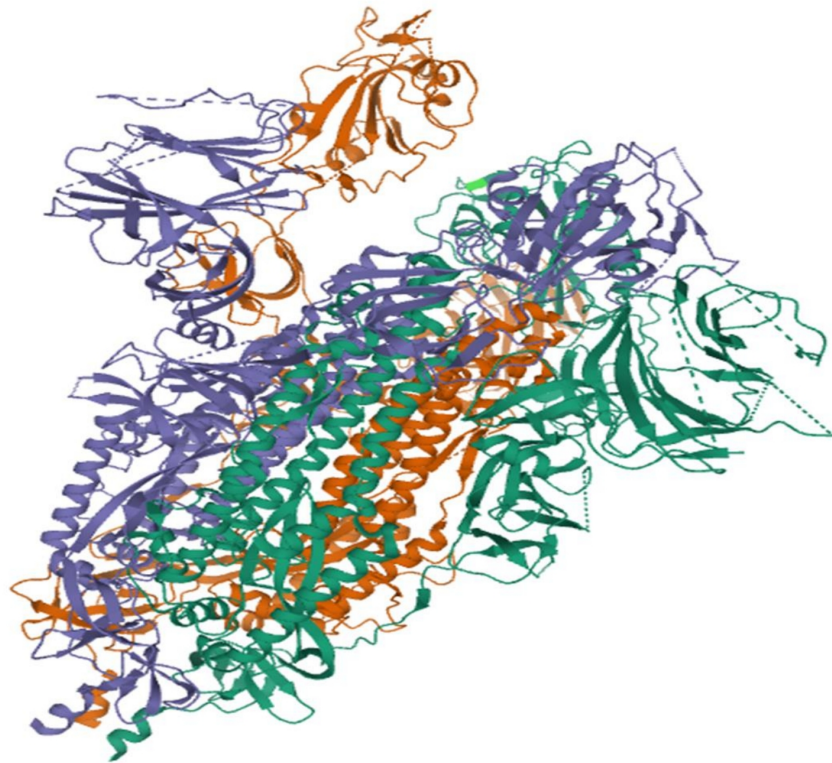


Spike ectodomain protein



Papain-like protease protein

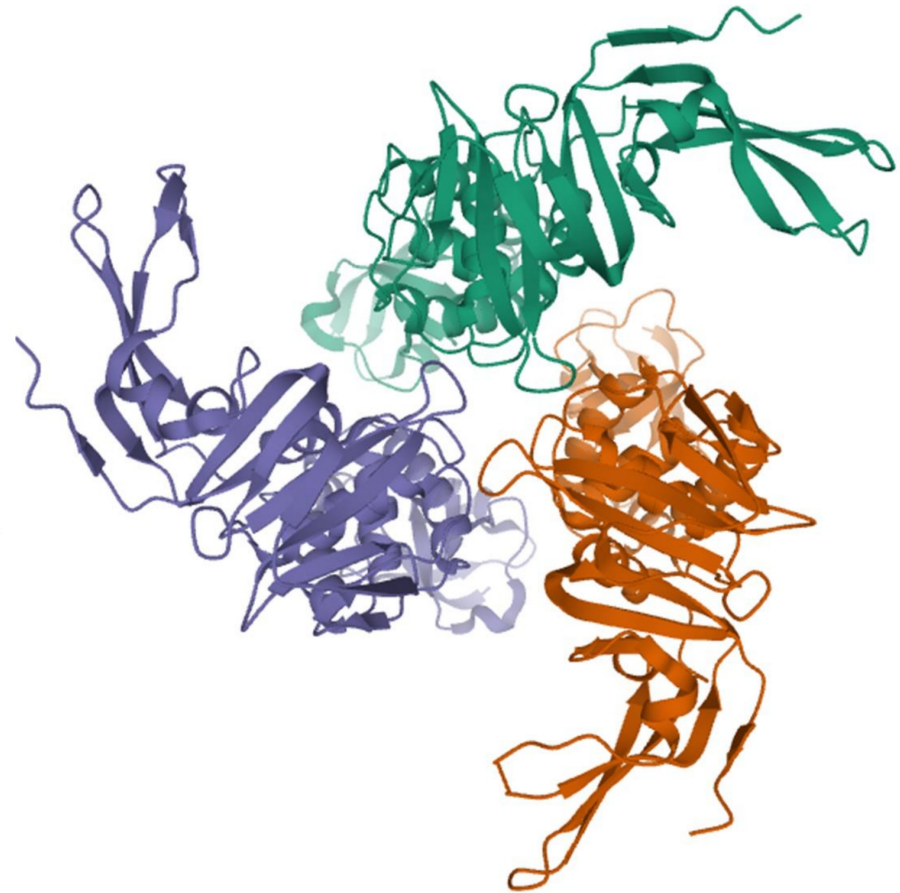
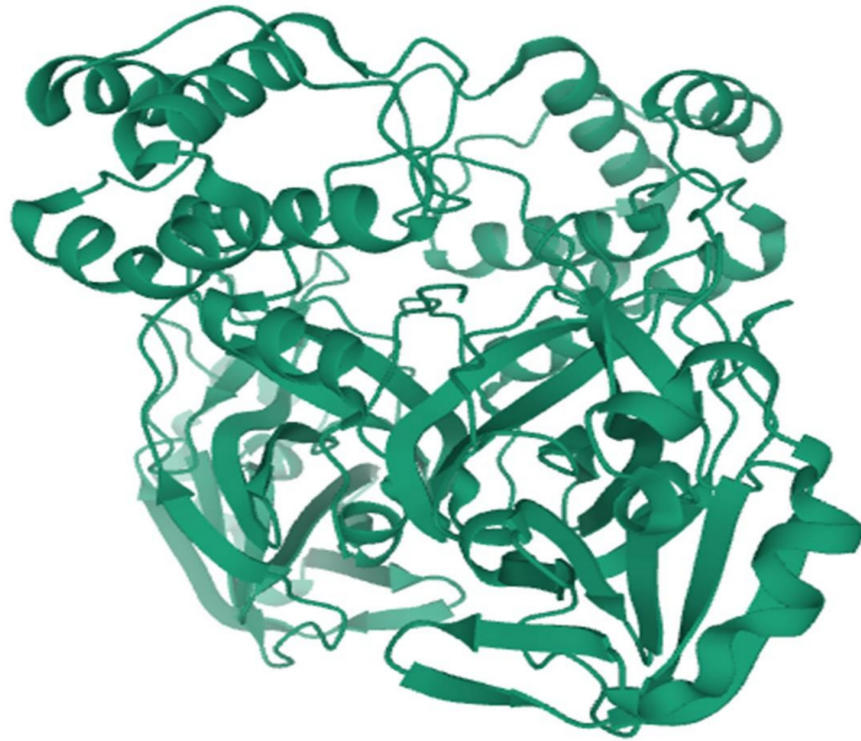


