

Docking

Prof. Dr. Diego Mariano

Atracamento molecular

Docagem molecular prediz a orientação e as interações formadas entre uma molécula em relação a outra, descrevendo de forma computacional o possível complexo alvo-ligante que acontece no ambiente biológico.

Santos (2021)

Ferramentas usadas na aula

Resumo

- SwissDock
- Autodock Vina (interface SwissDock)
- Prodigy
- AlphaFold server
- AlphaFold-Multimer (ColabFold)
- HDOCK
- DockThor

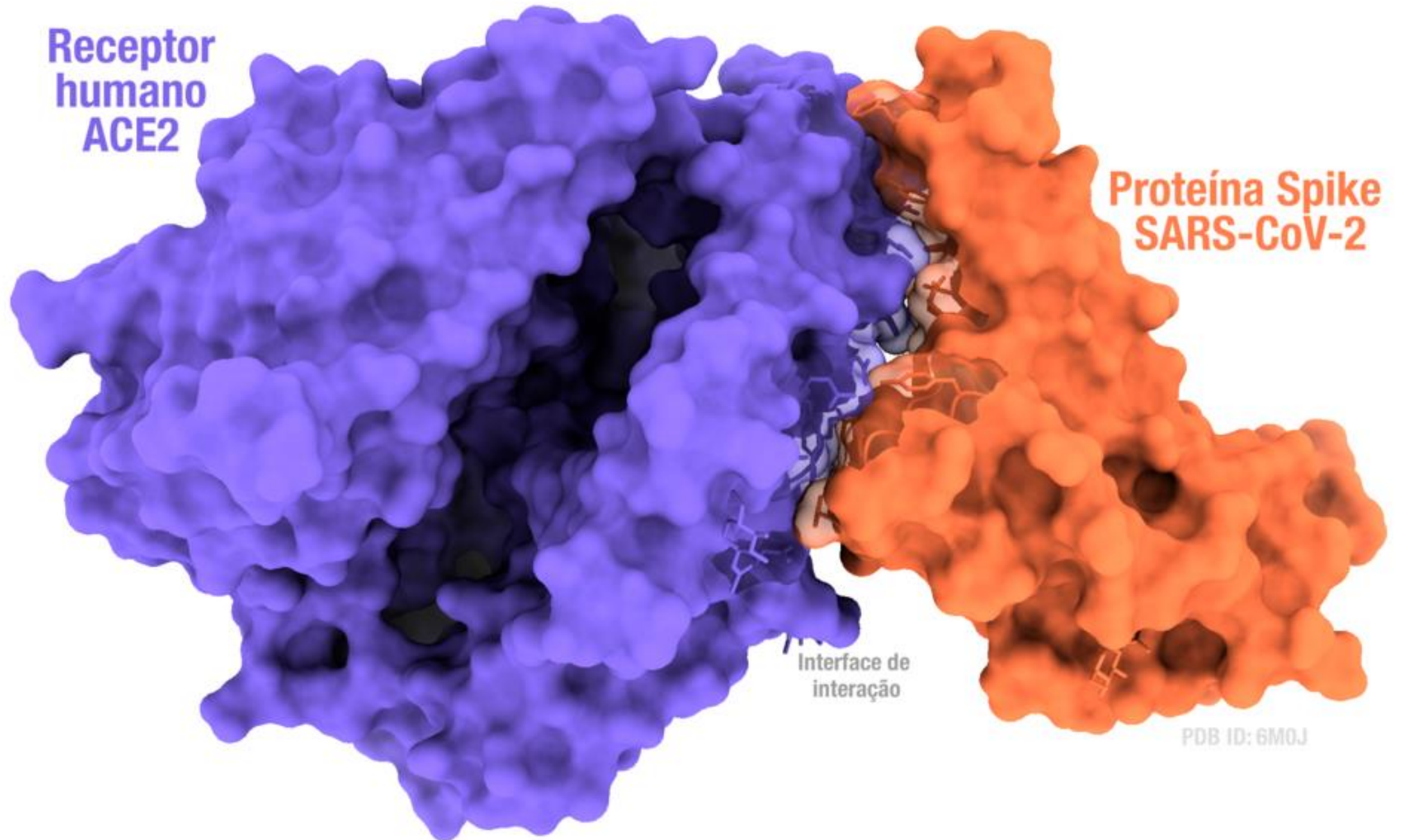
Importância

Entender
mecanismos
moleculares

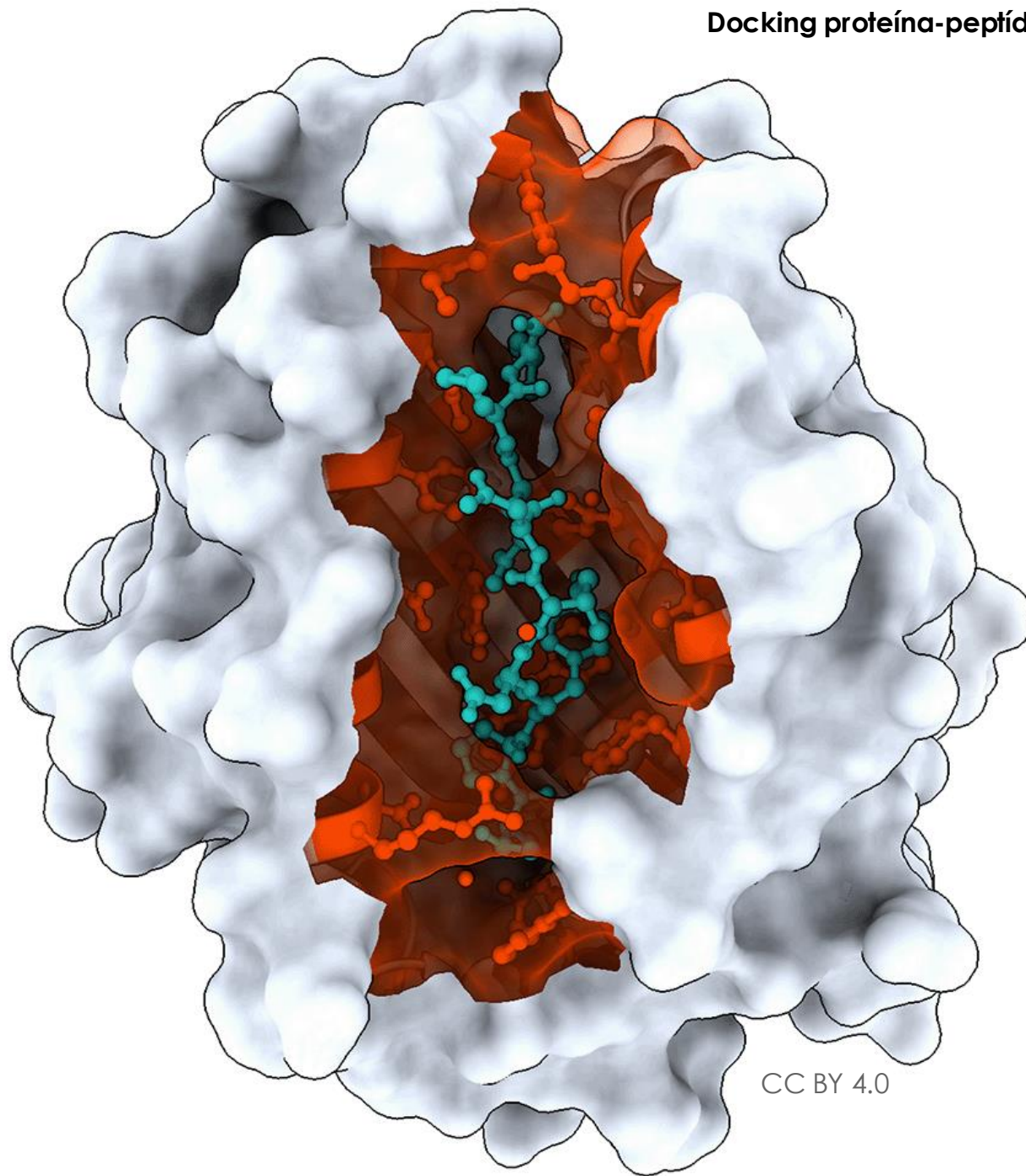


Compreender
os modos de
interações entre
moléculas

Exemplo: entender a posição de interação da proteína spike e o receptor humano ACE2

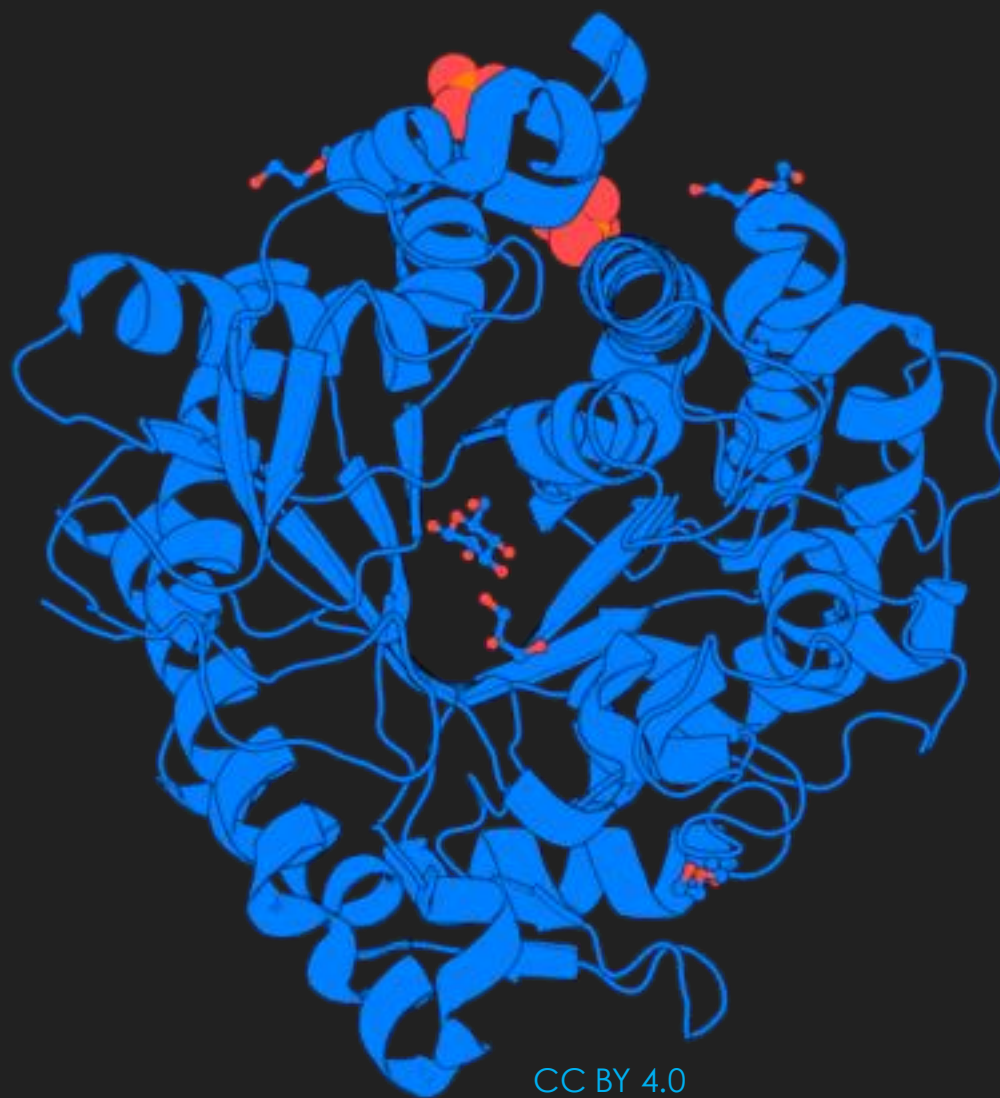


Docking proteína-peptídeo



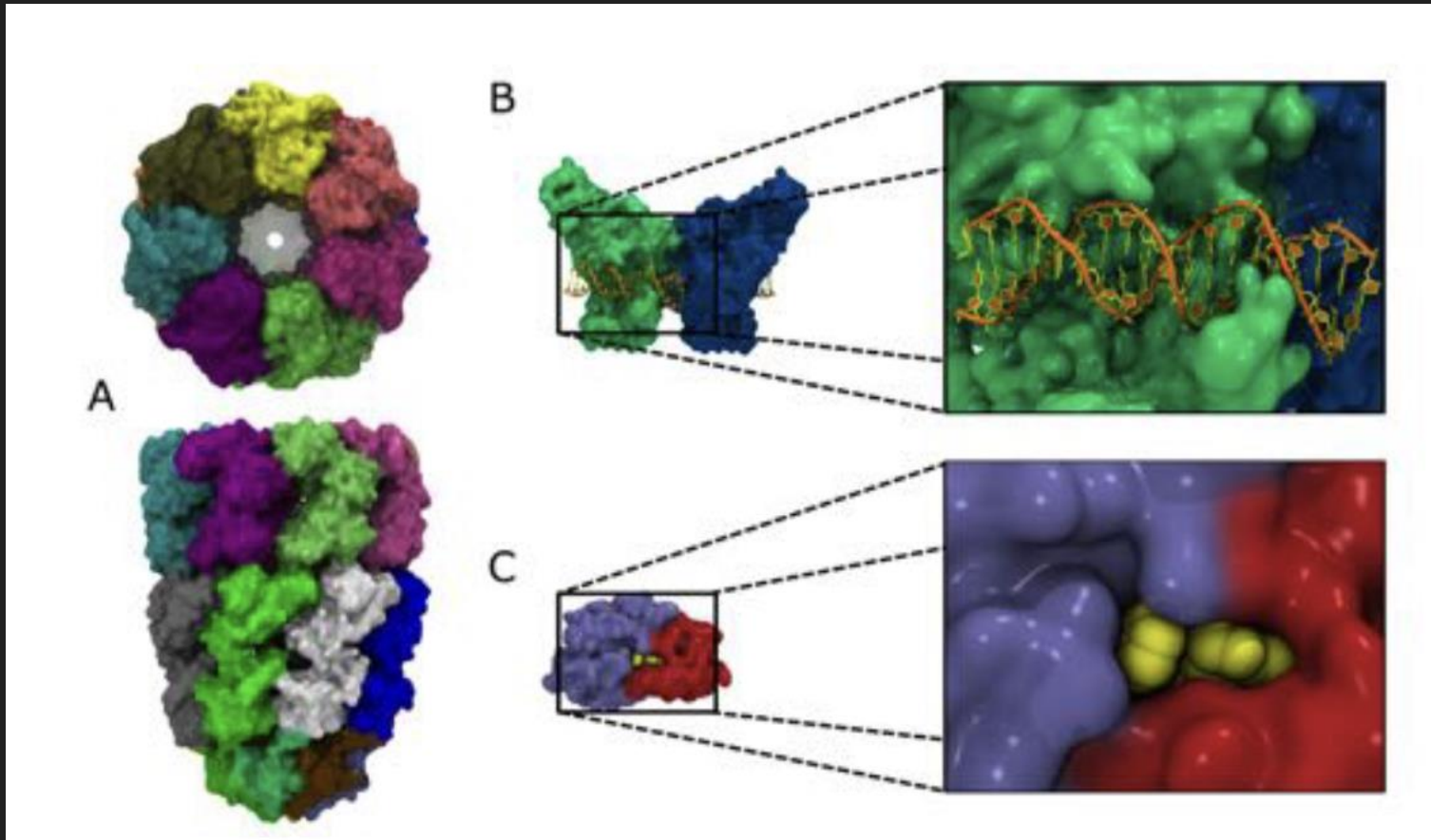
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Exemplo 2:
Entender a ligação de
um peptídeo a uma
proteína



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Exemplo 3:
Compreender a
inibição de uma
enzima usada na
produção de
biocombustíveis



Exemplos de complexos moleculares:

(A) chaperona GroEL (PDB ID1AON), (B) complexo DNA com proteína DMT1 (PDB ID 3PT6) e (C) complexo da enzima HIV-1 protease com o inibidor indinavir (PDB ID1HSG).

Fonte: <https://lume.ufrgs.br/bitstream/handle/10183/166105/001012172.pdf>

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Atracamento molecular

- *Molecular docking* (em inglês)
- Simulação computacional das ligações entre moléculas
- Previsão do modo de ligação e reconhecimento molecular:

Tipos de docking

01

Proteína-
ligante

02

Proteína-
proteína

03

Proteína-
peptídeo

04

Proteína-
DNA

05

Proteína-
RNA

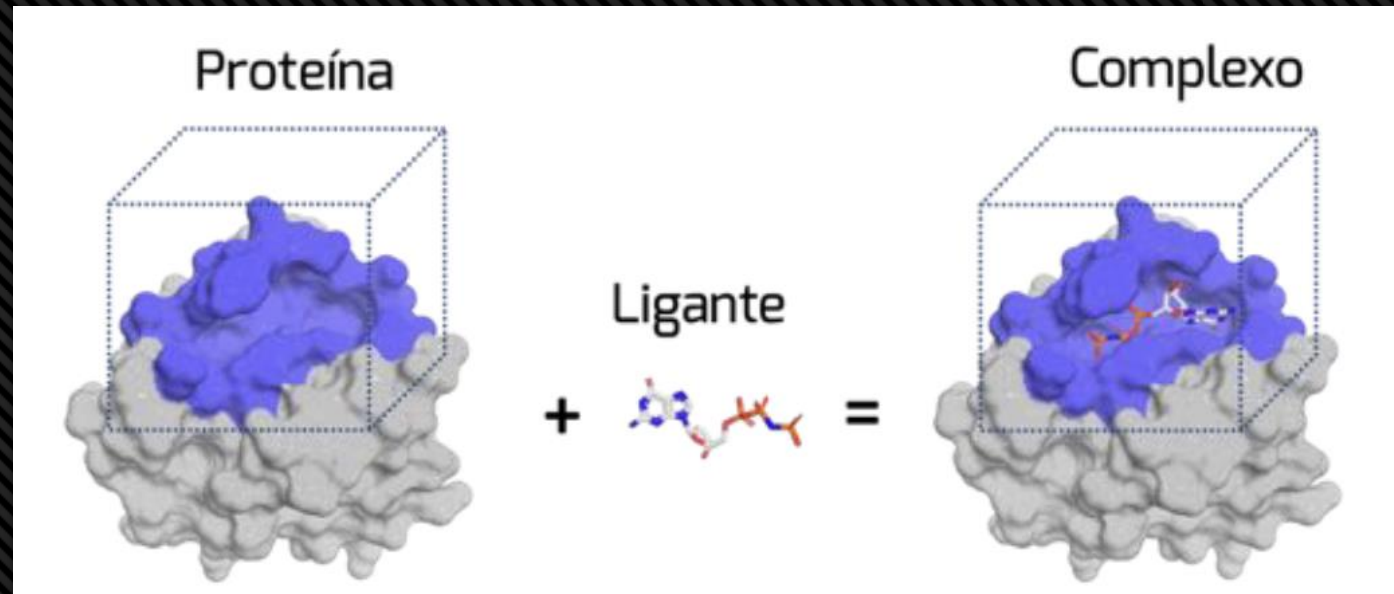
06

Outros

Carboidratos +
pequenos ligantes

Conceitos

Verli (2014)

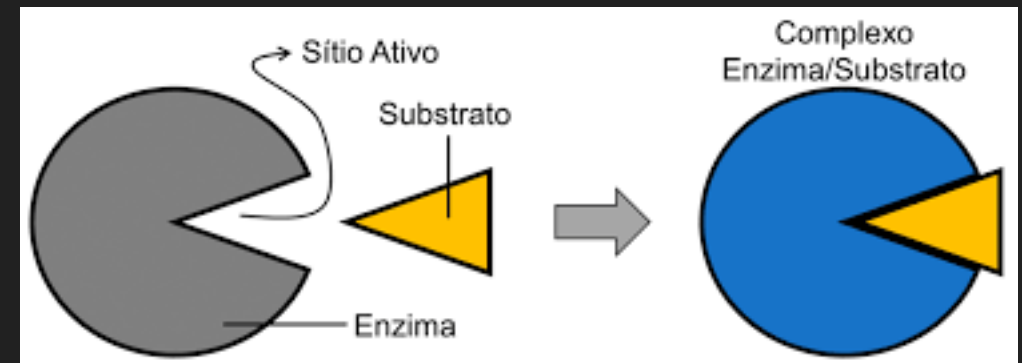


Fonte: <https://lume.ufrgs.br/bitstream/handle/10183/166105/001012172.pdf>

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Modelo chave-fechadura

- Proposto por Emil Fischer em 1894
- **Receptor proteico:** fechadura
- **Ligante:** chave
- Problemas:
 - no meio biológico, tanto ligante quanto a proteína são flexíveis



<https://bioinfo.com.br/docagem-molecular-em-busca-do-encaixe-perfeito-e-acessivel/>

