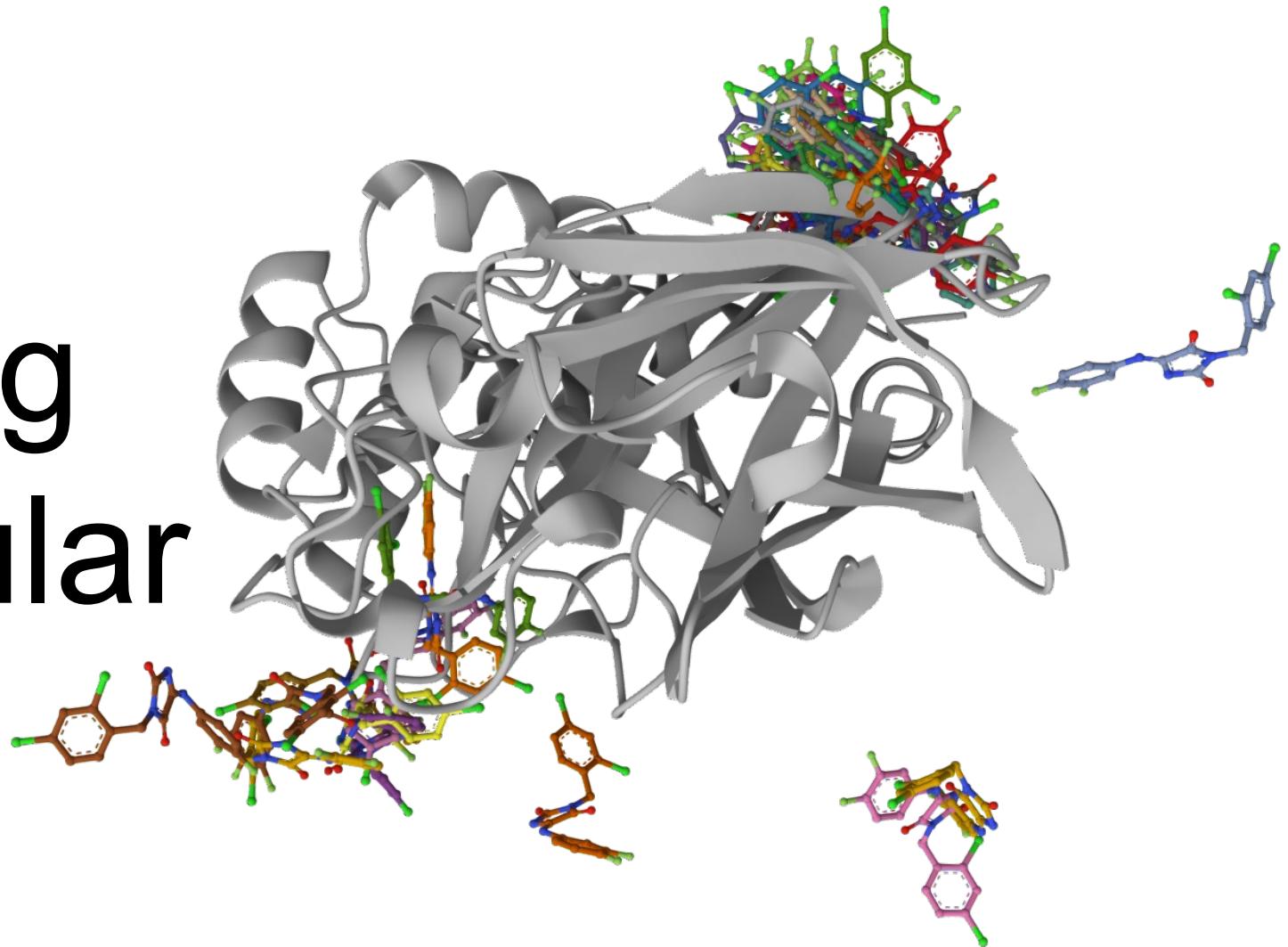
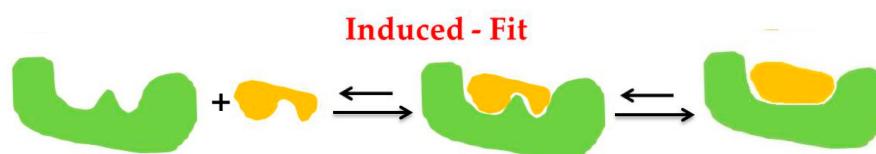
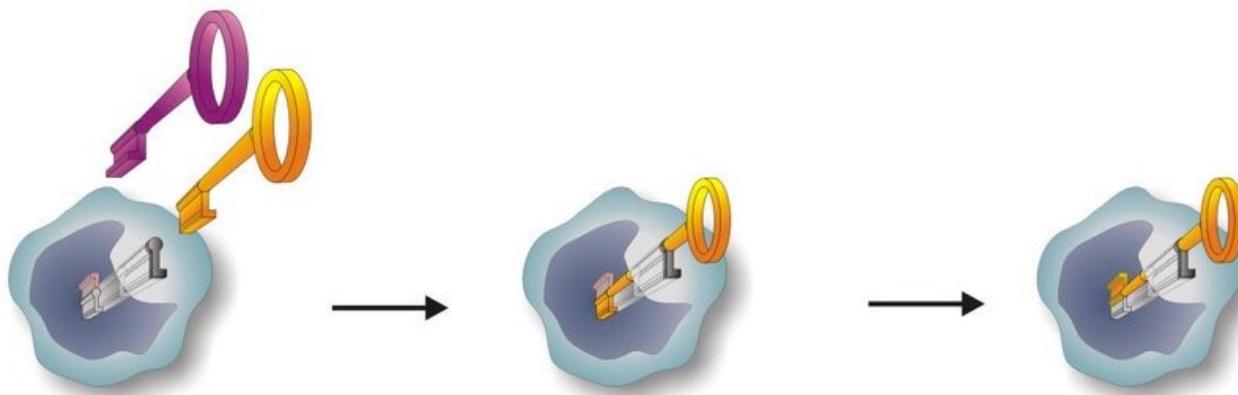


Docking Molecular

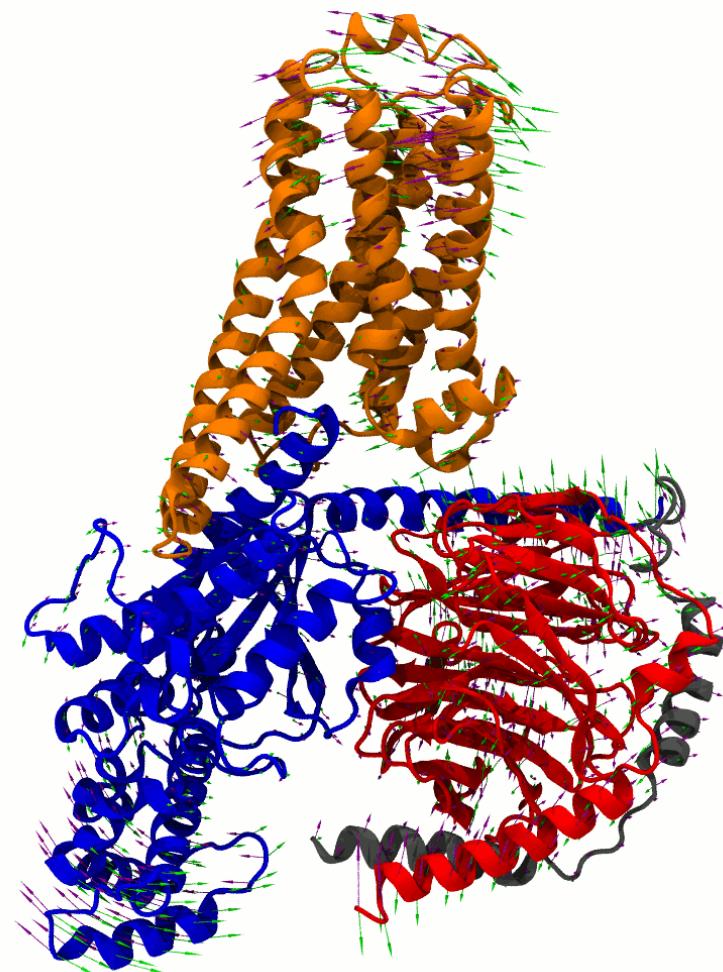
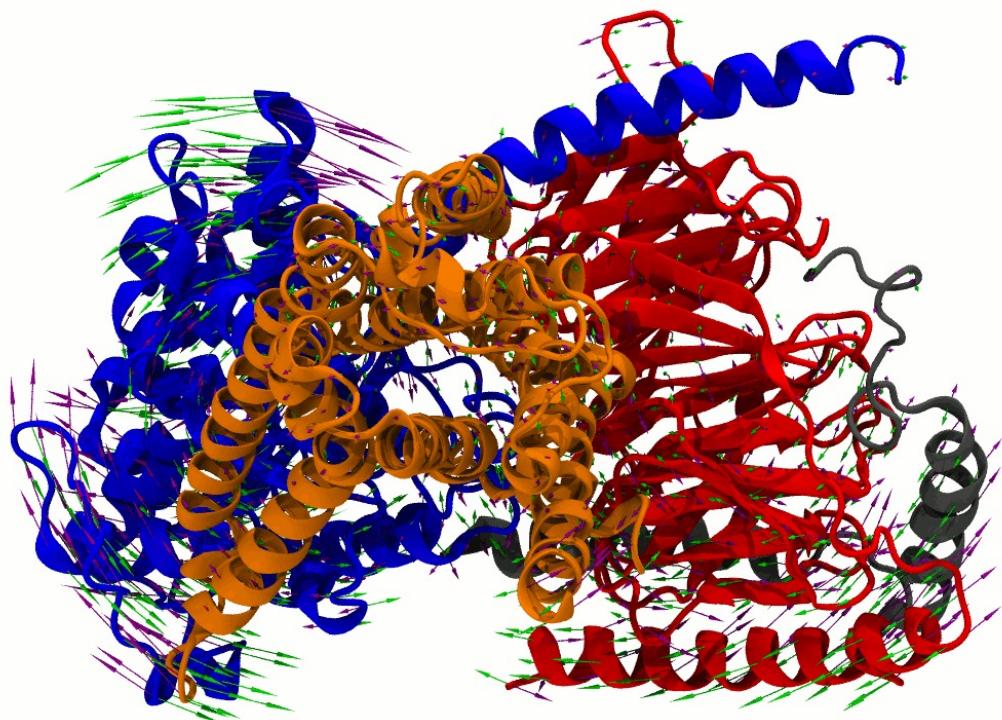
Madson Aragão
Bioinformática, UFMG
Data Science, PUC-Rio
Genética & Biologia Molecular, UFPE
Belo Horizonte, 2025



ANTES DE TUDO

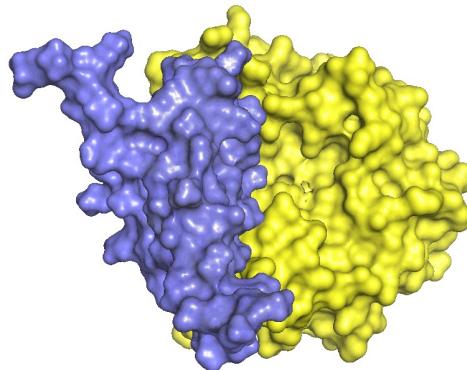


ANTES DE TUDO



DOCKING/ANCORAGEM/ATRACAMENTO MOLECULAR

- Técnica *in silico* utilizada para prever a interação entre duas moléculas, geralmente uma **proteína** e um **ligante**;
- Essa técnica desempenha um **papel fundamental na modelagem de interações biomoleculares**, sendo amplamente aplicado no **desenvolvimento de fármacos** e compressão de **interações em processos biológicos**;
- A metodologia envolve a **simulação de diferentes conformações** moleculares para encontrar a **melhor orientação e afinidade de ligação**.
- **Exemplos** incluem a identificação de inibidores enzimáticos e o estudo de interações proteína-proteína.

