Identification of and Mechanistic Insights into SARS-CoV-2 Main Protease Non-Covalent Inhibitors: An In-Silico Study

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Table S1. ZINC IDs of the 593 hit compounds and their respective score values (kcal/mol) of the top-ranked docking pose (see the file Table_S1.xlsx).

Table S2. Predicted parameters of Lipinski's rule of five (Ro5) and ADMET for the 78 potential candidate compounds (PCCs) and the reference compound ML188 (see the file Table_S2.xlsx).
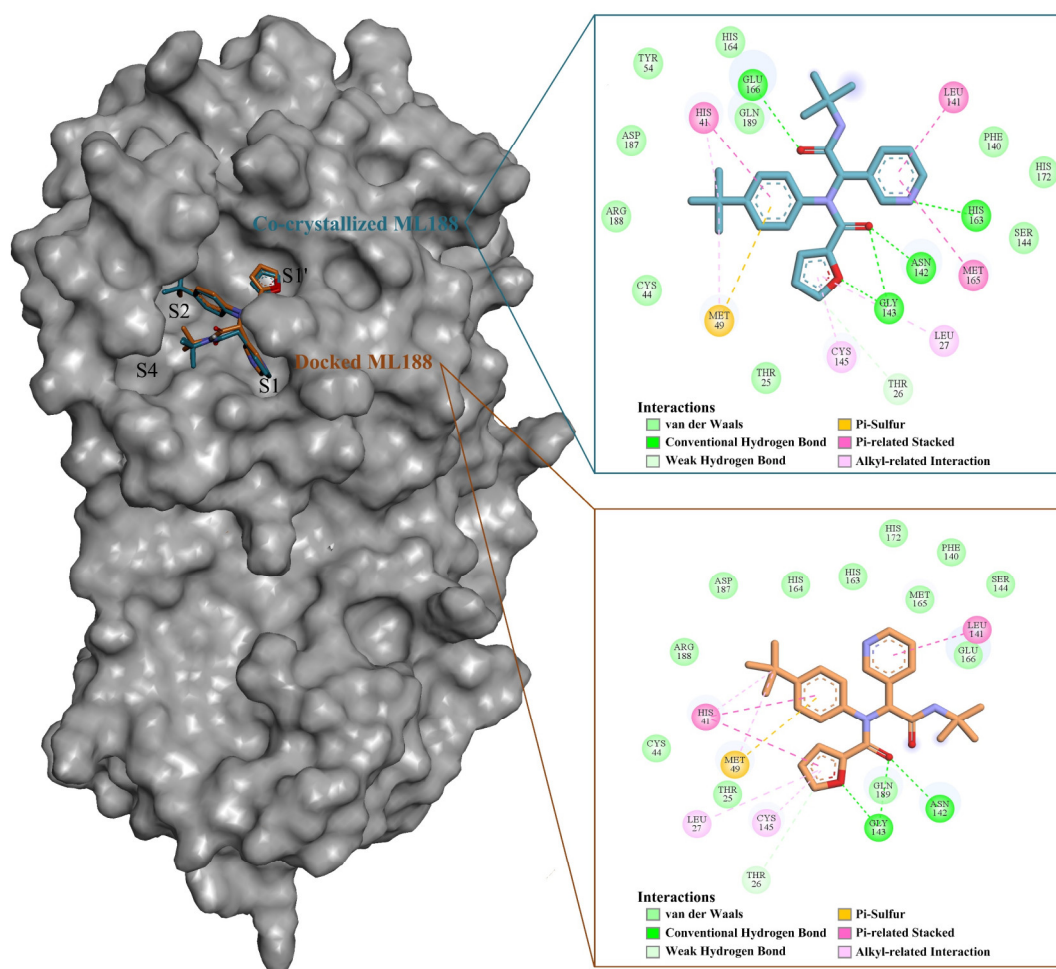
Figure S1. The co-crystallized and docked ML188 within the substrate-binding cavity of the SARS-CoV-2 Mpro. The two enlarged panels show the 2D representations of the binding modes of the co-crystallized ML188 (in dark cyan) and docked ML188 (in orange) with Mpro residues, respectively.
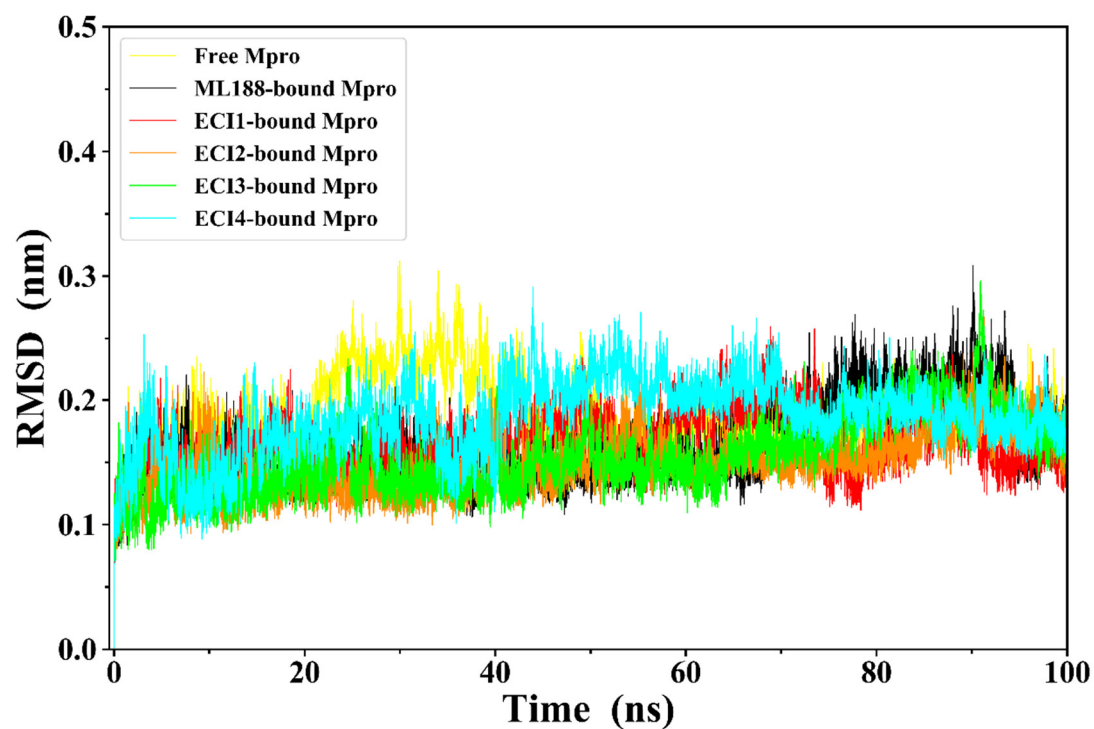
Figure S2. Time-dependent C_α root mean square deviation (RMSD) values of the free Mpro (without ligand) and the ligand-bound Mpro with respect to their respective starting structures during the 100-ns MD simulation.

File S1. Python script for constructing free energy landscapes (FELs) of the reference complex Mpro-ML188 and the three effective complexes Mpro-ECI2, Mpro-ECI3, and Mpro-ECI4 (see the file File_S1.py).