Fig. 1 (a): Crystal structure of SARS-CoV2 spike ectodomain protein (open state) (PDB ID: 6VYB) and papain-like protease protein (PDB ID: 6W9C)

Main protease protein



RNA-dependent RNA polymerase

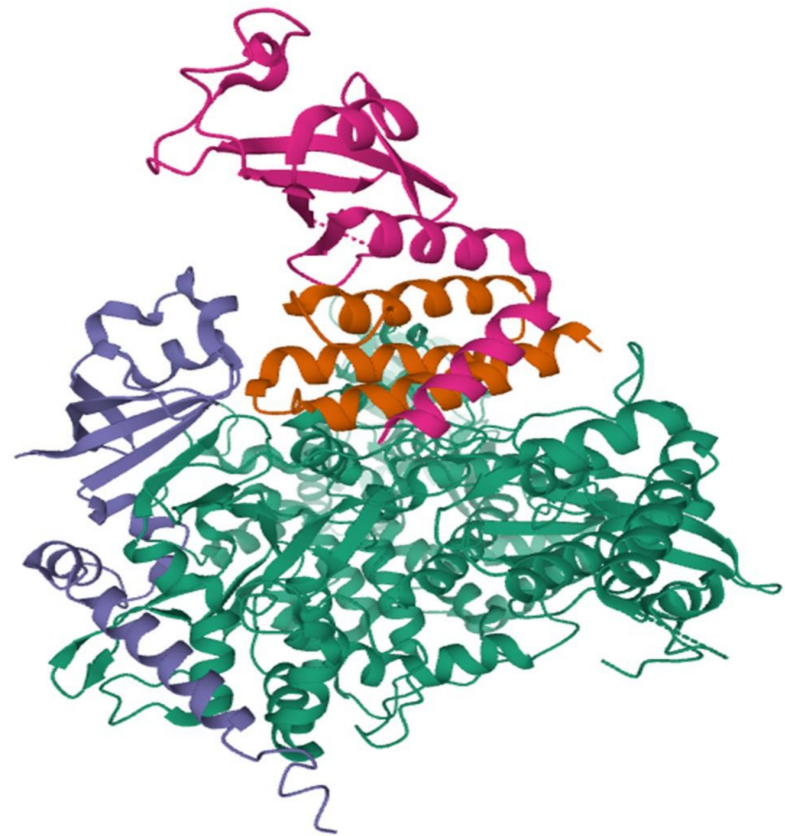


Fig. 1 (b): Crystal structure of SARS-CoV2 main protease protein (PDB ID: 6YB7) and RNA-dependent RNA polymerase (PDB ID: 7BTF)