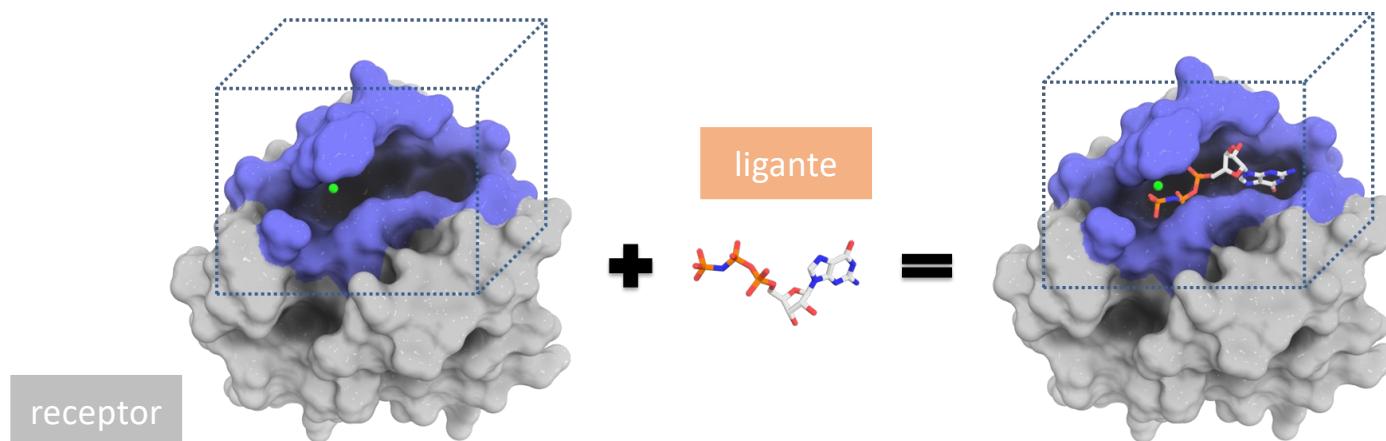


NOMECLATURAS USADAS NO DOCKING MOLECULAR

Para compreender o docking molecular, é essencial conhecer algumas nomenclaturas básicas:

Receptor: Geralmente, uma proteína ou macromolécula que interage com um ligante.

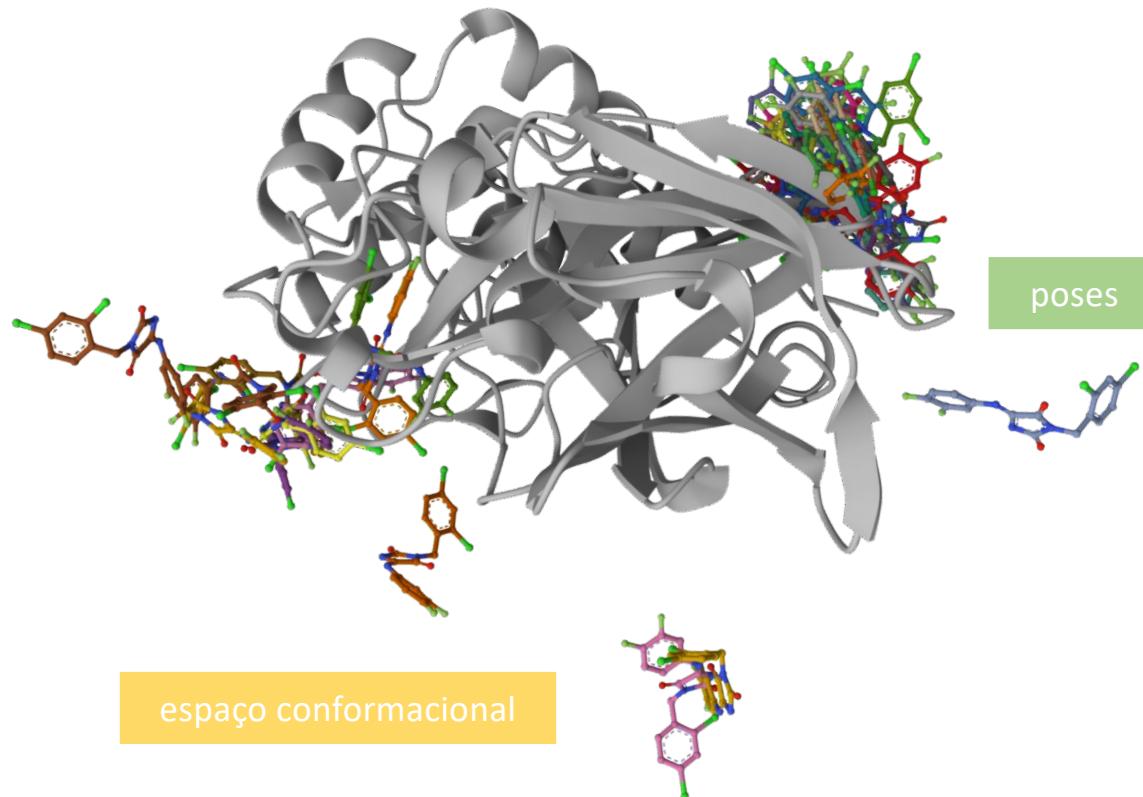
Ligante: Pequena molécula que se liga ao receptor, podendo ser um fármaco, peptídeo ou outra biomolécula.



NOMECLATURAS USADAS NO DOCKING MOLECULAR

Pose: Diferentes conformações assumidas pelo ligante ao se encaixar no sítio de ligação do receptor.

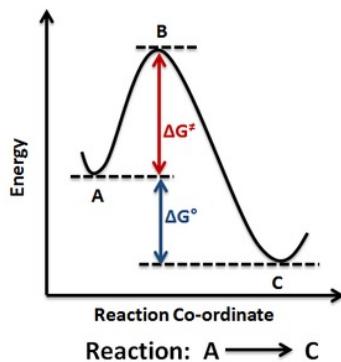
Espaço Conformacional: Conjunto de possíveis orientações e conformações de um ligante em relação ao receptor.



NOMECLATURAS USADAS NO DOCKING MOLECULAR

Energia de Ligação (ΔG): Valor que indica a estabilidade do complexo formado, geralmente expresso em kcal/mol.

Scoring Function: Função matemática que avalia a afinidade entre ligante e receptor com base na energia de ligação, essa medida pode variar de acordo com a ferramenta que está sendo utilizada.

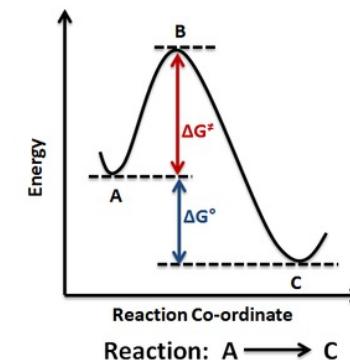


**energia de ligação
(simplificada/conceitual)**

$$E_{\text{binding}} = E_{\text{complexo}} - (E_{\text{receptor}} + E_{\text{ligante}})$$

variação da energia livre de Gibbs (ΔG)

$$\Delta G_{\text{binding}} = G_{\text{complexo}} - (G_{\text{receptor}} + G_{\text{ligante}})$$



Em muitos estudos de docking, a **energia de ligação é definida como a diferença entre a energia do complexo formado e a soma das energias dos componentes isolados**. Em alguns contextos, essa energia é considerada equivalente ao **ΔG de ligação**, no entanto, pode ser uma estimativa simplificada, dependendo do método utilizado, já que nem sempre incorpora todos os termos entálpicos e entrópicos.

NOMECLATURAS USADAS NO DOCKING MOLECULAR

Energia de Ligação (ΔG): Valor que indica a estabilidade do complexo formado, geralmente expresso em kcal/mol.

Scoring Function: Função matemática que avalia a afinidade entre ligante e receptor com base na energia de ligação, essa medida pode variar de acordo com a ferramenta que está sendo utilizada.

$\Delta\Delta G$ (diferença de ΔG entre dois sistemas)

Essa medida é usada para comparar, por exemplo, um sistema wild type com um sistema mutante:

$$\Delta\Delta G = \Delta G_{\text{mutante}} - \Delta G_{\text{wild-type}}$$

Um $\Delta\Delta G$ positivo indica que a mutação tornou a ligação menos favorável (o ΔG do mutante é menos negativo), enquanto um $\Delta\Delta G$ negativo sugere uma melhoria na afinidade de ligação.



quanto mais negativo



quanto menos negativo

ΔG (DIFERENÇA DE ΔG ENTRE DIFERENTES POSES)

POSE	ΔG
1	-11.6
2	-11.4
3	-11.3
4	-11.1
5	-10.9
6	-10.8
7	-10.7
8	-10.7
9	-10.7

ΔG (DIFERENÇA DE ΔG ENTRE DIFERENTES POSES)

