## D3Targets-2019-nCoV manual

This manual will help you become familiar with the basic operation procedures and precautions of D3Targets-2019-nCoV as soon as possible.

## 1. Registration and login

If this is your first time to use D3Targets-2019-nCoV, please register your account and log in to protect your files, or your results will be visible to other users.

Note: Asterisk (\*) indicates required fields.

REGISTER		
Username:		*
Your first name:		*
Your middle name:		
Your last name:		*
Your Title:		*
(e.g. Dr., Mr., Mrs., Prof.)		
Research Advisor's Title:		
Laboratory/University Web Address: (For example: www.dddc.ac.cn)		
Department:		
Name of Institute/University:		
(no abbreviations, please)		,
Address:		
Country:		*
E-mail address:		*
Re-enter E-mail address		*
Password:		*
Re-enter password:		*
	I HAVE READ AND A CONDITIONS FOR D accept	THE LICENCE TERMS AND
SIGN IN		
Username:		
Password:		
signin		

## 2. Submit Job

Example: remdsivir-meta.sdf (The drug's SDF file can be downloaded from "Sample File 1" in step 2 of the web page.)

Step1: To set job title

Edit the name of the job.



Step2: To upload ligand file (.sdf or .mol2)

The input small molecule file should be in sdf or mol2 format. Please note that we strongly recommend the users submitting 3D chemical structure, especially for the compounds with at least one chiral center.



Step3: To select proteins

There are two ways to select proteins.

Method 1: For selecting specific targets, enter the target names, protein ID or PDB ID into the search box. Then click the "Select" button, your selected will be uploaded into the table as shown below, provided that your interested target proteins are collected in our database.

Step 3. To select proteins									
Target Name:	spike		(Format: target1; ta	(Format: target1; target2; e.g. ORF1ab; Spike)					
Protein ID:			(Format: Protein_id	(Format: Protein_id1; Protein_id2;)					
Template PDB I	D:		(Format: PDB_ID1; I	(Format: PDB_ID1; PDB_ID2;)					
All Select Clear									
There are 2 targets selected. <u>hide</u>									
<b></b> all Ta	arget_Full_Name	Protein_Id		Template PDB_ID					
<b>✓</b> Sp	oike proteinClose	QHD43416.1		5x58					
<b>⊘</b> Sp	pike proteinOpen	QHD43416.1		5x5b					

Method 2: For selecting all the target proteins in our database, click the "All" or "Select" button to select all protein targets as shown in the table below.

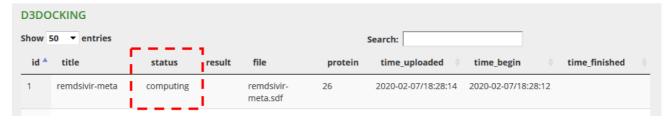
After the selection is completed, click the "Submit" button to submit the job.

Step 3. To select proteins							
Target Name: (Format: target1; target2; e.g. O Protein ID: (Format: Protein_id1; Protein_id2; Template PDB ID: (Format: PDB_ID1; PDB_ID2;)  All Select Clear There are 26 targets selected, hide							
<b></b> all	Target_Full_Name	Protein_Id Te	emplate PDB_ID				
•	Transmembrane protease serine 2	AAD37117.1					
•	Cathepsin L	AAN87068.1 1c	:58				
•	Angiotensin converting enzyme 2	AAT45083.1 6a	acg				
•	ORF1ab 5325-5925 HelicaseDimer	QHD43415.1 6jy	yt				
•	ORF1ab polyprotein 1-180 Host translation inhibitor nsp1	QHD43415.1 2h	nsx				
•	ORF1ab polyprotein 819-2763 Papain-like proteinase Monomer	QHD43415.1 3e	99s				
•	ORF1ab polyprotein 3264-3569 3C-like proteinase Dimer	QHD43415.1 2z	·9j				
•	ORF1ab polyprotein 3264-3569 3C-like proteinase Monomer	QHD43415.1 1z	:1i				
•	ORF1ab polyprotein 3860-3942 Non-structural protein 7	QHD43415.1 1y	/sy				

## 3. Result

Click the "Results" button to check the status of the job. There are three types of task status, namely "computing", "waiting" and "finished".

- Computing: The job you submitted is ongoing.
- Waiting: There are other jobs in progress before your job, and your job is in the queue waiting for calculation.
- Finished: The job you submitted has been completed.



If your task has been completed, click "result" to obtain the molecular docking results.



You can download the detailed result file from "download" in File link, which involves the scores of each pocket on each selected protein.



In the result report, you can click on the corresponding pocket under the "Pocket" header to view the corresponding position of the pocket on the protein.

