

Supplementary data

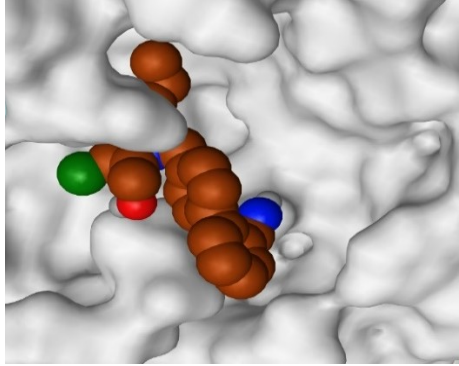
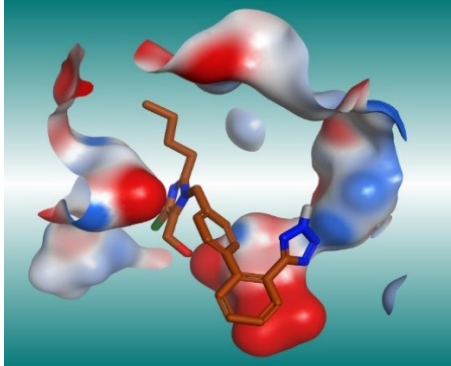
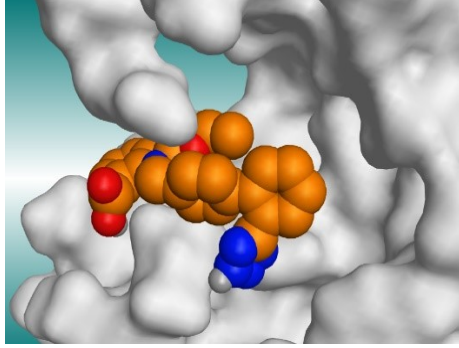
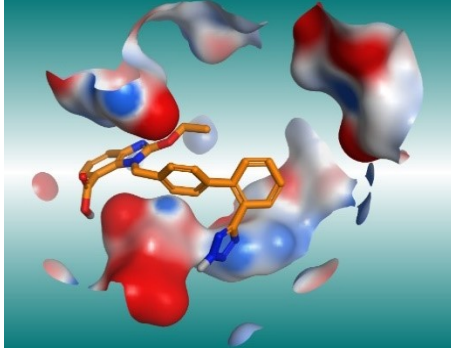
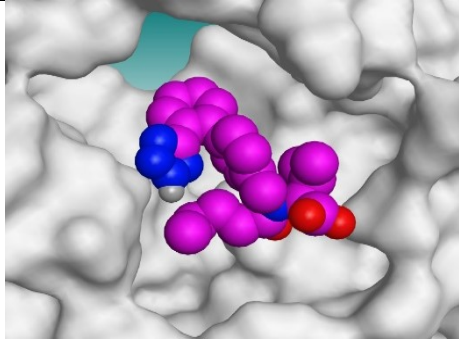
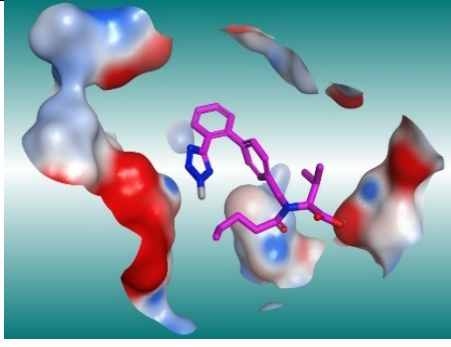
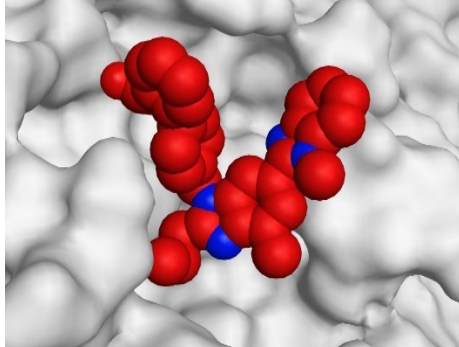
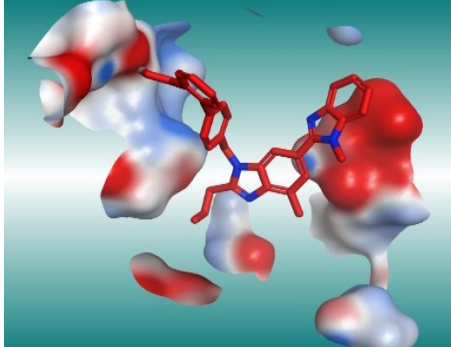
Fig. 1: 2D and 3D docking representations of ARBs and N3 inhibitor against the binding site of the COVID-19 main protease.

