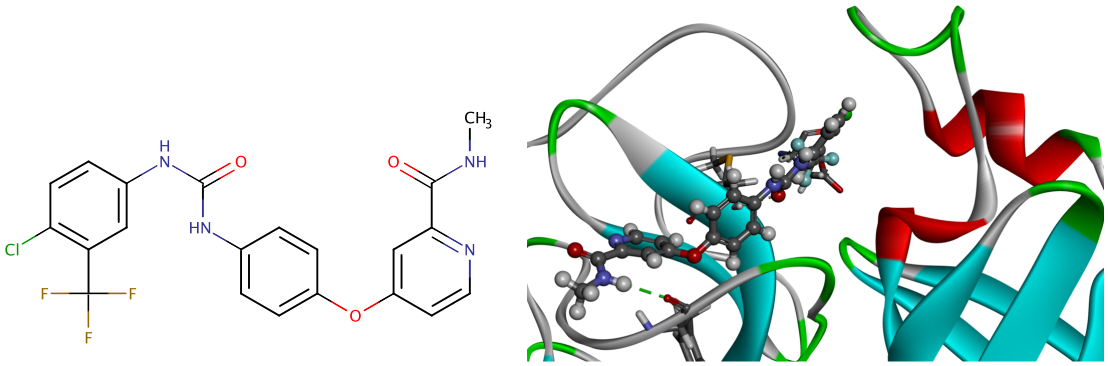
Supplementary Materials
Potentially highly potent drugs for 2019-nCoV

Duc Duy Nguyen[1], Kaifu Gao[1], Jiahui Chen[1], Rui Wang[1], and Guo-Wei Wei[1,2,3] *
[1] Department of Mathematics, Michigan State University, MI 48824, USA
[2] Department of Biochemistry and Molecular Biology
Michigan State University, MI 48824, USA
[3] Department of Electrical and Computer Engineering
Michigan State University, MI 48824, USA

Contents

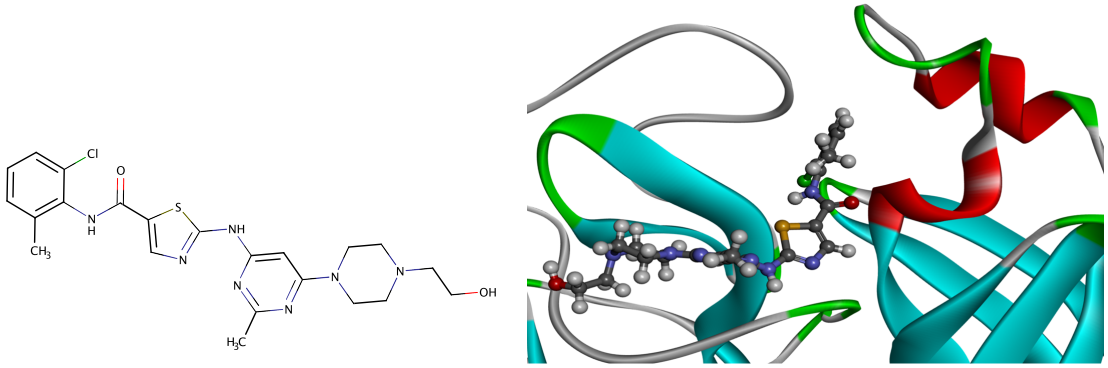
*Address correspondences to Guo-Wei Wei. E-mail:wei@math.msu.edu