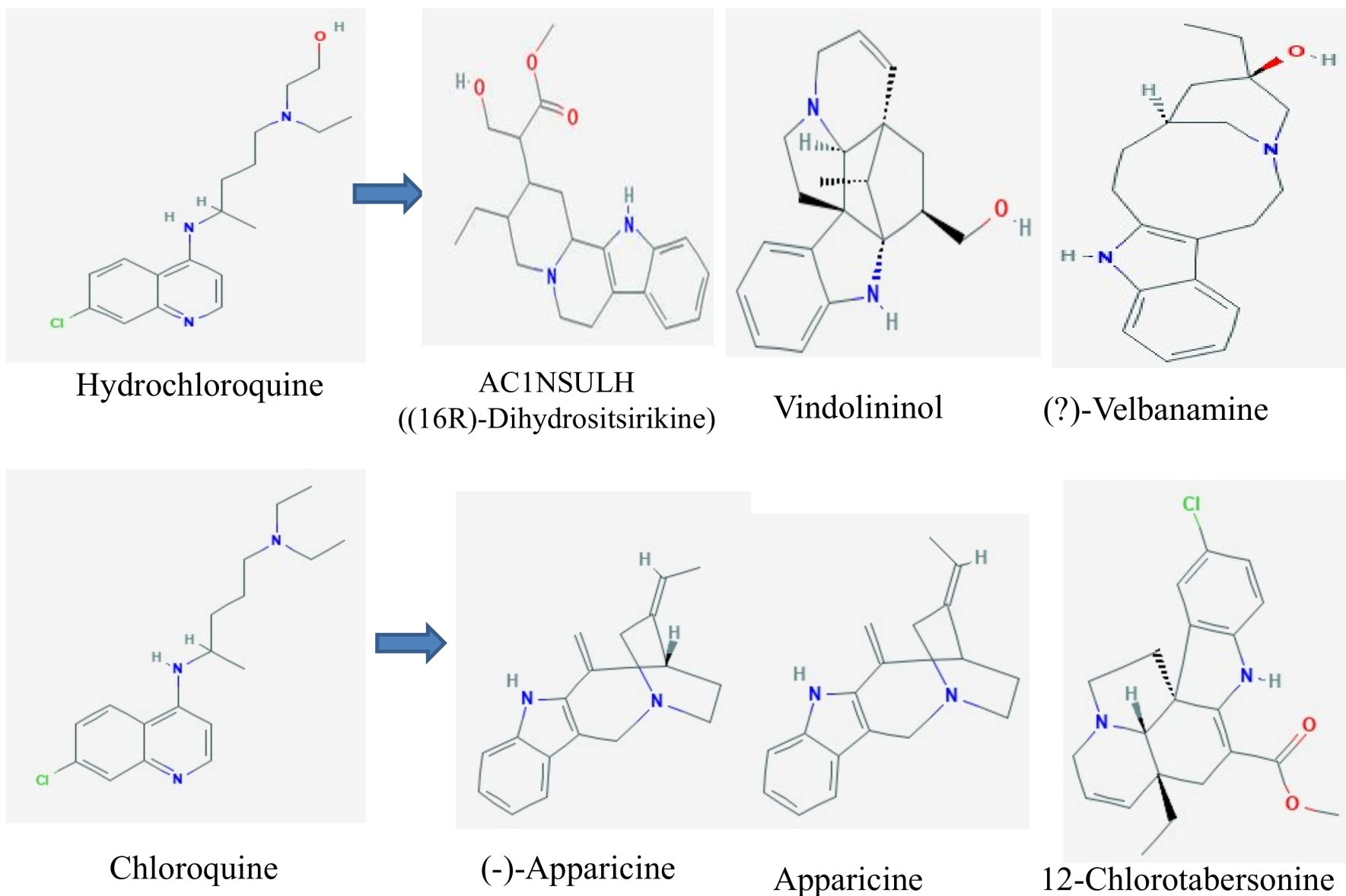
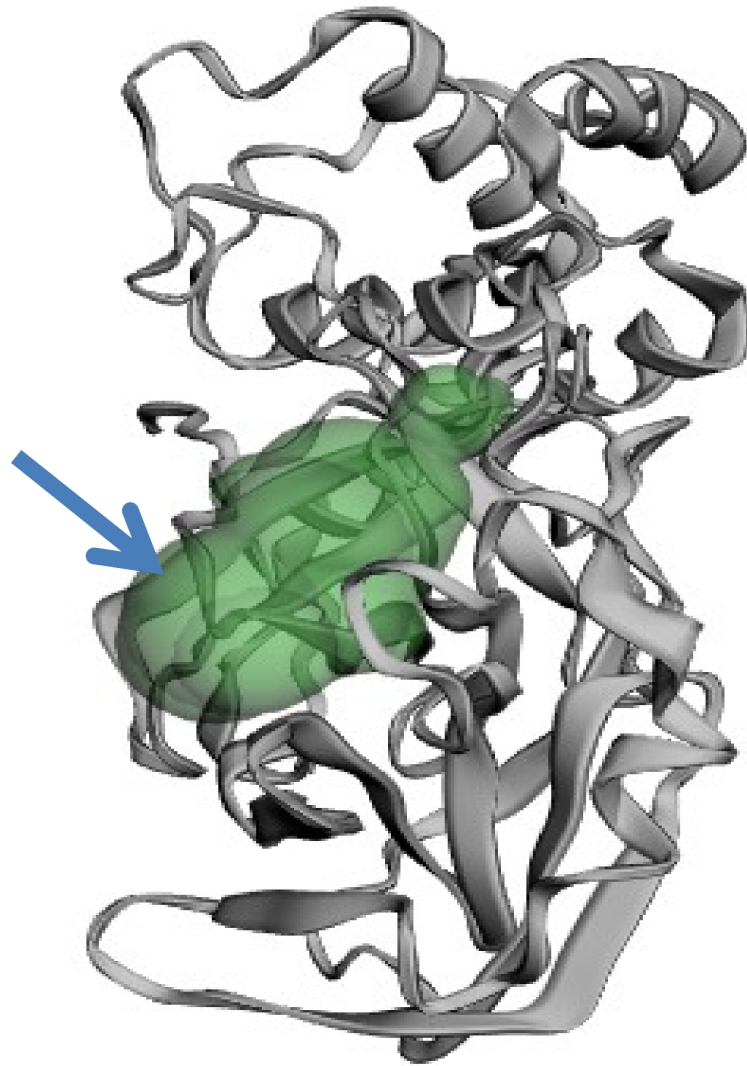


