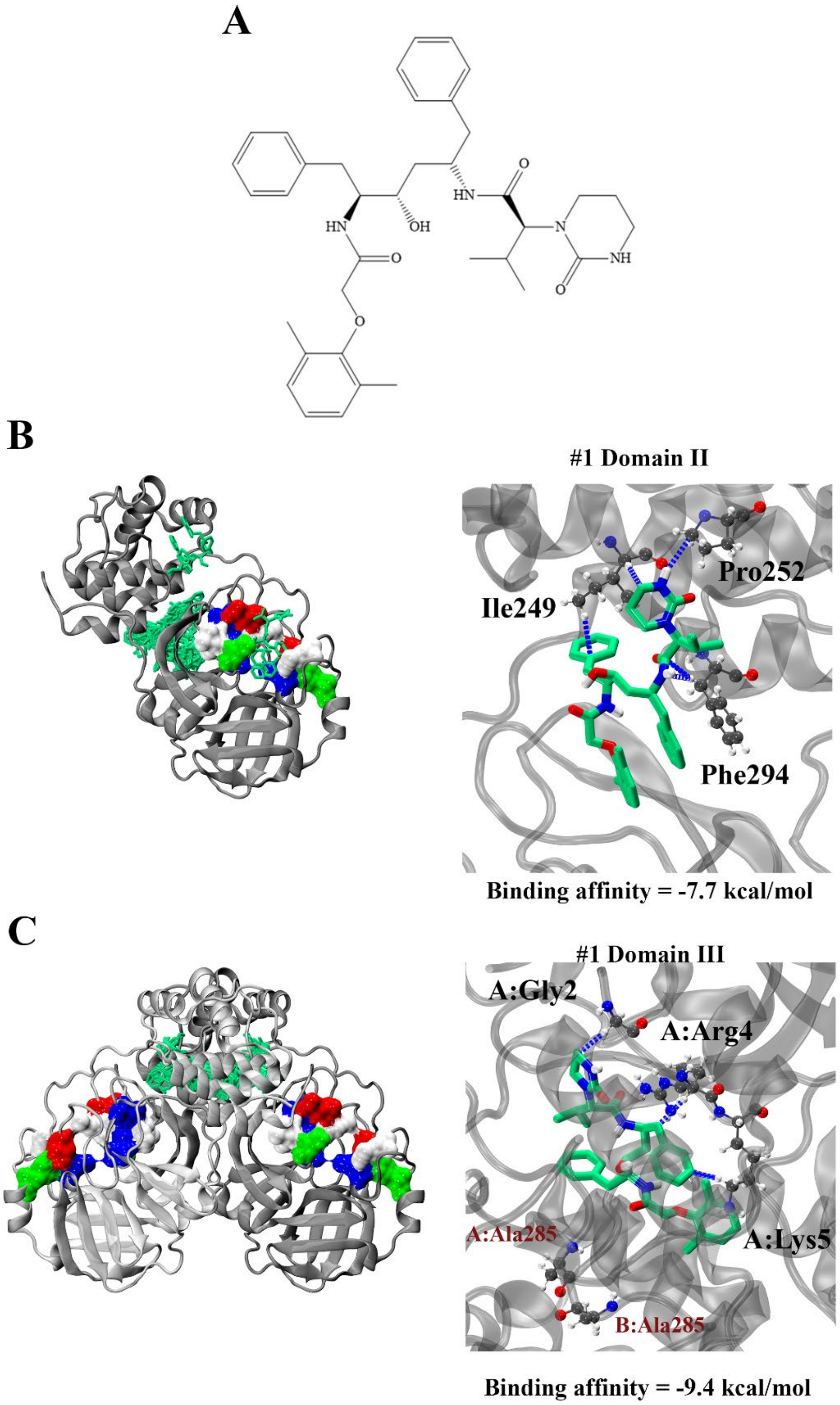

Figure S1. Blind docking of lopinavir (A) to SARS-CoV-2 main protease monomer (B) and dimer (C).

Figure. S2.

