

Prática de Docking

Introdução a modelagem, docking e dinâmica molecular

(Foco em Doenças

Negligenciadas)



Prepare o Ligante

- Abra sua estrutura com ligante (4CYQ) no Pymol
- Selecione seu ligante de interesse
- Exporte a molécula

Encontre o centro da caixa

- . Abra o PDB do ligante no bloco de notas
- . Encontre as coordenadas XYZ de alguma das moléculas
- . Guarde essa informação

Prepare a Proteína

- Ainda com a estrutura anterior aberta, abra o PDB do seu modelo
- Alinhe seu modelo à estrutura de referência
- Exporte a proteína

Selecione o Arquivo da sua Proteína

Na página <https://dockthor.lncc.br/v2/index.php#>

The screenshot displays the 'Protein' tab of the DockThor v2 interface. At the top, there are five tabs: Protein, Cofactors, Ligand, Docking, and Results. Below the tabs, a section titled '1 Upload your protein file' contains a green '+ Add File' button and a 'Select Test File' link. The '+ Add File' button is highlighted with a red rectangle. Below this, there is a 'New COVID-19 resources' section with three dropdown menus labeled 'Target', 'Variant', and 'Structure', followed by three colored circular icons (blue, orange, and blue). At the bottom, a table lists uploaded files. The first row shows a file named '1_donovani.pdb' with a size of '550.49 KB' and a status of a loading spinner. The 'Actions' column for this row contains a blue 'Send' button and a red trash icon, both of which are highlighted with red rectangles.

File name	Size	Status	Actions
1_donovani.pdb	550.49 KB		

Protone e envie a Estrutura




② Select the protonation states ⓘ

➤ Chain A

Apply Preset

③ Prepared protein file

View 3D Download **Send to DockThor**

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Se Necessário, Adicione Cofatores

The screenshot displays the dockThor web interface, a receptor-ligand docking program. The top navigation bar includes links for Home, Docking (active), References, About, and Support. A Login/Register link is also present. The main workflow is divided into five steps: Protein, Cofactors (current), Ligand, Docking, and Results. Under the 'Cofactors' step, the instruction '1 Upload your cofactor file' is shown. Two options are available: '+ Add file' (highlighted with a red box) and 'Select Test File'. Below these, the word 'Or' is displayed, followed by a button labeled 'Do not use cofactors' (also highlighted with a red box). The footer contains logos for GMMSB, SENAPAD, Inct, FAPERJ, CNPq, and the Laboratório Nacional de Computação Científica.

Selecione Seu Ligante

The screenshot displays the DockThor web interface, a receptor-ligand docking program. The top navigation bar includes links for Home, Docking (selected), References, About, and Support. A 'Login | Register' link is also present. The main interface is divided into five tabs: Protein, Cofactors, Ligand (selected), Docking, and Results. Under the 'Ligand' tab, the first step is 'Upload your ligand file'. A red box highlights the '+ Add file' button. Below this, there is a section for 'Compounds Datasets' with input fields for 'Dataset', 'pH range', and 'Version'. A table below shows a single entry with file name 'lig.pdb', size '4.02 KB', and an 'Add H' toggle. The table also includes a 'Status' column and an 'Actions' column with buttons for 'Send' and 'Remove all'. A footer section contains logos for GMMSB, SITAPAD, Inct, FAPERJ, CNPq, and Laboratório Nacional de Computação Científica.

① Upload your ligand file

+ Add file Select Test File -

New Compounds Datasets

Dataset - pH range - Version -

* Attention: some datasets are available exclusively for approved projects and registered users. You can sign up submitting your project on the Login tab.

#	File name	Size	Add H	Status	Actions
1	lig.pdb	4.02 KB	<input type="checkbox"/>		

Send Remove all

Void structures: 0 (max: 200)

GMMSB SITAPAD Inct FAPERJ CNPq Laboratório Nacional de Computação Científica

Defina Quais Ligações Devem Ser Consideradas Rotáveis

② Rotatable bond editor

Rotatable bonds: 9

#	Atom 1	Atom 2	Disable/Enable
1	C6	C2	<input checked="" type="checkbox"/>
2	N7	C18	<input checked="" type="checkbox"/>
3	C13	C4	<input checked="" type="checkbox"/>
4	C19	C20	<input checked="" type="checkbox"/>
5	C20	C21	<input checked="" type="checkbox"/>