S1 Supplementary Figures



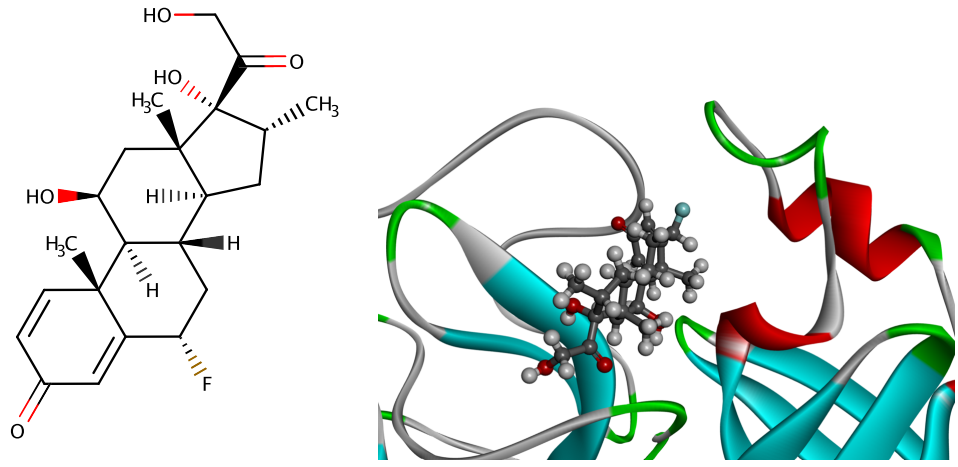
(a) Sorafenib, -10.01 kcal/mol (b) 2019-nCoV protease and Sorafenib complex

Figure 1: Sorafenib and its complex with 2019-nCoV protease.



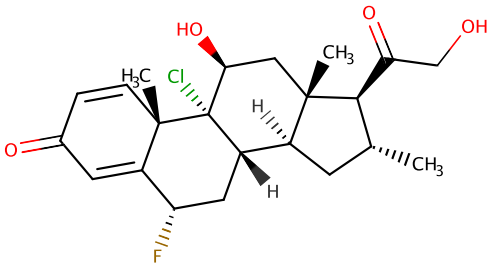
(a) Dasatinib, -9.87 kcal/mol (b) 2019-nCoV protease and Dasatinib complex

Figure 2: Dasatinib and its complex with 2019-nCoV protease.

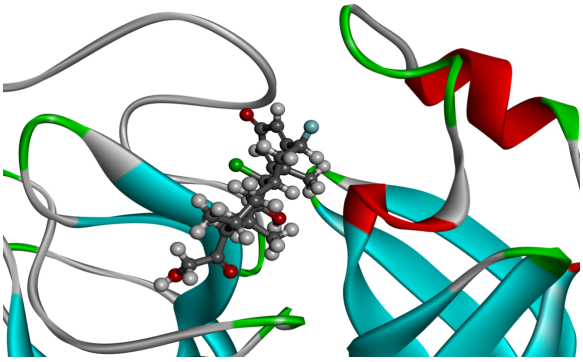


(a) Paramethasone, -9.71 kcal/mol (b) 2019-nCoV protease and Paramethasone complex

Figure 3: Paramethasone and its complex with 2019-nCoV protease.

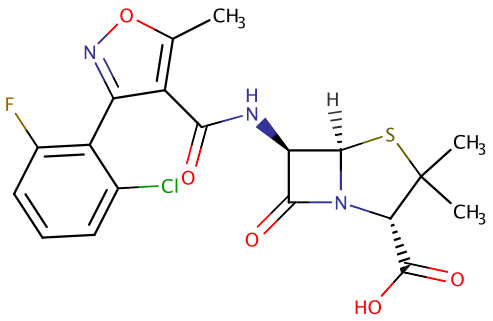


(a) Clocortolone, -9.58 kcal/mol

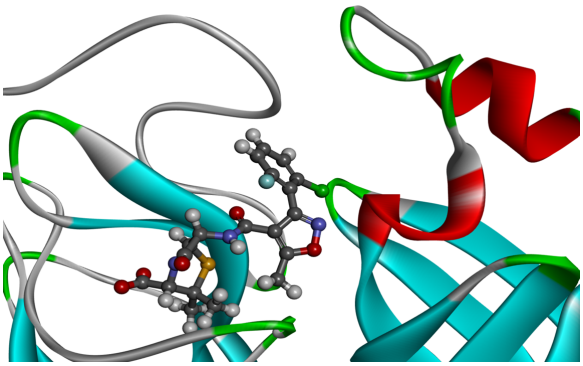


(b) 2019-nCoV protease and Clocortolone complex

Figure 4: Clocortolone and its complex with 2019-nCoV protease.