Fig. 2: 2D structures of Hydrochloroquine and chloroquine with its analog as phytochemicals from Medicinal Plants IMPPAT database

spike ectodomain protein



papain-like protease protein

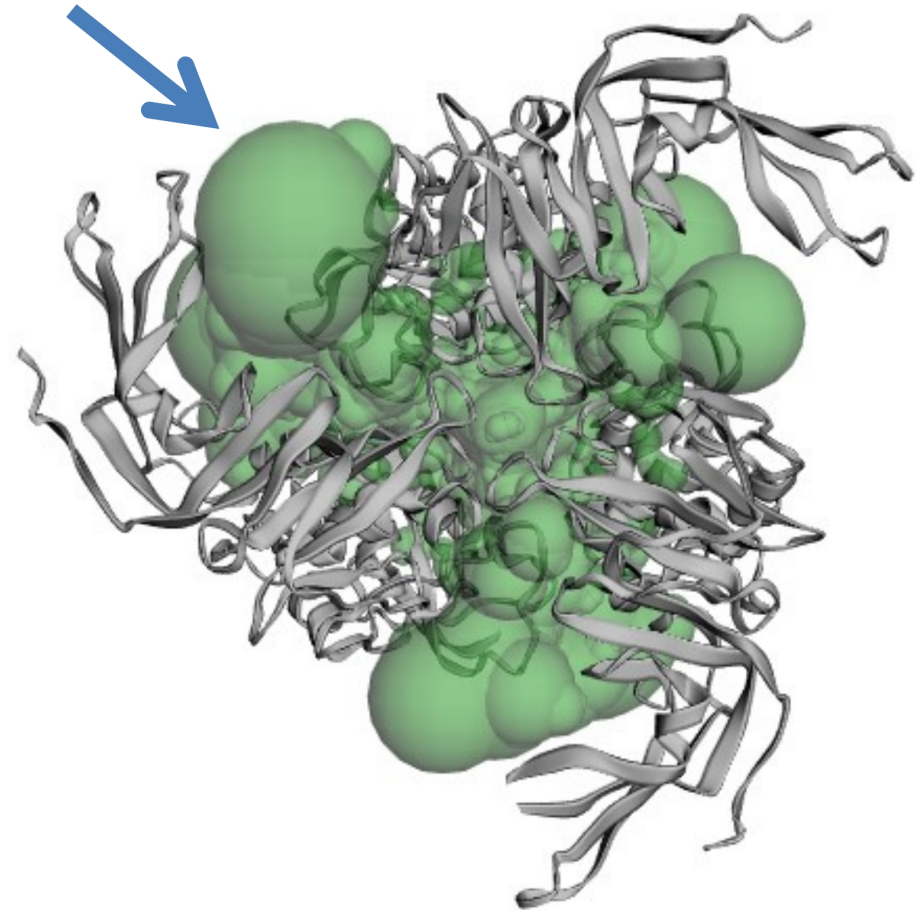


Fig. 3 (a): Active site of spike and papain-like protease protein of SARS-CoV2 using CASTp server

