

### Project No. 3. Due date: Dec 16, Monday

This project is a protein-ligand docking experiment on the SwissDock webserver. You need to dock small molecules against the influenza virus hemagglutinin. If scientists search for new antiviral drugs against influenza, they may start with this step.

So, the target protein is 1TI8. The ligand molecules are listed below:

Name	ID Number	Project 3 ZINC code	bonus code1	bonus code 2
Mohammed A. Mustafa	209115739	ZINC03873936	ZINC03647770	ZINC03815424
Omar Feras Sabti	2111130410	ZINC19632834	ZINC03817234	ZINC03871612
Yousef Alhashemi		ZINC03871613	ZINC03871614	ZINC03823475
Abdulrhman Khalid Ali	209115499	ZINC19632891	ZINC03871615	ZINC00000135
Sarah Mohammad	208217331	ZINC00001380	ZINC19632912	ZINC03830255
Aber Almutairi	207114878	ZINC03830256	ZINC03830257	ZINC00897089
Suliman Abd Almonem	210116435	ZINC11680943	ZINC03650334	ZINC19632927
Moody Al-Hudaib	209222891	ZINC33342870	ZINC18167382	ZINC00113386
Omar Alobaid	208113395	ZINC00113378	ZINC00000070	ZINC11680943
Meriam Al-Hasawi	211221984	ZINC03650334	ZINC19632927	ZINC33342870

**For project 3:** You need to submit the best docked configuration of your ligand to 1TI8 in graphical form (screenshot is fine). You need to choose the best cluster. This is 100% if performed correctly.

**For 50% bonus points:** Dock also the bonus codes 1 and 2. Choose the best from the three ligands. (Which is the best? How do you know it?) Give the name of the best ligand with the graphical docking configuration printed.

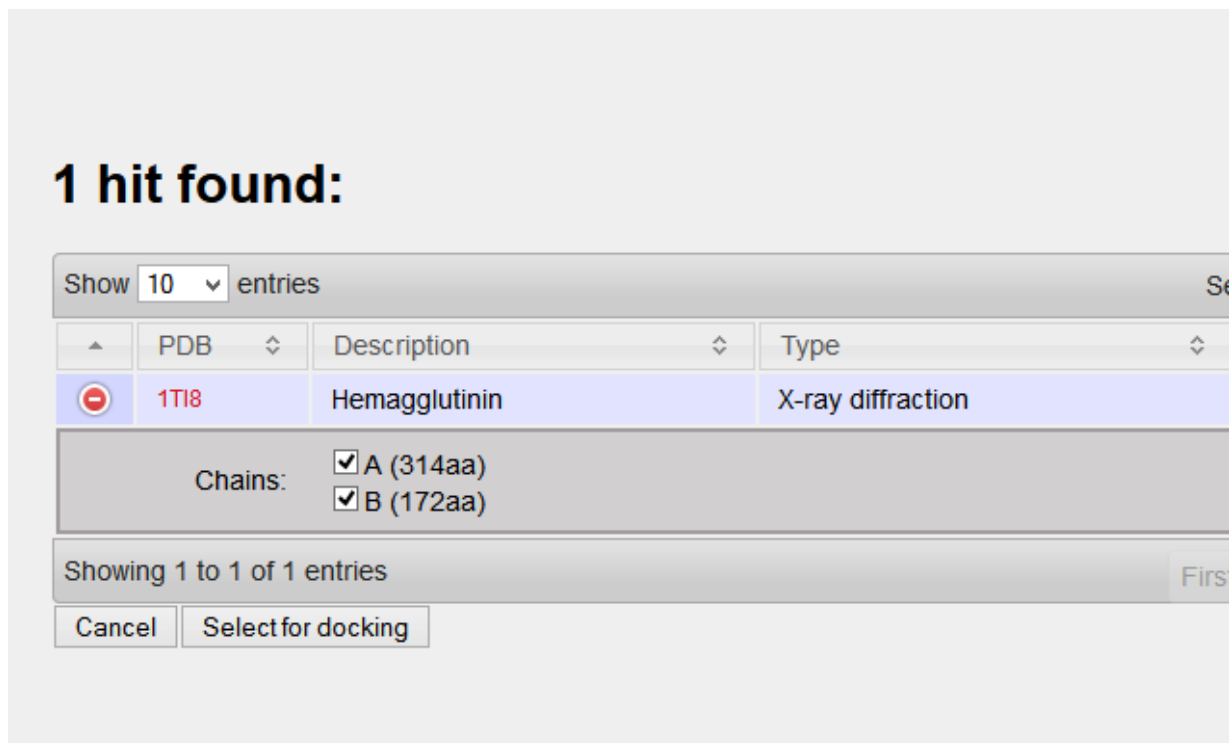
Submit the results electronically and on paper, too.

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## Guidance:

Input 1TI8 in <http://www.swissdock.ch/docking> in the field "search targets", hit search.