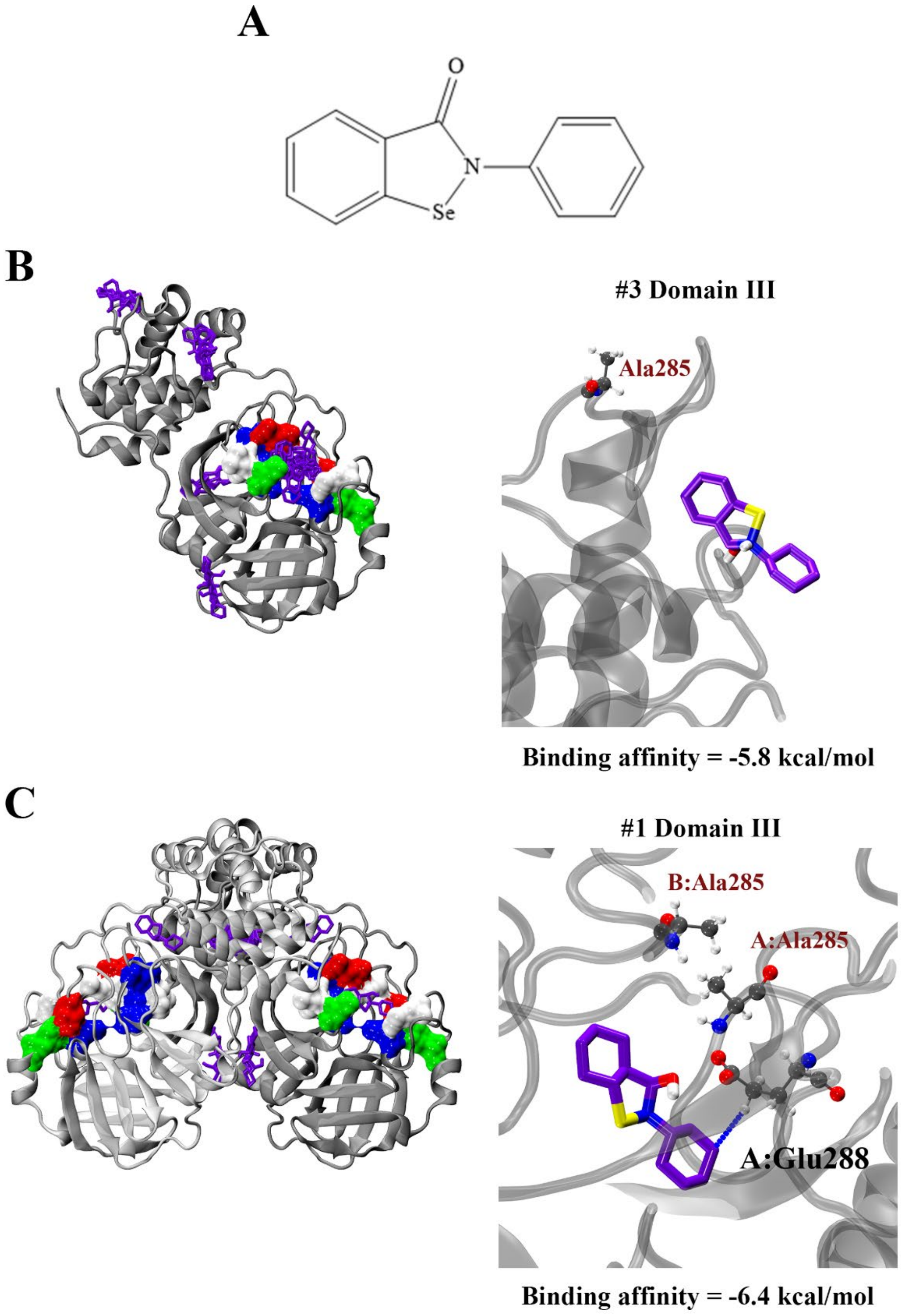

Figure S2. Blind docking of ebselen (A) to SARS-CoV-2 main protease monomer (B) and dimer (C).

Table S1: Average energy contribution of ligands bound to different regions of SARS-CoV-2 M^{pro} in kcal/mol

Ligand	Binding location	Van der Waal	Electrostatic	Polar solvation	SASA energy	Binding energy
α-ketoamide 13b	**Protomer A**	-44.0	-11.0	37.5	-5.2	**-22.7**
	Protomer B	-49.6	-15.3	47.0	-5.5	**-23.5**
	Domain III	-59.9	-23.8	84.9	-6.5	**-5.2**
SRT1720	**Protomer A**	-51.4	-77.9	77.9	-5.4	**-56.8**
	Protomer B	-40.1	-67.1	53.8	-4.4	**-57.8**
	Domain III	-30.2	-4.9	22.1	-3.4	**-16.4**
Ritonavir	**Protomer A**	-38.7	-5.9	31.6	-4.9	**-17.9**
	Protomer B	-40.8	-9.3	37.9	-5.0	**-17.2**
	Domain III	-74.4	-14.3	72.1	-7.8	**-24.4**

Movie S1.

100 ns trajectory of the apo form of the SARS-CoV-2 main protease

Movie S2.

100 ns trajectory of ritonavir bound to the active site of the SARS-CoV-2 main protease

Movie S3.

100 ns trajectory of ritonavir bound to the top binding pose in domain III of the SARS-CoV-2 main protease

Movie S4.

100 ns trajectory of α-ketoamide 13b to the active site of the SARS-CoV-2 main protease

Movie S5.

100 ns trajectory of α-ketoamide 13b to the top binding pose in domain III of the of the SARS-CoV-2 main protease

Movie S6.

100 ns trajectory of SRT1720 bound to the active site of the SARS-CoV-2 main protease

Movie S7.

100 ns trajectory of SRT1720 bound in domain III (binding pose #3) of the SARS-CoV-2 main protease