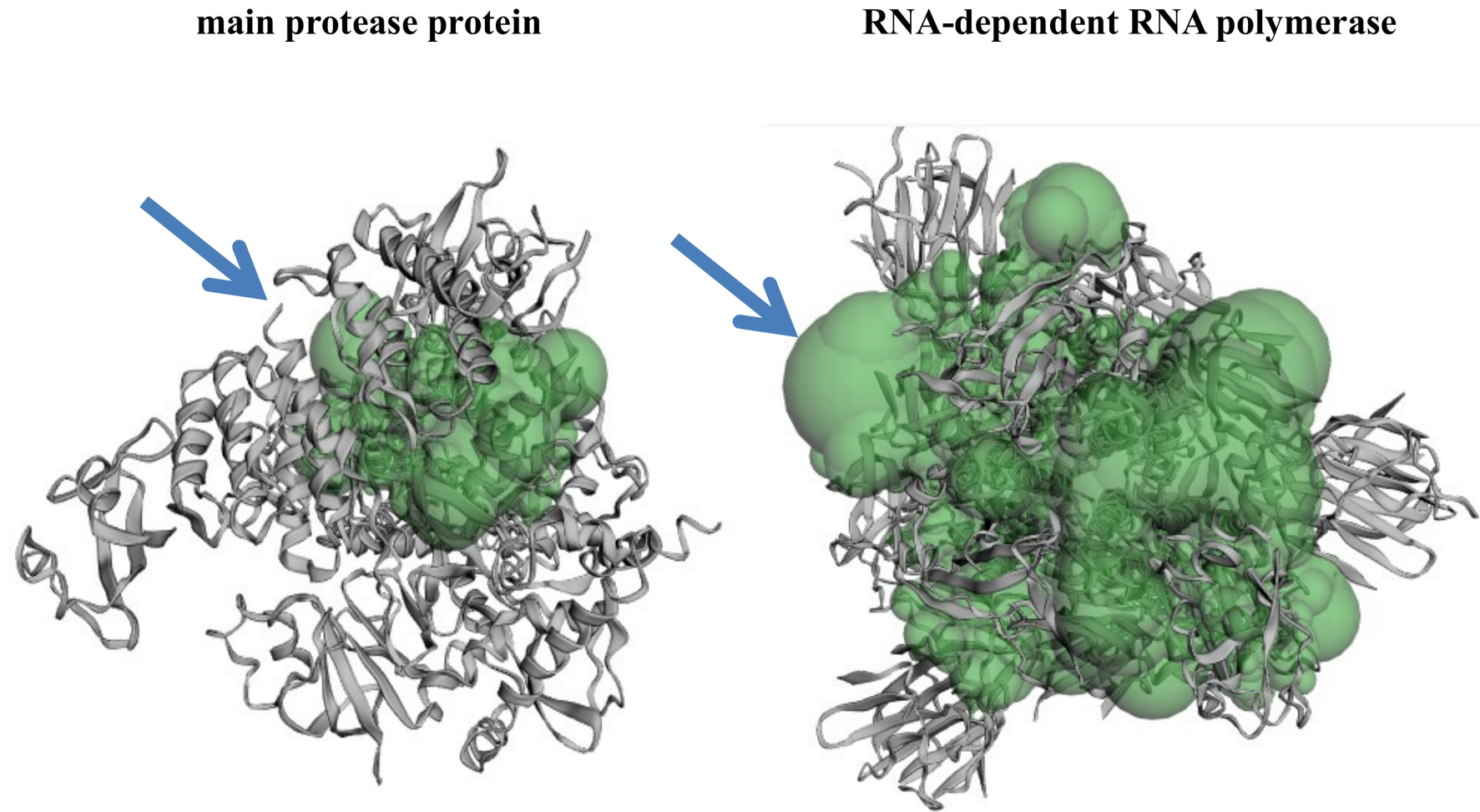
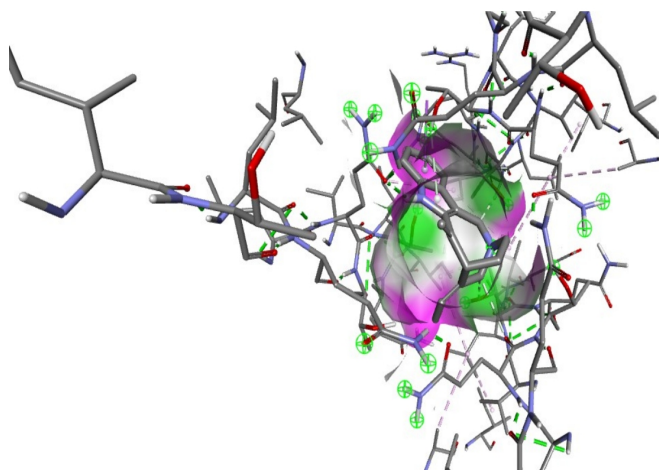


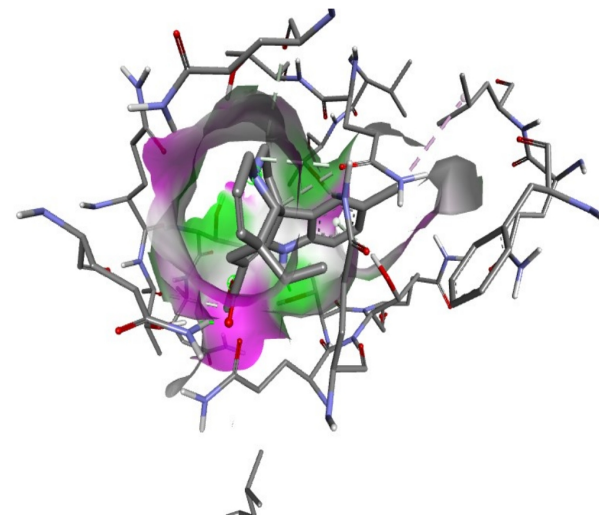
Fig. 3 (b): Active site of main protease protein and RNA-dependent RNA polymerase of SARS-CoV2 using CASTp server