POSE	ΔG
1	-11.6
2	-11.4
3	-11.3
4	-11.1
5	-10.9
6	-10.8
7	-10.7
8	-10.7
9	-10.7



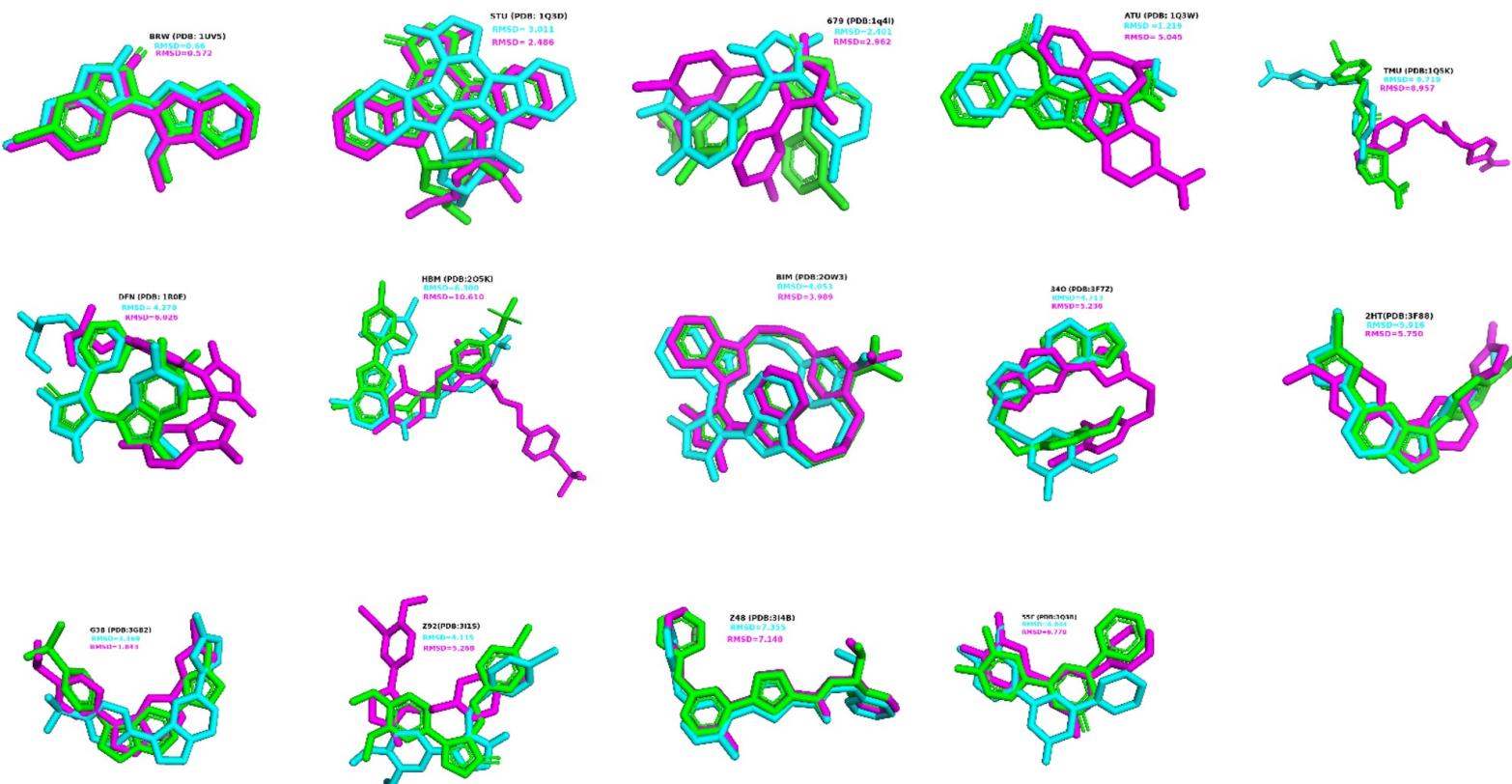
quanto mais negativo



quanto mais perto de zero

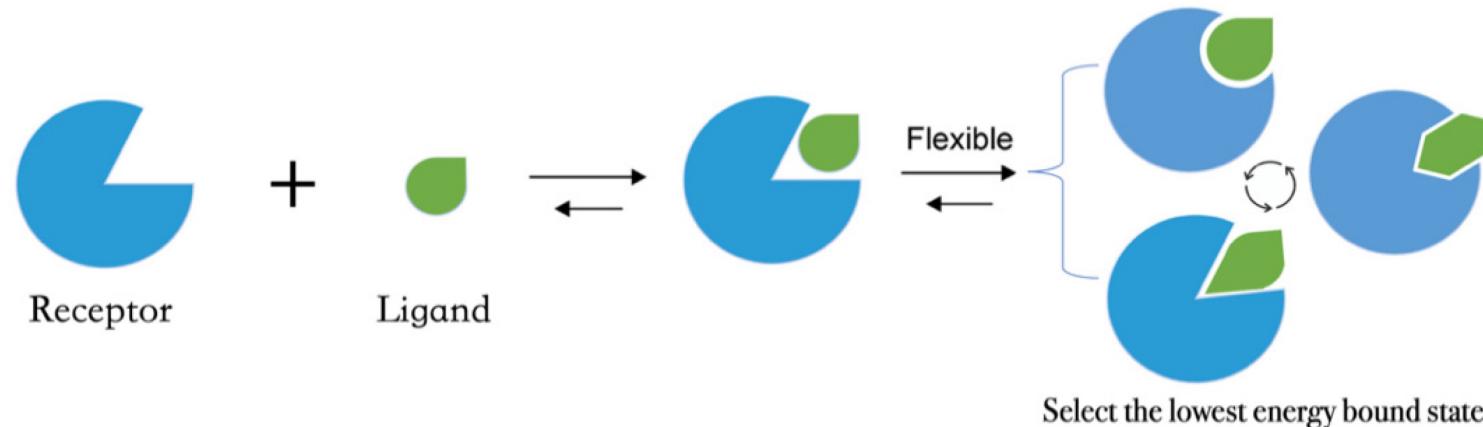
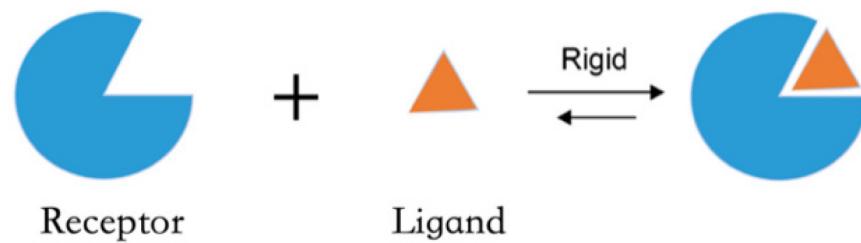
NOMECLATURAS USADAS NO DOCKING MOLECULAR

RMSD (Root Mean Square Deviation): Mede a diferença entre duas conformações moleculares, sendo utilizado para comparar poses do docking.



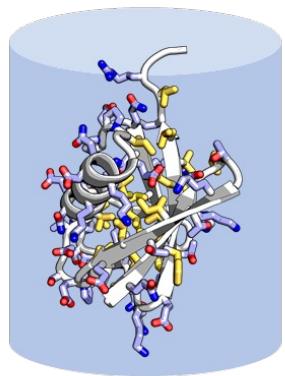
NOMECLATURAS USADAS NO DOCKING MOLECULAR

Flexibilidade Molecular: Alguns algoritmos permitem que o receptor e/ou o ligante tenham movimentos estruturais durante o docking.

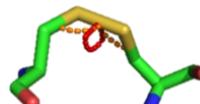


FATORES QUE INFLUENCIAM NO DOCKING

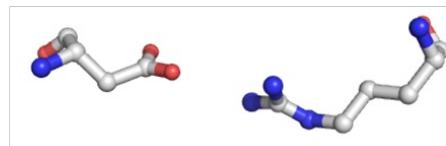
Solvation



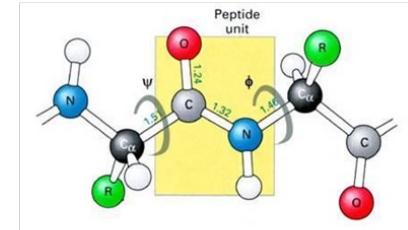
Disulfide bond



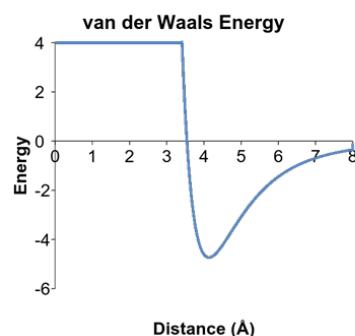
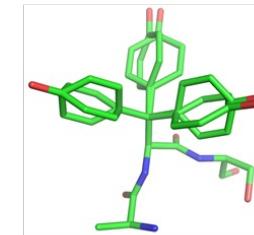
Ionic bond



Backbone conformations

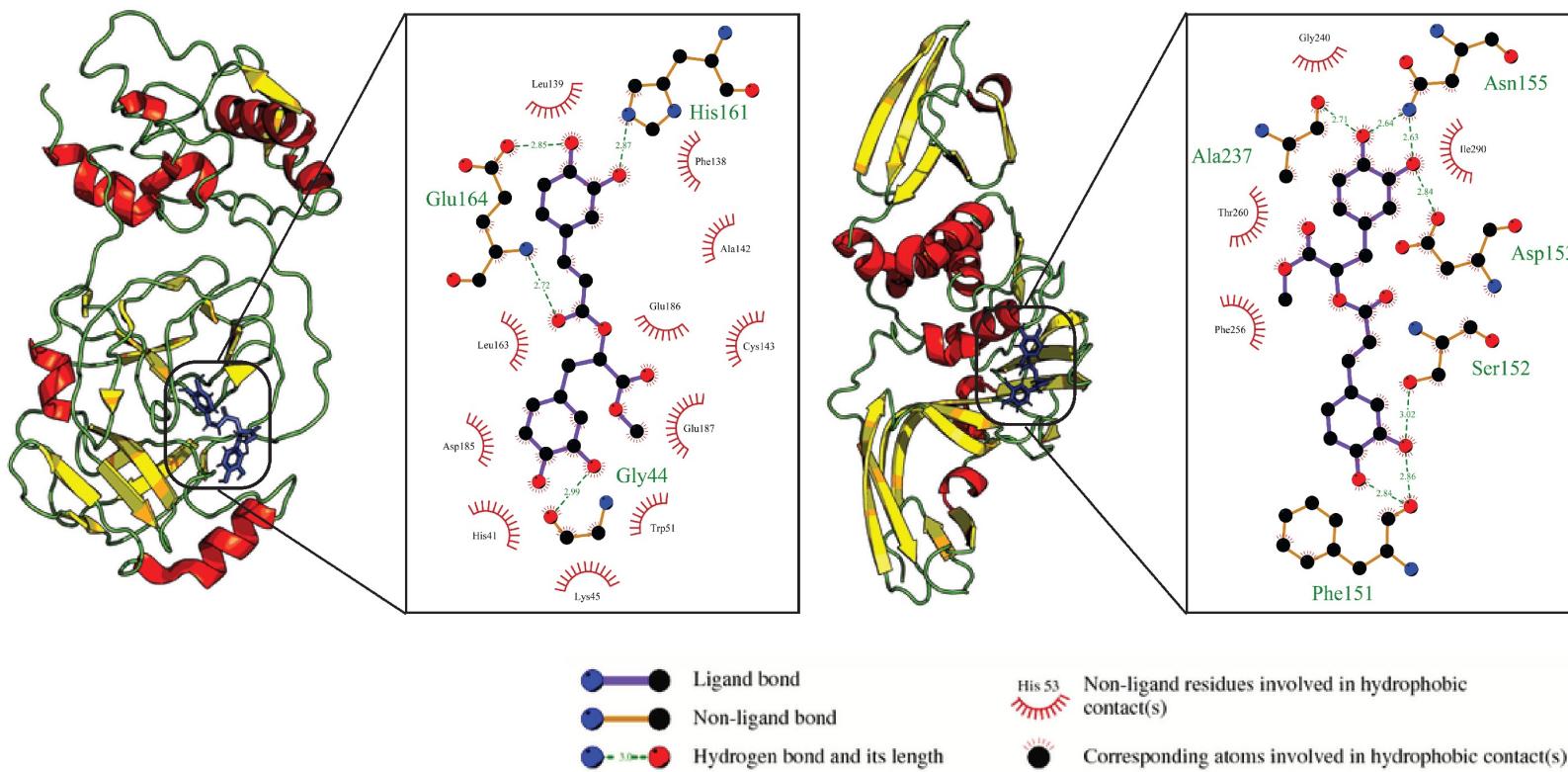


Sidechain conformations



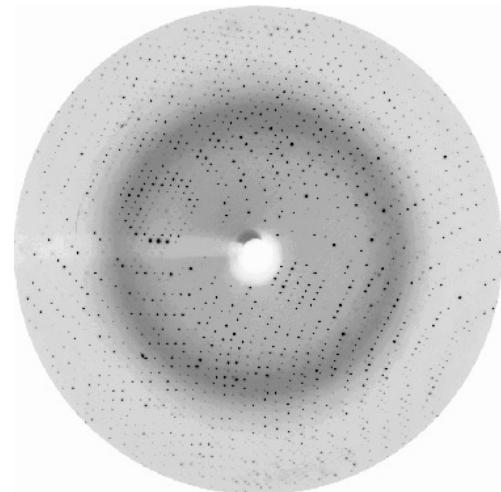
Inspired by a Sergey Ovchinnikov class

FATORES QUE INFLUENCIAM NO DOCKING



ORIGEM DAS ESTRUTURAS (RECEPTORES):

