

## 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:	<input type="text"/>	*
Your first name:	<input type="text"/>	*
Your middle name:	<input type="text"/>	
Your last name:	<input type="text"/>	*
Your Title: (e.g. Dr., Mr., Mrs., Prof.)	<input type="text"/>	*
Research Advisor's Title:	<input type="text"/>	
Laboratory/University Web Address: (For example: www.dddc.ac.cn)	<input type="text"/>	
Department:	<input type="text"/>	
Name of Institute/University: (no abbreviations, please)	<input type="text"/>	*
Address:	<input type="text"/>	
Country:	<input type="text"/>	*
E-mail address:	<input type="text"/>	*
Re-enter E-mail address	<input type="text"/>	*
Password:	<input type="text"/>	*
Re-enter password:	<input type="text"/>	*

I HAVE READ AND ACCEPT THE LICENCE TERMS AND CONDITIONS FOR DDB

#### SIGN IN

Username:	<input type="text"/>
Password:	<input type="text"/>

### 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.

## D3DOCKING

### Step 1. To set job title

Job Title:

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.

### Step 2. To upload ligand file (.sdf or .mol2)

#### Molecule File:

没有选择文件

Sample File 1

File : The three-dimensional molecular structure file(sdf file or mol2 file).

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:  (Format: target1; target2; ... e.g. ORF1ab; Spike)  
Protein ID:  (Format: Protein\_id1; Protein\_id2; ...)  
Template PDB ID:  (Format: PDB\_ID1; PDB\_ID2; ...)

There are 2 targets selected. [hide](#)

<input checked="" type="checkbox"/> all	Target_Full_Name	Protein_Id	Template PDB_ID
<input checked="" type="checkbox"/>	Spike protein--Close	QHD43416.1	5x58
<input checked="" type="checkbox"/>	Spike protein--Open	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. ORF1ab; Spike)  
Protein ID:  (Format: Protein\_id1; Protein\_id2; ...)  
Template PDB ID:  (Format: PDB\_ID1; PDB\_ID2; ...)

There are 26 targets selected. [hide](#)

<input checked="" type="checkbox"/> all	Target_Full_Name	Protein_Id	Template PDB_ID
<input checked="" type="checkbox"/>	Transmembrane protease serine 2	AAD37117.1	-
<input checked="" type="checkbox"/>	Cathepsin L	AAN87068.1	1cs8
<input checked="" type="checkbox"/>	Angiotensin converting enzyme 2	AAT45083.1	6acg
<input checked="" type="checkbox"/>	ORF1ab 5325-5925 Helicase--Dimer	QHD43415.1	6jyt
<input checked="" type="checkbox"/>	ORF1ab polyprotein 1-180 Host translation inhibitor nsp1	QHD43415.1	2hsx
<input checked="" type="checkbox"/>	ORF1ab polyprotein 819-2763 Papain-like proteinase--Monomer	QHD43415.1	3e9s
<input checked="" type="checkbox"/>	ORF1ab polyprotein 3264-3569 3C-like proteinase--Dimer	QHD43415.1	2z9j
<input checked="" type="checkbox"/>	ORF1ab polyprotein 3264-3569 3C-like proteinase--Monomer	QHD43415.1	1z1i
<input checked="" type="checkbox"/>	ORF1ab polyprotein 3860-3942 Non-structural protein 7	QHD43415.1	1ysy

### 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.

**D3DOCKING**

Show  entries Search:

id	title	status	result	file	protein	time_uploaded	time_begin	time_finished
1	remdsivir-meta	computing		remdsivir-meta.sdf	26	2020-02-07/18:28:14	2020-02-07/18:28:12	

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

**D3DOCKING**

Show  entries Search:

id	title	status	result	file	protein	time_uploaded	time_begin	time_finished
1	remdsivir-meta	finished	result	remdsivir-meta.sdf	26	2020-02-07/18:28:14	2020-02-07/18:28:12	2020-02-07/18:53:31

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

**D3DOCKING**

Job Title:  
remdsivir-meta6744

Job File:  
remdsivir-meta.sdf

File link:  
[download](#)

Score:

id	Protein_ID	score	Target_Full_Name	Pocket	Template PDB_ID
1	QHD43415.1	-10.7071562	ORF1ab polyprotein 4393-5324 RNA-directed RNA polymerase	Pocket1	6nur
2	QHD43415.1	-9.8777914	ORF1ab polyprotein 6453-6798 Uridylate-specific endoribonuclease--Monomer	Pocket1	2h85
3	QHD43415.1	-9.78340435	ORF1ab polyprotein 819-2763 Papain-like proteinase--Dimer	Pocket3	5y3e

**Results file**

**Sort protein targets by score**

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.

**D3Targets**

**D3DOCKING**

Job Title:  
remdsivir-meta6744

Job File:  
remdsivir-meta.sdf

File link:  
[download](#)

Score:

id	Protein_ID	score	Target_Full_Name	Pocket	Template PDB_ID
1	QHD43415.1	-10.7071562	ORF1ab polyprotein 4393-5324 RNA-directed RNA polymerase	Pocket1	6nur
2	QHD43415.1	-9.8777914	ORF1ab polyprotein 6453-6798 Uridylate-specific endoribonuclease--Monomer	Pocket1	2h85
3	QHD43415.1	-9.78340435	ORF1ab polyprotein 819-2763 Papain-like proteinase--Dimer	Pocket3	5y3e
4	QHD43415.1	-9.67866516	ORF1ab polyprotein 5926-6452 Guanine-N7 methyltransferase	Pocket1	5nfy
5	QHD43415.1	-9.14918137	ORF1ab polyprotein 3264-3569 3C-like proteinase--Dimer	Pocket1	2z9j

**Click to show pocket position**

