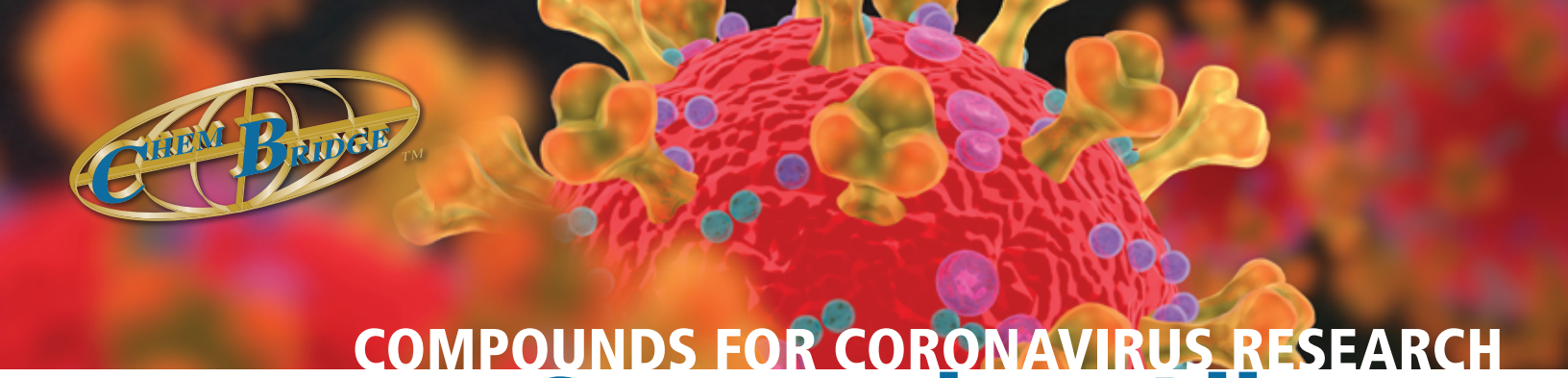


COMPOUNDS FOR CORONAVIRUS RESEARCH

# Coronavirus Library

## Highlights

- Generated in collaboration with a leading academic group
- High quality, PAINS free, lead-like and drug-like, small molecule compounds
- For SARS-CoV-2 and other coronavirus research
- Custom select from more than 14,000 compounds covering 17 targets

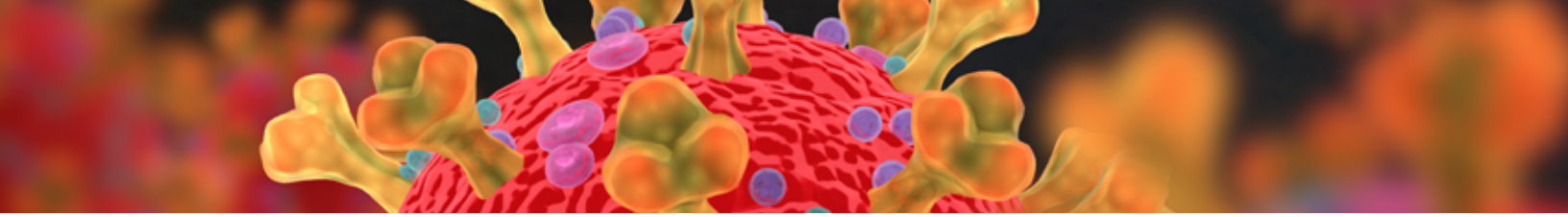
## Introduction

The ChemBridge® Coronavirus Library offers more than 14,000 compounds with potential to interact with SARS-CoV-2 viral targets or the host target ACE2. Compounds in the Coronavirus Library were selected in collaboration with the Wagner Lab at Harvard using the Virtual Flow methodology developed and published by the Wagner Lab. Details on the Virtual Flow methodology are published in Gorgulla, C., Boeszoermenyi, A., Wang, Z. et al. "An open-source drug discovery platform enables ultra-large virtual screens" Nature 580, 663–668 (2020).