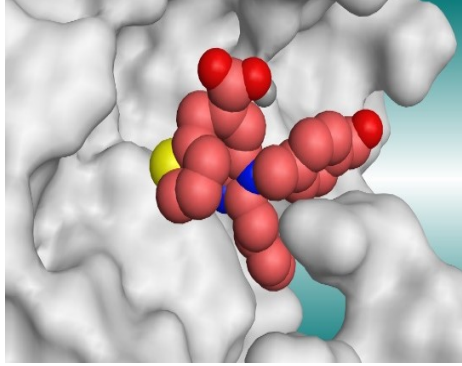
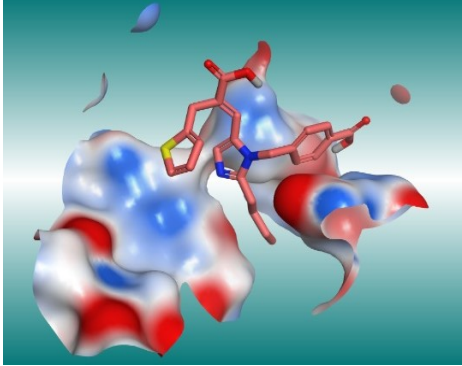
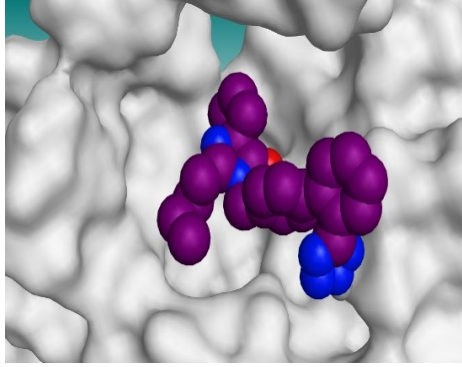
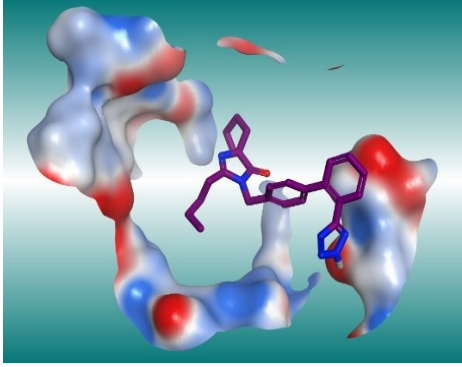
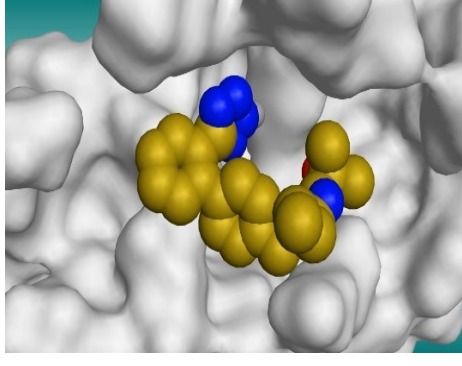
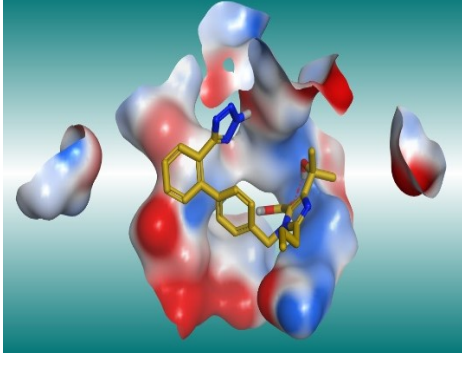
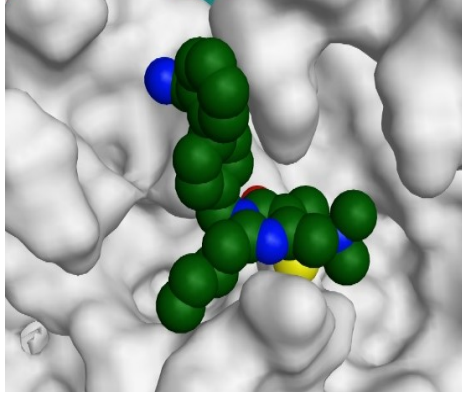
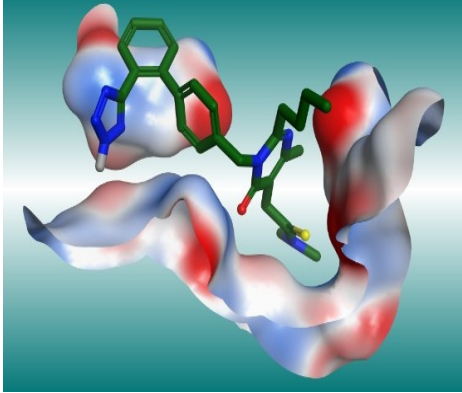
No.	ARB drug	2D	3D
		<p> ○ polar → sidechain acceptor ○ solvent residue ○ arene-arene ○ acidic ← sidechain donor ○ metal complex ○ arene-H ○ basic → backbone acceptor ○ solvent contact ○ arene-cation ○ greasy ← backbone donor ○ metal/ion contact ○ proximity ● ligand exposure ○ receptor exposure ○ contour </p>	<p>Red dashed lines refer to hydrogen bonds, while the black ones denote hydrophobic interactions.</p>
1	Losartan		
2	Candesartan		
3	Valsartan		