A1

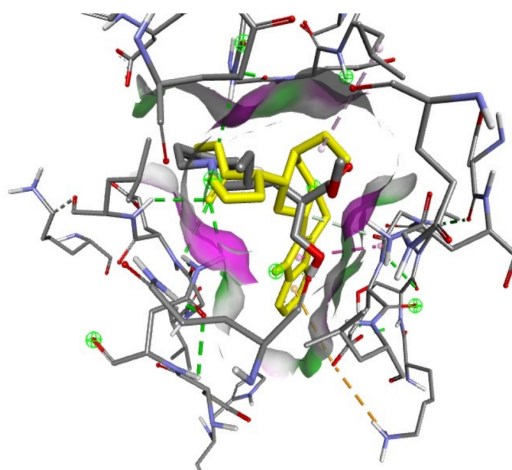
H-Bonds
Donor
Acceptor


**A2**

H-Bonds
Donor
Acceptor


**B1**

H-Bonds
Donor
Acceptor


**B2**

H-Bonds
Donor
Acceptor

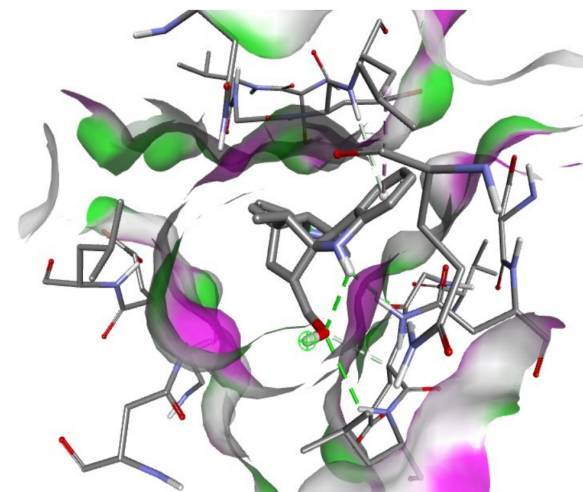
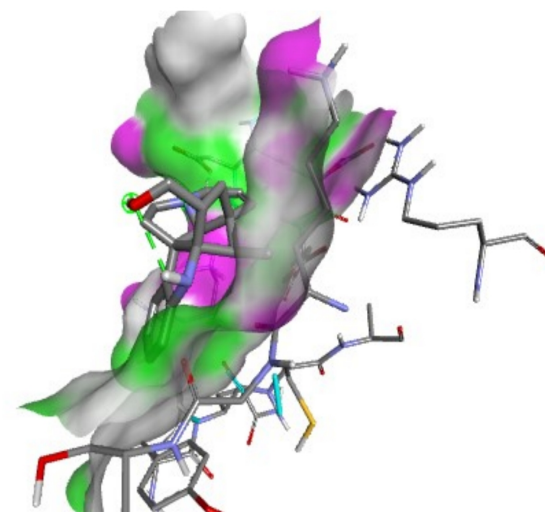



Fig. 4 (a): Three-dimensional representation of intermolecular interaction between SARS-CoV2 proteins and phytochemicals A) spike ectodomain protein with 1) Apparicine 2) 12-Chlorotabersonine , B) papain-like protease protein with 1) AC1NSULH 2) Vindolinol,

C1

H-Bonds
Donor
Acceptor



D1

H-Bonds
Donor
Acceptor

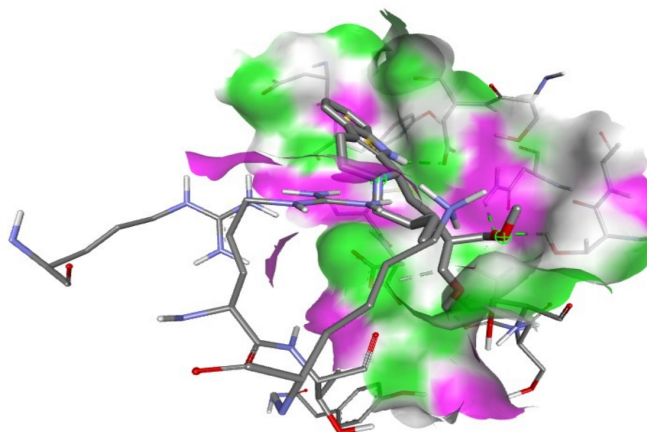


Fig. 4 (b): Three-dimensional representation of intermolecular interaction between SARS-CoV2 proteins and pytochemicals C) main protease protein with 1) Vindolinol and D) RNA-dependent RNA polymerase 1) AC1NSULH