Choose both chains:



The screenshot displays the search results for PDB ID 1TI8. The interface shows a table with one entry, 'Hemagglutinin', which is an X-ray diffraction target. Below the table, the 'Chains' section is expanded, showing two chains: 'A (314aa)' and 'B (172aa)', both of which are selected with checkmarks. At the bottom of the interface, there are two buttons: 'Cancel' and 'Select for docking'.

**1 hit found:**

▲	PDB	Description	Type
⊖	1TI8	Hemagglutinin	X-ray diffraction

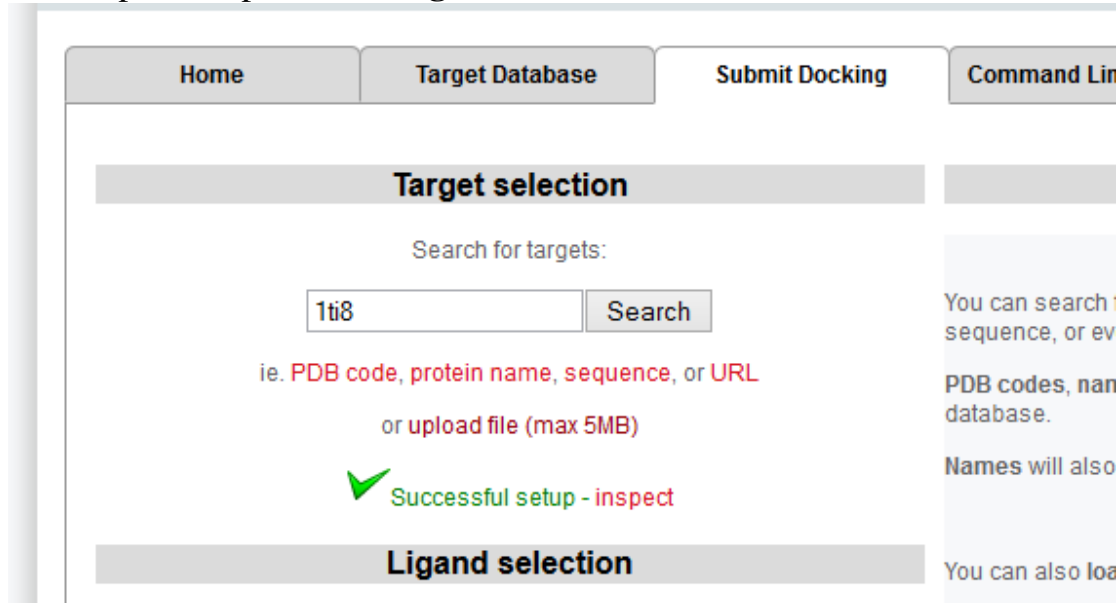
Chains:  A (314aa)  
 B (172aa)

Showing 1 to 1 of 1 entries

Cancel Select for docking

Hit "select for docking".

This step is completed **if the green checkmark is visible:**




Home Target Database Submit Docking Command Lin

### Target selection

Search for targets:

ie. PDB code, protein name, sequence, or URL

or upload file (max 5MB)

 Successful setup - inspect

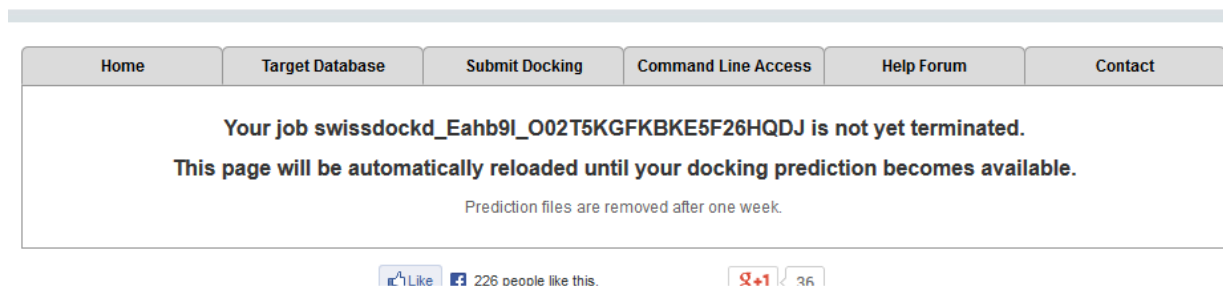
### Ligand selection

You can search for a target by PDB code, protein name, sequence, or even a URL. You can also search for a target by PDB codes, name, or database. Names will also be used to search for a target. You can also load a target from a file.

Input the ligand name. If more than one hits are present then check-mark that with your ZINC number.





Give a job name and your email address. The docking may take hours.

You probably did everything right if you see something similar:



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Your job swissdockd\_Eahb9I\_O02T5KGFKBKE5F26HQDJ is not yet terminated.  
This page will be automatically reloaded until your docking prediction becomes available.  
Prediction files are removed after one week.

 Like  226 people like this.  +1  36