## Methodology

ChemBridge's stock of more than 1.3 million compounds were prepared and docked against each of 40 different target sites on 17 different potential viral and host targets using the Virtual Flow screening platform. Top ranked compounds were further filtered to ensure that the Coronavirus Library included only high quality, lead-like or drug-like compounds free of undesirable chemical functionalities and free of PAINS structural alerts. The compound count per target ranges from 1,000 to 5,000 with 1,000 to 2,000 compounds per site screened.

Structures from ChemBridge stock were prepared with VirtualFlow for Ligand Preparation (VFLP)[1]. For each virtual screen a single target structure was used, and the protein was held rigid. QuickVina-W[2] was used to perform a blind docking procedure for the HR1 domain of the spike protein, the RNA binding interface of the nucleoprotein, the RNA binding site of nsp12, as well as for nsp7 and ORF7a. For all the other site specific docking routines, QuickVina 2[3] was used. Both docking programs are based on AutoDock Vina[4]. The receptor structures were prepared with AutoDockTools[5] from the PDB format to the PDBQT format. The proteins targeted are listed on the on the reverse.



## Targets

| Protein | Alternname Name(s) | Site(s) Docked |
|---|---|---|
| Spike | S-protein | Spike RBD–ACE2 interface, HR1 domain |
| TMPRSS2 | Transmembrane protease serine 2 | Active site |
| ORF7a | Protein 7a | Blind docking |
| Phosphatase | (macro) X domain | Closed active site, open active site |
| PLpro | Papain-like protease | Active site, accessory pocket, DUB binding site |
| Mpro | Main protease | Active site, dimerization site, alpha-helix 5 attachment site |
| nsp7 | Replicase polyprotein 1ab | Blind docking of nsp8 and nsp12 binding interfaces |
| nsp8 | Primase complex | nsp7 binding interface, nsp12 binding interface |
| nsp9 | Replicase | Dimerization interface |
| nsp10 | N/A | nsp14 binding interface, nsp16 binding interface |
| nsp12 | RNA dependent RNA-polymerase | RNA binding interface, nucleotide binding site, nsp8 binding interface, nsp7 binding interface |
| nsp13 | Helicase | RNA binding interface, active site |
| nsp14 | Exoribonuclease or N7 methyltransferase | nsp10 binding interface, ExoN active site, N7-MT active site |
| nsp15 | Endoribonuclease | Active site |
| nsp16 | 2′-O methyltransferase | 2′-O MT active site, nsp10 binding interface |
| Nucleoprotein | Ribonucleocapsid protein | NTD RNA binding site, NTD oligomerization site, CTD dimerization interface, CTD oligomerization site |
| ACE2 | Angiotensin-converting enzyme 2 | Spike RBD binding region, dynamic pocket 1 near spike RBD, dynamic pocket 2 near spike RBD |

## Format

- Custom select from more than 14,000 Coronavirus Library compounds
- Available in 384-well and 96-well formats including 384-well acoustic qualified plates
- Amounts as low as 0.25 micromole (25ul of 10mM DMSO solution) available
- Available as DMSO solutions or dry in micromole or mg amounts

## Structure File

For a file of structures, please email **sales@chembridge.com**


**References**

1. Gorgulla C et al. An open-source drug discovery platform enables ultra-large virtual screens. Nature 2020 580, 663–668.

2. Hassan NM et al. Protein-Ligand Blind Docking Using QuickVina-W With Inter-Process Spatio-Temporal Integration. Nature Sci. Reports 2017 7(1), 15451

3. Alhossary A et al. Fast, Accurate, and Reliable Molecular Docking with QuickVina 2. Bioinformatics 2015 31(13), 2214-2216.

4. Trott O. et al. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, J Computational Chem 2010 31, 455-461.

5. Morris GM et al. Autodock4 and AutoDockTools4: automated docking with selective receptor flexibility. J Computational Chem 2009 16, 2785-91.



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