Target



+

Ligand



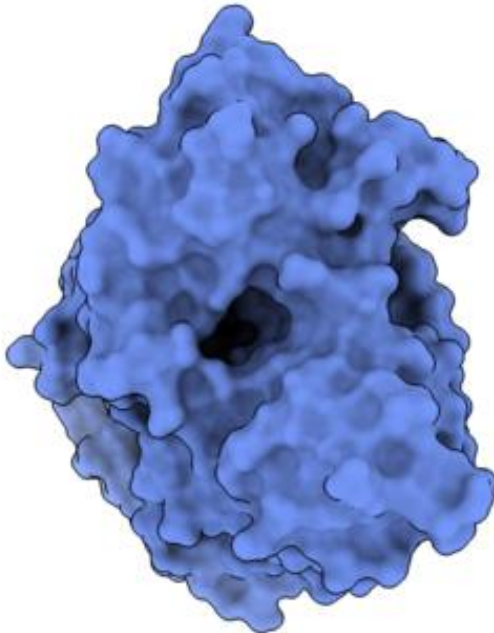
Docking



Complex



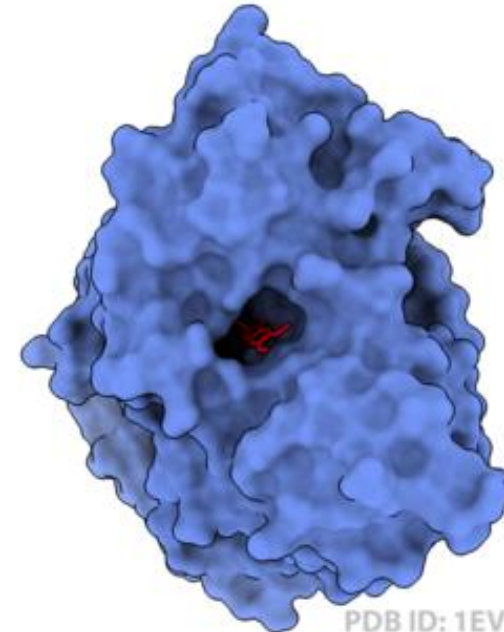
Molecular docking



+



Docking

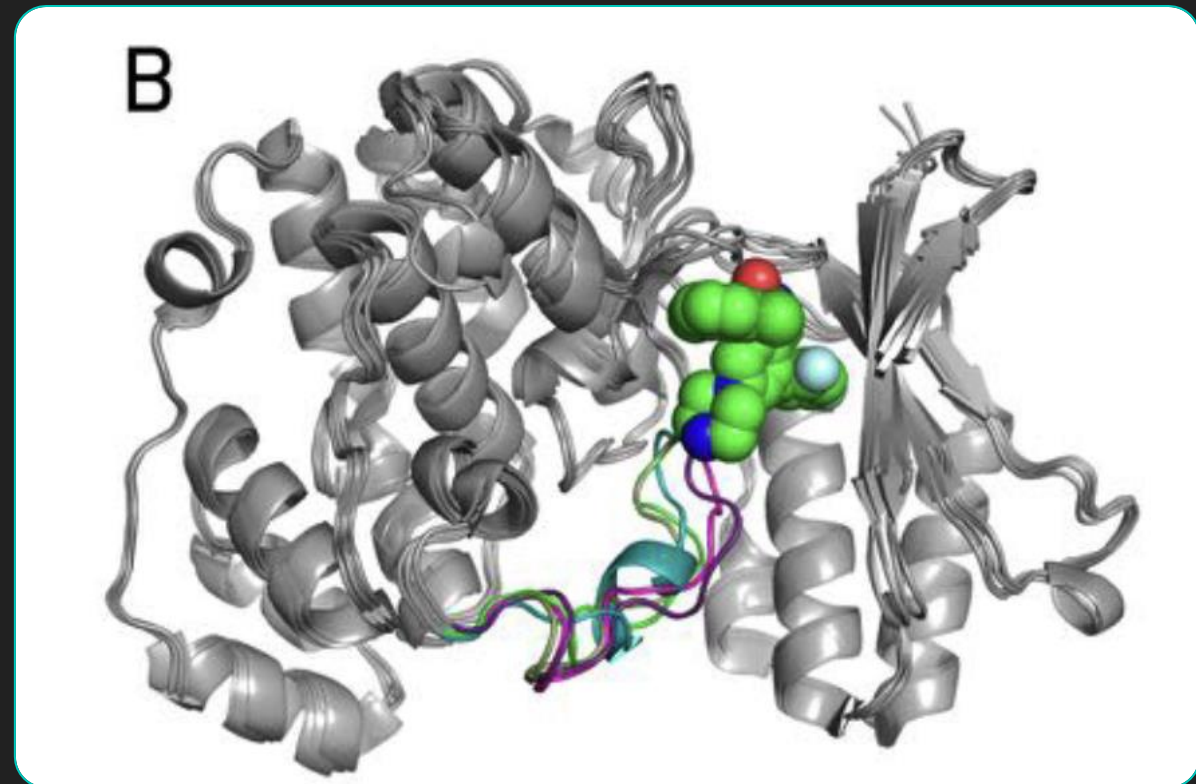


PDB ID: 1EVE

Encaixe induzido

- Modelo que prevê que ligante e receptor podem ser flexíveis

Verli (2014)

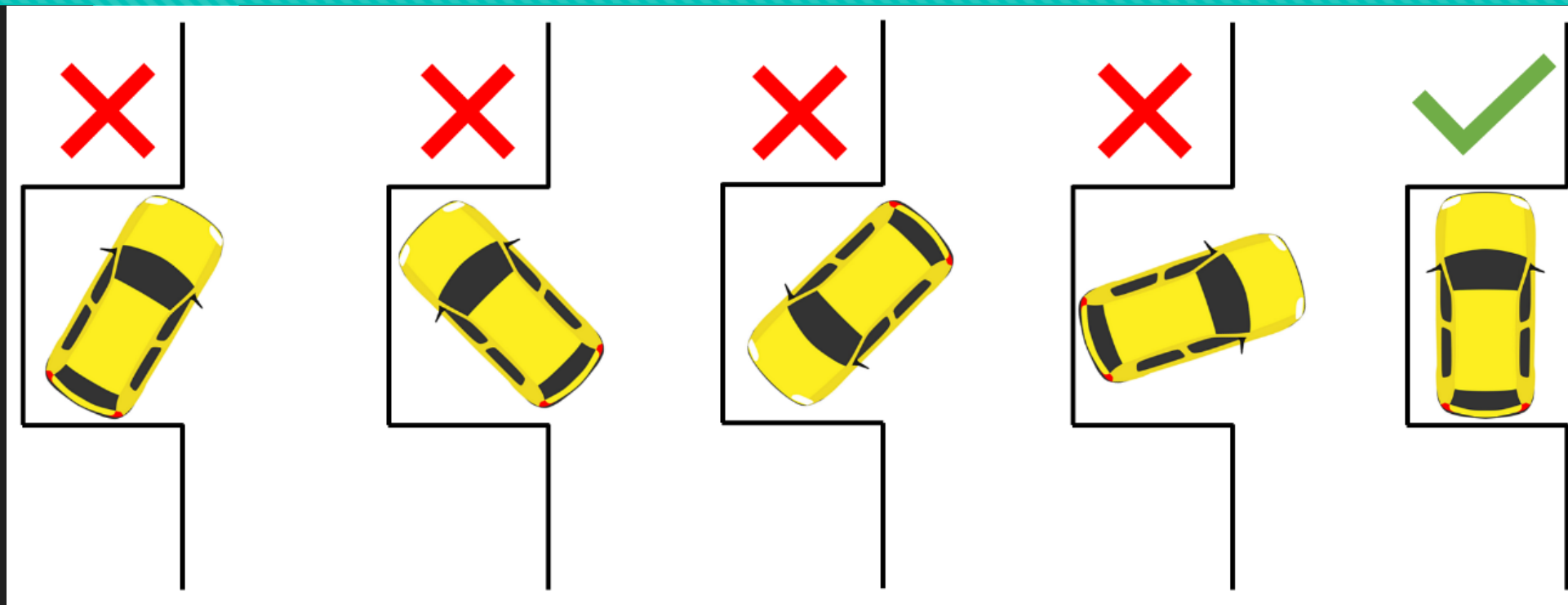


Fonte: <https://lume.ufrgs.br/bitstream/handle/10183/166105/001012172.pdf>

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Diversas conformações de alça no sítio de ligação do ATP à enzima MAP cinase p38

Como funcionam os programas de docking?



Fonte: <https://bioinfo.com.br/docagem-molecular-em-busca-do-encaixe-perfeito-e-acessivel/>

O processo de amostragem na docagem pode ser pensada como uma pessoa aprendendo a colocar o carro em uma vaga de estacionamento, onde várias tentativas são feitas até o carro ficar perfeitamente alinhado na vaga, ganhando assim uma boa pontuação.

Etapas do docking

01

Preparação
do receptor
e ligante

02

Definição
da caixa

03

Seleção de
poses

04

Cálculo de
energia de
ligação

Preparação do receptor

- **Remover moléculas que não participam da interação**
 - Remoção de água cristalográfica (a menos que seja funcional)
 - Íons desnecessários
 - Ligantes co-cristalizados (exceto quando usados como referência)
- **Corrigir e completar a estrutura**
 - Adicionar hidrogênios (especialmente polares)
 - Completar resíduos faltantes
 - Corrigir estados de tautomeria e protonação em resíduos críticos
 - Ajustar cargas parciais
- **Minimização leve da estrutura**
 - Remover clashes atômicos
 - Ajustar geometrias inconsistentes

Preparação do ligante

1. Definir a estrutura química correta

- Conectividade
- Aromaticidade
- Estereoquímica
- Estados de protonação corretos (pH fisiológico)
- Tautômeros mais prováveis

2. Adicionar cargas e tipos de átomos

- Cargas parciais (Gasteiger, MMFF, etc.)
- Tipos de átomos do force field (AutoDock, OpenMM, etc.)

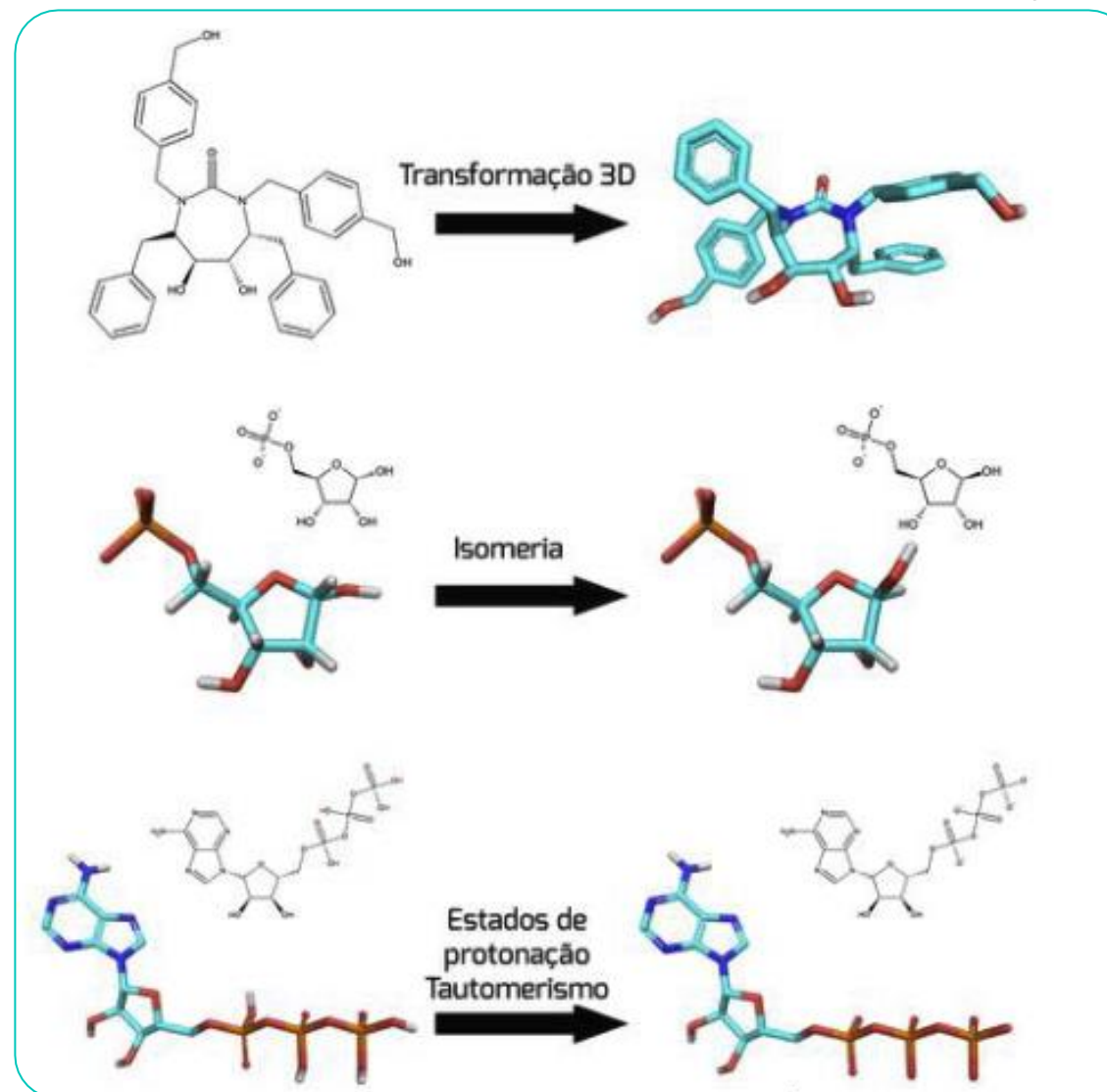
3. Flexibilidade do ligante

- Identificar ligações rotacionáveis
- Definir ângulos que o docking pode explorar

4. Minimizar energia

- Relaxar geometrias ruins
- Gerar a melhor conformação inicial

Verli (2014)



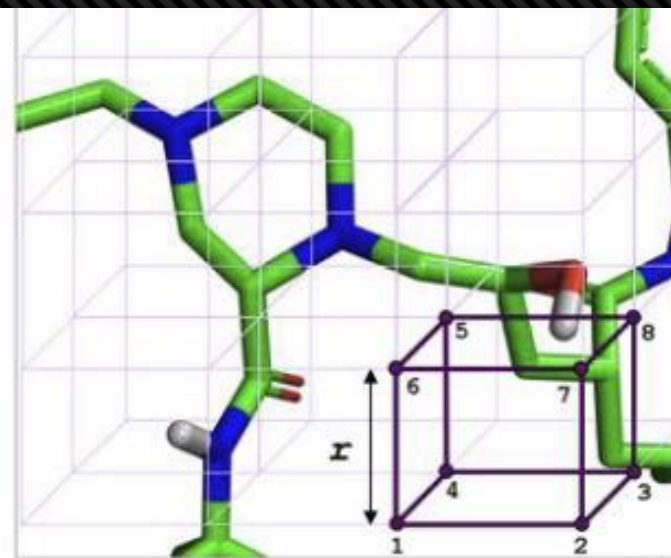
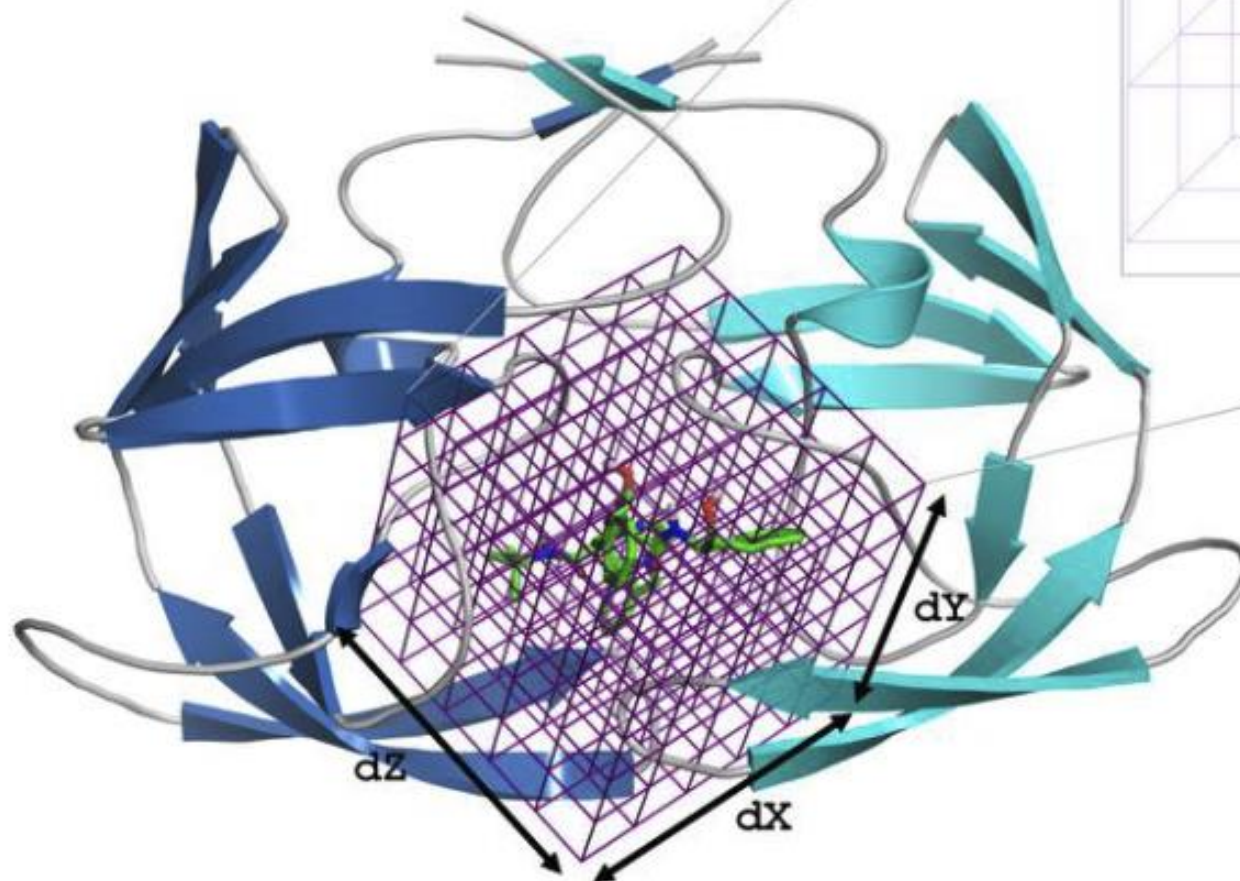
Fonte: <https://lume.ufrgs.br/bitstream/handle/10183/166105/001012172.pdf>

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Formato pdbqt

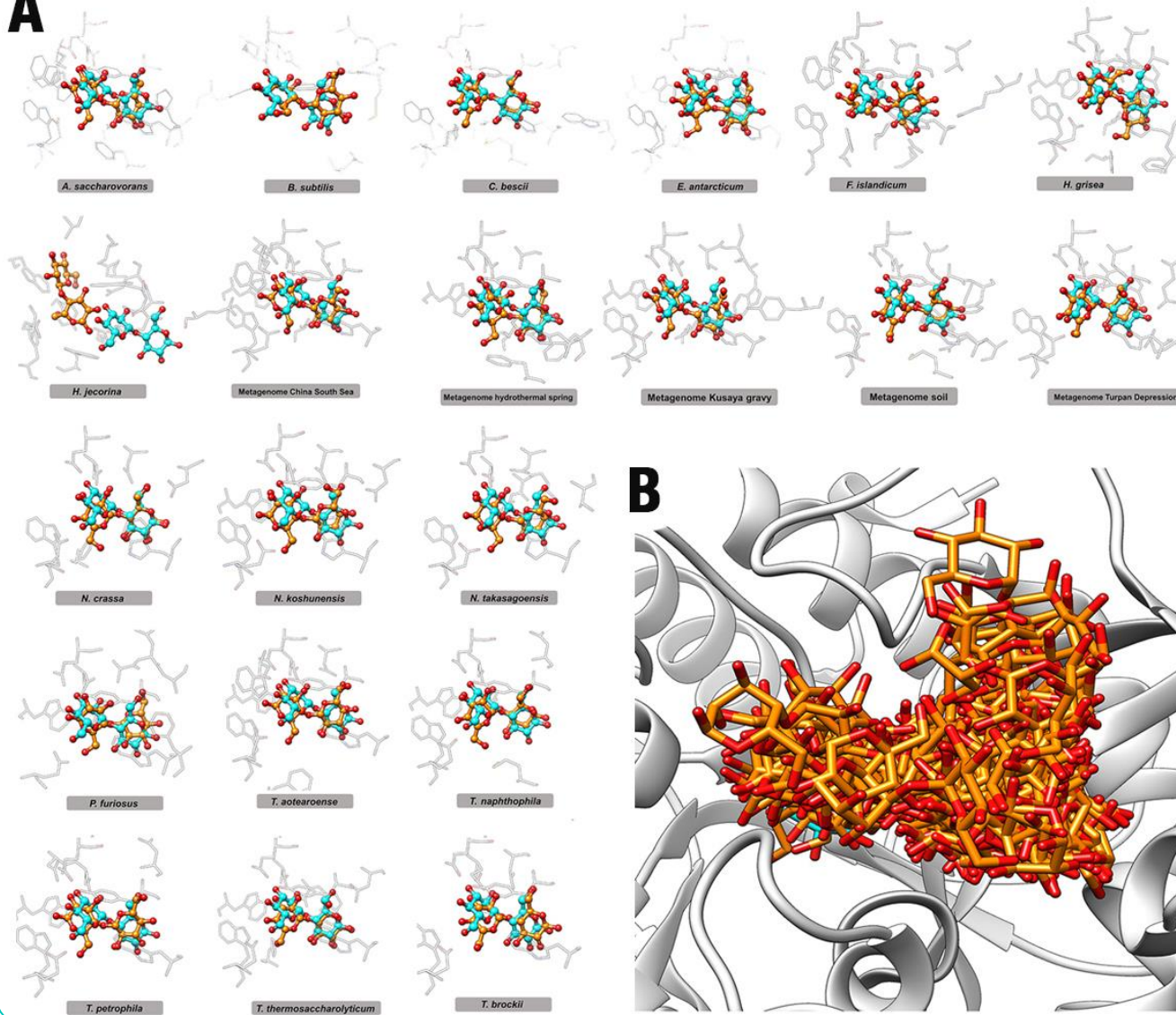
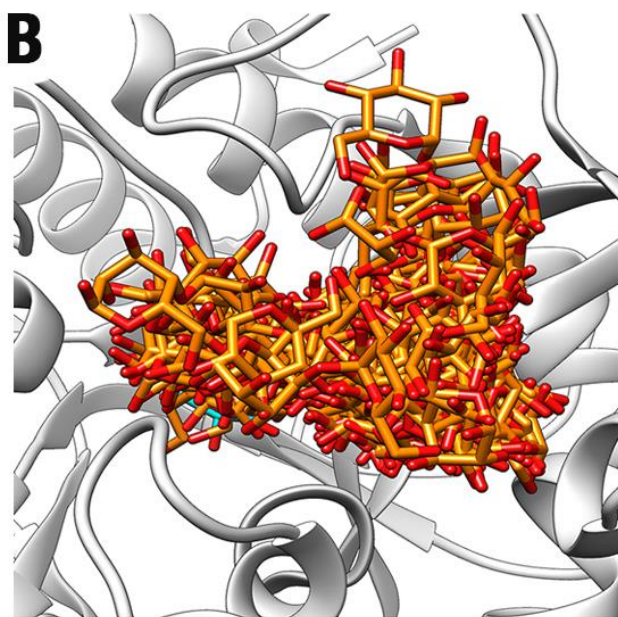
Onde o algoritmo de docking irá tentar posicionar o ligante?

