Table S1. List of CoV protease structures in the homology analysis.

| Protein                                | Group | Pdb ID  | Ligand       |
|----------------------------------------|-------|---------|--------------|
| SARS-CoV-2 main protease               | beta  | 7RFW    | PF-07311332  |
| SARS-CoV-2 main protease               | beta  | 6LU7    | PRD_002214   |
| SARS-CoV-1 main protease               | beta  | 2AMQ    | PRD_002214   |
| MERS-CoV                               | beta  | 4RSP    | PRD_002174   |
| MHV (Murine hepatitis virus)           | beta  | 6JIJ    | PRD_002214   |
| HKU1                                   | beta  | 3D23    | PRD_002214   |
| HKU4 (Tylonycteris bat coronavirus)    | beta  | 4YOG    | 4F5          |
| 229E                                   | alpha | 2ZU2    | apo          |
| PEDV (Porcine epidemic diarrhea virus) | alpha | 5GWZ    | PRD_002214   |
| FIPV (Feline infectious peritonitis virus) | alpha | 5EU8    | PRD_002214   |
| NL63                                   | alpha | 5GWY    | PRD_002214   |
| IBV (infectious bronchitis virus)      | gamma | 2Q6F    | PRD_002214   |