- Cristalografia por raio-x
- Ressonância magnética nuclear
- Microscopia crio-eletrônica



+210 mil proteínas depositadas





Biological Assembly 1

Explore in 3D: [Structure](#) | [Sequence Annotations](#) |
[Electron Density](#) | [Validation Report](#) | [Ligand Interaction \(PIO\)](#) |
[Predict Membrane](#)

4CQK

Crystal structure of ligand-bound NaD1

PDB DOI: <https://doi.org/10.2211/pdb4CQK/pdb>

Classification: PLANT PROTEIN

Organism(s): Nicotiana alata

Mutation(s): No

Membrane Protein: Yes OPM

Deposited: 2014-02-17 Released: 2014-04-16

Deposition Author(s): Lay, F.T., Mills, G.M., Poon, I.K.H., Baxter, A.A., Hulett, M.D., Kvansakul, M.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.60 Å

R-Value Free: 0.183

R-Value Work: 0.155

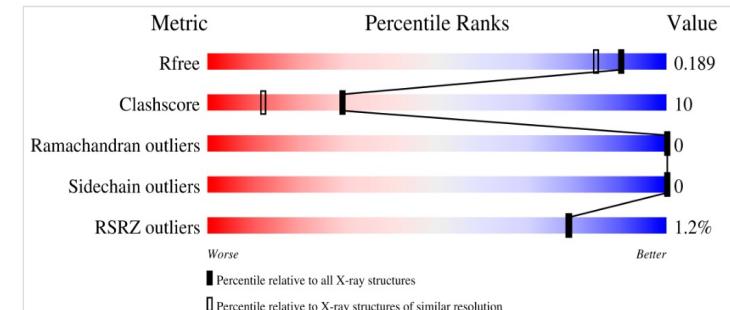
R-Value Observed: 0.156

Starting Model: experimental

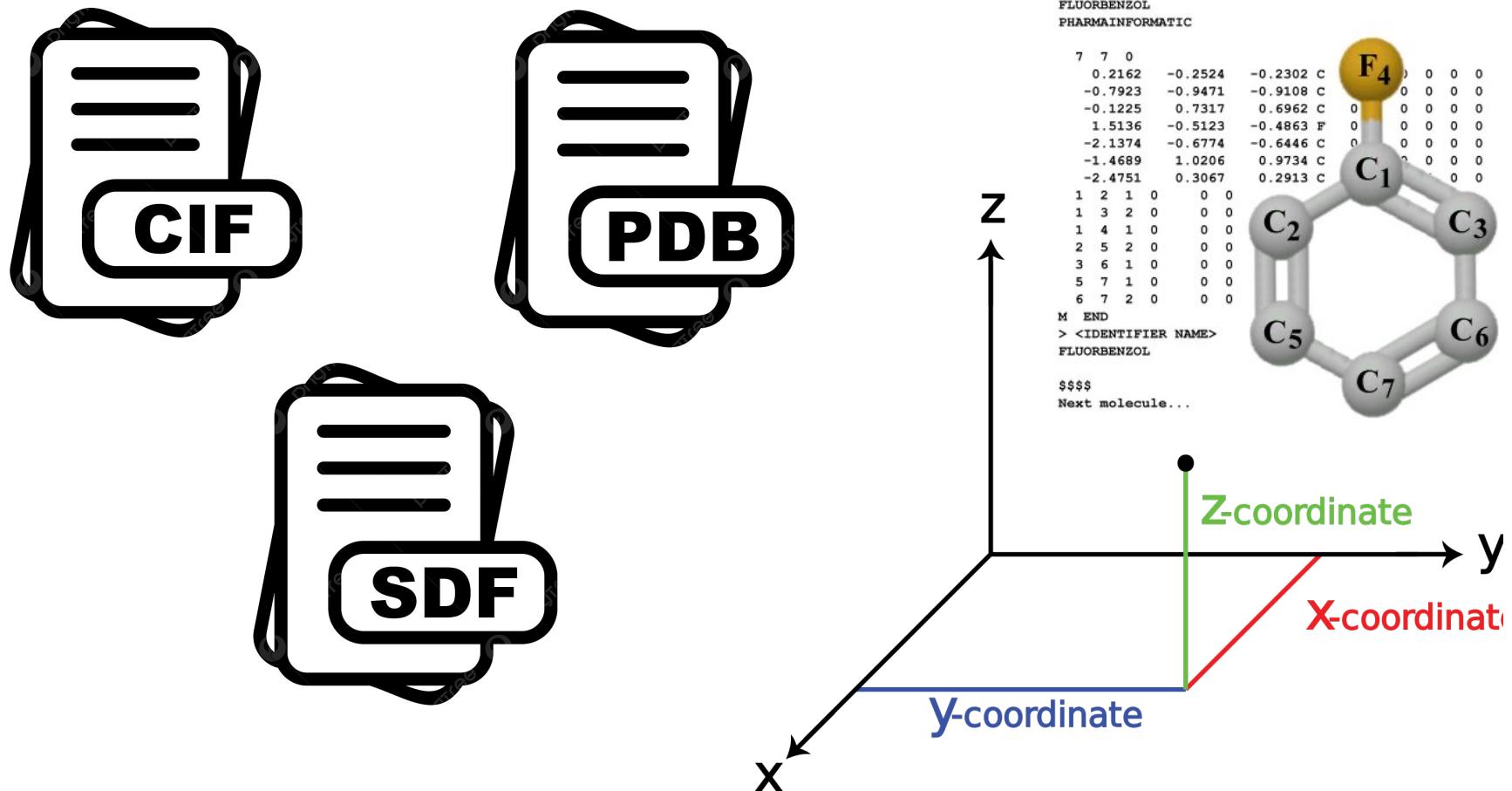
[View more details](#)

wwPDB Validation

[3D Report](#) [Full Report](#)



MAS ONDE/COMO ESSAS COORDENADAS SÃO ARMAZENADAS?



MAS ONDE/COMO ESSAS COORDENADAS SÃO ARMAZENADAS?

HEADER CELL CYCLE
 TITLE P53 CHARGED CORE
 COMPD MOL_ID: 1;
 COMPD 2 MOLECULE: CELLULAR TUMOR ANTIGEN P53;
 COMPD 3 CHAIN: A;
 COMPD 4 SYNONYM: ANTIGEN NY-CO-13, PHOSPHOPROTEIN P53, TUMOR SUPPRESSOR P53;
 COMPD 5 ENGINEERED: YES;
 COMPD 6 MUTATION: YES
 SOURCE MOL_ID: 1;
 SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
 SOURCE 3 ORGANISM_COMMON: HUMAN;
 SOURCE 4 GENBANK_ACCESSION: 9666;
 SOURCE 5 GENBANK_PDB: P53;
 SOURCE 6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
 SOURCE 7 EXPRESSION_SYSTEM_TAXID: 562
 KEYWDS TUMOR SUPPRESSOR, AGGREGATION PRONE, MUTANT P53, CELL CYCLE
 EXPDTA X-RAY DIFFRACTION
 AUTHOR R.GALLARDO,T.LANGENBERG,J.SCHYMKOWITZ,F.ROUSSEAU,C.ULENS
 REVDAT 3 -24-JAN-24 65L6 1 REMARK
 REVDAT 2 -23-SEP-24 65L6 1 JRNL
 REVDAT 1 -11-MAR-20 65L6 0
 JRNL AUTH T.LANGENBERG,R.GALLARDO,R.VAN DER KANT,N.LOUROS,E.MICHEILS,
 JRNL AUTH 2 R.DURAN-ROMANA,B.HOUBEN,R.CASSIO,H.WILKINSON,T.GARCIA,
 JRNL AUTH 3 C.ULENS,J.VAN DURME,F.ROUSSEAU,J.SCHYMKOWITZ
 JRNL TITL THERMODYNAMIC AND EVOLUTIONARY COUPLING BETWEEN THE NATIVE
 JRNL TITL 2 AND AMYLOID STATE OF GLLOBULAR PROTEINS.
 JRNL REF CELL REP
 JRNL REFL 31 07512 2020
 JRNL ESSN 2211-1247
 JRNL PMID 32994448
 JRNL DOI 10.1016/J.CELREP.2020.03.076
 REMARK 2
 REMARK 2 RESOLUTION, 1.67 ANGSTROMS.
 REMARK 3
 REMARK 3 REFINEMENT.
 REMARK 3 PROGRAM : PHENIX 1.15.2_3472
 REMARK 3 AUTHORS : PAUL ADAMS,PAVEL AFONINE,VINCENT CHEN,IAN
 REMARK 3 : DAVIS,KRISHNA GOPAL,RALF GROSSE-KUNSTLEVE,
 REMARK 3 : LI-WEI HUNG,ROBERT IMMORNING,TOM IOERGER,
 REMARK 3 : AIRLINE MCCOY,ERIK MCKEE,NIGEL MORTIARY,
 REMARK 3 : REETAL PAI,RANDY READ,JANE RICHARDSON,
 REMARK 3 : DAVID RICHARDSON,TOD ROMO, JIM SACCHETTINI,
 REMARK 3 : NICHOLAS SAUTER,JACOB SMITH,LAURENT
 REMARK 3 : STORONI,TOM TERWILLIGER,PIETER ZWART
 REMARK 3
 REMARK 3 REFINEMENT TARGET : NULL
 REMARK 3
 REMARK 3 DATA USED IN REFINEMENT.
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.67
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 42.48
 REMARK 3 MIN(FOBS/SIGMA_FOBS) : 1.930
 REMARK 3 COMPLETENESS FOR RANGE (%) : 97.9
 REMARK 3 NUMBER OF REFLECTIONS : 28523
 REMARK 3
 REMARK 3 FIT TO DATA USED IN REFINEMENT.
 REMARK 3 R VALUE (WORKING + TEST SET) : 0.164
 REMARK 3 R VALUE (WORKING SET) : 0.163
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 REMARK 3 FREE R VALUE TEST SET SIZE (%) : 4.976
 REMARK 3 FREE R VALUE TEST SET COUNT : 1419
 REMARK 3
 REMARK 3 FIT TO DATA USED IN REFINEMENT (IN BINS).
 REMARK 3 BIN RESOLUTION RANGE COMPL. NWORK NFREE RWORK RFREE
 REMARK 3 1 42.4810 - 3.5939 0.99 2883 159 0.1599 0.1641
 REMARK 3 2 3.5939 - 2.8528 0.99 2788 139 0.1461 0.1656
 REMARK 3 3 2.8528 - 2.4922 0.99 2753 142 0.1597 0.1826
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 REMARK 3 8 1.8791 - 1.7973 0.98 2681 136 0.1697 0.2028