Definição da caixa



Centro da caixa
Tamanho das bordas

Verli (2014)

A**B**

Como definir a melhor pose de ligação

- Encontrar a melhor pose do ligante não é trivial
- Existem diversas estratégias para isso
 - Algoritmo de Monte Carlo
 - Algoritmo genético

Fonte: Mariano (2019) – tese de doutorado

Algoritmo de Monte Carlo

- Baseia-se em amostragem aleatória para explorar um espaço de busca
- Em docking, o objetivo é encontrar a melhor pose do ligante no sítio ativo.
- MC é usado para explorar aleatoriamente:
 - translação do ligante
 - rotação do ligante
 - conformações flexíveis (ligações rotacionáveis)

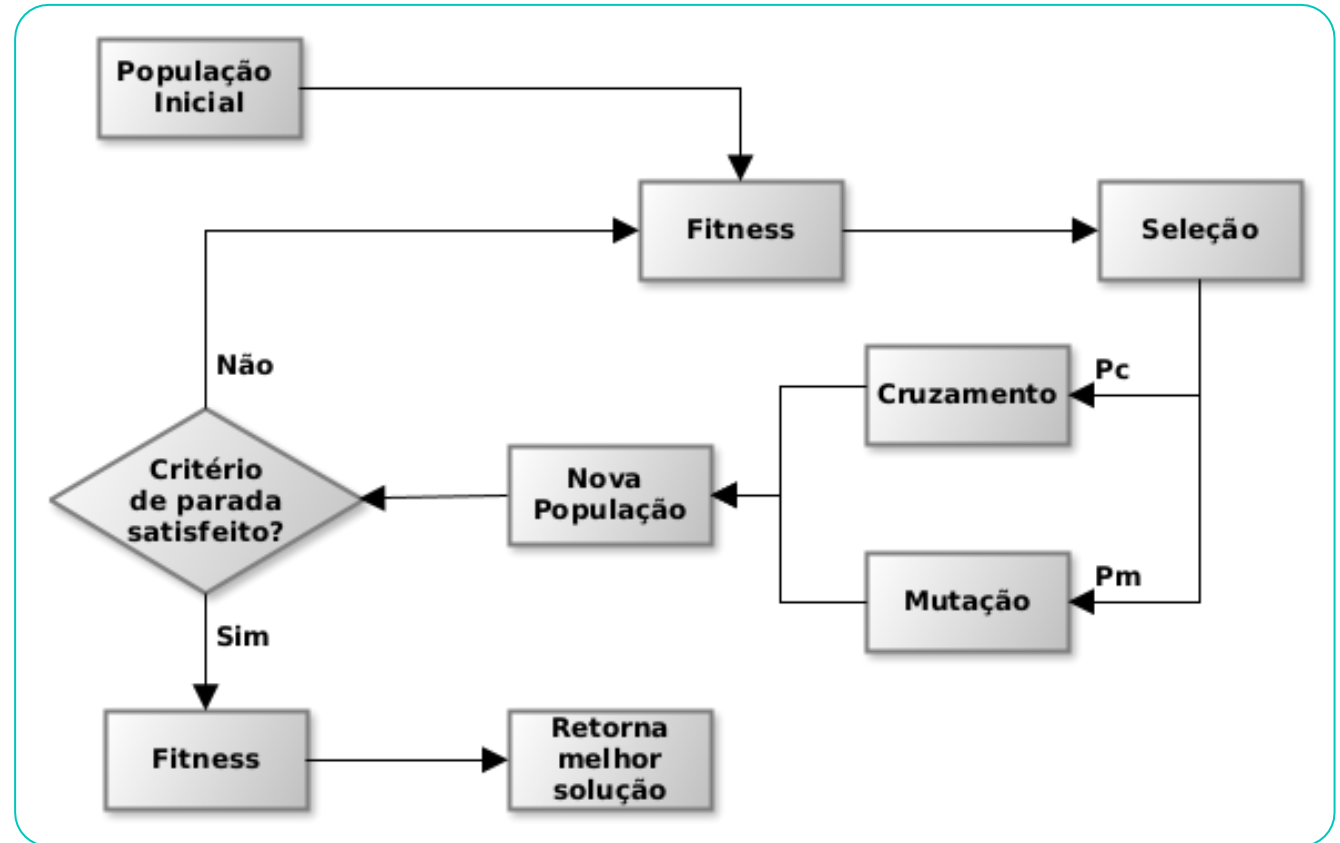


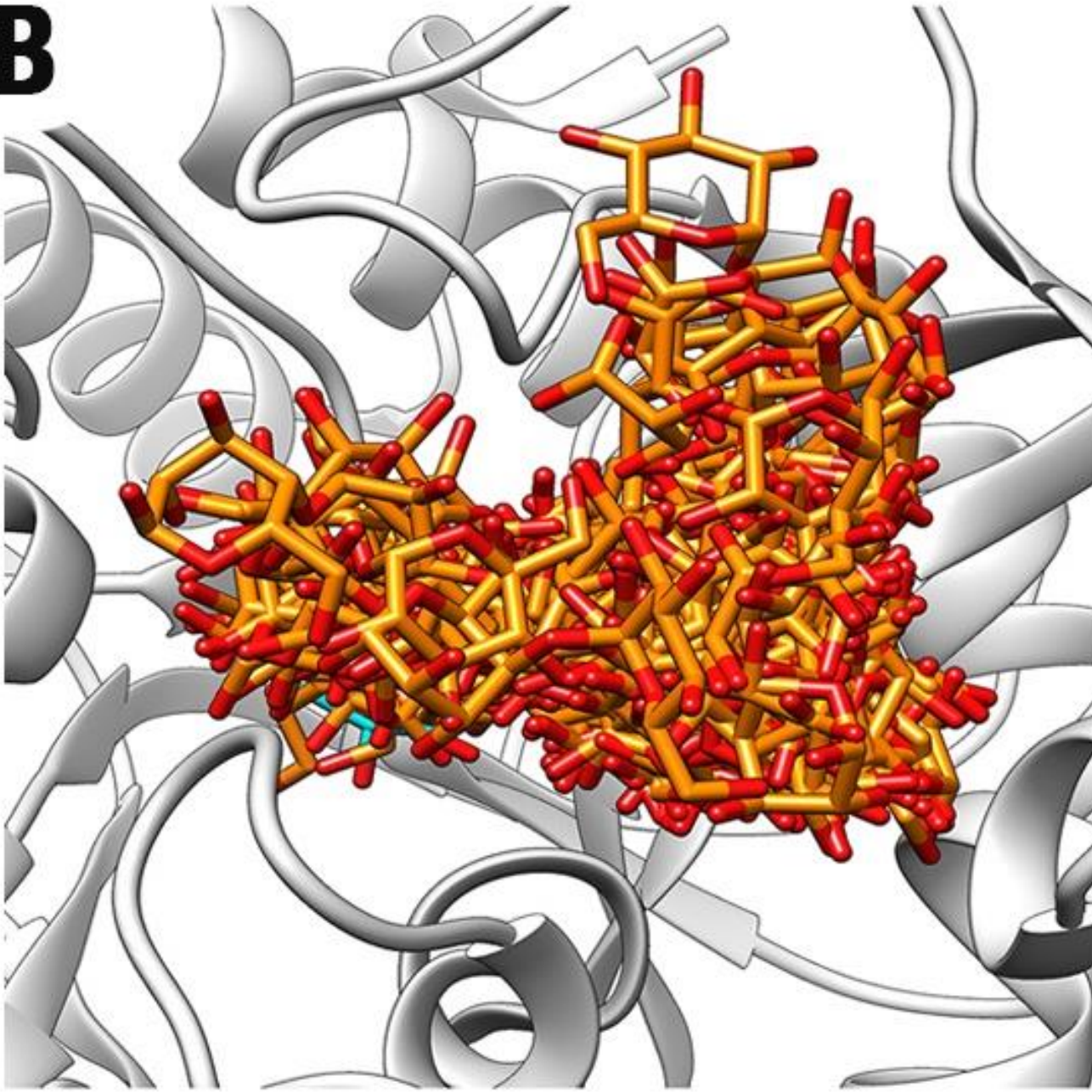
Nome é inspirado no Cassino Monte Carlo em Mônaco

Algoritmo genético

- No docking, uma pose inicial é definida aleatoriamente
- Em seguida, a posição do ligante é alterada por meio de mutações ou cruzamento
- Por fim, o algoritmo avalia a energia de ligação
- Isso é feito sucessivas vezes até se obter um melhor resultado

“Algoritmos Genéticos (AGs) são métodos meta-heurísticos baseados na teoria de seleção natural de Charles Darwin” (Kato et al.,2021)



B

Várias poses são testadas

- Os algoritmos testam várias poses
- Avaliam o resultado por meio do cálculo de energia de ligação

Como saber qual o melhor resultado?

- Basta medir a energia de ligação entre o complexo receptor-ligante
- Resultado é dado em kcal/mol
- Quanto mais negativo mais forte é a ligação

Energia de ligação de Gibbs

$$\Delta G_{\text{lig}} = \Delta H - T\Delta S = -RT \ln K_{eq}$$

$$K_d = ([R][L])/[RL] \quad K_a = [RL]/([R][L])$$

Constante de dissociação e associação

$$\Delta G_{\text{lig}} = \alpha(\langle V^{LJ} \rangle_{\text{lig}} - \langle V^{LJ} \rangle_{\text{livre}}) + \beta(\langle V^{el} \rangle_{\text{lig}} - \langle V^{el} \rangle_{\text{livre}})$$

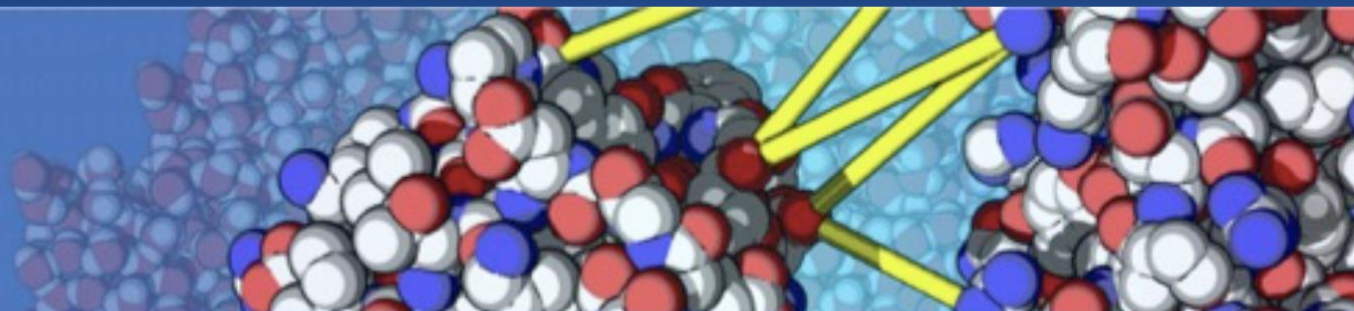
Delta G: variação da energia livre

Existem programas para predição de energia de ligação

Propõem scores (pontuações) para avaliar a ligação. Entretanto, os resultados não são muito confiáveis.

PRODIGY

@Bonvinlab



PRODIGY ▾

Home

Manual

Method

Dataset

Example

Reference

Login

Ferramentas para mensurar a energia de ligação

<https://rascar.science.uu.nl/prodigy/>

Três tipos

PRODIGY
(protein-protein)

PRODIGY-LIGAND
(protein-small molecule)

PRODIGY-CRYSTAL
(biological or crystallographic)

PRODIGY
(protein-protein)

PRODIGY-LIGAND
(protein-small molecule)

PRODIGY-CRYSTAL
(biological or crystallographic)

Please provide the PDB ID of the protein-small molecule complex or submit a file in [PDB](#) or [mmCIF](#) format.

An archive of multiple PDB/mmCIF files can also be provided (as a multi-model PDB), together with the interacting chains.

Information about the predictive approach can be found at the online [method page](#).

Structure(s)*

3PTB

OR

Escolher arquivo Nen...lhido

Protein Chain ID*

A

Ligand ID*

A:BEN

Electrostatic Energy

HADDOCK electrostatic energy - Optional



Electrostatic Interaction (from HADDOCK)

Job ID

Tripsina

Add a custom Job ID to identify your run.

Email

Email

Optional email address to which the results will be send.



Não sou um robô

Os Termos de Serviço do reCAPTCHA estão mudando. [Acesse](#).



reCAPTCHA
Privacidade - Termos

Load Sample Data

Submit Prodigy-Ligand

Exemplo:
tripsina + Benzamidina



Resultado

BINDING AFFINITY

Complex	$\Delta G_{\text{prediction}}$ (Kcal/mol)	ΔG_{noelec} (Kcal/mol)	ΔG_{score}	CC	CO	CN	CX	OO	OX	NO	NN	NX	XX
3PTB	-	-6.21	-	822	279	505	23	0	0	85	74	6	0

- A energia livre de ligação predita entre a tripsina e a Benzamidina é de -6,21 kcal/mol

PRODIGY
(protein-protein)

PRODIGY-LIGAND
(protein-small molecule)

PRODIGY-CRYSTAL
(biological or crystallographic)

Please provide the PDB ID of the target complex or submit a file in [PDB](#) or [mmCIF](#) format.

An archive of multiple PDB/mmCIF files can also be provided (as a multi-model PDB), together with the interacting chains.

Information about the predictive approach can be found at the online [method page](#).

Structure(s)*

OR

Interactor 1*

Interactor 2*

Temperature (in °C)*

Job ID

Add a custom Job ID to identify your run.

Email

Optional email address to which the results will be send.

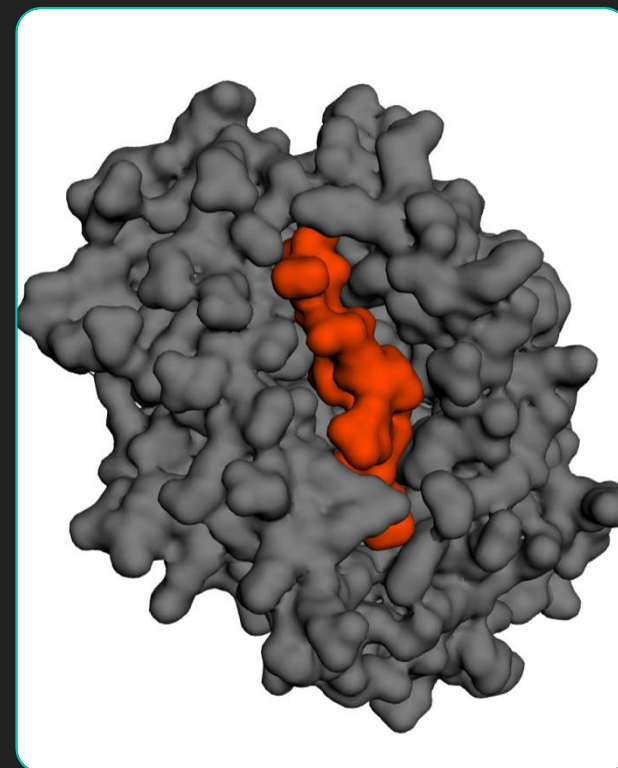
Não sou um robô

Os Termos de Serviço do reCAPTCHA estão mudando. [Acesse](#).



reCAPTCHA
Privacidade - Termos

Exemplo com Interação proteína- proteína



Complexo proteína-peptídeo
(1a1m)

Resultado

BINDING AFFINITY AND K_D PREDICTION

Protein-protein complex	ΔG (kcal mol ⁻¹)	K_d (M) at °C	ICs charged-charged	ICs charged-polar	ICs charged-apolar	ICs polar-polar	ICs polar-apolar	ICs apolar-apolar	NIS charged	NIS apolar
1A1M	-11.2	6.1e-09	1.0	3.0	10.0	5.0	26.0	25.0	33.67	32.66

- A energia livre de ligação predita entre proteína-peptídeo é de -11,2 kcal/mol

Exemplos de ferramentas de docking

- DockThor
- SwissDock
- DOCK
- AutoDock Vina

Estudo de caso: tripsina

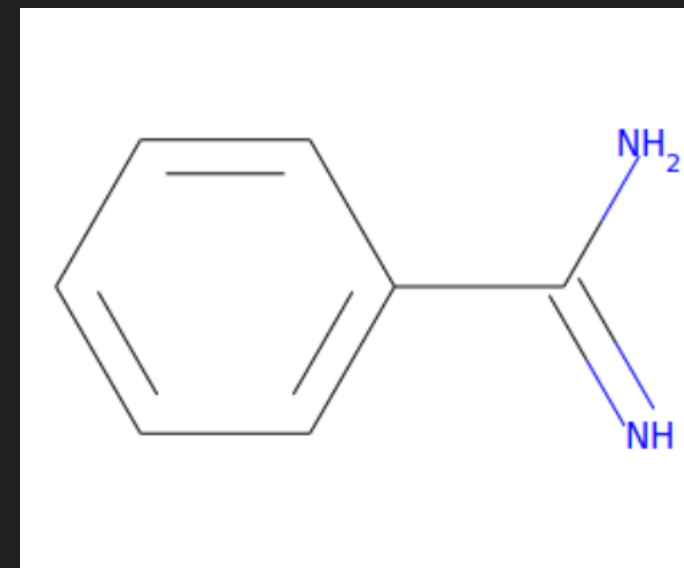
- A **tripsina** é uma enzima digestiva **crucial** no organismo
- Pertencente à família das **serino proteases**
- Ela é amplamente utilizada tanto **biologicamente** quanto **industrialmente** e também é um alvo clássico em **bioquímica estrutural, enzimologia e docking molecular**.
- Benzamidina é um inibidor conhecido



1S0Q

Prática 1

- **Tripsina + Benzamidina (benzamidine)**
- Estrutura sem ligante: 1S0Q
- Estrutura com ligante: 3PTB
- Ligante:
 - <https://zinc.docking.org/substances/ZINC000000036634>
- Smiles:
 - N=C(N)c1ccccc1



www.swissdock.ch



SwissDock
SwissDrugDesign

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Welcome to the new SwissDock, based on the Attracting cavities and Autodock Vina docking engines. Please, note that the old version, based on EADock DSS, is still available at the address <http://old.swissdock.ch> and will be maintained for several months. Consider transitioning your projects from the old to the new server. Thank you!


Docking with Attracting Cavities

Docking with AutoDock Vina

Duas opções

Attracting cavities

- Algoritmo de docking criado pela equipe do SwissDock (mesmo grupo do Swiss-model)
- Vamos testá-lo primeiro

▶ J Chem Inf Model. 2023 Jun 7;63(12):3925–3940. doi: [10.1021/acs.jcim.3c00054](https://doi.org/10.1021/acs.jcim.3c00054) 

Attracting Cavities 2.0: Improving the Flexibility and Robustness for Small-Molecule Docking

[Ute F Röhrig](#)^{†,*}, [Mathilde Goullieux](#)[†], [Marine Bugnon](#)[†], [Vincent Zoete](#)^{†,‡,*}

▶ Author information

PMCID: PMC10305763

Docking with Attracting Cavities

Passo 1: envie o ligante

1 - Submit a ligand

Provide a SMILES

... or upload a Mol2 file 

... or input, or modify, or check the molecule **using the sketcher**

... or use the **advanced search**



- Podemos enviar o código SMILES do ligante ou um arquivo no formato Mol2

Envie a proteína

2 - Submit a target

Provide a PDB id (e.g. 5hie)

Choose chain(s) to keep*:

Choose heteroatom(s) to keep*: ?

... or upload a PDB file

... or use the **advanced search**



Prepare target

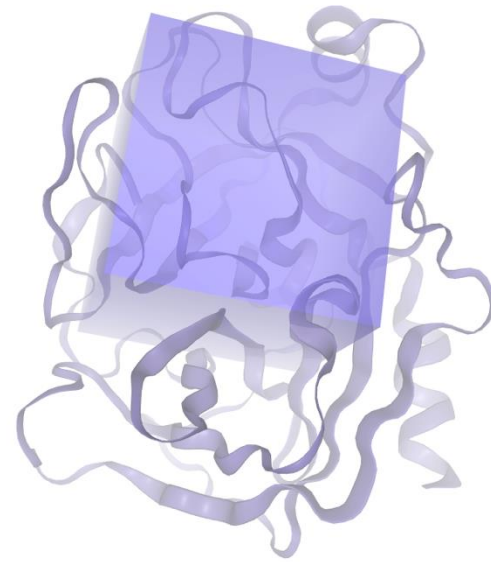
Reset target

- Podemos enviar um arquivo pdb ou fornecer o pdb id (aponte a cadeia logo abaixo)

3 - Define search space

Search box center Å

Search box size Å



Precisamos definir o centro da caixa

Hydrogen
bonds

Ionic
interactions

Cation- π
interactions

Hydrophobic
contacts

π -stacking
interactions

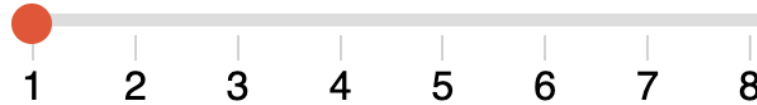
Show protein
surface

Reset

Não altere esses parâmetros

4 - Select parameters

Number of RIC ?



Show extra parameters



Check parameters



This job is estimated to take 0:03:54 (h:mm:ss)

Inicie o docking

5 - Start docking

Enter an email (optional)

Enter a docking name (optional)

START DOCKING

Reset form

Docking sendo processado



SwissDock 
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Parameters:

Submission date: December 2, 2025, 2:37 am UTC
Docking name: Tripsina Benzamidina benzamidine
Ligand: N=C(N)c1ccccc1
Target: 1s0q_modified.pdb
Box center: 55 - 40 - 15
Box size: 20 - 20 - 20
Docking method: AC
Sampling exhaustivity: medium
Cavity prioritization: buried
Number of RIC: 1
This job is estimated to take 0:03:54 (h:mm:ss)

Query

Ligand N=C(N)c1ccccc1
Target 1s0q_modified.pdb
Method Attracting Cavities 2.0
Date December 2, 2025, 2:37 am UTC

Parameters:

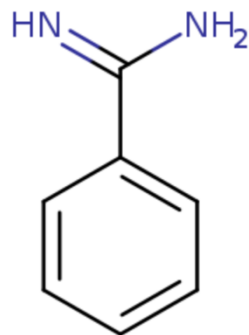
Box center: 55 - 40 - 15 Sampling exhaustivity: medium Number of RIC: 1
 Box size: 20 - 20 - 20 Cavity prioritization: buried

If you publish these results, please, cite the following papers:

Bugnon M, Röhrig UF, Goullieux M, Perez MAS, Daina A, Michielin O, Zoete V. SwissDock 2024: major enhancements for small-molecule docking with Attracting Cavities and AutoDock Vina. *Nucleic Acids Res.* **2024**

Röhrig UF, Goullieux M, Bugnon M, Zoete V. Attracting Cavities 2.0: improving the flexibility and robustness for small-molecule docking. *J. Chem. Inf. Model.*, **2023**

Ligand



Export your results:  

Results

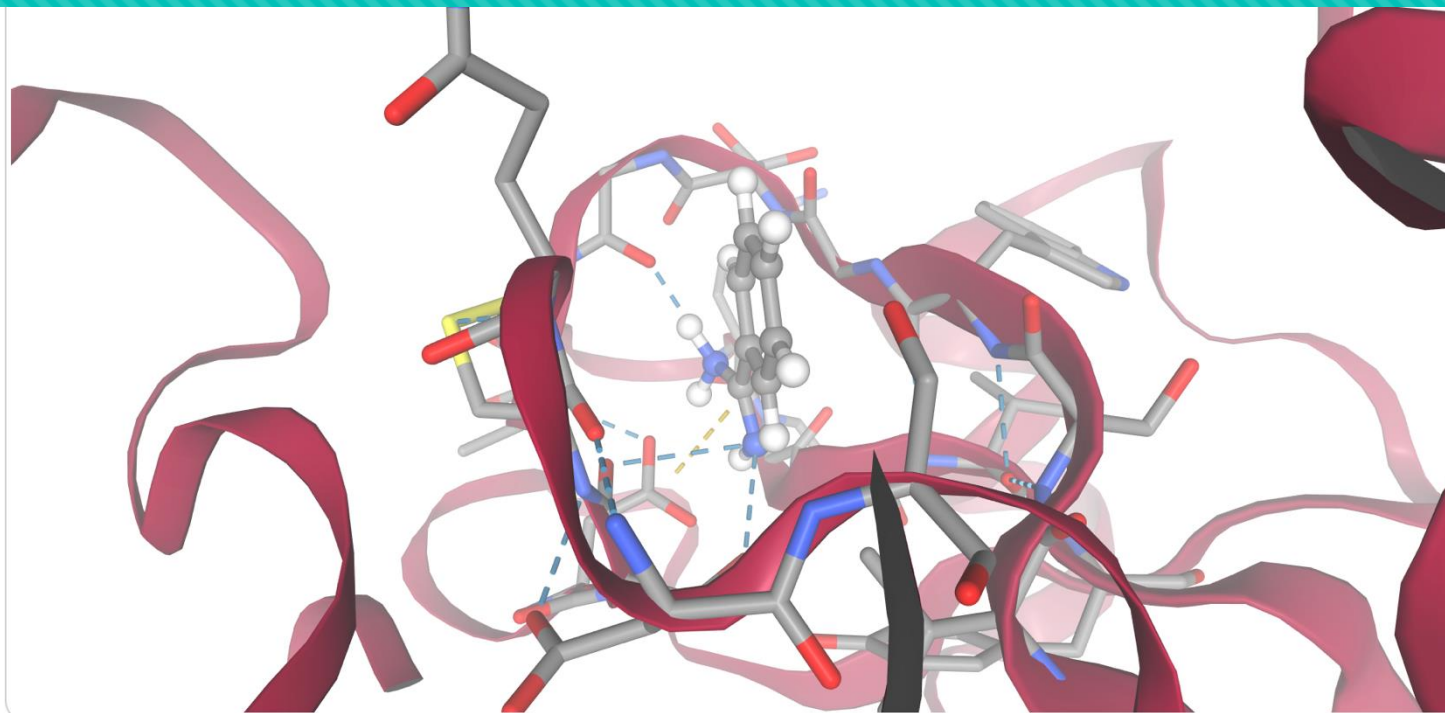
 Resultado

Best members

By cluster

Number of displayed clusters: 

