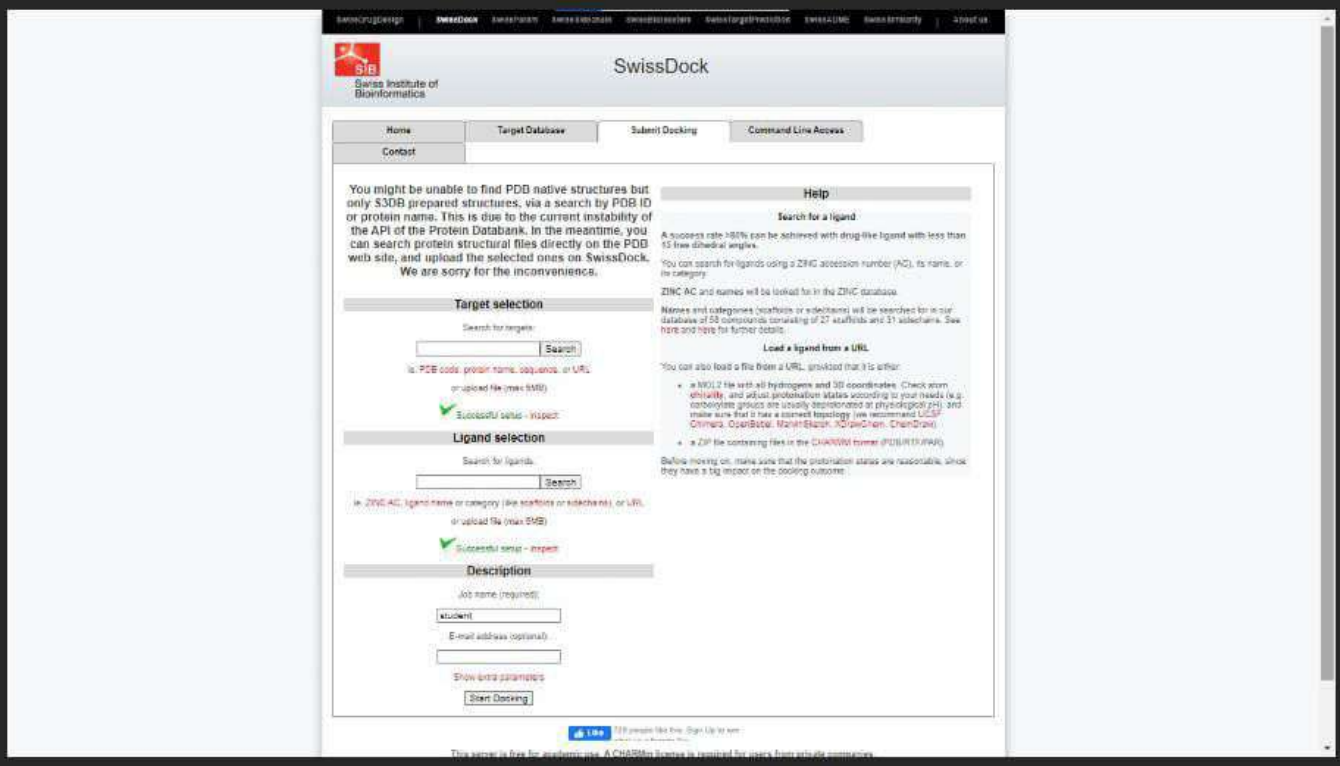

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The SwissDock team maintains a high-quality database of manually curated protein structures forming a complex with their ligands, if any.

Usage:

- **search** by target protein name or PDB code
- **start docking jobs** by clicking on the dock links
- **download structures** in PDB and CHARMM format, as well as Mol2 format for ligands

Show 10 entries Search: adenosine

Target Family name	PDB id	Details	Target	Ligand	Complex
Adenosine deaminase	1add	view	dock download	dock download	download

Showing 1 to 1 of 1 entries (filtered from 264 total entries) First Previous 1 Next Last

If you use these structures, please cite this article.

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Congratulation! When terminated, your docking results will be available here