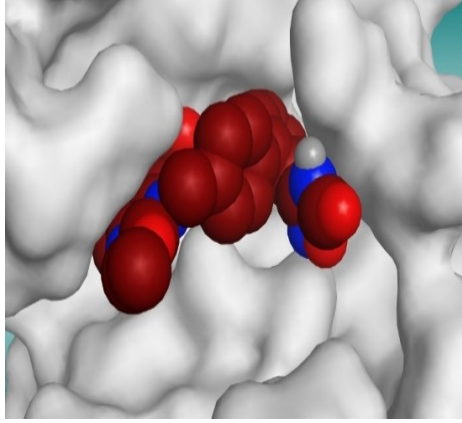
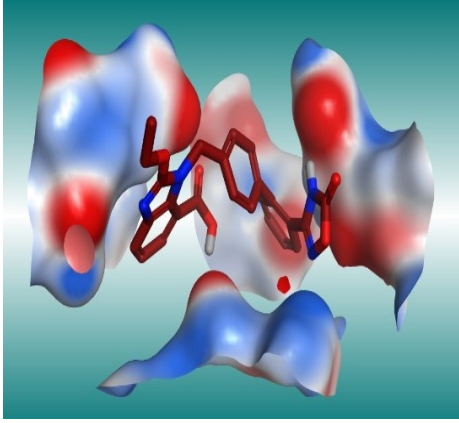
4	Telmisartan		
5	Eprosartan		
6	Irbesartan		
7	Olmesartan		

8	Fimasartan		
9	Azilsartan		
10	N3		

Fig. 2: A) Surface of M^{pro} showing the positioning and fitting of tested compounds, B) surface and maps of the tested compounds compared to N3 inhibitor

No.	ARB drug	A	B
1	Losartan	 A 3D molecular model of Losartan (represented by brown, green, red, and blue spheres) docked into the grey surface of the M ^{pro} protein.	 A 3D comparison of Losartan (brown sticks) and the N3 inhibitor (blue sticks) overlaid on a red and blue electrostatic potential map.
2	Candesartan	 A 3D molecular model of Candesartan (represented by orange, red, and blue spheres) docked into the grey surface of the M ^{pro} protein.	 A 3D comparison of Candesartan (orange sticks) and the N3 inhibitor (blue sticks) overlaid on a red and blue electrostatic potential map.
3	Valsartan	 A 3D molecular model of Valsartan (represented by purple, blue, and red spheres) docked into the grey surface of the M ^{pro} protein.	 A 3D comparison of Valsartan (purple sticks) and the N3 inhibitor (blue sticks) overlaid on a red and blue electrostatic potential map.
4	Telmisartan	 A 3D molecular model of Telmisartan (represented by red and blue spheres) docked into the grey surface of the M ^{pro} protein.	 A 3D comparison of Telmisartan (red sticks) and the N3 inhibitor (blue sticks) overlaid on a red and blue electrostatic potential map.

5	Eprosartan		
6	Irbesartan		
7	Olmesartan		
8	Fimasartan		

9	Azilsartan		
10	N3	