Disable/Enable all: ☒

Apply

③ Prepared ligand file



GMMSB
GRUPO DE MODELAGEM E SIMULAÇÃO DE MOLECULAS



Laboratório
Nacional de
Computação
Científica


Defina As Coordenadas XYZ E Dimensões Da Caixa

② Define the binding site

Attention: the current version of DockThor (released on April 13, 2020), requires the **total size** of the grid box instead of the half value on each dimension. For example, now the input grid size for the docking with the test files are X = 20, Y = 20 and Z = 20 instead of 10 Å on each axis.

Grid center:		Grid size:		Discretization:	
X	<input type="text" value="1.720"/>	X	<input type="text" value="20"/>		<input type="text" value="0.25"/>
Y	<input type="text" value="50.643"/>	Y	<input type="text" value="20"/>	Total Grid Points:	<input type="text" value="53184"/>
Z	<input type="text" value="59.596"/>	Z	<input type="text" value="20"/>		

Use your mouse to drag, rotate, and zoom in and out of the structure:
☐ auto view ☐ shift + left mouse = drag zoom ☐ ctrl + right mouse = drag rotate



X = 1.720
Y = 50.643
Z = 59.596

Selecione Os Parâmetros De Docking E Coloque Identificadores

③ Select the search algorithm precision

Standard Virtual Screening Explorer

Number of Evaluations:

1000000

Population Size:

750

Initial Seed:

-1985

Number of Runs:

24

Soft Docking 



④ Identify your docking job

Job name:

INIB



E-mail:

visalpi1@hotmail.com



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Parâmetros de Análise e download

① Select the parameters for analyses of docking results:

RMDS to cluster conformers :

Number of binding modes :

Compare docking poses with a reference conformation? ☐

② Analyze your docking results:

AnalyzeDownloadDelete Job

Observe os Resultados

Table

Rank

File ID

Compound

Affinity

Total Energy

vdw Energy

Elec. Energy

1

c7a6c75a89

ligand 1

-10.214

58.685

-38.701

0.613

<

1

>

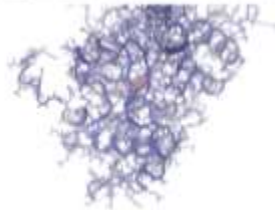
3D View

Use your mouse to drag, rotate, and zoom in and out of the structure:

⌘ auto view

shift + left mouse + drag zoom

ctrl + right mouse + drag rotate



3D é muito difícil ver todas as interações

- Abra o site proteins.plus
- Coloque o arquivo .pdb da proteína e .sdf do ligante
- Envie os dados pra plataforma



The screenshot shows the Proteins Plus website interface. On the left is the logo, which consists of a blue wireframe sphere with a black plus sign and the text "PROTEINS PLUS" in bold black letters. On the right is the main form area. At the top of the form is a text input field with the placeholder text "PDB-Code (PDB Database) or UniProt accession number (AlphaFold Database) or search term:". Below this field are two rows of upload options. The first row is "Upload Protein (PDB format):" followed by a button labeled "Escolher arquivo" and the text "Nenhum arquivo escolhido". The second row is "Upload Ligand (SDF format):" followed by a button labeled "Escolher arquivo" and the text "Nenhum arquivo escolhido". At the bottom right of the form area are two links: "Advanced search" and a blue button labeled "Go!".

Selecione o PoseView e a Molécula De Interesse

The screenshot displays the ProteinPlus web interface, a tool for protein-ligand complex analysis. The main window shows a 3D ribbon representation of a protein structure in red, with a ligand molecule (a complex organic molecule) docked in the binding pocket. The ligand is shown in a stick representation with green and blue atoms. Below the main view, there are several control panels for representation options, surface options, view options, and more options. The right sidebar contains a list of analysis tools, including Protein-Hydrogen prediction, DefAbleScore, DefAble, PoseView 3D Interaction Diagrams, SINA, PyPI, IDA, METAL, Alpha-Motion, LIGANDS, WATPO, MoleculeFlow, and GEMME. The bottom of the interface features a navigation bar with buttons for Home, About, Contact, and other links.

Analise o Gráfico 2D