Cluster number	Cluster member	AC Score	SwissParam Score
0	1	-33.903193	-6.3445
1	1	-29.436369	-6.1856
2	1	-28.451408	-6.3144
3	1	-27.385242	-6.0611
4	1	-27.017753	-6.0230
5	1	-27.010609	-5.9395
6	1	-26.346690	-5.9072
7	1	-25.860985	-5.6696
8	1	-25.849083	-5.8635
9	1	-25.467528	-5.7559



- Hydrogen bonds
- Ionic interactions
- Cation- π interactions
- Hydrophobic contacts
- π -stacking interactions
- Show protein surface
- Reset

- Best members
- By cluster

Number of displayed clusters:

Cluster number	Cluster member	AC Score	SwissParam Score
0	1	-33.945389	-6.3333
1	1	-29.502184	-6.1840

Baixe o resultado

files	Hoje, 23:35	--	Pasta
extra.par	Hoje, 23:28	2 KB	Documento
extra.rtf	Hoje, 23:28	4 KB	Documento RTF
ligand.pdb	Hoje, 23:35	2 KB	Docum...ext.app
receptor.crd	Hoje, 23:31	229 KB	Documento
receptor.pdb	Hoje, 23:31	248 KB	Docum...ext.app
receptor.psf	Hoje, 23:31	916 KB	Protein...ructure
parameters	Hoje, 23:35	219 bytes	Documento
result.dock4	Hoje, 23:44	184 KB	Documento

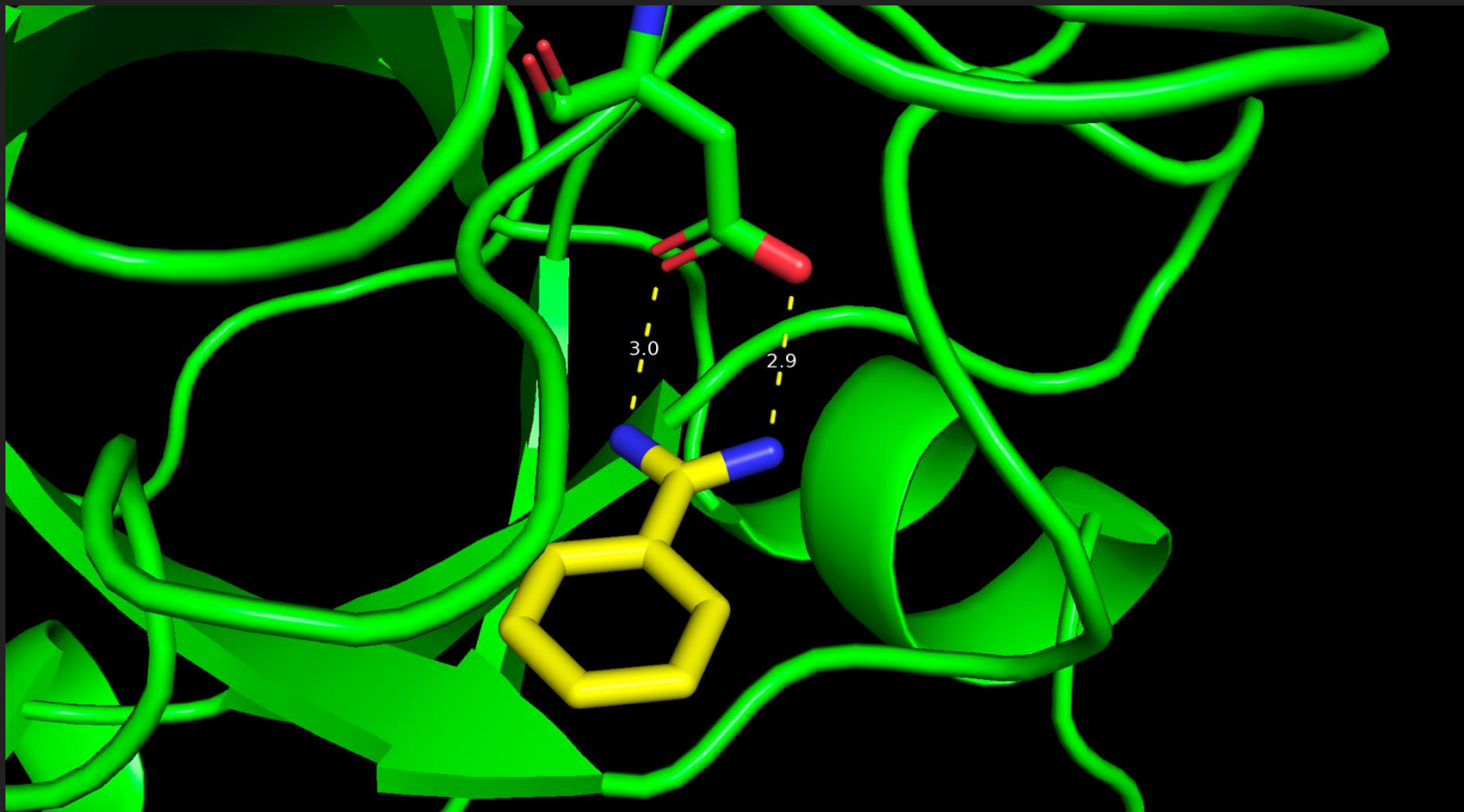
Altere o nome deste arquivo

files	Hoje, 23:35	--	Pasta
extra.par	Hoje, 23:28	2 KB	Documento
extra.rtf	Hoje, 23:28	4 KB	Documento RTF
ligand.pdb	Hoje, 23:35	2 KB	Docum...ext.app
receptor.crd	Hoje, 23:31	229 KB	Documento
receptor.pdb	Hoje, 23:31	248 KB	Docum...ext.app
receptor.psf	Hoje, 23:31	916 KB	Protein...ructure
parameters	Hoje, 23:35	219 bytes	Documento
result.pdb	Hoje, 23:44	184 KB	Docum...ext.app

```
result.pdb
1  REMARK FILE_NAME : seed-1-1-1-0-0.crd
2  REMARK CLUSTER_NUM : 0
3  REMARK CLUSTER_MEMBER : 1
4  REMARK MEMBER_ENERGY : -33.903193
5  REMARK MEMBER_SCORE : -33.903193
6  REMARK SP-dG : -6.3445
7  REMARK Polar : -2.9785
8  REMARK Nonpolar : -22.9619
9  REMARK Inter : -25.9404
10 REMARK Polar15 : -27.4297
11 REMARK RMSD : 75.4859
12 ATOM 3223 N1 LIG 1 57.013 43.537 19.577 1.00 1.85 LIG
13 ATOM 3224 C1 LIG 1 56.429 43.092 18.439 1.00 2.00 LIG
14 ATOM 3225 N2 LIG 1 56.079 41.865 18.420 1.00 1.85 LIG
15 ATOM 3226 C2 LIG 1 56.293 43.926 17.207 1.00 1.99 LIG
16 ATOM 3227 C3 LIG 1 55.986 43.299 15.986 1.00 1.99 LIG
17 ATOM 3228 C4 LIG 1 55.897 44.050 14.812 1.00 1.99 LIG
18 ATOM 3229 C5 LIG 1 56.106 45.430 14.848 1.00 1.99 LIG
19 ATOM 3230 C6 LIG 1 56.401 46.063 16.058 1.00 1.99 LIG
20 ATOM 3231 C7 LIG 1 56.494 45.316 17.236 1.00 1.99 LIG
21 ATOM 3232 H1 LIG 1 57.607 44.363 19.516 1.00 0.22 LIG
22 ATOM 3233 H2 LIG 1 57.400 42.813 20.191 1.00 0.22 LIG
23 ATOM 3234 H3 LIG 1 56.393 41.450 19.312 1.00 0.22 LIG
24 ATOM 3235 H4 LIG 1 55.817 42.228 15.941 1.00 1.32 LIG
25 ATOM 3236 H5 LIG 1 55.659 43.553 13.879 1.00 1.32 LIG
26 ATOM 3237 H6 LIG 1 56.025 46.016 13.940 1.00 1.32 LIG
27 ATOM 3238 H7 LIG 1 56.547 47.137 16.094 1.00 1.32 LIG
28 ATOM 3239 H8 LIG 1 56.691 45.824 18.172 1.00 1.32 LIG
29 TER
30
```

Vamos usar apenas a primeira pose, então apague as outras linhas após TER

Sticks amarelos indicam o resultado do docking (BEN)



Estrutura inicial:
1S0Q

Abra as estruturas no PyMOL

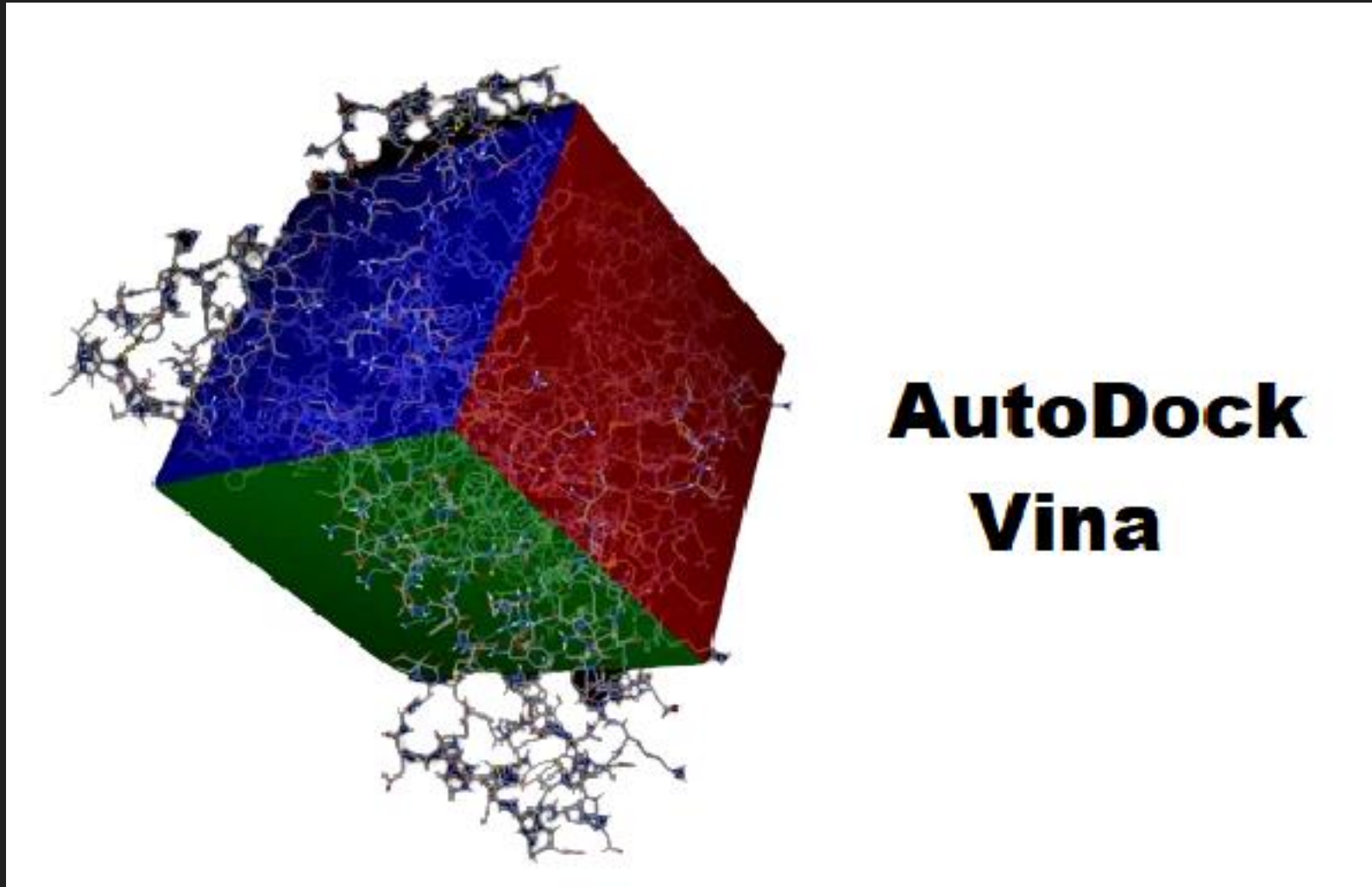
Estrutura sem ligante: 1S0Q

Estrutura com ligante: 3PTB



Comparação com a pose real

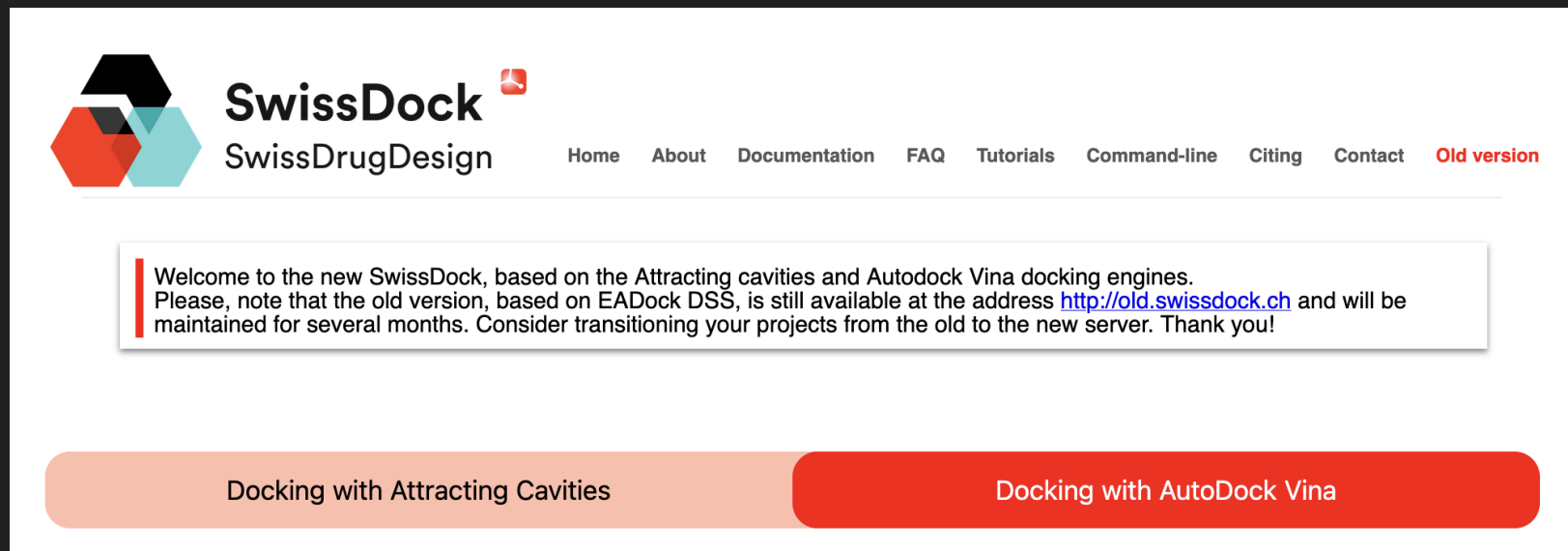
Agora vamos testar outra ferramenta bastante popular:




AutoDock Vina

- **AutoDock Vina** é um dos programas de **docking molecular** mais usados no mundo
- **Rápido, gratuito e de fácil uso**
- Funciona via linha de comandos
- Incorporado por outros software
- **Parâmetros:**
 - **center_x, center_y, center_z**
 - Centro da caixa de busca.
 - **size_x, size_y, size_z**
 - Dimensões da região onde o ligante pode explorar.
 - **exhaustiveness**
 - Define intensidade da busca (padrão: 8). Quanto maior, mais completo (mas mais lento).
 - **num_modes**
 - Número máximo de poses retornadas.

VINA



The screenshot shows the SwissDock website. At the top left is the logo, which consists of three overlapping hexagons in black, red, and teal. To the right of the logo is the text "SwissDock" in a large, bold, black font, with a small red square icon to its right. Below "SwissDock" is the text "SwissDrugDesign" in a smaller, black font. To the right of the logo and text is a horizontal navigation menu with the following items: "Home", "About", "Documentation", "FAQ", "Tutorials", "Command-line", "Citing", "Contact", and "Old version" (which is highlighted in red). Below the navigation menu is a white rectangular box with a thin border containing the following text: "Welcome to the new SwissDock, based on the Attracting cavities and Autodock Vina docking engines. Please, note that the old version, based on EADock DSS, is still available at the address <http://old.swissdock.ch> and will be maintained for several months. Consider transitioning your projects from the old to the new server. Thank you!". At the bottom of the page are two rounded rectangular buttons. The left button is light orange and contains the text "Docking with Attracting Cavities". The right button is red and contains the text "Docking with AutoDock Vina".

SwissDock 
SwissDrugDesign

Home About Documentation FAQ Tutorials Command-line Citing Contact **Old version**

Welcome to the new SwissDock, based on the Attracting cavities and Autodock Vina docking engines. Please, note that the old version, based on EADock DSS, is still available at the address <http://old.swissdock.ch> and will be maintained for several months. Consider transitioning your projects from the old to the new server. Thank you!

Docking with Attracting Cavities

Docking with AutoDock Vina

- SwissDock possui o Vina embutido (basta clicar na aba correspondente)

Repita a configuração anterior

1 - Submit a ligand

Provide a SMILES

... or upload a Mol2 file

... or input, or modify, or check the molecule **using the sketcher**

... or use the **advanced search**



2 - Submit a target

Provide a PDB id (e.g. 5hie)

Choose chain(s) to keep*:

Choose heteroatom(s) to keep*:

... or upload a PDB file

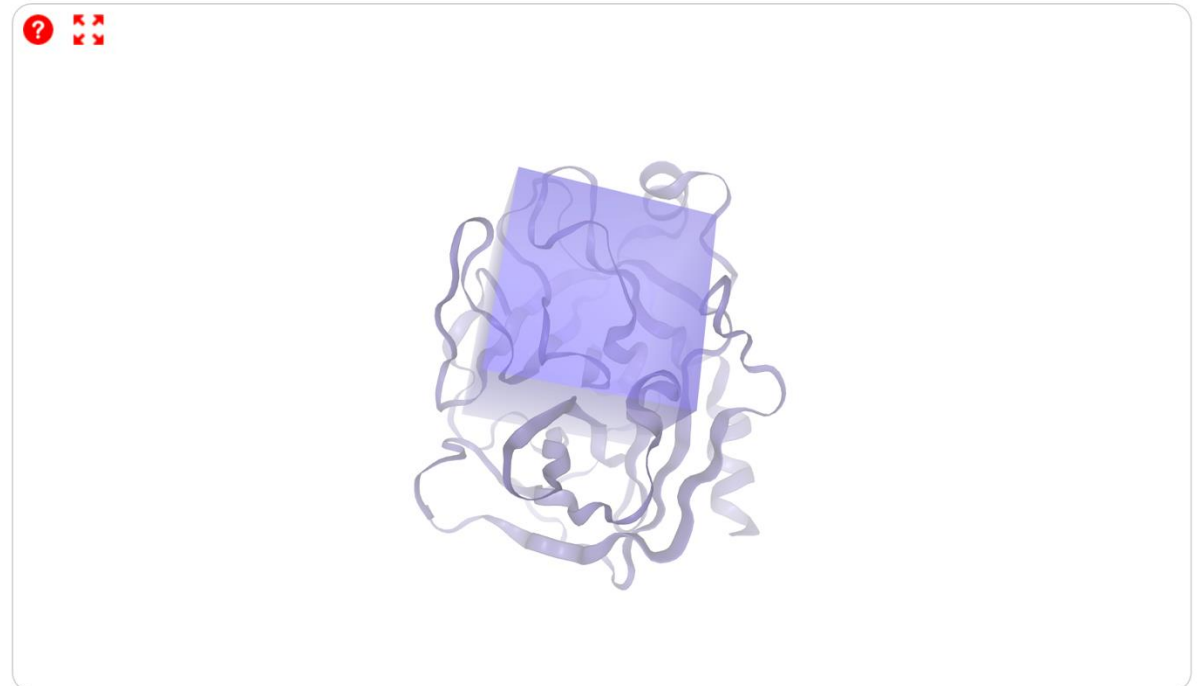
... or use the **advanced search**



3 - Define search space

Search box center Å

Search box size Å



VINA

○ Execute



[Home](#) [About](#) [Documentation](#) [FAQ](#) [Tutorials](#) [Command-line](#) [Citing](#) [Contact](#) [Old version](#)

Parameters:

Submission date: December 2, 2025, 2:40 am UTC
Docking name: VINA - Tripsina Benzamidina benzamidine
Ligand: N=C(N)c1ccccc1
Target: 1s0q_modified.pdb
Box center: 55 - 40 - 15
Box size: 20 - 20 - 20
Docking method: Vina
Sampling exhaustivity: 4
This job is estimated to take 0:00:10 (h:mm:ss).