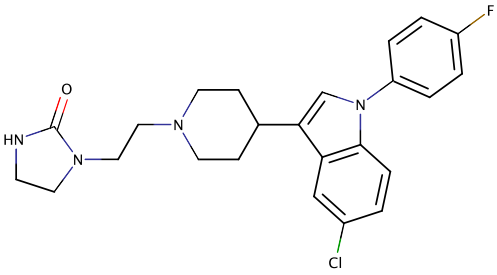


(a) Flucloxacillin, -9.57 kcal/mol

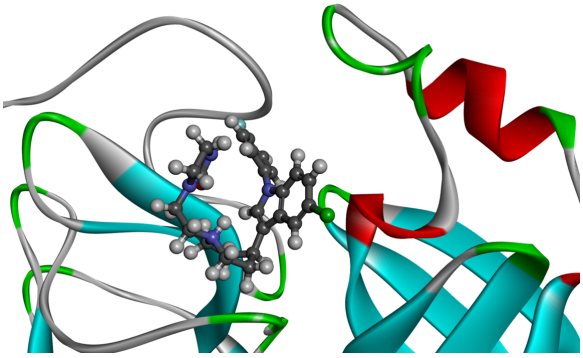


(b) 2019-nCoV protease and Flucloxacillin complex

Figure 5: Flucloxacillin and its complex with 2019-nCoV protease.

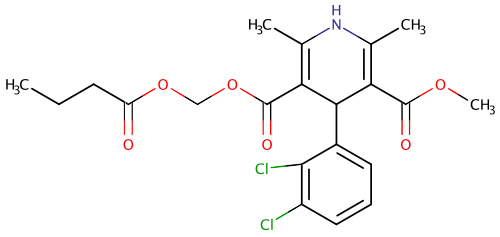


(a) Sertindole, -9.54 kcal/mol

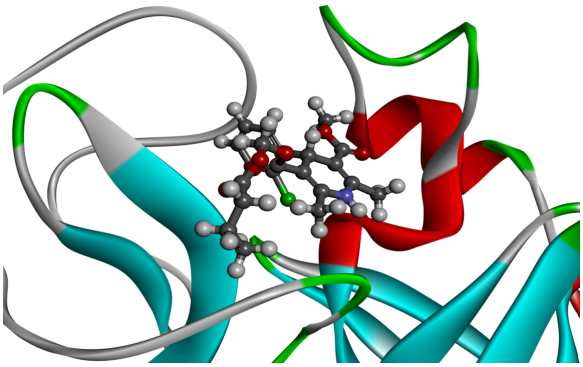


(b) 2019-nCoV protease and Sertindole complex

Figure 6: Sertindole and its complex with 2019-nCoV protease.

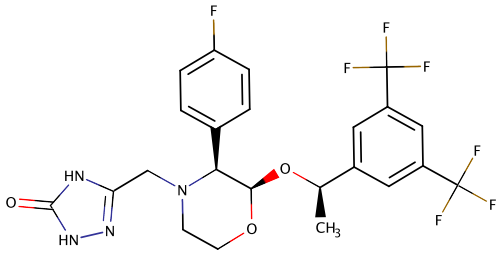


(a) Clevidipine, -9.52 kcal/mol

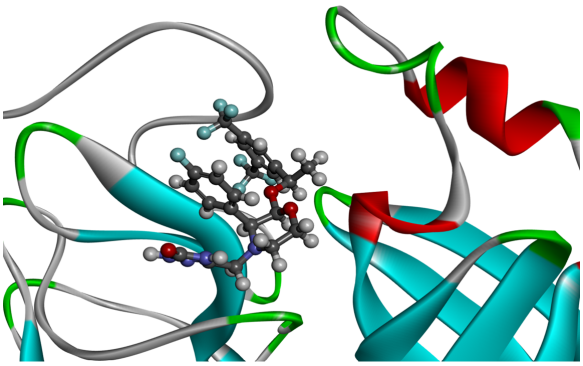


(b) 2019-nCoV protease and Clevidipine complex

Figure 7: Clevidipine and its complex with 2019-nCoV protease.