Help us improve SwissDock by telling us more about you

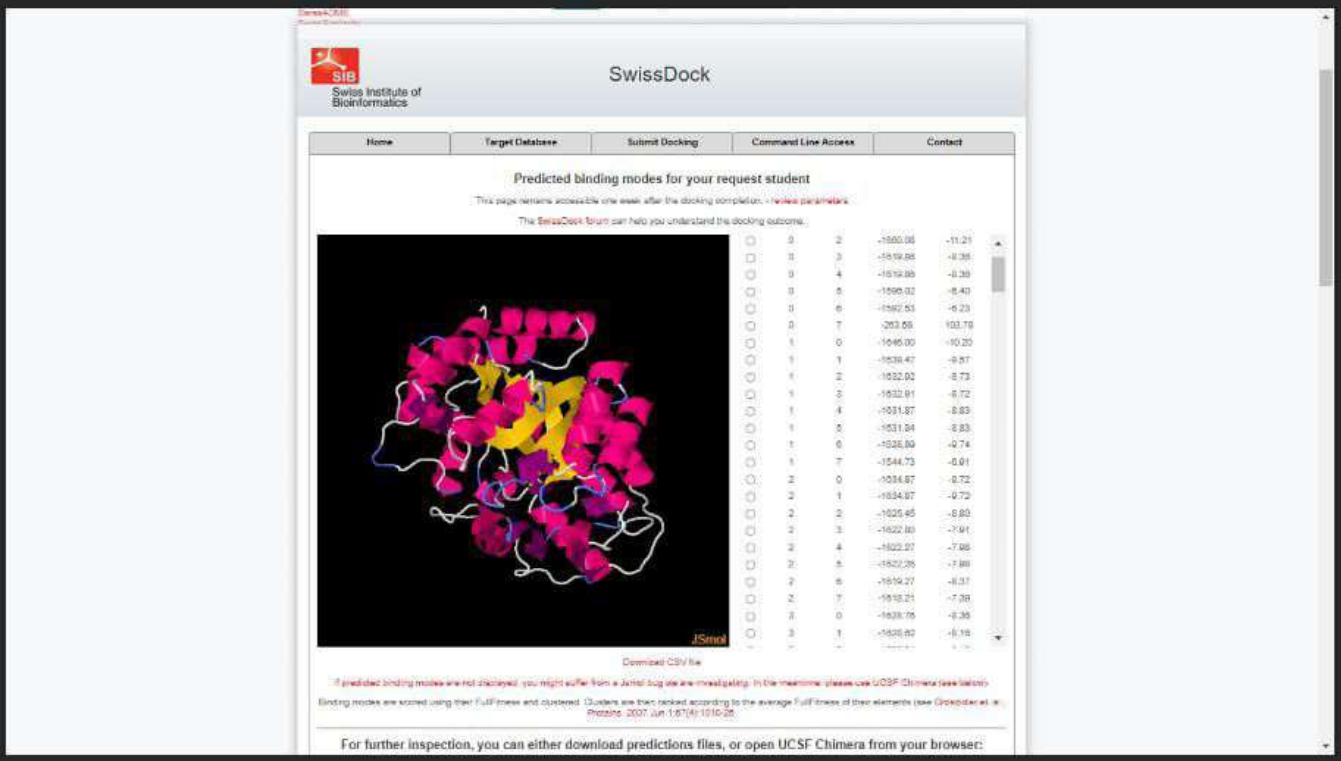
This survey is not mandatory. If you choose to answer it, please do it only once.

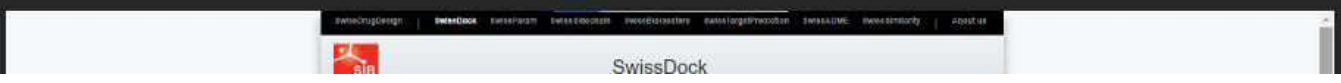
Sign in to Google to save your progress. Learn more

* Indicates required question

What is your email address? *

Your answer





*) Choose files in target selection & Ligand selection description entry is optional.
*) Click on start docking results will be displayed after sometime and if email id is provided the results will be mailed as well.

Result & Discussion :-

The tool is used for docking is SWISSDock under SBI it is used to predict the molecular Interaction that may occur between target protein & ligand. Molecule of adenosine deaminase was done.

The result will be displayed protein target. In its tertiary structure format. Alongside a list of ligands for predicted binding modes are displayed. The user can select any ligand along with parameters Number of clusters & number of elements can be selected by clicking on show option Full fitness (energy) is indicated in K Cal/mol and estimated ΔG (force energy changes) referred as shown in K Cal/mol for docking interaction specified by the user the docking score is highest negative (-ve) free energy Change which is obtained as a best fit for given binding pocket.

Name of Experiment..... Date 24/1/24

Experiment No. 8 Experiment Result..... Page No. 24

Docking studies - Analysis of Substrate / Ligand binding using homologues Structure.

Aim:- To carryout docking studies using SWISSDOCK Software tool.

Introduction:-

SWISSDOCK a web service to predict the molecular interaction that may occur between a target protein & a small molecule SDB a database of manuals created target & ligand structure are available SwissDock allows the user to do the following. Propose a binding mode for ligand, create, figure for your article generate a complex to perform subsequent calculation. Design inhibition for the target of your choice It is based on EADOCK DSS.

Query:- Adenosine Deaminase.

URL:- www.SWISSDOCK.ch

Procedure:-

* Log on to www.SWISSDOCK.ch the homepage of SWISSDOCK is opened which is under SIB.
* Click on target database select any the pair of target & ligand click dock download
* The files will be downloaded in zip format, next select submit docking upload