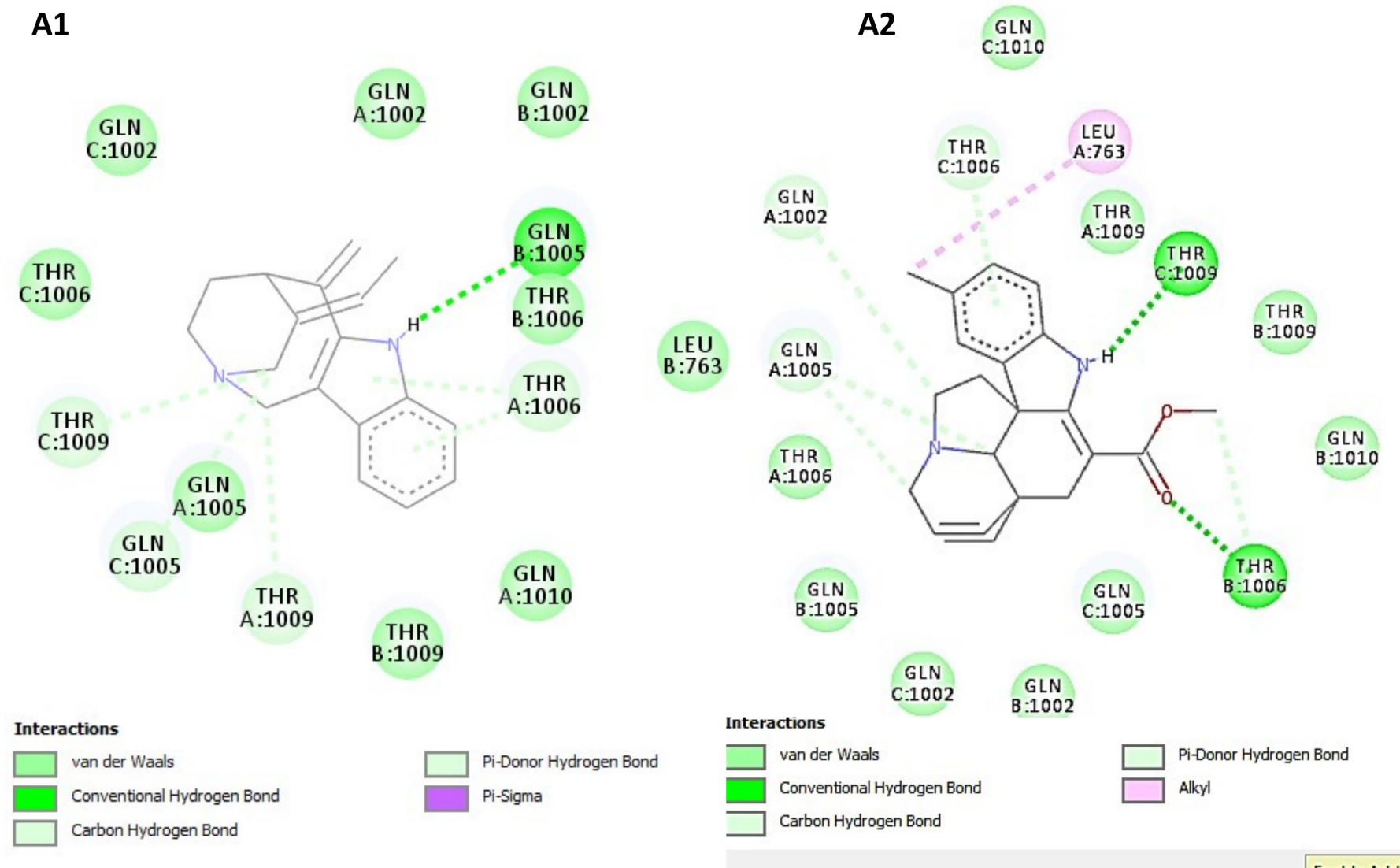


Fig. 5 (a): ‘Two-dimensional’ representation of SARS-CoV2 proteins residues forming hydrogen bonds (labelled bold) during interaction with atoms of phytochemicals A) spike ectodomain protein with 1) Appiricine 2) 12-Chlorotabersonine

