



**Figure S1.** Non-covalent interactions among the GWS ligand and amino acid residues from the active site of SARS-CoV-2 M<sup>pro</sup>. **(A)** Interactions of the co-crystallized ligand. **(B)** Interactions after redocking with Smina and the flexible docking approach **(B)**. Hydrogen bonds are represented by dashed green lines together with the estimated length in Angstroms (Å). Other non-covalent interactions are represented with red arches.