Resultado



SwissDock
SwissDrugDesign



[Home](#) [About](#) [Documentation](#) [FAQ](#) [Tutorials](#) [Command-line](#) [Citing](#) [Contact](#) [Old version](#)

Query

Ligand N=C(N)c1ccccc1
Target 1s0q_modified.pdb
Method AutoDock Vina
Date December 2, 2025, 2:40 am UTC

Parameters:

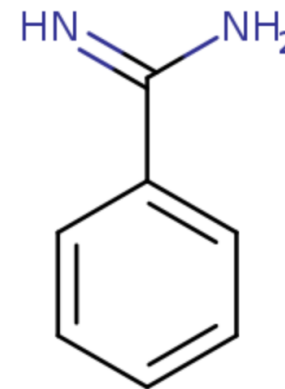
Box center: 55 - 40 - 15 Sampling exhaustivity: 4
Box size: 20 - 20 - 20

If you publish these results, please, cite the following papers:

Bugnon M, Röhrig UF, Goullieux M, Perez MAS, Daina A, Michielin O, Zoete V. SwissDock 2024: major enhancements for small-molecule docking with Attracting Cavities and AutoDock Vina. *Nucleic Acids Res.* **2024**

Eberhardt J, Santos-Martins D, Tillack AF, Forli S.. AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *J. Chem. Inf. Model.*, **2021**

Ligand



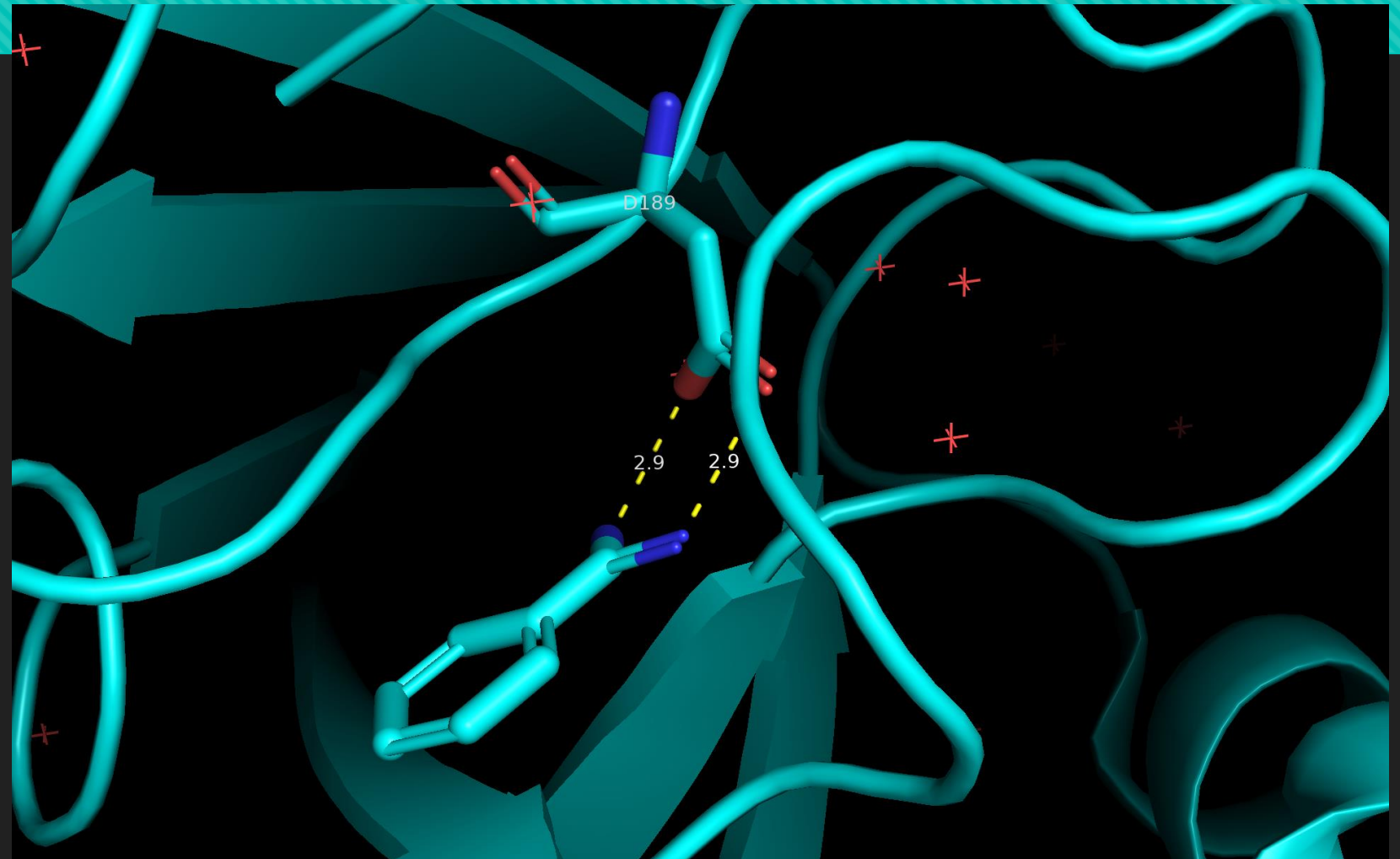
Resultado

- Vina retorna as energias de ligação das principais poses

Model	Calculated affinity (kcal/mol)
1	-5.496
2	-4.820
3	-4.477
4	-4.153
5	-4.050
6	-3.889
7	-3.530
8	-3.481
9	-3.481
10	-3.392
11	-3.195
12	-3.150
13	-2.618

Interação com D189

- Avaliar o resultado depende do contexto
- No caso da tripsina, sabemos que a ligação ocorre entre D189 e o ligante

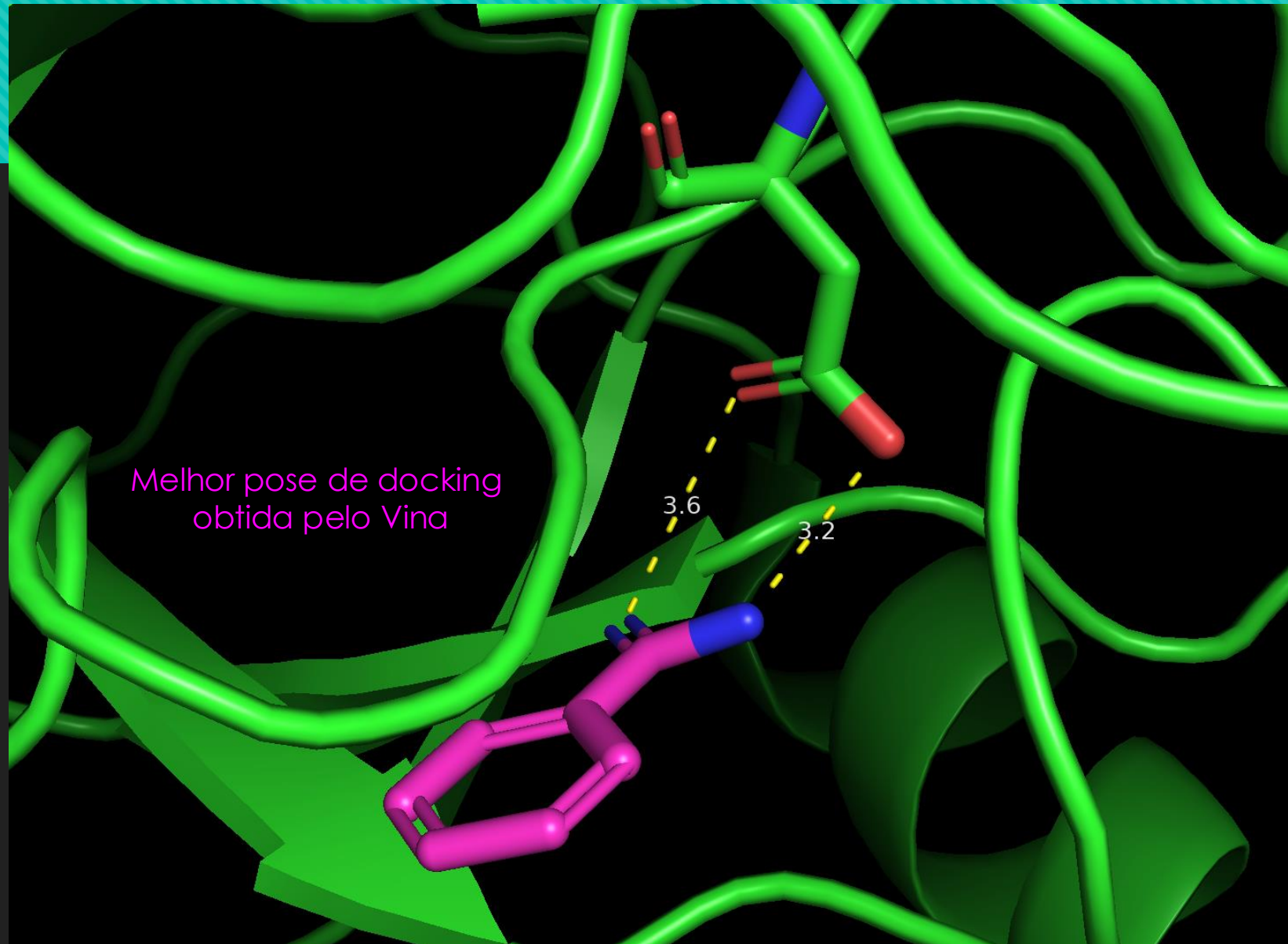


Estrutura com ligante: 3PTB

Dados reais

D830

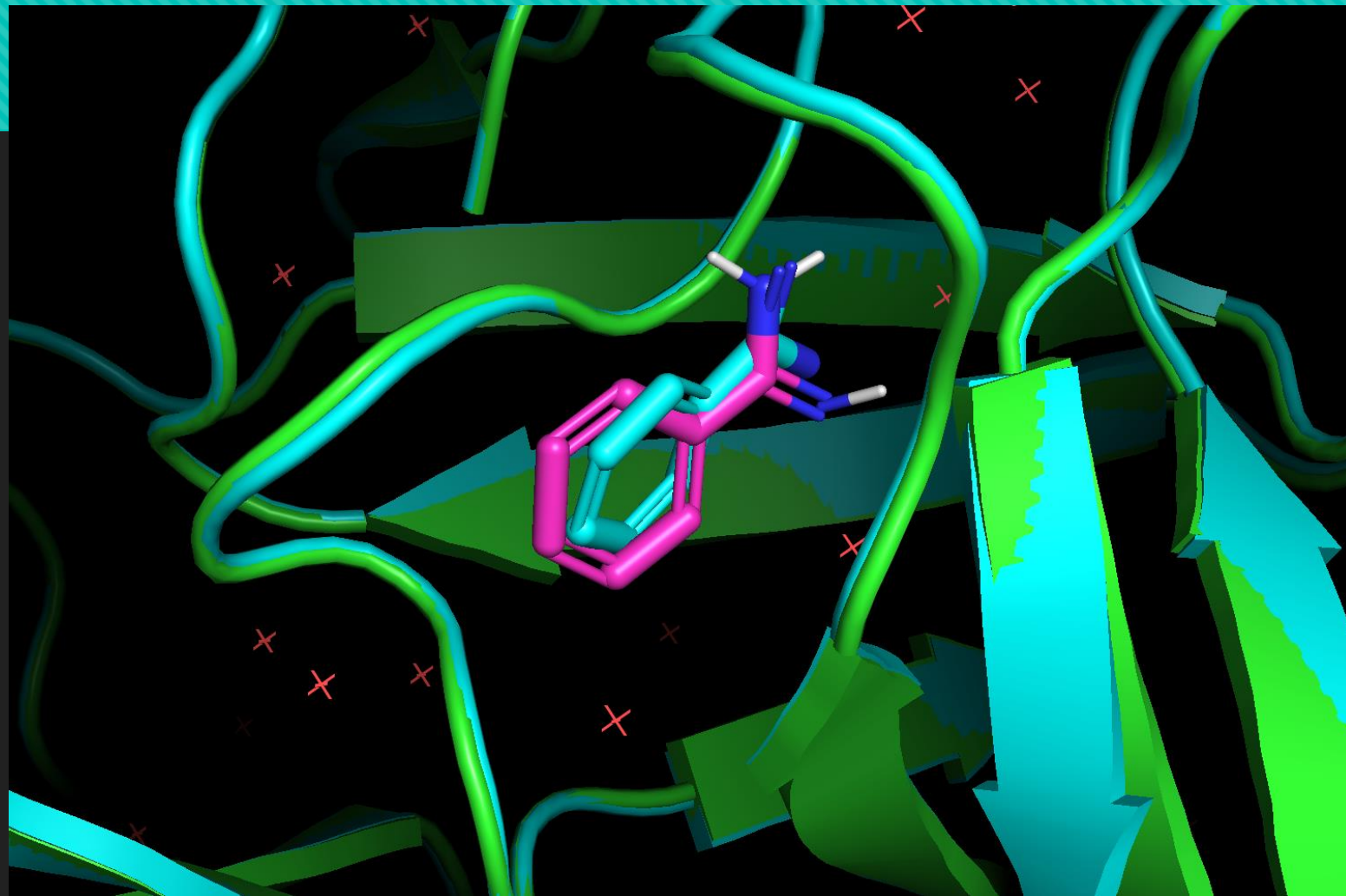
- Observe que o resíduo equivalente a D189 em 1s0q é D830



Estrutura sem ligante: 1S0Q

Comparação

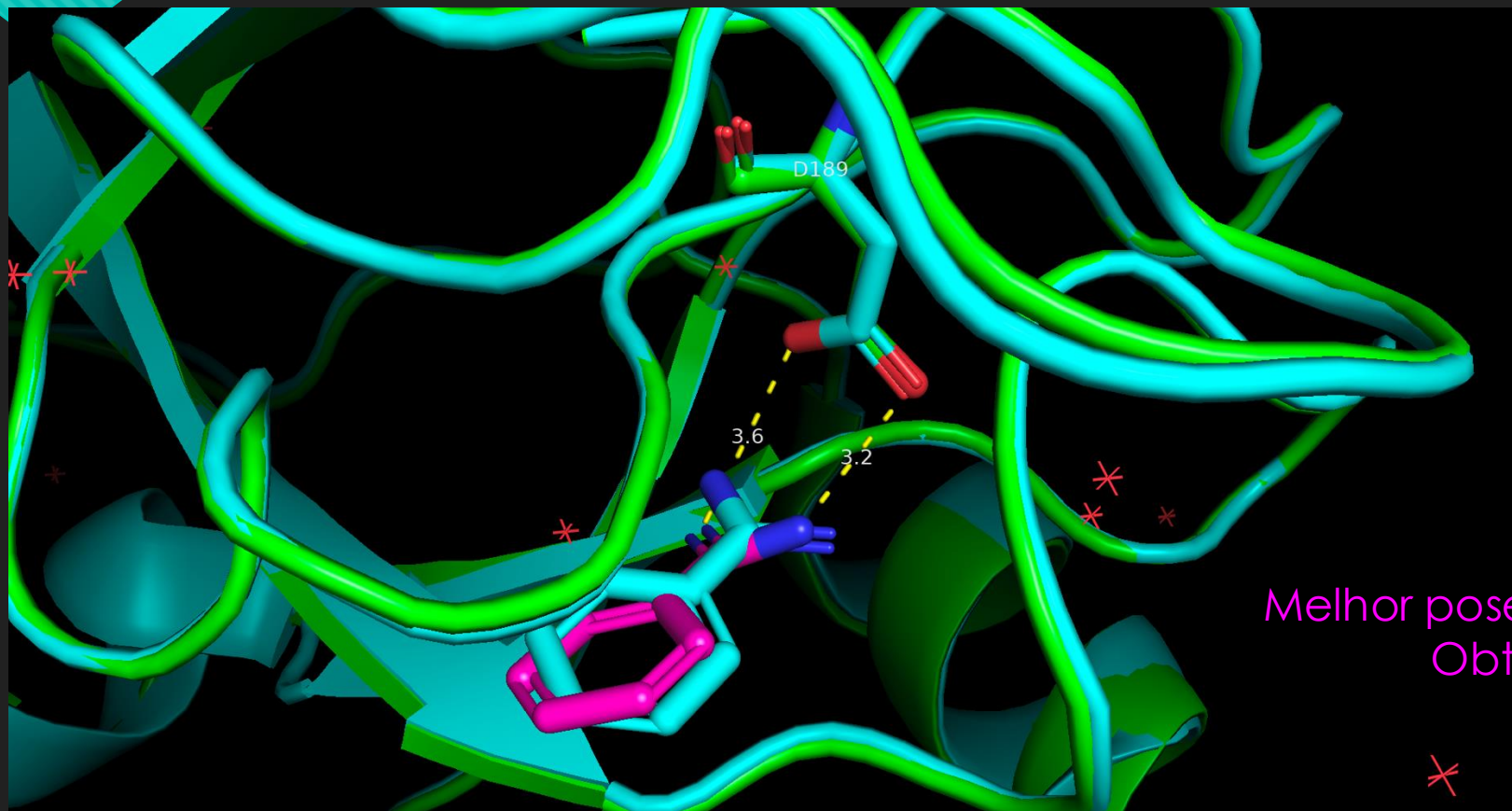
Melhor pose de docking
Obtida pelo Vina



Estrutura sem ligante: 1S0Q
Estrutura com ligante: 3PTB

hide sticks, hydro

Comparação

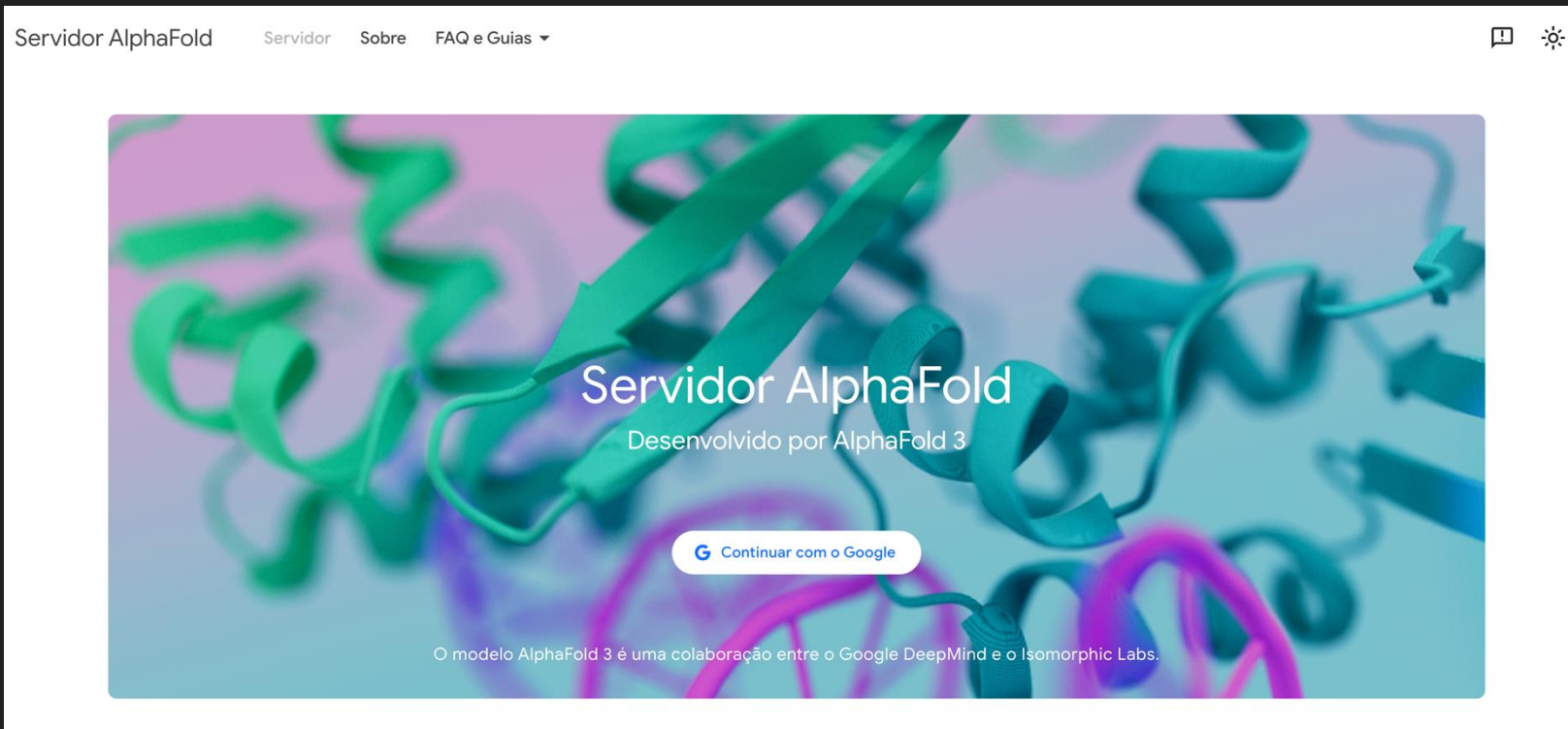


Estrutura sem ligante: 1S0Q
Estrutura com ligante: 3PTB

Melhor pose de docking
Obtida pelo Vina

Prática 2

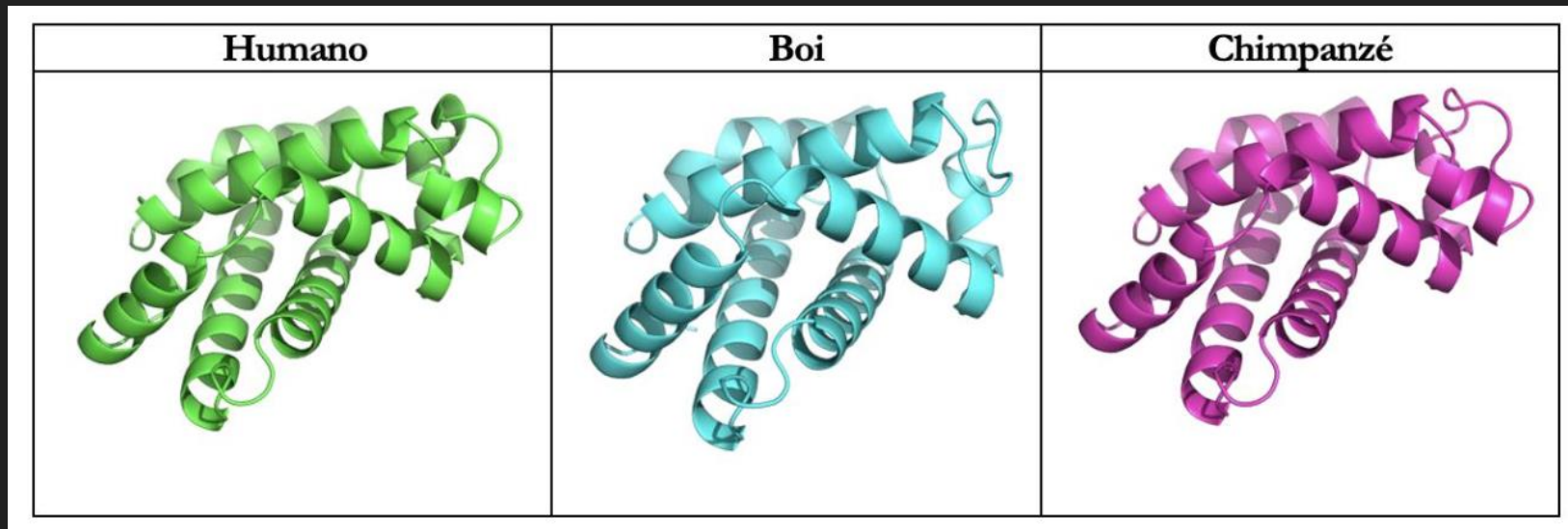
- “Docking” com AlphaFold
- Não é um docking, mas uma modelagem completa da estrutura prevendo a pose de ligação do ligante



<https://alphafoldserver.com>




Exemplo: hemoglobina

- Anteriormente modelamos a hemoglobina bovina, mas ela não tinha um grupo **heme**