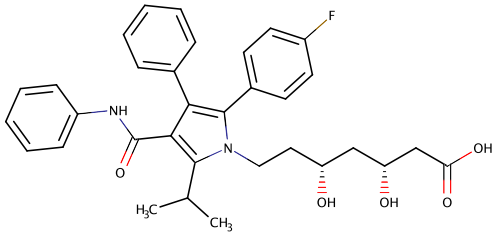


(a) Aprepitant, -9.49 kcal/mol

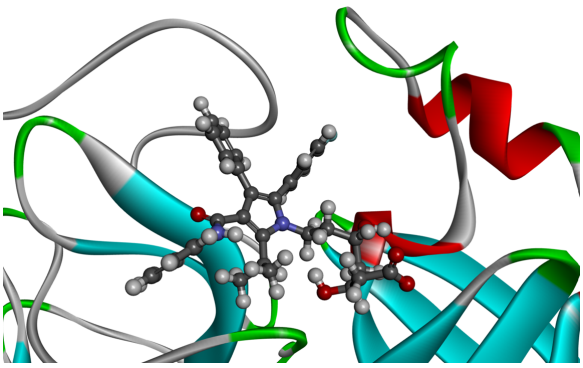


(b) 2019-nCoV protease and Aprepitant complex

Figure 8: Aprepitant and its complex with 2019-nCoV protease.

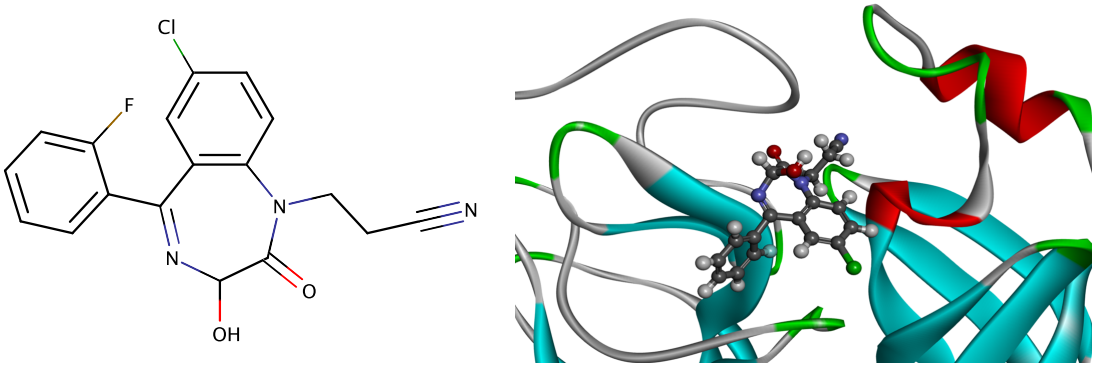


(a) Atorvastatin, -9.49 kcal/mol



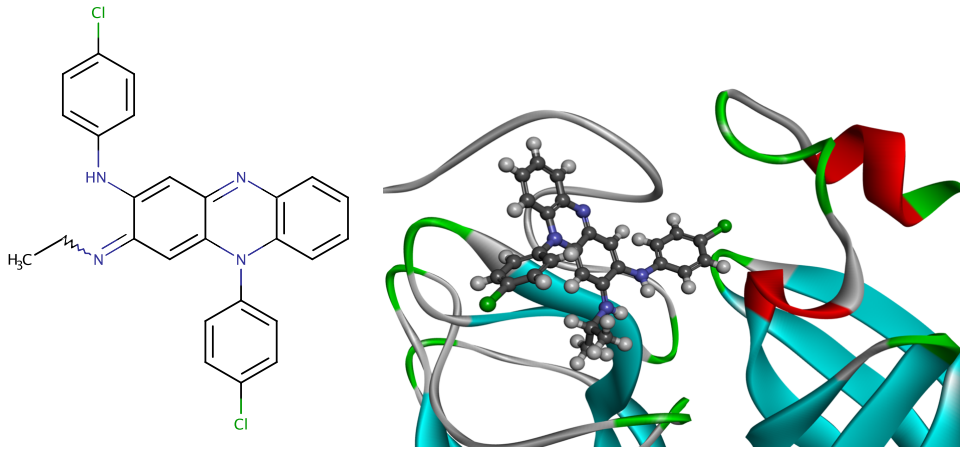
(b) 2019-nCoV protease and Atorvastatin complex