6sl6.pdb — Edited

Downloads — vi 6sl6.pdb — 80x24

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COMPND 3 CHAIN: A; ←
COMPND 4 SYNONYM: ANTIGEN NY-CO-13, PHOSPHOPROTEIN P53, TUMOR SUPPRESSOR P53; ←
COMPND 5 ENGINEERED: YES;
COMPND 6 MUTATION: YES ←
SOURCE MOL_ID: 1;
SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS; ←
SOURCE 3 ORGANISM_COMMON: HUMAN;
SOURCE 4 ORGANISM_TAXID: 9606;
SOURCE 5 GENE: TP53, P53; ←
SOURCE 6 EXPRESSION_SYSTEM: ESCHERICHIA COLI; ←
SOURCE 7 EXPRESSION_SYSTEM_TAXID: 562 ←
KEYWDS TUMOR SUPPRESSOR, AGGREGATION PRONE, MUTANT P53, CELL CYCLE
EXPDTA X-RAY DIFFRACTION
AUTHOR R.GALLARDO, T.LANGENBERG, J.SCHYMKOWITZ, F.ROUSSEAU, C.ULENS
REVDAT 3 24-JAN-24 6SL6 1      REMARK
REVDAT 2 23-SEP-20 6SL6 1      JRNL
REVDAT 1 11-MAR-20 6SL6 0
JRNL      AUTH T.LANGENBERG, R.GALLARDO, R.VAN DER KANT, N.LOUROS, E.MICHEELS,
JRNL      AUTH 2 R.DURAN-ROMANA, B.HOUBEN, R.CASSIO, H.WILKINSON, T.GARCIA,
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CIF OU PDB? O HÁ DE NOVO? QUEM ESTÁ USANDO

 **PDB**
PROTEIN DATA BANK

 **230,444** Structures from the PDB
 **1,068,577** Computed Structure Models (CSM)

 Advanced Search | Browse Annotations

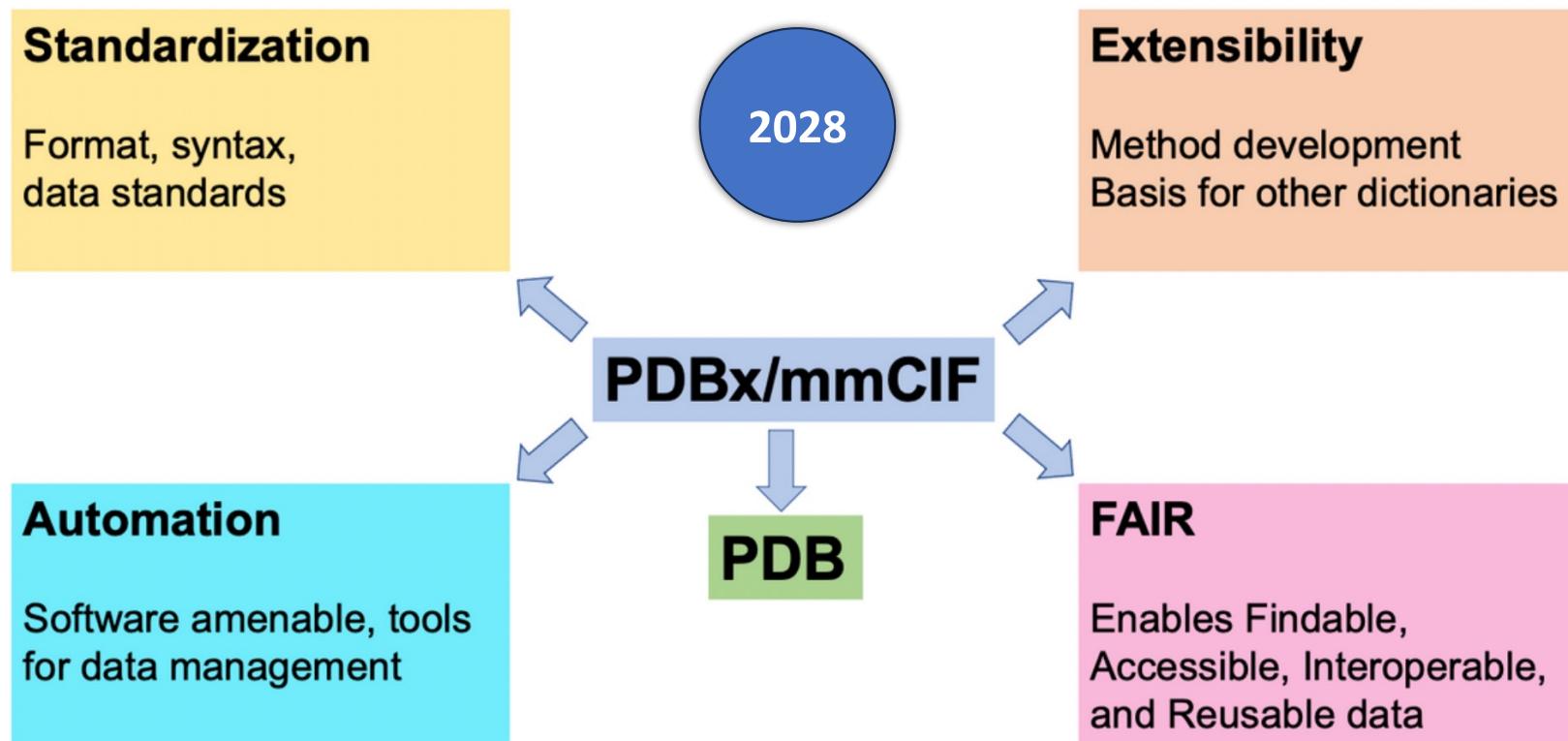
News

[2025](#) [2024](#) [2023](#) [2022](#) [2021](#) [2020](#) [2019](#) [2018](#) [2017](#) [2016](#) [2015](#) [2014](#) [2013](#) [2012](#) [2011](#) [2010](#) [2009](#) [2008](#)

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Announcing the New PDBx/mmCIF User Guide

CIF OU PDB? O HÁ DE NOVO? QUEM ESTÁ USANDO



ORIGEM DAS ESTRUTURAS (LIGANTES):

- CIF
- PDB
- SDF

<https://www.rcsb.org/>



<https://go.drugbank.com/>

The screenshot shows the DrugBank Online homepage. At the top, there are navigation links: 'Explore', 'For Drug Discovery', 'For Clinical Software', and 'For Academic Research'. A search bar is centered with the placeholder 'Search our knowledgebase's 500,000+ drugs and drug products'. Below the search bar, there is a dropdown menu set to 'Drugs' and a text input field with the placeholder 'Type your search...'. To the right of the search area is a pink button labeled 'CHAT WITH AN EXPERT'. The main content area features a large illustration of a scientist working at a desk with a computer monitor, surrounded by various scientific icons like DNA, a lightbulb, and a microscope. The text 'The pharmaceutical data you've been looking for' is overlaid on this illustration. Below the illustration, a paragraph reads: 'DrugBank is a vital resource for your pharmaceutical research, offering comprehensive & reliable drug data, structured for immediate use or easy software integration.' A small link 'SCROLL TO SEE OUR SOLUTIONS' with a downward arrow is located at the bottom of this section.

<https://www.ebi.ac.uk/chembl/>

The ChEMBL homepage has a teal header with the ChEMBL logo and a search bar. Below the header are navigation links for UNICHEM, CHEMBL-NTD, SURECHEMBL, MALARIA INHIBITOR PREDICTION, DOWNLOADS, and MORE. A descriptive text states: 'ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs.' Below this is a 'Explore ChEMBL' section featuring a circular diagram with data points: 1.7M Assays, 2.5M Compounds, 15.5k Drugs, 782 Targets, 16.0k Targets, 6.9k Drug Descriptions, 2.1k Drug Lines, 48.8k Drug Descriptions, 1.4k Drug Descriptions, and 95.1k Documents.

<https://pubchem.ncbi.nlm.nih.gov/>

The PubChem homepage has a dark blue header with the NIH National Library of Medicine logo. Below the header is a search bar with placeholder 'Try aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2h3' and a 'Use Entrez' checkbox. Below the search bar are buttons for 'Draw Structure', 'Upload ID List', 'Browse Data', and 'Periodic Table'. The main content area features a large blue hexagonal background with the text 'Explore Chemistry' and 'Quickly find chemical information from authoritative sources'. At the bottom, there are statistics: 119M Compounds, 328M Substances, 297M Bioactivities, 43M Literature, 51M Patents, and 1029 Data Sources.

ORIGEM DAS ESTRUTURAS (LIGANTES):

<https://go.drugbank.com/>

Explore a selection of our essential drug information below, or:

[CREATE FREE ACCOUNT](#)

Full Drug Profiles

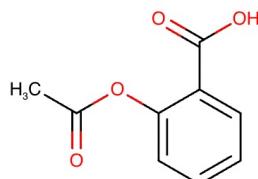
Unlock enhanced features & extensive drug insights, including detailed interaction data & regulatory status. [Create a free account.](#)

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Data Packages

Explore the full scope of our drug knowledge tailored for pharmaceutical research needs in our data library. [Learn more.](#)

Structure



Description

A painkiller used to treat pain, fever, inflammation, and migraines, as well as reduce the risk of heart attacks, strokes, and other events.

DrugBank ID

DB00945 [Small Molecule](#)

US Approved

[YES](#)

Other Approved

[YES](#)

Patents

14

Indicated Conditions

55

Clinical Trials

Phase 0	Phase 1	Phase 2	Phase 3	Phase 4
47	159	252	358	465

Therapeutic Categories

[Anti-Inflammatory Agents, Non-Steroidal](#)

[Antiplatelet agents](#)

[Salicylates](#)

Mechanism of Action

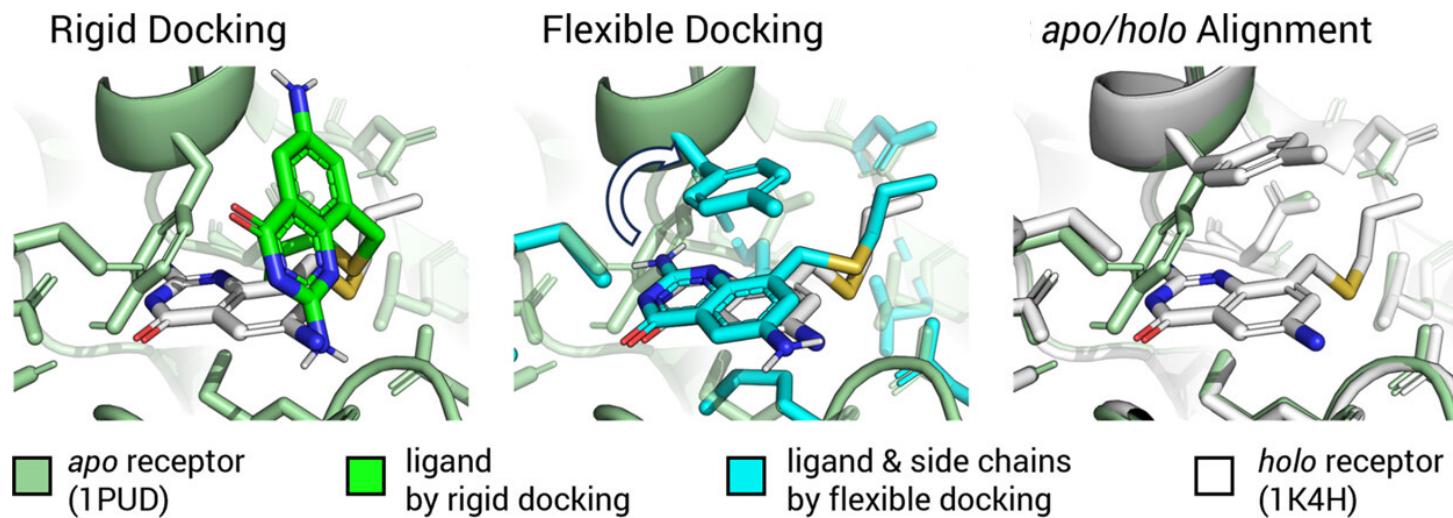
[Prostaglandin G/H synthase 1 Inhibitor](#)

