Coronavirus Screening Tools

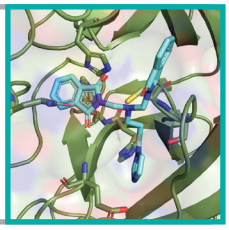
Cayman has developed a SARS-CoV-2 Screening Library in which over 70,000 unique drugs and small molecules have been screened *in silico* for binding to SARS-CoV-2 targets including the spike glycoprotein, proteases, and non-structural proteins (nsps), and human angiotensin-converting enzyme 2 (ACE2). These are available as both a data pack and a library of the chemical entities in a 96-well format.

- Cayman's unique set of compounds
- FDA-approved drugs
- Diverse commercial compounds

Virtual screening against SARS-CoV-2 targets

Hit selection criteria:

- Docking scores
- Intermolecular hydrogen bonds within the amino acid residues of the binding pockets



Library Data Package

Parameter	HTS02812	JFD03677
GlideScore/Glide Emodel	-9.38/-85.955	-9.60/-98.831
MW	369.463	452.509
Number of H Donors	3	4
Number of H Acceptors	7.4	6
PSA	82.08	97.04
ClogS	-2.18	-5.376
ClogPo/w	2.57	4.867
ClogBB	-0.56	-1.69
ClogHERG	-6.29	-7.64

Docking score units are in kcal/mol.

Library Preparation

- Can be customized to your selected compounds/targets
- Supplied in a 96-well Matrix™ format

Hit-to-Lead and Lead Optimization Services

- *In vitro*/*In vivo* Screening
- SBDD/MedChem

SARS-CoV-2 Screening Library

Item No. 9003509

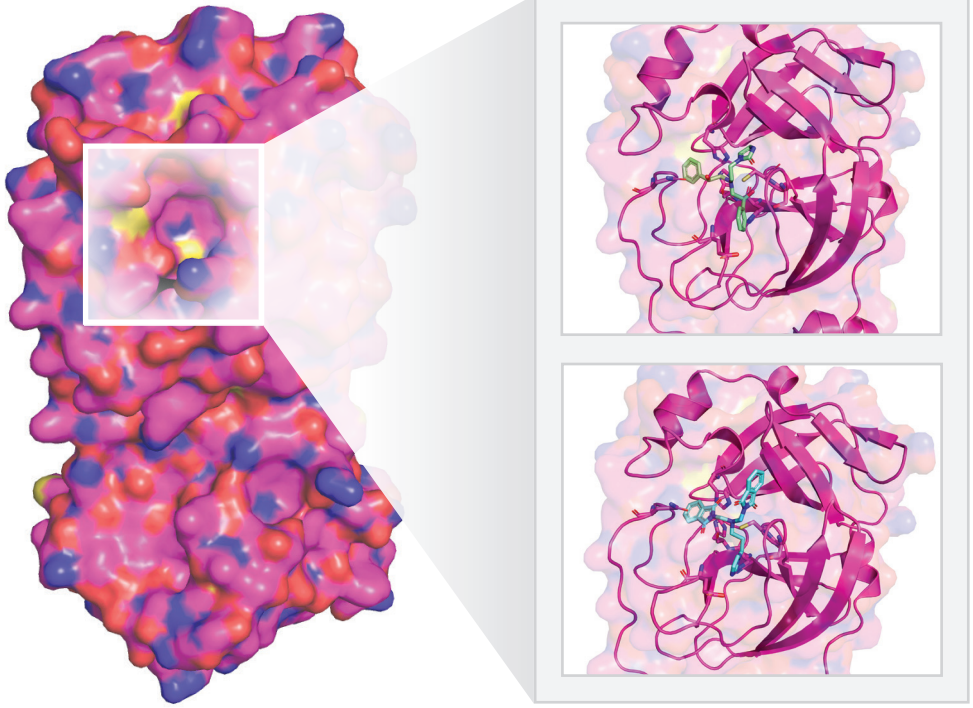
The SARS-CoV-2 Screening Library is a custom, made-to-order library that features a diverse set of FDA-approved and drug-like compounds identified from *in silico* modeling using Maestro (Schrödinger Suite) software. Choose from the entire library of 2,000+ compounds or a custom built library to your preferred target and specifications. The data package for all SARS-CoV-2 targets is also available. SARS-CoV-2 targets include:

- Main protease (M^{pro}), also known as 3C-like protease ($3CL^{pro}$; nsp5)
- Spike glycoprotein
- ACE2 (human)
- RNA-dependent RNA polymerase (RdRp; nsp12)
- Endoribonuclease (nsp15)
- Guanine-N7 methyltransferase (Guanine-N7 MTase; nsp14)
- Exoribonuclease domain (ExoN domain; nsp14)
- Papain-like protease (PL^{pro}; nsp3)
- ADP-ribose phosphatase (ADRP; nsp3)
- Nucleocapsid protein

SARS-CoV-2 Library Data Package

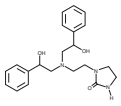
The SARS-CoV-2 Library Data Package includes compound characteristics, docking scores (per target), and predicted physicochemical properties for ten SARS-CoV-2 targets. It is available for purchase, and the cost can be applied towards your next screening, lead optimization, or compound synthesis project with Cayman.

Sample Data:

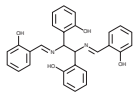


M^{pro} (PDB ID 6LU7)

Key Residues in M^{pro} SARS-CoV-2: His41 motif, His163-Glu166 motif, and catalytic Cys145



HTS02812



JFD03677

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To learn more about our Medicinal Chemistry & Structural Biology services, visit **www.caymanchem.com/medchem**