Boi
MVLSAADKGNVKAAWGKVG
GHAAEYGAEALERMFLSFP
TTKTYFPHFDLSHGSAQVK
GHGAKVAAALTKAVEHLDD
LPGALSELSDLHAHKLRVD
PVNFKLLSHSLLVTLASHL
PSDFTPAVHASLDKFLANV
STVLTSKYR

Docking do grupo heme usando AlphaFold

AlphaFold Server [Server](#) [About](#) [FAQ & Guides](#)   

Entity type: Protein Copies: 1

Entity type: Ligand Copies: 1

[+ Add entity](#) [Save job](#)

[Continue and preview job](#)

Job name*

hemoglobina do boi docado com grupo heme

Seed: Auto

Seed



Type	Copies	Sequence
Protein	1	MVLSAADKGNVKAAWGKVGGHAAEYGA EAL... (length 142)
Ligand	1	HEM – Heme

Remaining jobs: 30

[Go back and edit this job](#)

[Confirm and submit job](#)

Resultado:

Search History			
<input checked="" type="checkbox"/> Completed <input checked="" type="checkbox"/> Saved draft <input checked="" type="checkbox"/> In progress <input checked="" type="checkbox"/> Examples <input checked="" type="checkbox"/> Failed			
<input type="checkbox"/>	Name	Modified	
<input type="checkbox"/>	hemoglobina do boi docado com grupo heme	2025-11-30 12:26	⋮
<input type="checkbox"/>	<input checked="" type="checkbox"/> 2024-05-08_19:09	2024-05-08 19:12	⋮

Items per page: 10

Resultado

AlphaFold Server

Server About FAQ & Guides

hemoglobina do boi docado com grupo heme

[← Back](#) [↓ Download](#) [📄 Clone and reuse](#) [📧 Feedback on structure](#)

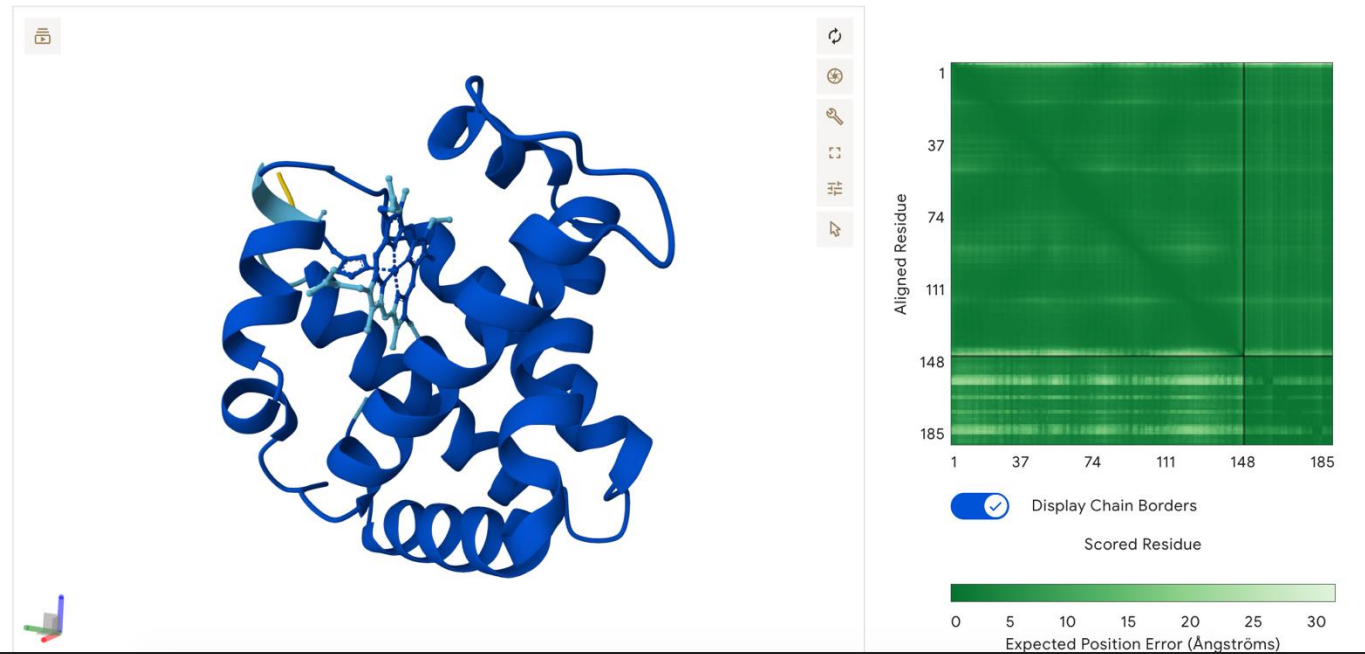
Very high (pLDDT > 90)

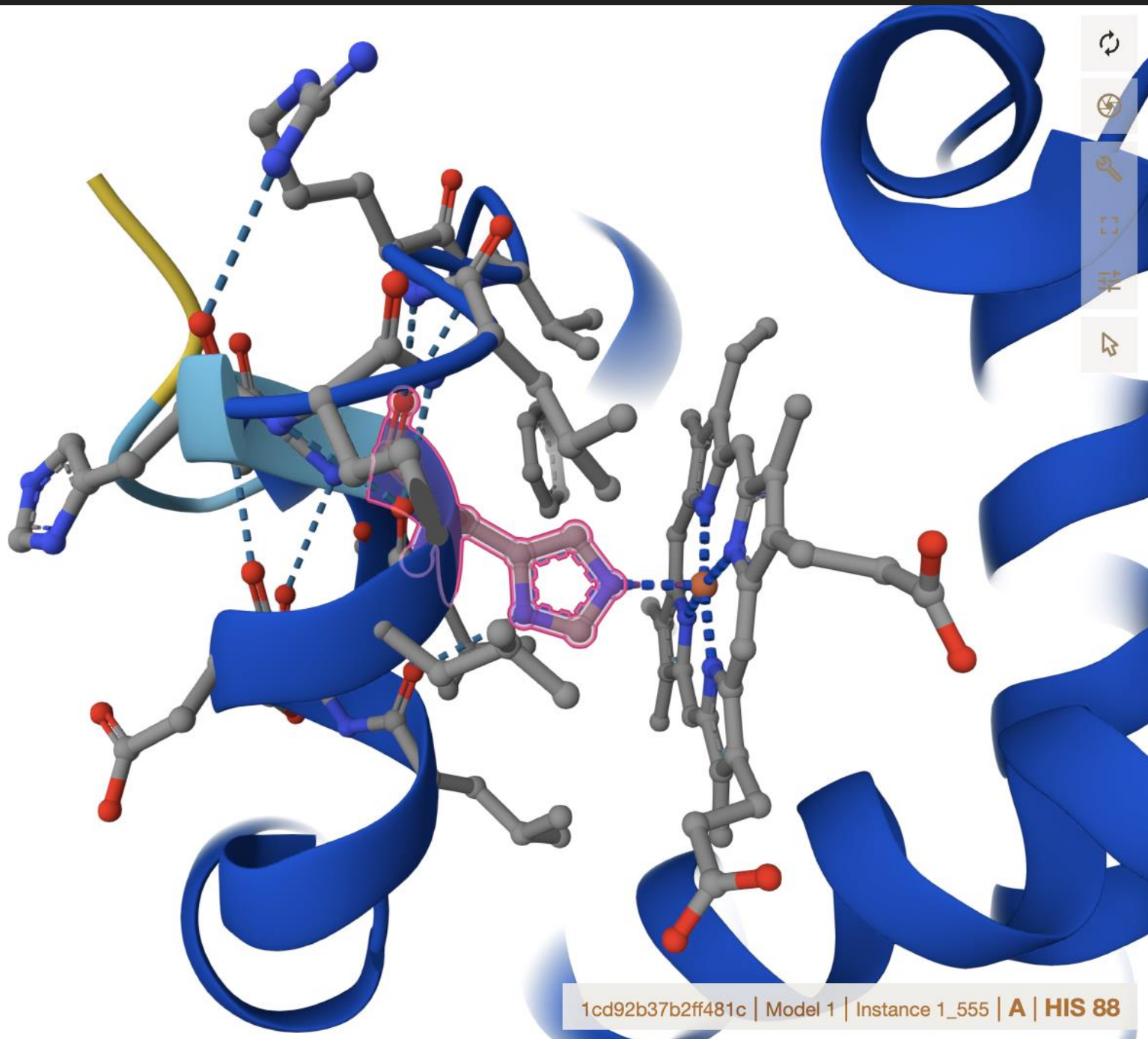
Confident (90 > pLDDT > 70)

Low (70 > pLDDT > 50)

Very low (pLDDT < 50)

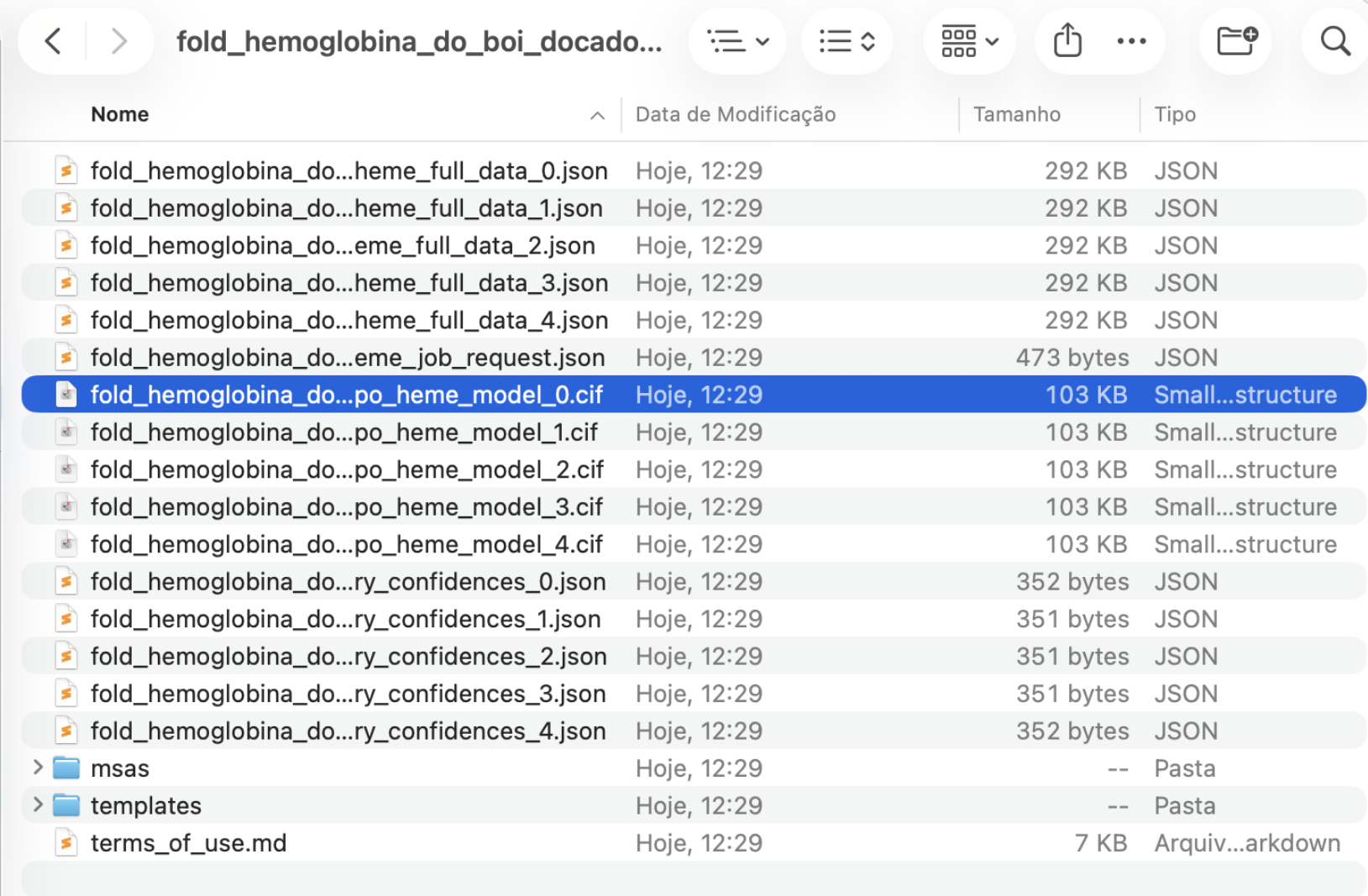
ipTM = 0.87 pTM = 0.91 [learn more](#)





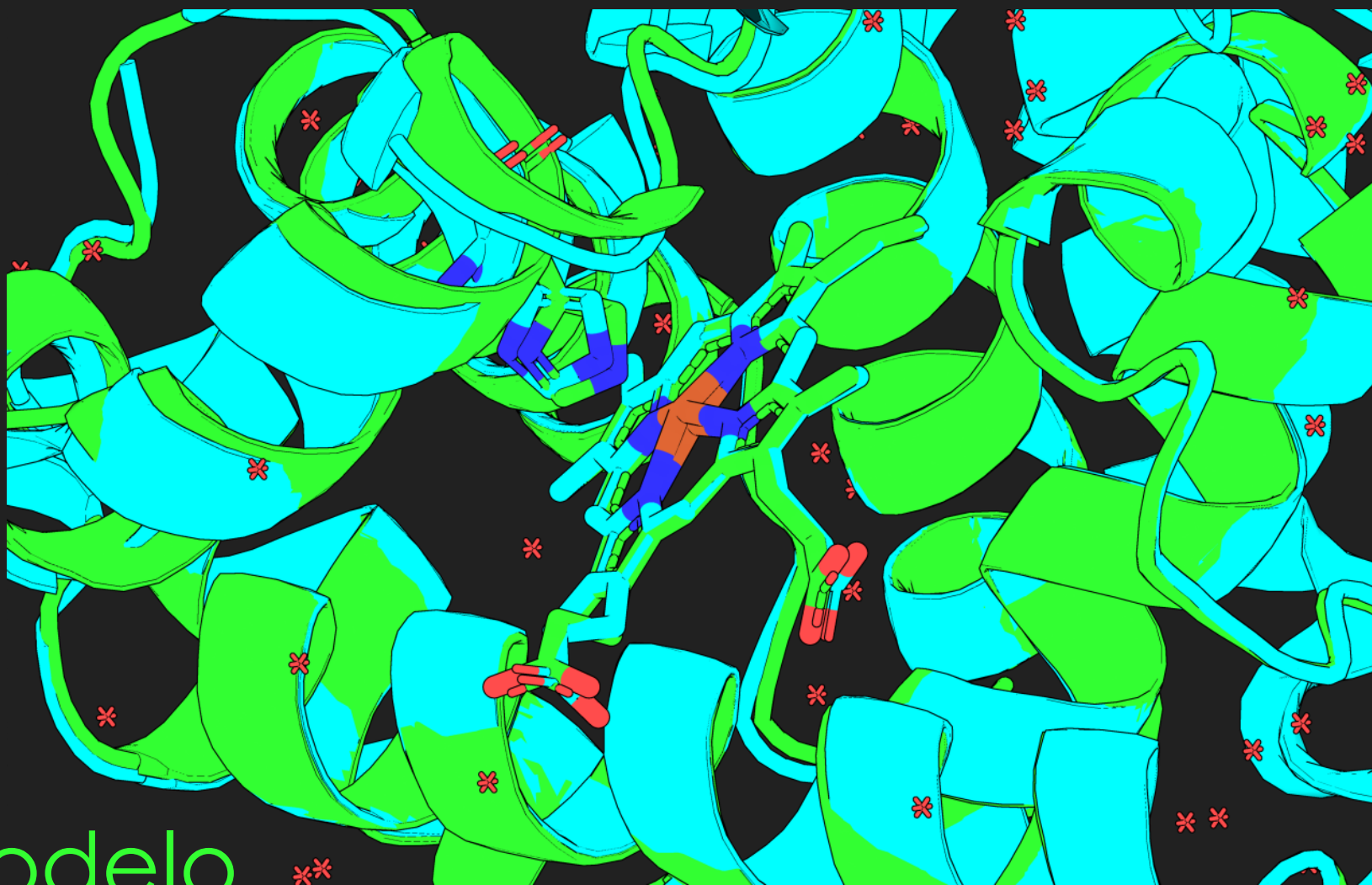
Observe a ligação com H88
(resíduo considerado importante)

hemoglobina do boi docado com grupo heme

[← Back](#)[Download](#)[Clone and reuse](#)[Feedback on structure](#)

fold_hemoglobina_do_boi_docado...

Nome	Data de Modificação	Tamanho	Tipo
fold_hemoglobina_do...heme_full_data_0.json	Hoje, 12:29	292 KB	JSON
fold_hemoglobina_do...heme_full_data_1.json	Hoje, 12:29	292 KB	JSON
fold_hemoglobina_do...eme_full_data_2.json	Hoje, 12:29	292 KB	JSON
fold_hemoglobina_do...heme_full_data_3.json	Hoje, 12:29	292 KB	JSON
fold_hemoglobina_do...heme_full_data_4.json	Hoje, 12:29	292 KB	JSON
fold_hemoglobina_do...eme_job_request.json	Hoje, 12:29	473 bytes	JSON
fold_hemoglobina_do...po_heme_model_0.cif	Hoje, 12:29	103 KB	Small...structure
fold_hemoglobina_do...po_heme_model_1.cif	Hoje, 12:29	103 KB	Small...structure
fold_hemoglobina_do...po_heme_model_2.cif	Hoje, 12:29	103 KB	Small...structure
fold_hemoglobina_do...po_heme_model_3.cif	Hoje, 12:29	103 KB	Small...structure
fold_hemoglobina_do...po_heme_model_4.cif	Hoje, 12:29	103 KB	Small...structure
fold_hemoglobina_do...ry_confidences_0.json	Hoje, 12:29	352 bytes	JSON
fold_hemoglobina_do...ry_confidences_1.json	Hoje, 12:29	351 bytes	JSON
fold_hemoglobina_do...ry_confidences_2.json	Hoje, 12:29	351 bytes	JSON
fold_hemoglobina_do...ry_confidences_3.json	Hoje, 12:29	351 bytes	JSON
fold_hemoglobina_do...ry_confidences_4.json	Hoje, 12:29	352 bytes	JSON
> msas	Hoje, 12:29	--	Pasta
> templates	Hoje, 12:29	--	Pasta
terms_of_use.md	Hoje, 12:29	7 KB	Arquiv...arkdown



Modelo **

PDB (1A00)

Docking proteína-peptídeo

- Visa detectar a interface de interação entre proteínas
- Orienta a posição de uma proteína em relação a outra
- Mais complexo

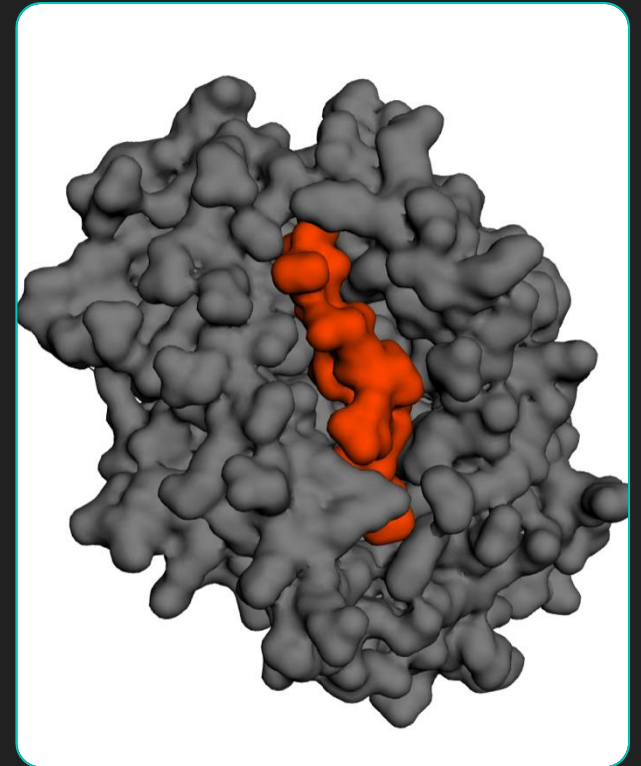
Docking usando AlphaFold-Multimer

- Podemos usar o ColabFold para modelar complexos proteína-proteína ou proteína-peptídeo
- AlphaFold-Multimer é uma versão do AlphaFold desenvolvida para prever estruturas de complexos proteicos
- Ou seja, interações entre duas ou mais proteínas (dímeros, trímeros, tetrâmeros etc.)
- Podemos usá-lo para prever complexos proteína-peptídeo

Exemplo

	Protein	Peptide
Chain ?	A	C
Description ?	HLA class I histocompatibility antigen, BW-53 B*5301 alpha chain	PEPTIDE TPYDINQML
Length (residues) ?	278	9

- Calmodulina complexada com um peptídeo da proteína quinase humana
- **PDB ID: 1A1M**



Sequências

○ Proteína

○ Peptídeo

Sequência ?