[Prostaglandin G/H synthase 2 Inhibitor](#)

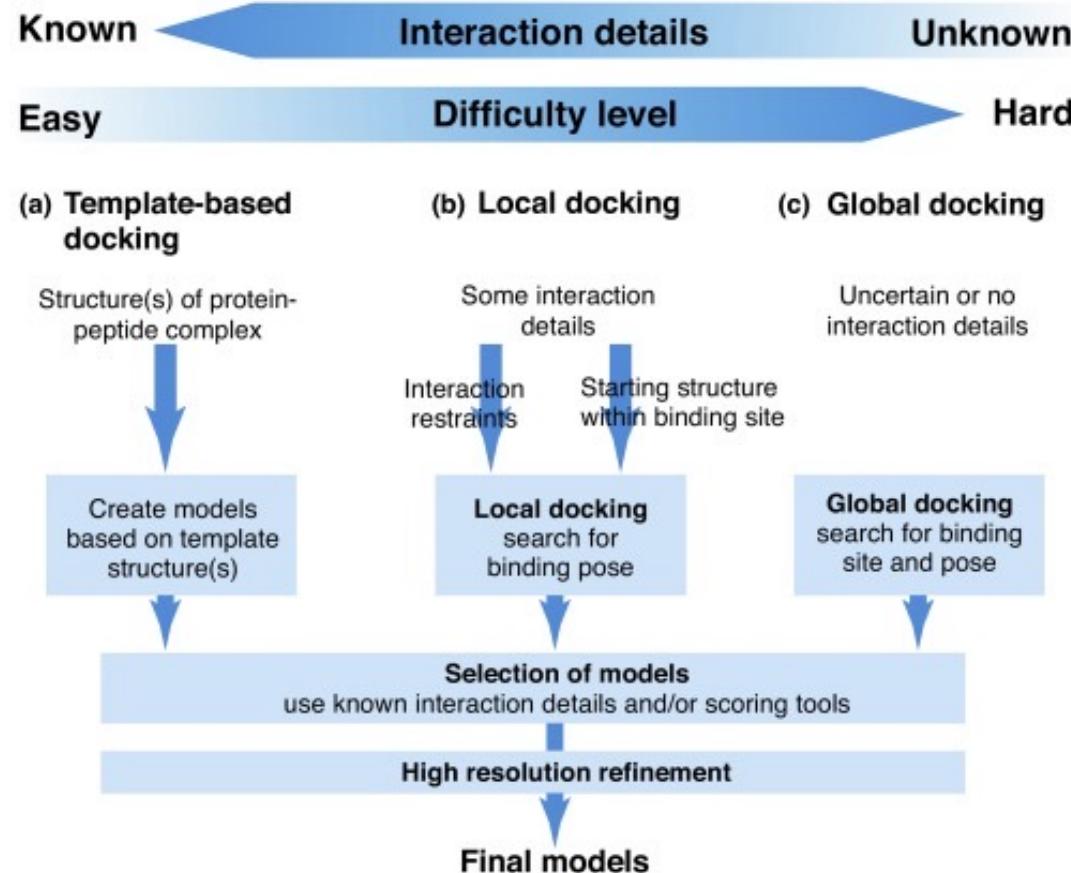
TIPOS DE DOCKING MOLECULAR

Existem diferentes tipos de docking molecular, cada um adequado para diferentes contextos biológicos:

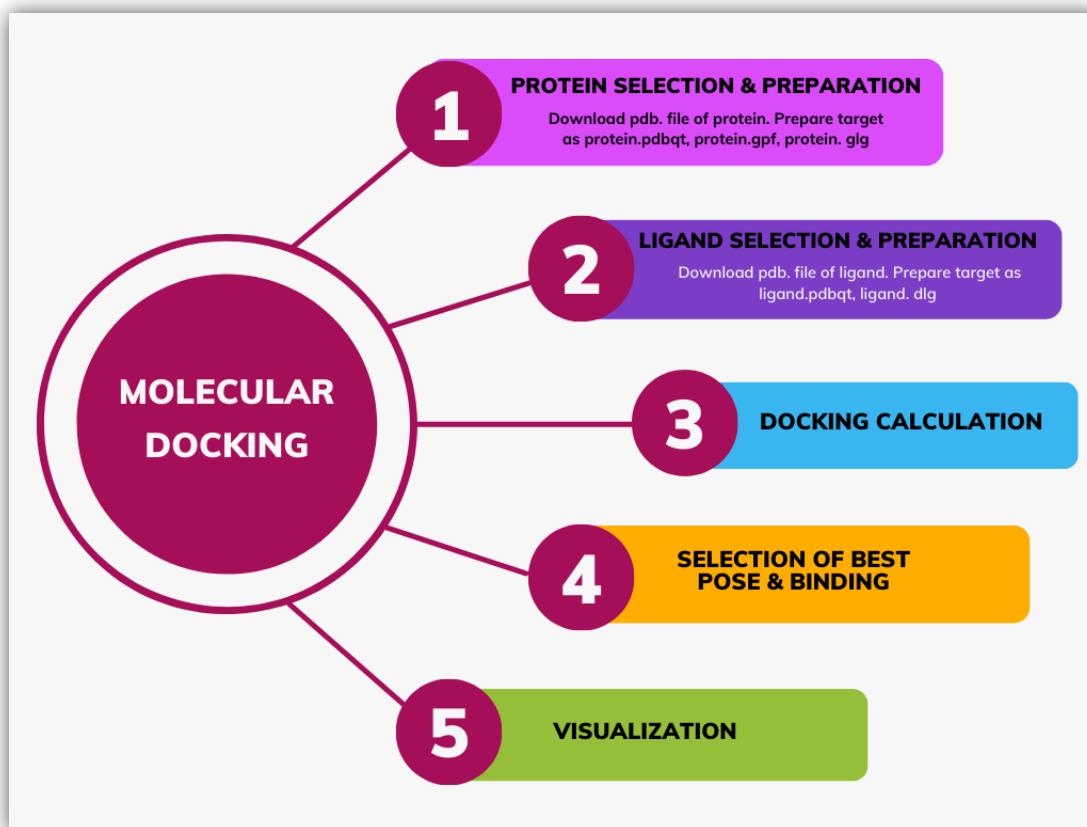
- **Docking rígido-rígido:** Tanto o receptor quanto o ligante são considerados estruturas rígidas, sem qualquer flexibilidade. É rápido, mas pode não representar bem sistemas biológicos dinâmicos.
- **Docking flexível-rígido:** O receptor é tratado como rígido, enquanto o ligante pode assumir diferentes conformações. Esse modelo melhora a precisão da predição sem aumentar muito o custo computacional.
- **Docking flexível-flexível:** Ambos o receptor e o ligante podem se mover e ajustar durante a simulação. Esse método é mais realista, mas também mais complexo e computacionalmente exigente.



TIPOS DE DOCKING MOLECULAR



ETAPAS DO DOCKING MOLECULAR

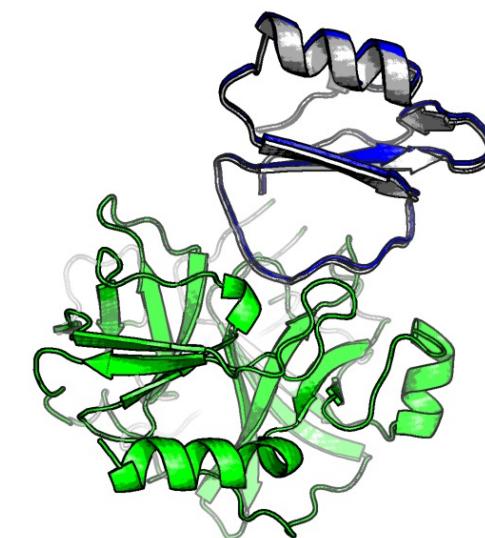
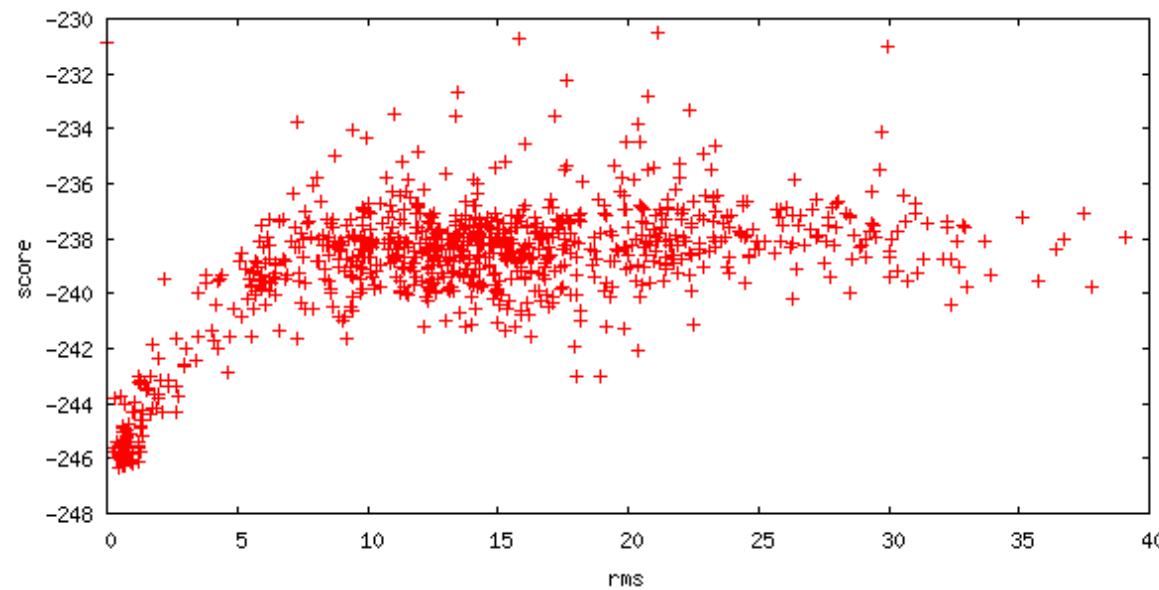


Antes de realizar o docking, é essencial preparar as estruturas. O processo inclui a **limpeza estrutural**, removendo solventes e ligantes indesejados. A **protonação** ajusta os estados de ionização dos resíduos para refletir condições fisiológicas. A **inspeção da qualidade estrutural** garante que não existam átomos ausentes ou distorções estruturais. Softwares como **Chimera**, **AutoDockTools** e **PDBFixer** auxiliam nessas etapas para otimizar os modelos que serão utilizados nas próximas etapas.