Figure 9: Atorvastatin and its complex with 2019-nCoV protease.



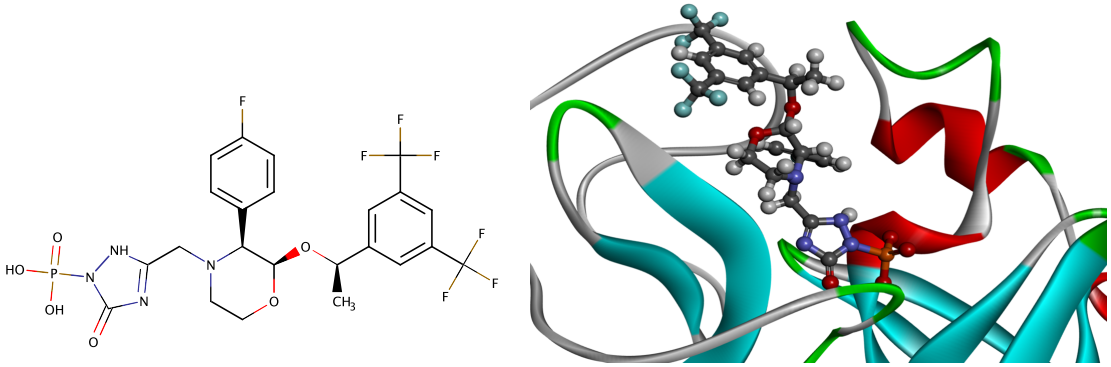
(a) Cinolazepam, -9.47 kcal/mol (b) 2019-nCoV protease and Cinolazepam complex

Figure 10: Cinolazepam and its complex with 2019-nCoV protease.



(a) Clofazimine, -9.43 kcal/mol (b) 2019-nCoV protease and Clofazimine complex

Figure 11: Clofazimine and its complex with 2019-nCoV protease.



(a) Fosaprepitant, -9.39 kcal/mol (b) 2019-nCoV protease and Fosaprepitant complex

Figure 12: Fosaprepitant and its complex with 2019-nCoV protease.

Figures 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 display top 4 to 15 molecules predicted by our 3D models. Their predicted binding affinities are given, together with their complexes with 2019-nCoV protease. These compounds are ranked according to their binding affinity values predicted by the consensus of 3DALL and 3DMT.

S2 Supplementary Data Guide

Supplementary data are given in TableS1.csv, TableS2.csv, TableS3.csv, FileS2.zip, and FileS1.zip.

S2.0.0.1 TableS1.csv Table of the experimental IC50 of 84 SARS-CoV inhibitors.

S2.0.0.2 TableS2.csv Table of predicted binding affinities of 1445 FDA-approved drugs and 2019-nCoV protease.

S2.0.0.3 TableS3.csv Table of PDBID and experimental affinities of 15,843 complexes in PDBbind v2018 general set.

S2.0.0.4 FileS1.zip 3D structures of 84 complexes of SARS-CoV protease inhibitors and 2019-nCoV protease.

S2.0.0.5 FileS2.zip 3D structures of 1445 complexes of FDA-approved drugs and 2019-nCoV protease.

S2.0.0.6 Software Codes for our deep learning models will be made available to ensure the full reproducibility of the present results.