GSMSRYFYTAMSRPGRGEPRIAVGYVDDTQFVRFSDA
ASPRTEPRPPWIEQEGPEYWRNTQIFKTNTQTYRENLRI
ALRYYNQSEAGSHIIQRMYGCDLGPDRLLRGHDQSAYDG
KDYIALNEDLSSWTAADTAAQITQRKWEARVAEQLRAYL
EGLCWEVLRRYLENGKETLQRADPPKTHVTHHPVSDHEAT
LRCWALGFYPAEITLTWQRDGEDQTQDTELVETRPAGDRT
FQKWA AVVPSGEEQRYTCHVQHEGLPKPLTLRWEPPH

TPYDINQML

Una as sequências usando um símbolo de
dois-pontos entre elas:

GSMSMRYFYTAMSRPGRGEPRIAVGYVDDTQFVRFDSDAASPRTEPRP
PWIEQEGPEYWRNTQIFKTNTQTYRENLRIALRYYNQSEAGSHIIQRM
YGCDLGPDGRLLRGHDQSAYDGKDYIALNEDLSSWTAADTAAQITQRKW
EAARVAEQLRAYLEGLCVELRRYLENGKETLQRADPPKTHVTHHPVSD
HEATLRCWALGFYPAEITLTWQRDGEDQTQDTELVETRPAGDRTFQKWA
AVVVPSGEEQRYTCHVQHEGLPKPLTLRWEPPH:TPYDINQML

AlphaFold2.ipynb [Salve no GitHub para manter as alterações](#)

Arquivo Editar Ver Inserir Ambiente de execução Ferramentas Ajuda

Comandos + Código + Teclados

- Executar tudo ⌘/Ctrl+F9
- Executar antes ⌘/Ctrl+F8

easy to use protein structure prediction

Input protein sequence(s), then hit `Runtime` -> `Run all`

query_sequence: "GSHSMRYFYTAMSRPGRGEPRIAVGYVDDTQFVRFSDAASPRTEPRPPWIEQEGPEYWRNTQIFKTNQTYRENLRALRYYNQSEAGSHIIQRMYGCDLGPDRLLRGHDQSAYDGKDYIAL"

- Use `:` to specify inter-protein chainbreaks for **modeling complexes** (supports homo- and hetro-oligomers). For example `PI...SK:PI...SK` for a homodimer

jobname: "proteina-peptideo"

num_relax: 0

- specify how many of the top ranked structures to relax using amber

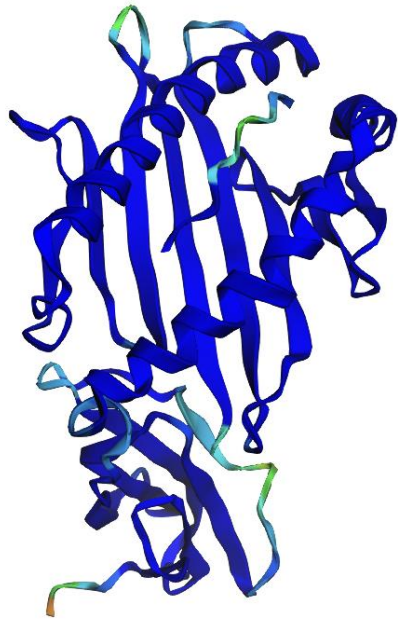
template_mode: none

- `none` = no template information is used. `pdb100` = detect templates in pdb100 (see [notes](#)). `custom` - upload and search own templates (PDB or mmCIF format, see [notes](#))

[Mostrar código](#)

<https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb>

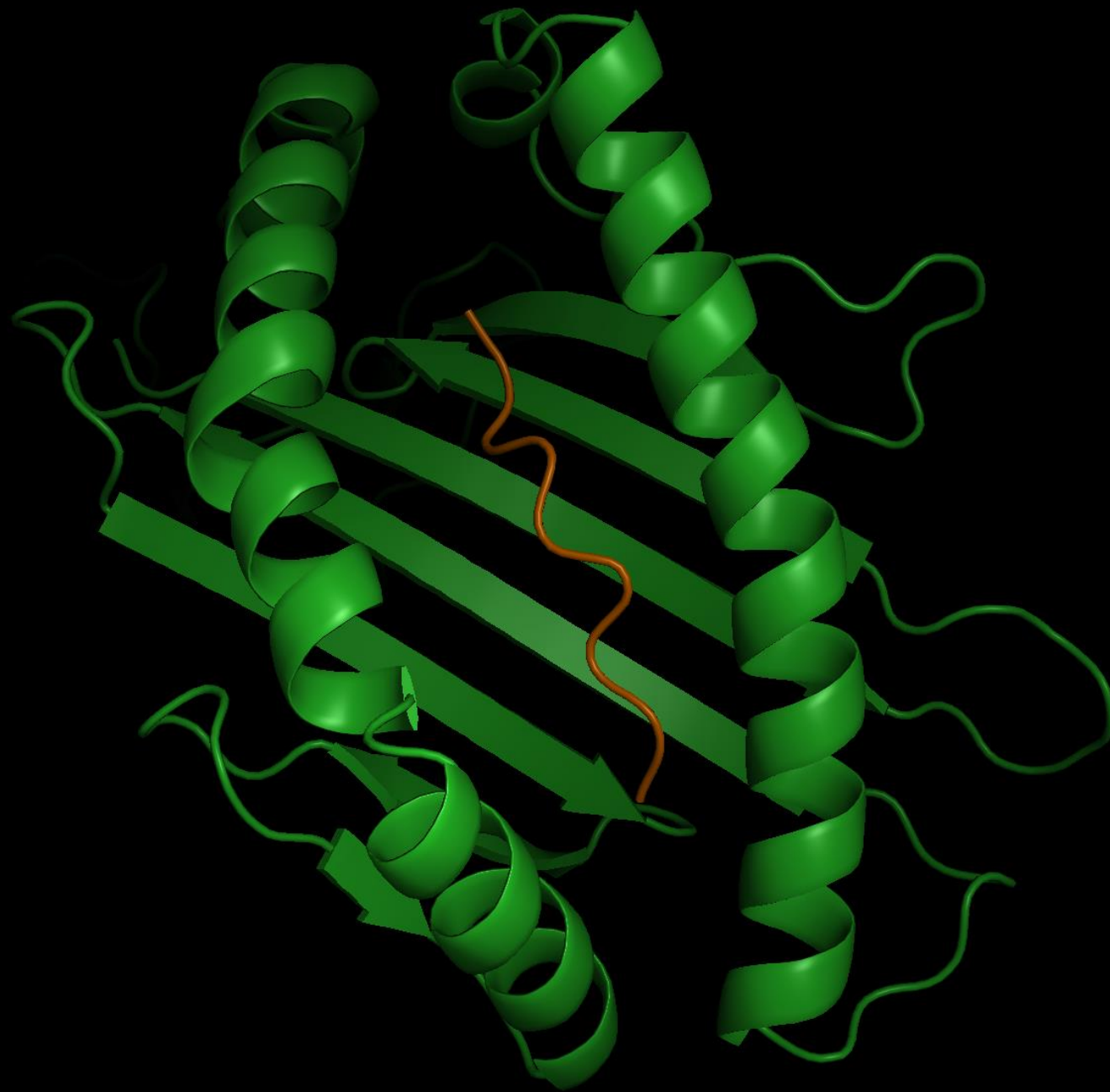
Resultado



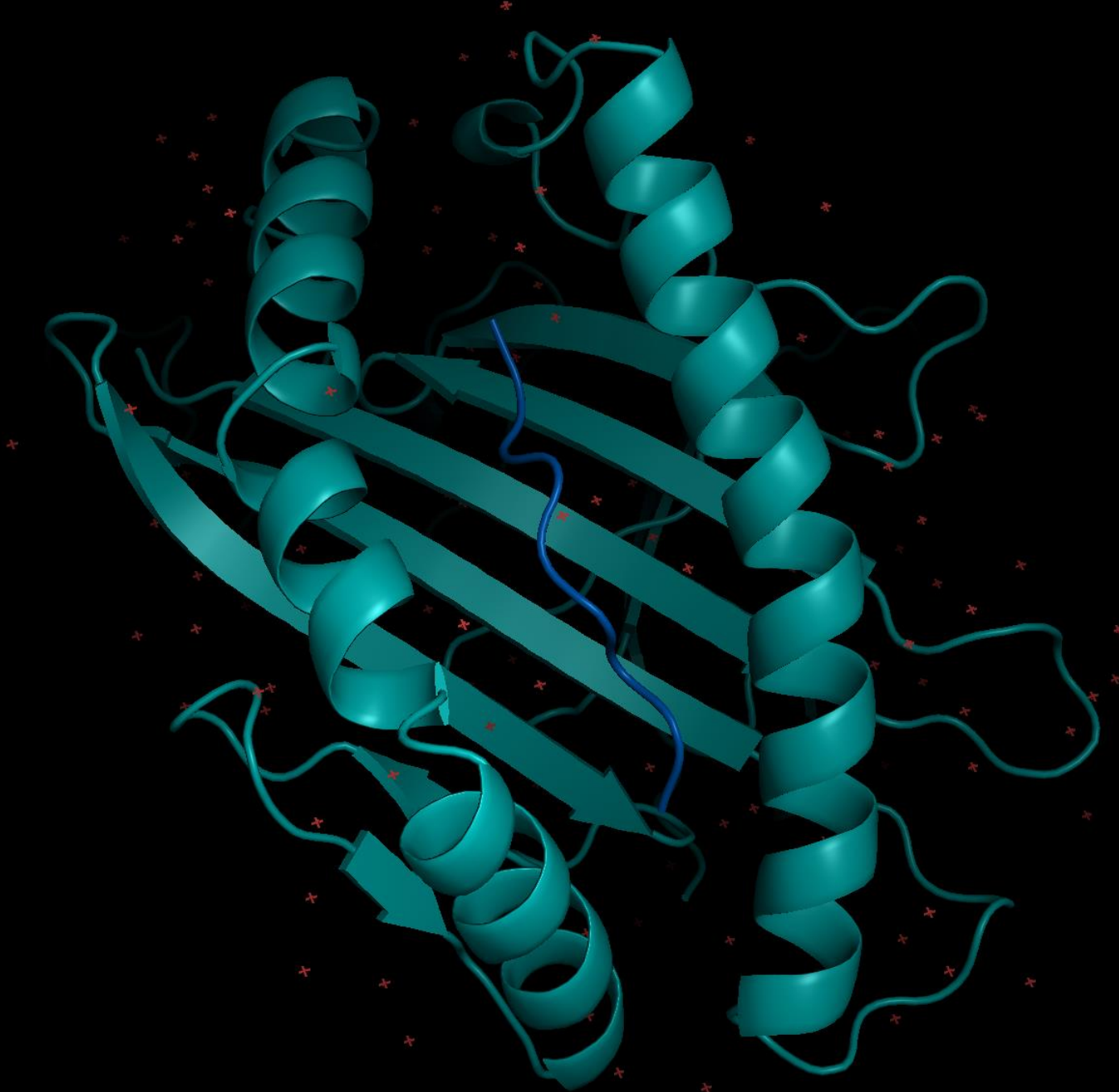
pI DDT: ■ Very low (<50) ■ Low (60) ■ OK (70) ■ Confident (80) ■ Very high (>90)

Baixe o resultado

Nome	Data de Modificação	Tamanho	Tipo
cite.bibtex	Hoje, 09:45	2 KB	BibTeX...cument
config.json	Hoje, 09:45	1 KB	JSON
log.txt	Hoje, 09:55	4 KB	texto
proteinapeptideo_a8c9e_coverage.png	Hoje, 09:47	89 KB	Imagem PNG
proteinapeptideo_a8c9e_env	Hoje, 09:47	--	Pasta
proteinapeptideo_a8c9e_pae.png	Hoje, 09:55	448 KB	Imagem PNG
proteinapeptideo_a8c9e_pairgreedy	Hoje, 09:47	--	Pasta
proteinapeptideo_a8c9e_plddt.png	Hoje, 09:55	125 KB	Imagem PNG
proteinapeptideo_a8c9e...ted_aligned_error_v1.json	Hoje, 09:55	505 KB	JSON
proteinapeptideo_a8c9e..._model_3_seed_000.json	Hoje, 09:52	507 KB	JSON
proteinapeptideo_a8c9e..._model_5_seed_000.json	Hoje, 09:55	502 KB	JSON
proteinapeptideo_a8c9e..._model_4_seed_000.json	Hoje, 09:54	500 KB	JSON
proteinapeptideo_a8c9e..._model_1_seed_000.json	Hoje, 09:50	501 KB	JSON
proteinapeptideo_a8c9e..._model_2_seed_000.json	Hoje, 09:51	502 KB	JSON
proteinapeptideo_a8c9e..._model_3_seed_000.pdb	Hoje, 09:52	191 KB	Docum...ext.app
proteinapeptideo_a8c9e..._model_5_seed_000.pdb	Hoje, 09:55	191 KB	Docum...ext.app
proteinapeptideo_a8c9e..._model_4_seed_000.pdb	Hoje, 09:54	191 KB	Docum...ext.app
proteinapeptideo_a8c9e..._model_1_seed_000.pdb	Hoje, 09:50	191 KB	Docum...ext.app
proteinapeptideo_a8c9e..._model_2_seed_000.pdb	Hoje, 09:51	191 KB	Docum...ext.app
proteinapeptideo_a8c9e.a3m	Hoje, 09:47	4,1 MB	Documento
proteinapeptideo_a8c9e.csv	Hoje, 09:42	323 bytes	valores...vírgula
proteinapeptideo_a8c9e.done.txt	Hoje, 09:55	Zero bytes	texto

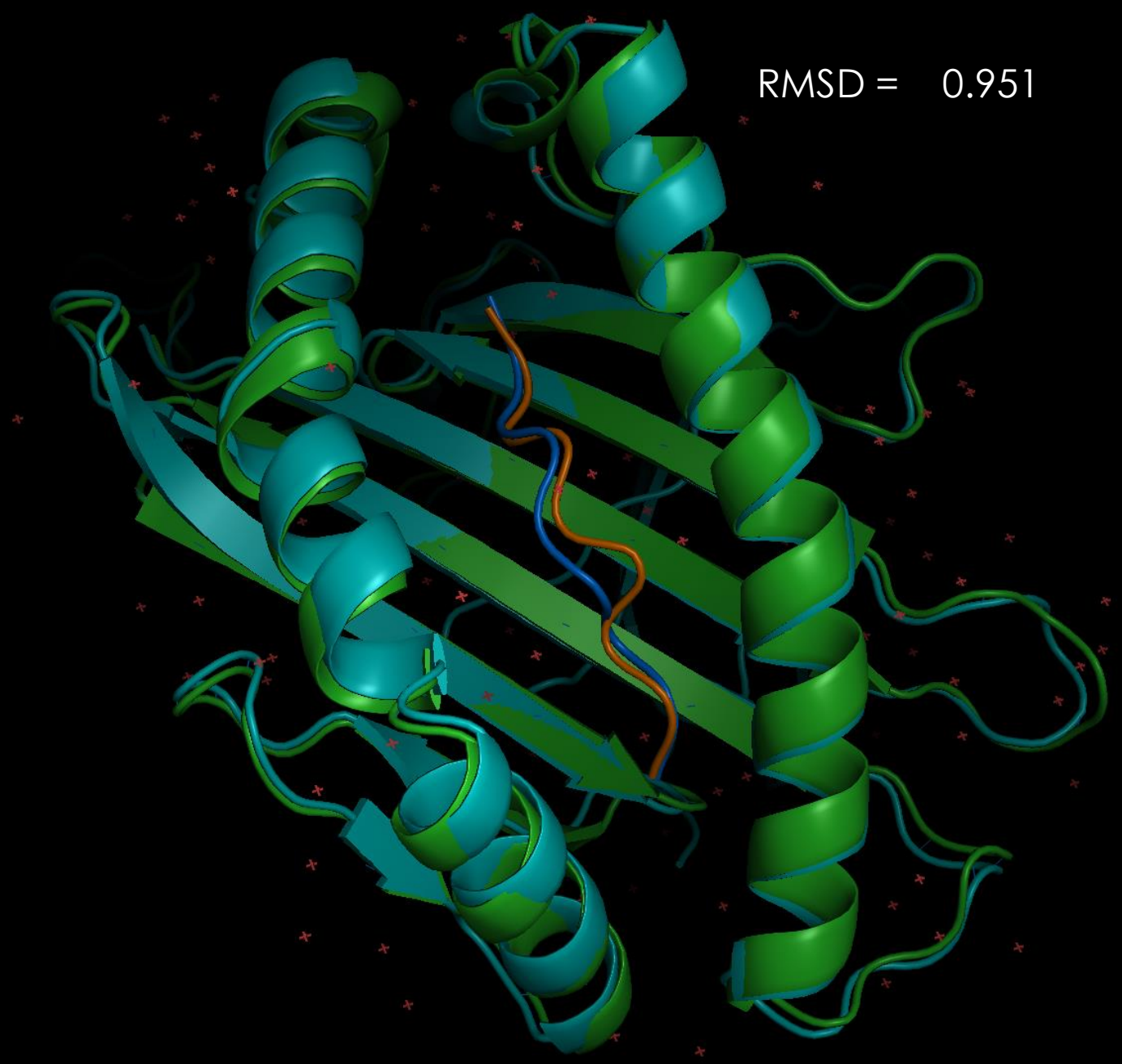


Estrutura predita pelo AlphaFold



Estrutura real (pdb: 1a1m)

RMSD = 0.951



Comparação

Exercício

Crie um peptídeo com o seu nome. Faça docking contra a proteína de 1a1m.

EXEMPLO:

GSHSMRYFYTAMSRPGRGEPRIAVGYVDDTQFVRFDSDAASPRTEPRPPW
IEQEGPEYWRNTQIFKTNTQTYRENLRIRYRNQSEAGSHIIQRMYGCD
LGPDGRLLRGHDQSAYDGKDYIALNEDLSSWTAADTAAQITQRKWEARVA
EQLRAYLEGLCVEWLRRYLENGKETLQRADPPKTHVTHHPVSDHEATLRW
ALGFYPAEITLTWQRDGEDQTQDTELVETRPAGDRTFQKWAAVVPSGEEQ
RYTCHVQHEGLPKPLTLRWEPHH:**DIEG**

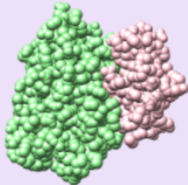
Docking proteína-peptídeo

com HDOCK

Advanced Options (Optional):

- Template-free docking only [Explanation]
- Symmetric multimer docking: (e.g., **C2** or **C3** for Cyclic; **D2** or **D3** for Dihedral) [Note]
- SAXS experimental data file: Nenhum ar...o escolhido [help] [example]
- Specify the residues of the binding site.

Não seguro hdock.phys.hust.edu.cn



HDOCK SERVER

Protein-protein and protein-DNA/RNA docking based on a hybrid algorithm of template-based modeling and *ab initio* free docking.

[\[Huang_Lab\]](#) [\[HDOCK\]](#) [\[Help\]](#) [\[Output example\]](#)

Input Receptor Molecule using **ONE** of the following four options: [\[help\]](#)

- Upload your **pdb** file in **PDB format**: Nenhum ar...o escolhido [\[example\]](#)
- OR** provide your **pdb** file in PDB ID:ChainID: (Example: **1CGI:E**)
- OR** copy and paste your **sequence** below in **FASTA format** (Sample input: **1CGI:E**, **1HCJ:A**)

```
GSMSRYFYTAMSRPGRGEPRFIAVGYVDDTQFVRFSDAASPRTEPRPPWIEQEGPEYWRNTQIFKNTQTYRENLRIALRYNQSEAGSHIIQRMYGC  
DLGPDGRLLRGHDQSAIDGKDYIALNEDLSSWTAADTAAQITQRKWEAARVAEQLRAYLEGLCWEVLRRLRYLENGKETLQRADPPKTHVTHHPVSDHEATLR  
CWALGFYPAEITLTWQRDGEDQTQDELVETRPAGDRTFQKWAAVVPSGEEQRYTCHVQHEGLPKPLTLRWEPHH
```
- OR** upload your **sequence** file in **FASTA format**: Nenhum ar...o escolhido [\[example\]](#)

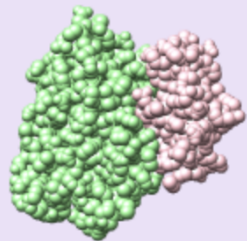
Input Ligand Molecule using **ONE** of the following four options: [\[help\]](#)

- Upload your **pdb** file in **PDB format**: Nenhum ar...o escolhido [\[example\]](#)
- OR** provide your **pdb** file in PDB ID:ChainID: (Example: **1CGI:I**)
- OR** copy and paste your **sequence** below in **FASTA format** (Sample input: **1CGI:I**) [\[help\]](#)

```
TPYDINQML
```
- OR** upload your **sequence** file in **FASTA format**: Nenhum ar...o escolhido [\[example\]](#)

TPYKINQML

mutação



HDOCK SERVER

Protein-protein and protein-DNA/RNA docking based on a hybrid algorithm of template-based modeling and *ab initio* free docking.

[\[Huang Lab\]](#) [\[HDOCK\]](#) [\[Help\]](#) [\[Output example\]](#)

Your HDOCK job *proteina-ligante* is QUEUED.

This page is automatically refreshed every 10 seconds. If the page hangs, you may press F5 to manually refresh this page anytime.

Your results will be shown on this page once your job is finished.

You can **bookmark this page** and access the results later.

If you have provided a valid email address, you will be also notified by email when your job is finished.

Your HDOCK results are stored for two weeks.



HDOCK SERVER

Protein-protein and protein-DNA/RNA docking based on a hybrid algorithm of template-based modeling and *ab initio* free docking.

[\[Huang Lab\]](#) [\[HDOCK\]](#) [\[Help\]](#) [\[Output example\]](#)

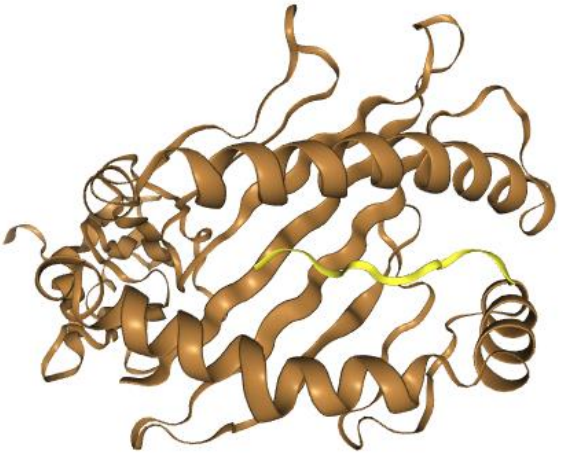
Your HDOCK results for job *proteina-ligante*

Download Files

[Receptor PDB file](#) [Ligand PDB file](#)

[\[1\]](#) [\[2\]](#) [\[3\]](#) [\[4\]](#) [\[5\]](#) [\[6\]](#) [\[7\]](#) [\[8\]](#) [\[9\]](#) [\[10\]](#) [\[11\]](#) [\[12\]](#) [\[13\]](#) [\[14\]](#) [\[15\]](#) [\[16\]](#) [\[17\]](#) [\[18\]](#) [\[19\]](#) [\[20\]](#)

[Top 10 Predictions](#) [Top 100 Predictions](#) [All the results in a package](#)