PACOTES/SERVIDORES PARA DOCKING MOLECULAR

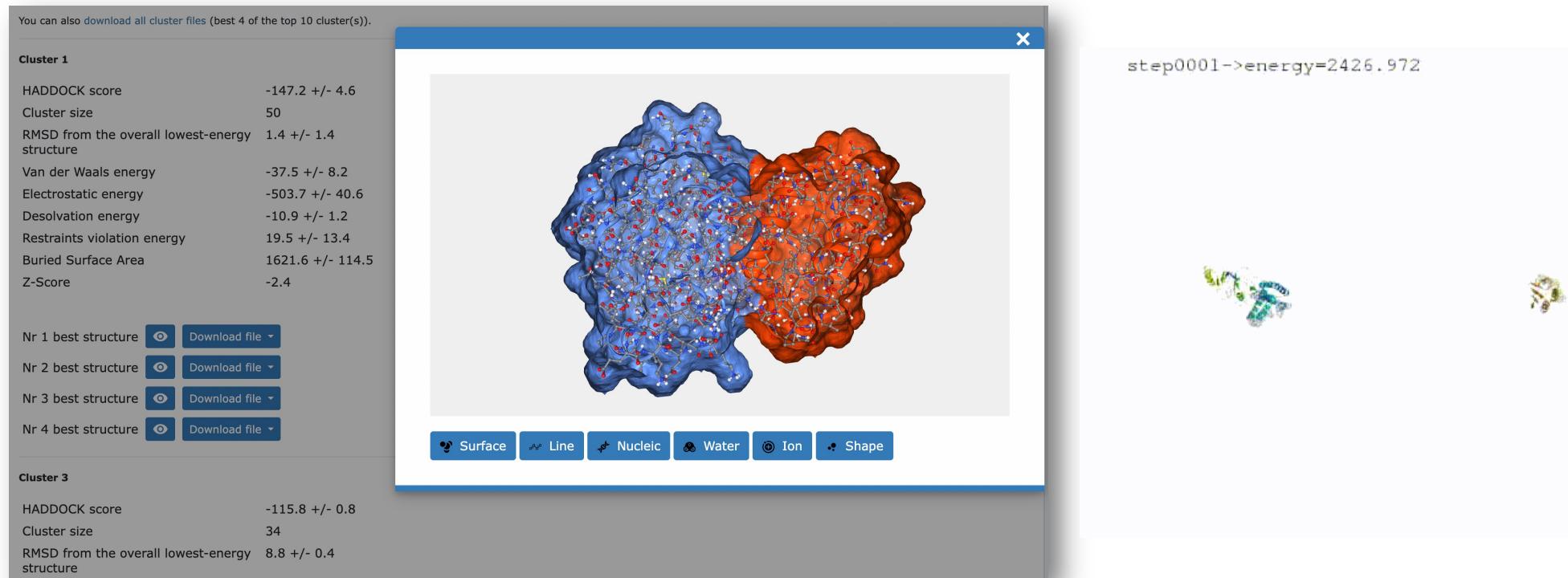
Existem diversas ferramentas computacionais para realizar docking molecular, cada uma com suas características e diferentes algoritmos e funções de energia:

Rosetta: Utilizado principalmente para **docking flexível-flexível**, permitindo o refinamento de interações moleculares com alta precisão. Sua principal vantagem é a modelagem detalhada de estruturas proteicas, mas seu alto custo computacional pode ser uma desvantagem.



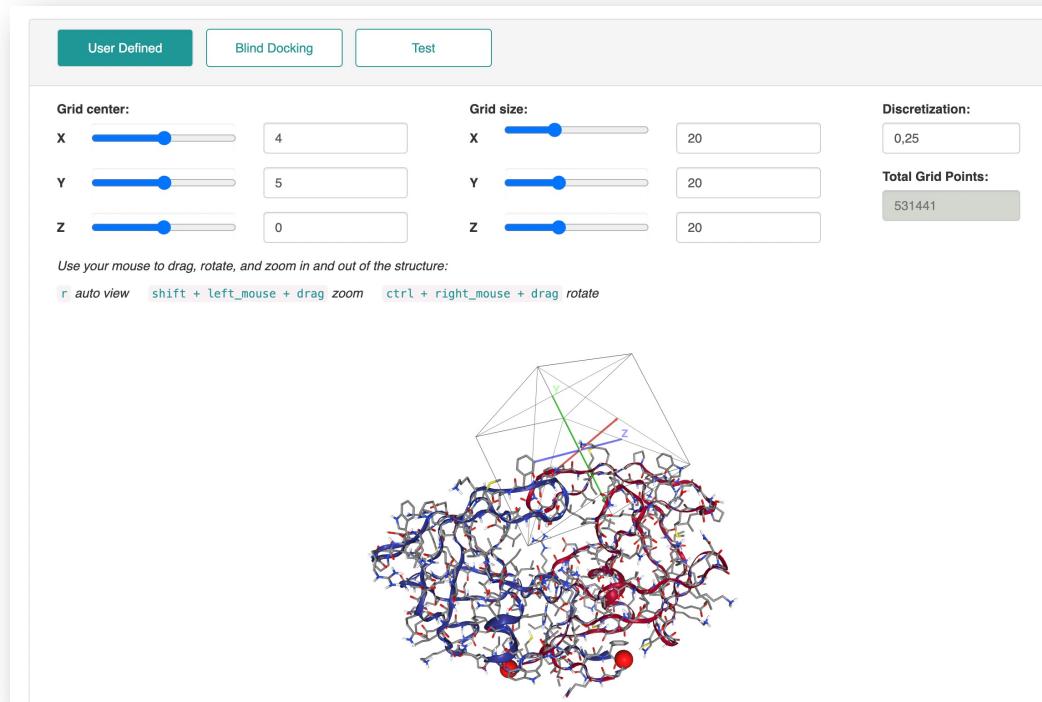
PACOTES/SERVIDORES PARA DOCKING MOLECULAR

Haddock: Especializado em docking proteína-proteína baseado em restrições experimentais. Ideal para **docking flexível-rígido ou flexível-flexível**, oferecendo alta precisão, mas exigindo alguns insights de informações experimentais prévias.



PACOTES/SERVIDORES PARA DOCKING MOLECULAR

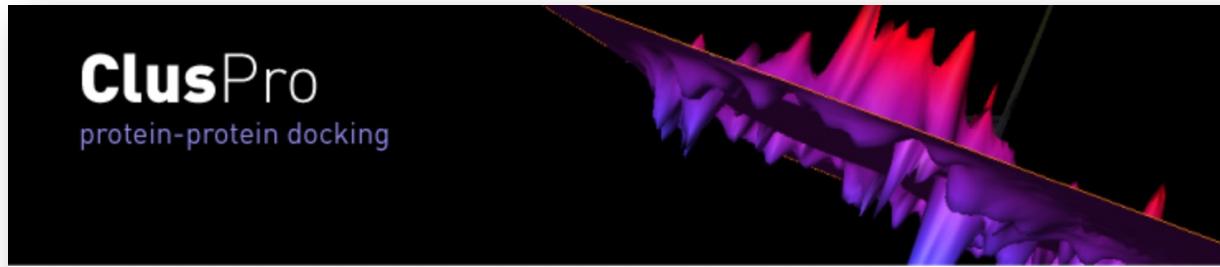
DockThor: Ferramenta que utiliza métodos de **docking flexível-rígido**, sendo eficiente e acessível para diversos usuários. Sua limitação está na menor flexibilidade do receptor.



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

PACOTES/SERVIDORES PARA DOCKING MOLECULAR

ClusPro: Realiza **docking rígido-rígido e flexível-rígido** para complexos proteína-proteína, com algoritmos de agrupamento para identificar interações estáveis. A vantagem é sua automação, mas ele pode não considerar todas as flexibilidades moleculares.



The screenshot shows the ClusPro software interface. At the top left, the logo "ClusPro" is displayed above the text "protein-protein docking". To the right of the logo is a 3D surface plot representing a protein-protein docking simulation, with color-coded regions of interaction energy. Below the main title, there is a "Help" button. Underneath the "Help" button, a text link reads: "For additional examples, please refer to our Nature Protocols publication [here](#)". Further down, there is a "Tutorials" section containing a list of links to various docking modes and methods.

Help

For additional examples, please refer to our Nature Protocols publication [here](#).

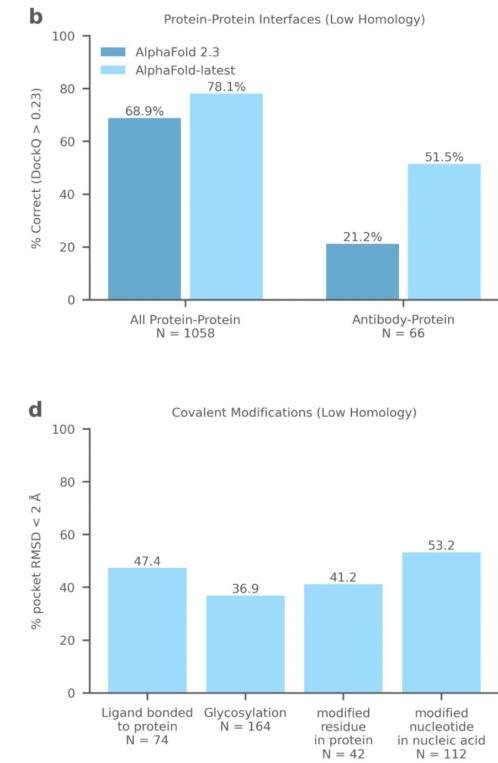
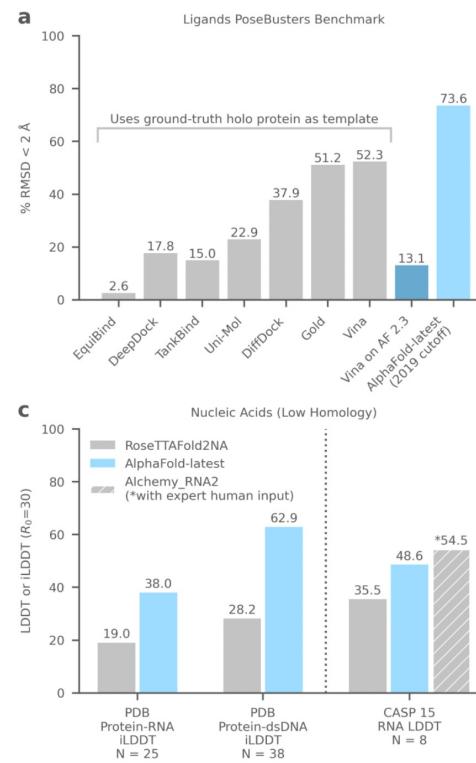
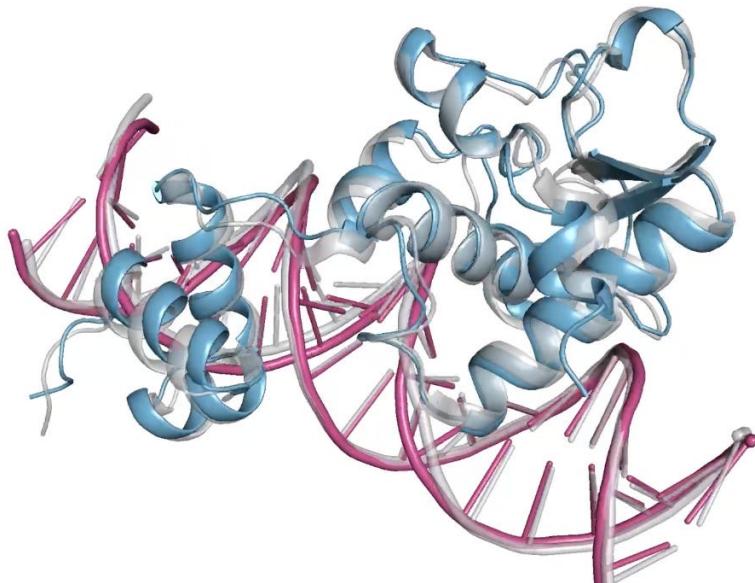
Tutorials

- [Beginning Docking](#)
- [Constraints: Attraction and Repulsion](#)
- [Tails & Unstructured Residues](#)
- [Antibody Mode](#)
- [Multimer Mode](#)
- [SAXS Mode](#)
- [Restraints Mode](#)
- [Dimer Classification](#)
- [Peptide Mode](#)

<https://cluspro.org/help.php>

PACOTES/SERVIDORES PARA DOCKING MOLECULAR

AlphaFold 3 (AF3): Embora seja conhecido por prever estruturas de proteínas, AF3 pode ser usado para prever interações moleculares e **docking flexível-flexível**, sendo uma ferramenta emergente para modelagem precisa de ligações.



