

Supplementary Information for

Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2

Mohammad M. Ghahremanpour,[†] Julian Tirado-Rives,[†] Maya Deshmukh,[‡] Joseph A. Ippolito,^{†‡} Chun-Hui Zhang,[†] Israel Cabeza de Vaca,[†] Maria-Elena Liosi,[†] Karen S. Anderson,^{‡,#,*} and William L. Jorgensen^{†,*}

[†]Department of Chemistry, Yale University, New Haven, Connecticut 06520-8107,

[‡]Department of Pharmacology, Yale University School of Medicine, New Haven, CT 06520-

8066, and [#]Department of Molecular Biophysics and Biochemistry, Yale University School of Medicine, New Haven, CT 06520-8066

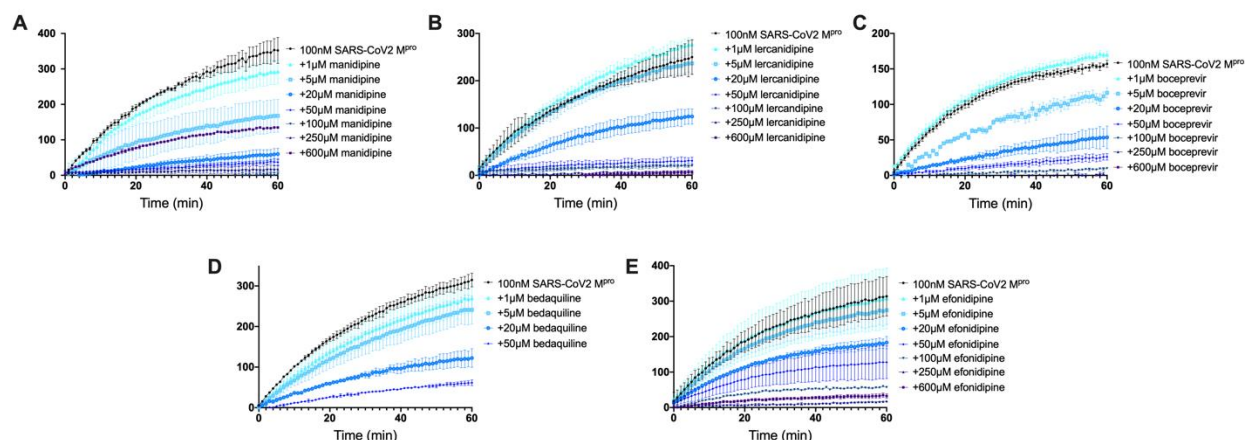
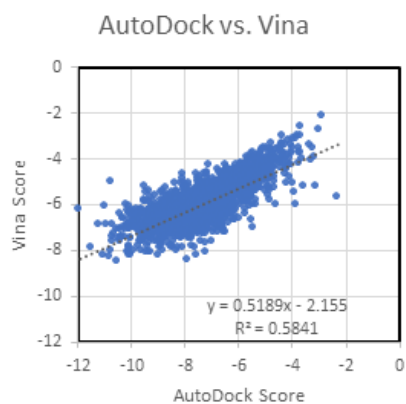
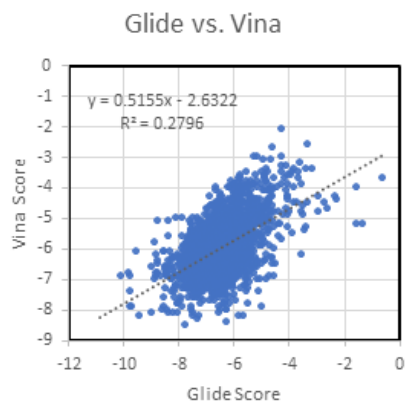
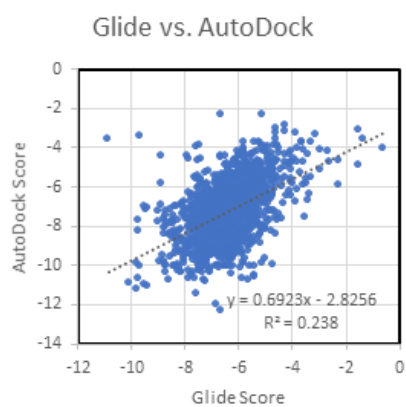


Figure S1. Kinetic data measuring activity of SARS-CoV2 M^{Pro} in the presence of A) manidipine, B) lercanidipine, C) boceprevir, D) bedaquiline, and E) efonidipine. All measurements were performed in triplicate, averaged, and plotted with standard deviation. Kinetic data for inhibition of M^{Pro} by bedaquiline was collected at concentrations up to 50 μ M due to solubility issues.

All Compounds



Consensus

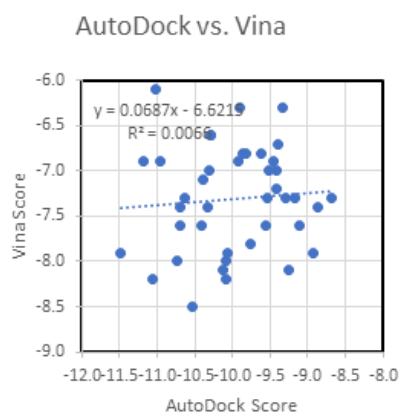
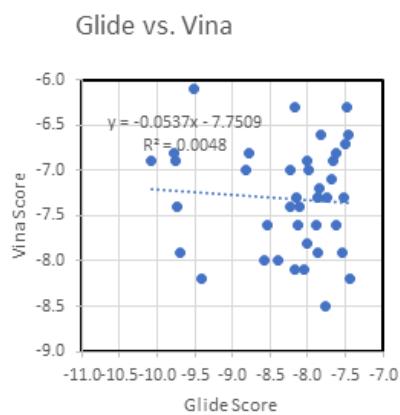
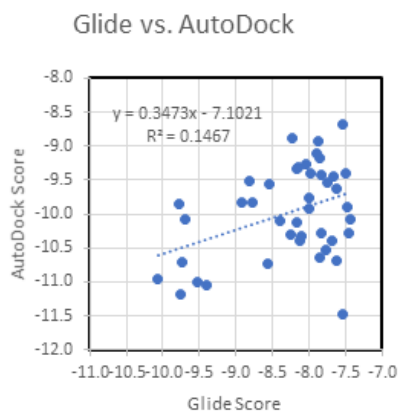


Figure S2. Correlation of docking scores for all drugs (left) and for the 42 consensus compounds (right).