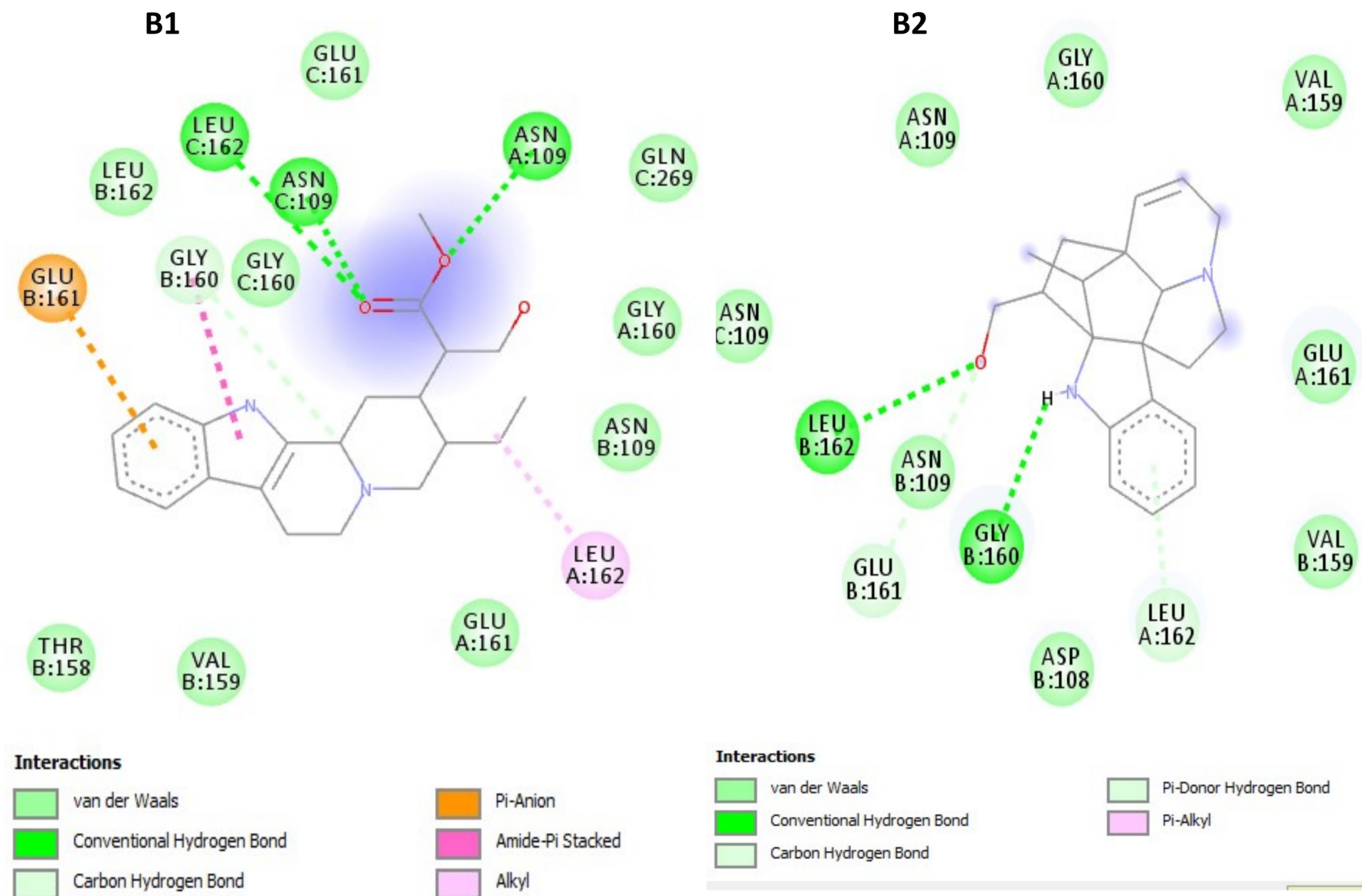


Fig. 5 (b): ‘Two-dimensional’ representation of SARS-CoV2 proteins residues forming hydrogen bonds (labelled bold) during interaction with atoms of phytochemicals B) papain-like protease protein with 1) AC1NSULH 2) Vindolinol

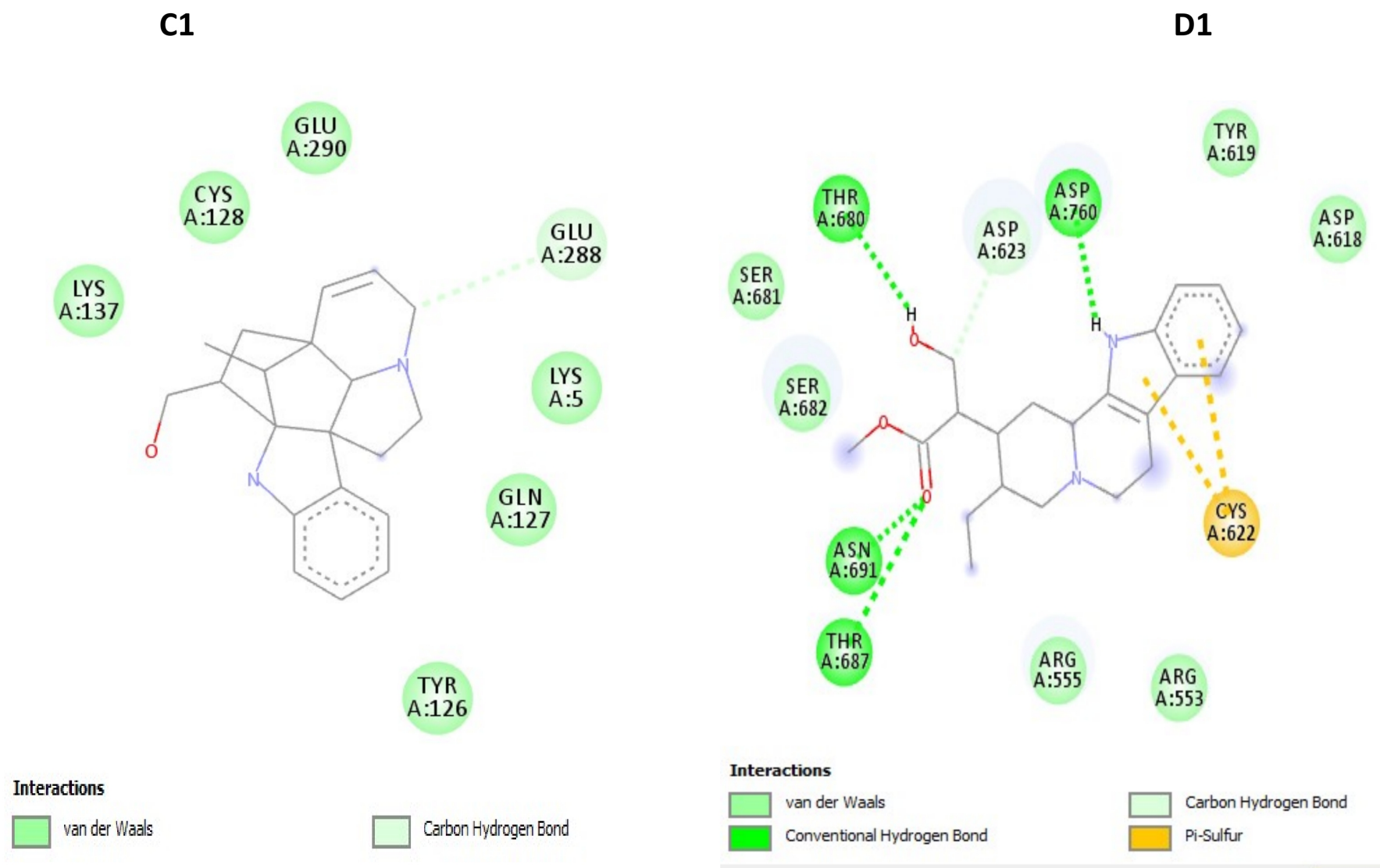


Fig. 5 (c): ‘Two-dimensional’ representation of SARS-CoV2 proteins residues forming hydrogen bonds (labelled bold) during interaction with atoms of phytochemicals C) main protease protein with 1) Vindolinol and D) RNA-dependent RNA polymerase 1) AC1NSULH

