

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