Receptor style
Cartoon

Receptor color
 Pure
 Rainbow

MODEL No.
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10

Ligand style
Cartoon

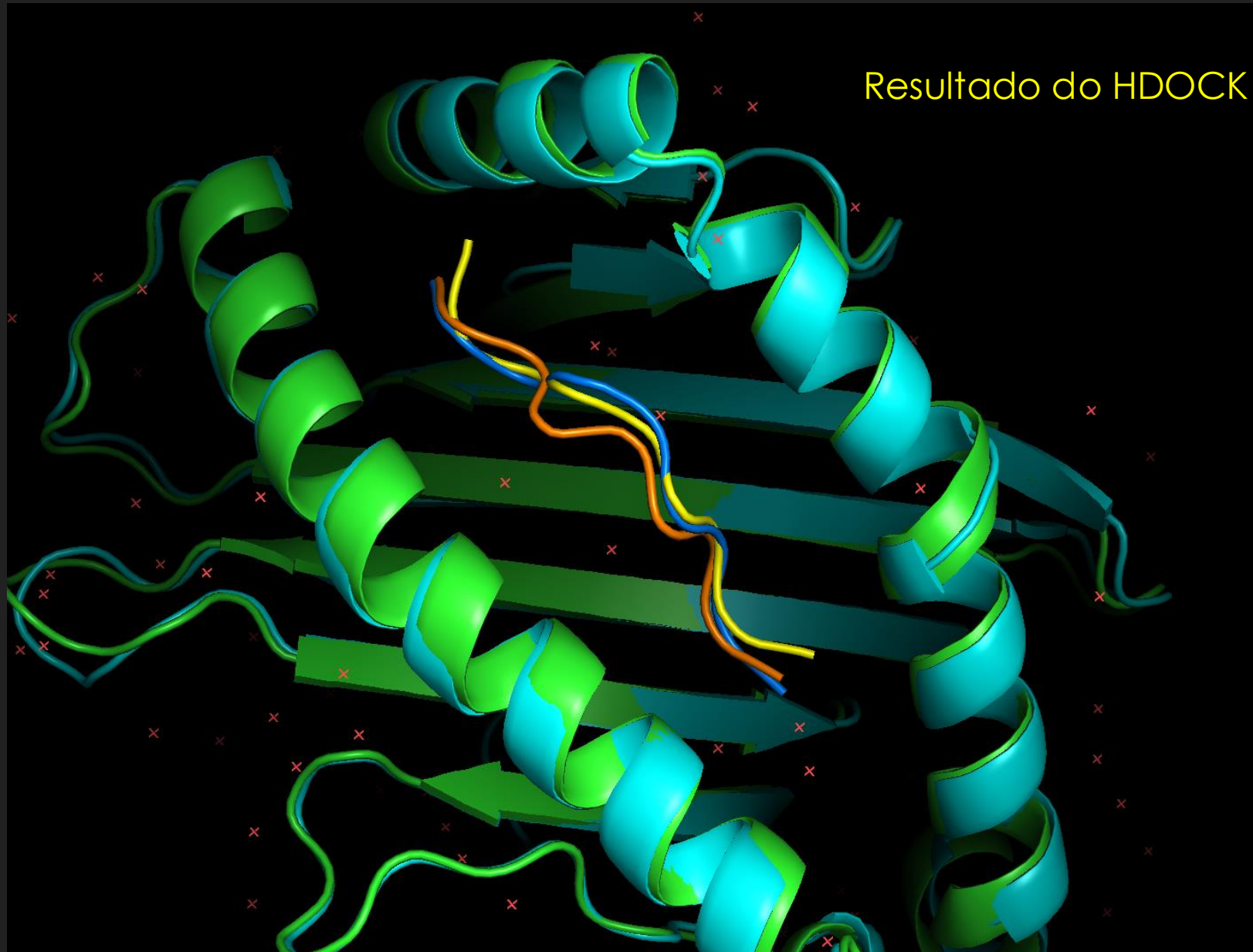
Action
Spin Reset

Complex Template Information ([Click to Show](#))

Summary of the Top 10 Models

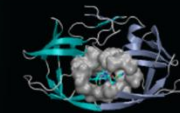
Rank	1	2	3	4	5	6	7	8	9	10
Docking Score	-254.53	-250.75	-235.03	-224.22	-208.43	-201.10	-199.28	-188.51	-186.84	-186.47
Confidence Score	0.8900	0.8824	0.8456	0.8152	0.7629	0.7354	0.7282	0.6836	0.6763	0.6747
Ligand rmsd (Å)	1.53	6.16	14.25	13.50	6.01	15.05	7.76	14.11	15.42	16.08

Resultado do HDock





Ferramenta de docking brasileira

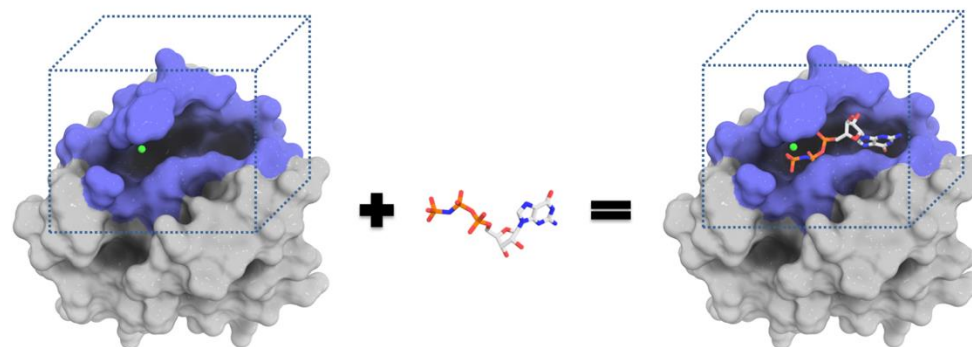


[COVID-19](#): We provide to the DockThor users structures of COVID-19 potential targets already prepared for docking at the Protein tab. New targets and structures will be available soon.

Guedes, I. A. et al. *Drug design and repurposing with DockThor-VS web server focusing on SARS-CoV-2 therapeutic targets and their non-synonym variants*. *Sci Rep* 11, 5543 (2021).

Welcome to DockThor

A Free Web Server for Protein-ligand Docking



<https://dockthor.lncc.br/v2/>

Clique em docking

Protein Cofactors Ligand Docking Results

① Upload your protein file

[+ Add file](#) [Select Test File](#)

New COVID-19 resources

Target ▾ Variant ▾ Structure ▾ ⓘ ↻ ⏸

File name	Size	Status	Actions
1hpv_protein.pdb	149.98 KB	⏸	Send Delete

Vamos usar os arquivos de teste da própria ferramenta.

Adicione cofatores

opcional

Protein Cofactors Ligand Docking Results

① Upload your cofactor file

+ Add file Select Test File

File name	Size	Add H	Status	Actions
1hpv_water.pdb	0.08 KB	<input checked="" type="checkbox"/>	✓	

Send Remove all

Valid structures: 1 (max. 10)

② Prepared cofactor file

View 3D Download Send to DockThor

Muitos cofatores podem ter uma papel importante na correta ligação com a proteína

Prepare o ligante

Protein Cofactors **Ligand** Docking Results

① Upload your ligand file

[+ Add file](#) [Select Test File](#)

New Compounds Datasets

Dataset pH range Version [i](#) [C](#) [O](#)

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

#	File name	Size	Add H	Status	Actions
1	1hvp_ligand.pdb	2.83 KB	<input checked="" type="checkbox"/>	✓	Remove

[Send](#) [Remove all](#)

Valid structures: 1 (max. 100)

① Check your docking input files

Protein (1)

+

Ligand (1)

+

Cofactor (1)

② Define the binding site

Attention: the current version of DockThor (released on April 17, 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.

User Defined

Blind Docking

Test

Grid center:

X	<input type="range"/>	<input type="text" value="10,387"/>
Y	<input type="range"/>	<input type="text" value="18,119"/>
Z	<input type="range"/>	<input type="text" value="8,484"/>

Grid size:

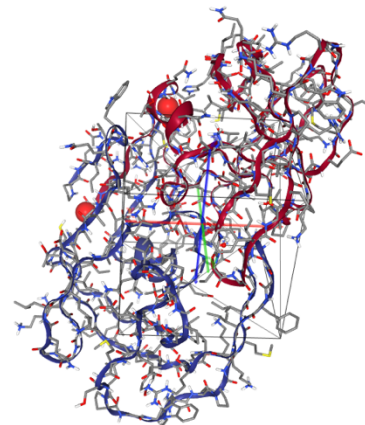
X	<input type="range"/>	<input type="text" value="20"/>
Y	<input type="range"/>	<input type="text" value="20"/>
Z	<input type="range"/>	<input type="text" value="20"/>

Discretization:**Total Grid Points:**

531441

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

`r` auto view `shift + left_mouse + drag` zoom `ctrl + right_mouse + drag` rotate



Defina o centro da caixa

Execute o docking

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: teste ✓

E-mail: seu@email.com ✓ +

Subscribe DockThor e-Newsletters

Accept [terms of use](#)


 Dock!

Você receberá um email confirmando o processo.

dockthor@lncc.br
Para: Você


Responder Responder a todos Encaminhar

Ter, 02/12/2025 12:27



Docking job submitted (id teste_692f05457f381).

We will send an e-mail when the job is finished.



If you do not receive an e-mail within 5 working days, please contact the support at
dockthor@lncc.br

This is an automatic message. Please do not reply to this e-mail.

DockThor is a service provided by LNCC.
Copyright © GMMSB 2017. All Rights Reserved.
Petrópolis, Rio de Janeiro, Brazil.

The screenshot displays the DockThor web application interface. At the top left is the logo "dockthor" with the tagline "A RECEPTOR-LIGAND DOCKING PROGRAM". To the right is a 3D molecular model of a protein-ligand complex. Below the logo is a navigation menu with "Home", "Docking" (highlighted), "References", "About", and "Support". On the far right of the menu are "Login" and "Register" links. A secondary navigation bar contains tabs for "Protein", "Cofactors", "Ligand", "Docking", and "Results", with "Results" being the active tab. The main content area features a "Job Status" section with a circled "1" icon. It displays the job ID "teste_692f05457f381" and the status "RUNNING". A small molecular icon is centered below the text. The footer contains logos for GMMSB, SINAPAD, INCT, FAPERJ, CNPq, and the Laboratório Nacional de Computação Científica. The version information "Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved." is located at the bottom center.

Aos 45 do segundo tempo...

dockthor@lncc.br
Para: Você

Responder Responder a todos Encaminhar

Qui, 04/12/2025 17:15

dockthor

Your docking job is done!

Click the link bellow to analyse and download your results.

[View Results](#)

Attention: Docking files will be available for 30 days. All files will be permanently deleted on **03/01/2026**.

This is an automatic message. Please do not reply to this e-mail.

DockThor is a service provided by LNCC.
Copyright © GMM5B 2017. All Rights Reserved.
Petrópolis, Rio de Janeiro, Brazil.

[Thank you!](#) [Here is the link.](#) [Great, thank you so much!](#)

② Analyze your docking results:

[Analyze](#)[Download](#)[Delete Job](#)[Table](#)[3D View](#)

Table

Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
1	17d0c4c0	ligand 1	-10.010	-1.670	-40.333	-19.878

« 1 »

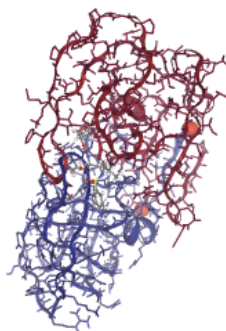
3D View

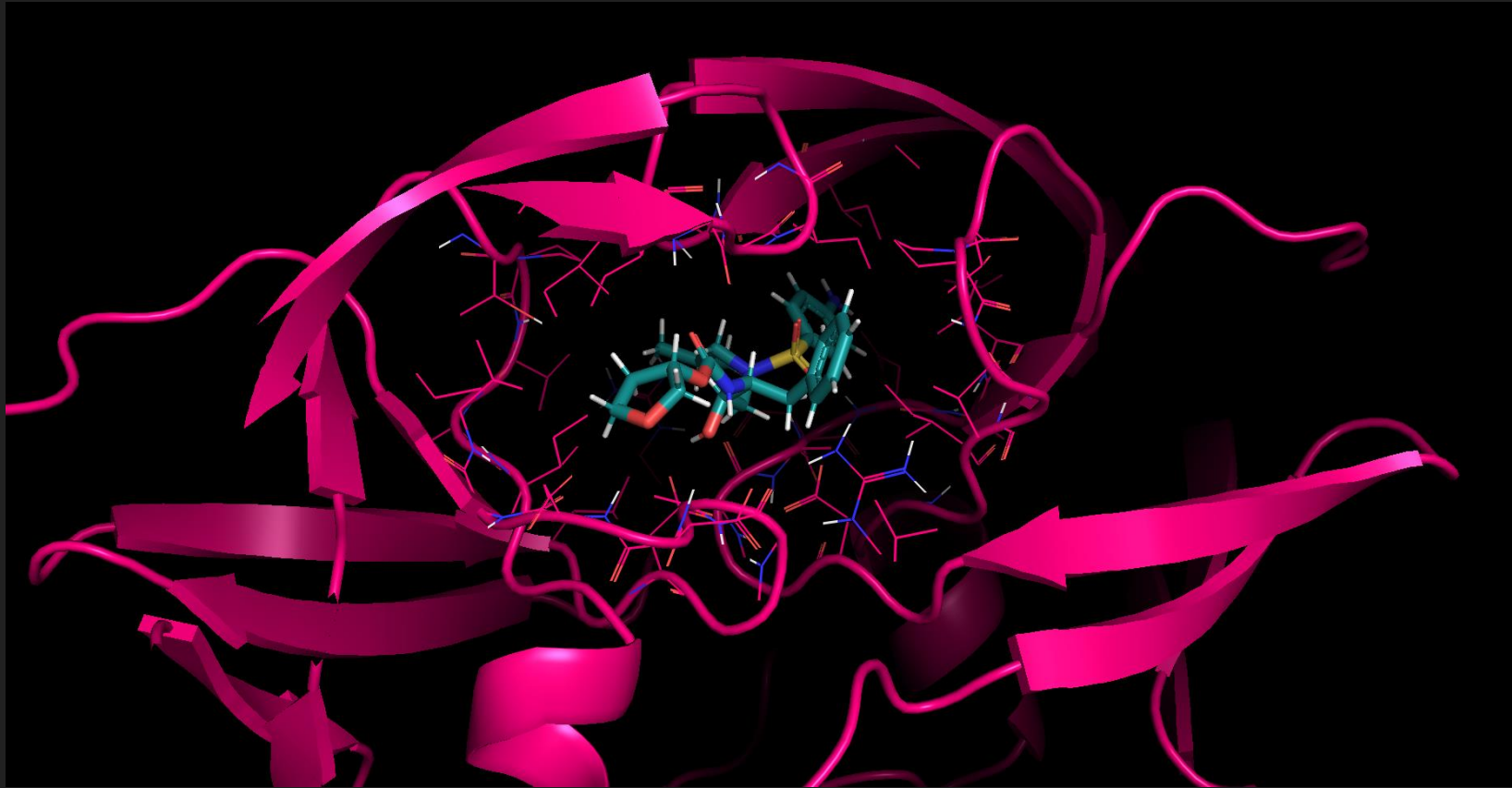
Use your mouse to drag, rotate, and zoom in and out of the structure:

auto view

shift + left_mouse + drag zoom

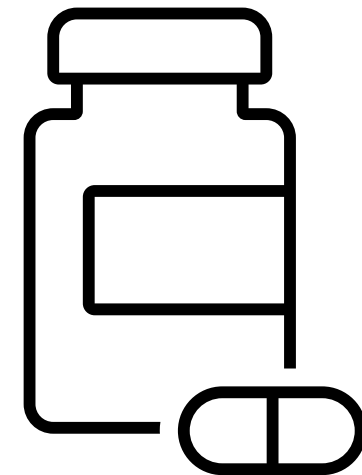
ctrl + right_mouse + drag rotate

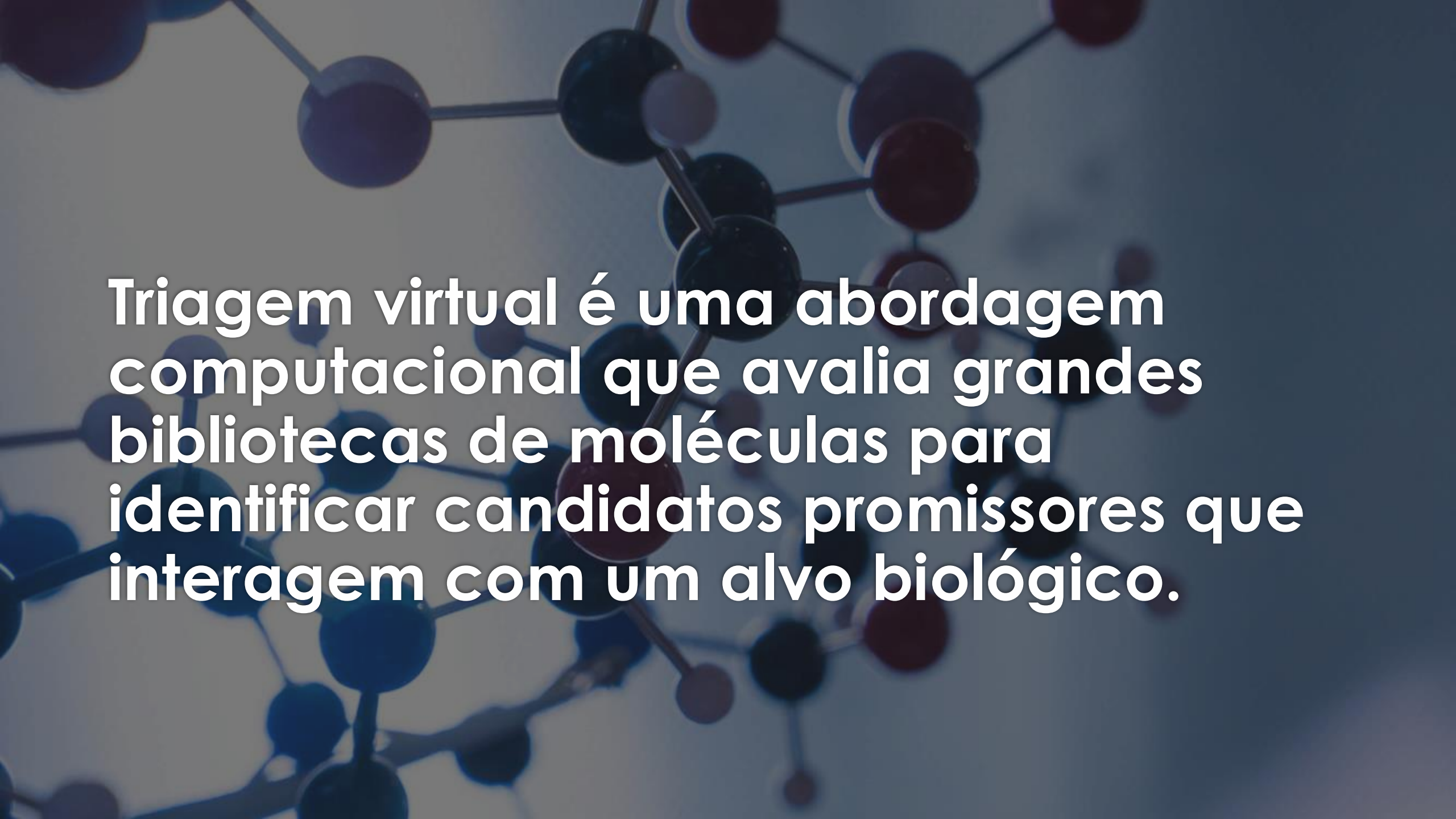




Desenvolvimento de novos medicamentos

- Desenvolver novos medicamentos é um processo complexo
- Pode levar de 10 a 15 anos
- Custar bilhões
- Técnicas computacionais podem auxiliar:
 - **Triagem virtual de fármacos**





Triagem virtual é uma abordagem computacional que avalia grandes bibliotecas de moléculas para identificar candidatos promissores que interagem com um alvo biológico.

Triagem virtual

- Técnica computacional para identificar compostos promissores antes de testes experimentais
- Avalia milhares ou milhões de moléculas rapidamente.
- Pode usar:
 - Docking
 - Abordagens baseadas em IA

Fundamentos do virtual screening

Encontre o alvo (proteína)

Selecione uma base de dados com
milhares ou milhões de moléculas



















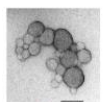





Realiza docking de todas as
estruturas contra o alvo

Selecione as melhores para
validação em bancada

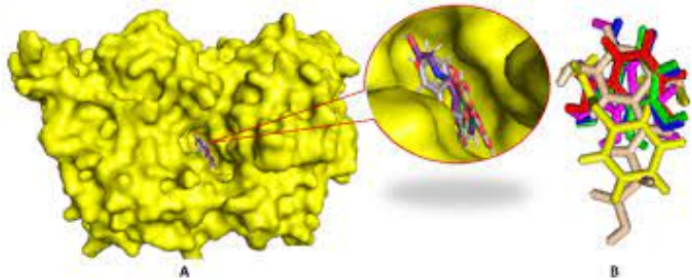
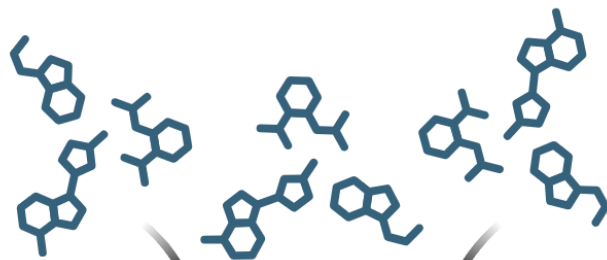
Testes com seres humanos

Bases de dados comerciais e abertas

The screenshot displays the ZINC database catalog page. At the top, there is a navigation bar with links for 'ZINC', 'Substances', 'Catalogs', 'Tranches', 'Biological', 'More', and 'About'. Below this is a search bar containing '450' and a 'Lookup' button. The main content area is a grid of 24 supplier logos and names, arranged in 4 rows and 6 columns. The suppliers listed are:

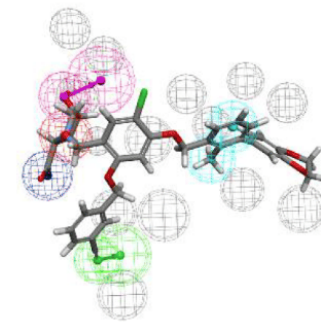
 OOI Chemical	 1PlusChem LLC	 A2B Chem Building Blocks	 AA Blocks	 AbovChem	 Accela ChemBio Inc
 AnalytiCon Discovery	 AnalytiCon Discovery Natural Derivatives	 AnalytiCon Discovery NP	 AnalytiCon Discovery NP BB	 Beijing Acemol Technology	 Aceschem
 AChemBlock	 Achemo BB	 Advanced Chemicals Intermediates	 Acros Organics	 ACT Chemical BB	 AfroDb Natural Products
 Aggregators	 AKOS	 AKOS (make-on-demand)	 AK Scientific, Inc. AK Scientific	 AK Scientific, Inc. AK Scientific Economical	 AK Scientific, Inc. AK Scientific Make on Demand Economical

ChEBI DATABASE (ALMOST 600,000 MOLECULES)

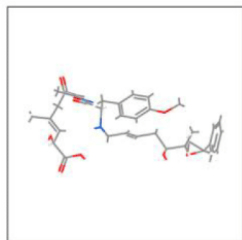


MOLECULAR DOCKING
(MORE THAN 1,500 FLAVONOIDS)

SELECTED HITS

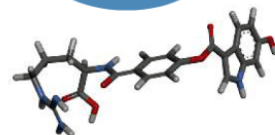
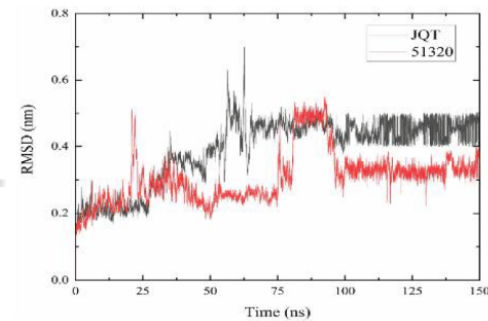


ADME AND TOXICITY PREDICTIONS



Predicted LD50: 765mg/kg	Name	User defined
Predicted Toxicity Class: 4	Molweight	620.73
1 2 3 4 5 6	Number of hydrogen bond acceptors	54
Average similarity: 46.29%	Number of hydrogen bond donors	5
Prediction accuracy: 54.26%	Number of atoms	89
	Number of bonds	91
	Number of rotatable bonds	19
	Molecular refractivity	170.98
	Topological Polar Surface Area	157.72
	octanol/water partition coefficient(logP)	4.43

MOLECULAR DYNAMICS



Docking vs. dinâmica molecular

- Docking te mostra uma "foto"
- Dinâmica te mostra um "filme"

Obrigado!

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