PACOTES/SERVIDORES PARA DOCKING MOLECULAR

NVIDIA Clara / DiffDock: Utiliza ML para otimizar docking molecular, especialmente para **docking flexível-flexível**. Sua vantagem está na velocidade de processamento, mas pode requerer hardware específico para um desempenho ideal.

The screenshot shows the NVIDIA Build interface for the "Build A Generative Virtual Screening Pipeline" blueprint. The top navigation bar includes "nvidia / Build", "Blueprints", "Experience", "Blueprint Card", and "NIM". The main title is "nvidia / Build A Generative Virtual Screening Pipeline". Below it, a sub-header states: "This blueprint shows how generative AI and accelerated NIM microservices can design optimized small molecules smarter and faster." The blueprint is categorized under "ALPHAFOLD2 • MOLMIM-GENERATE • DIFFDOCK" and includes tags for "biology", "blueprint", "healthcare", "molecular docking", "molecular generation", "protein folding", "nvidia bionemo", and "drug discovery". A prominent green button on the right says "Download Blueprint".

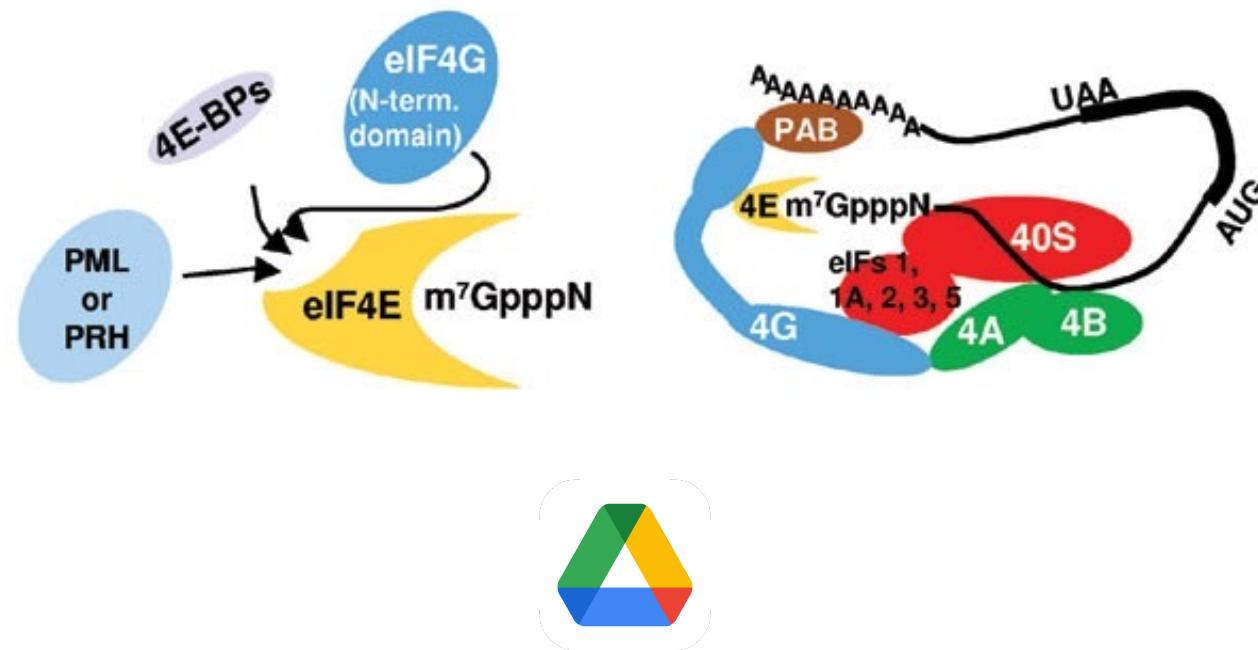
The interface is divided into sections: "Input" and "Output". The "Input" section contains a "View Examples" link and a "AlphaFold2 Inputs" section. It includes a dropdown menu for "Cached AlphaFold2 folded proteins" with "SARS-CoV-2 Main Protease" selected. Below this, a note says: "Choose which cached model you want to use for this blueprint". The "Output" section displays five generated molecules with scores: 0.81, 0.76, 0.75, 0.73, and 0.0. A "Download" button is located next to the last molecule. A warning message at the bottom of the screen reads: "AI models generate responses and outputs based on complex algorithms and machine learning techniques, and those responses or outputs may be inaccurate, harmful, biased or indecent. By testing this model, you assume the risk of any harm caused by any response or output of the model. Please do not upload any confidential information or personal data unless expressly permitted. Your use is logged for security purposes." A "x" icon is next to the message.

<https://build.nvidia.com/mit/difffdock>

<https://build.nvidia.com/nvidia/generative-virtual-screening-for-drug-discovery>

HANDS-ON COM O DiffDock

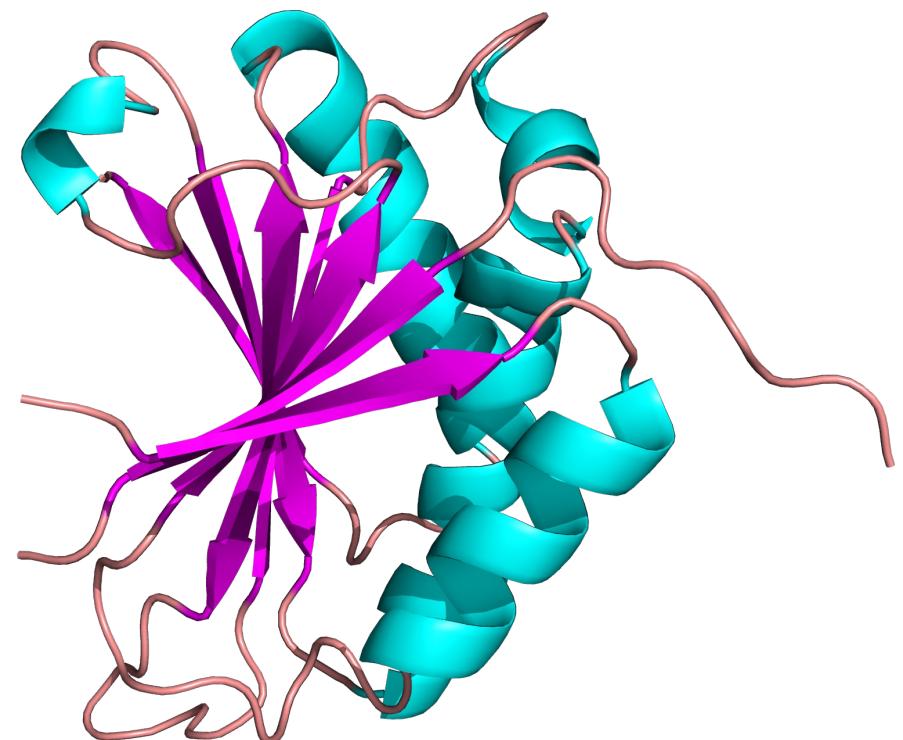
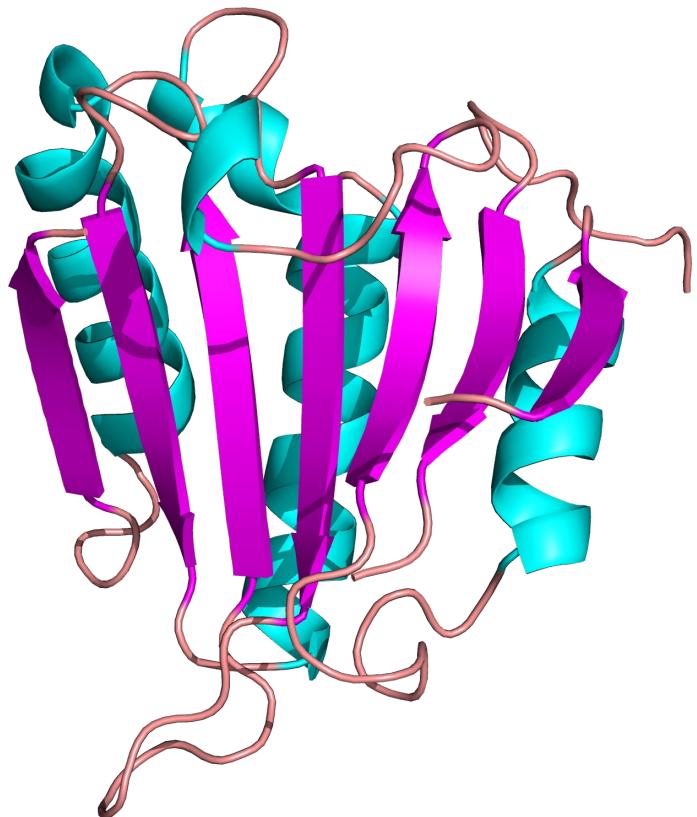
<https://build.nvidia.com/mit/diffdock>



<https://drive.google.com/drive/folders/14NIxbxxEwj6f1hKakTVgFh5jchan0YX?usp=sharing>

RECEPTOR (eIF4E)

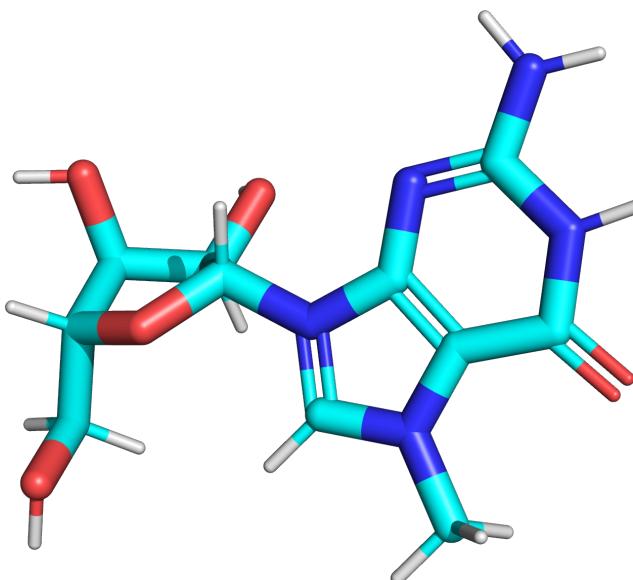
<https://www.rcsb.org/structure/8UH1>



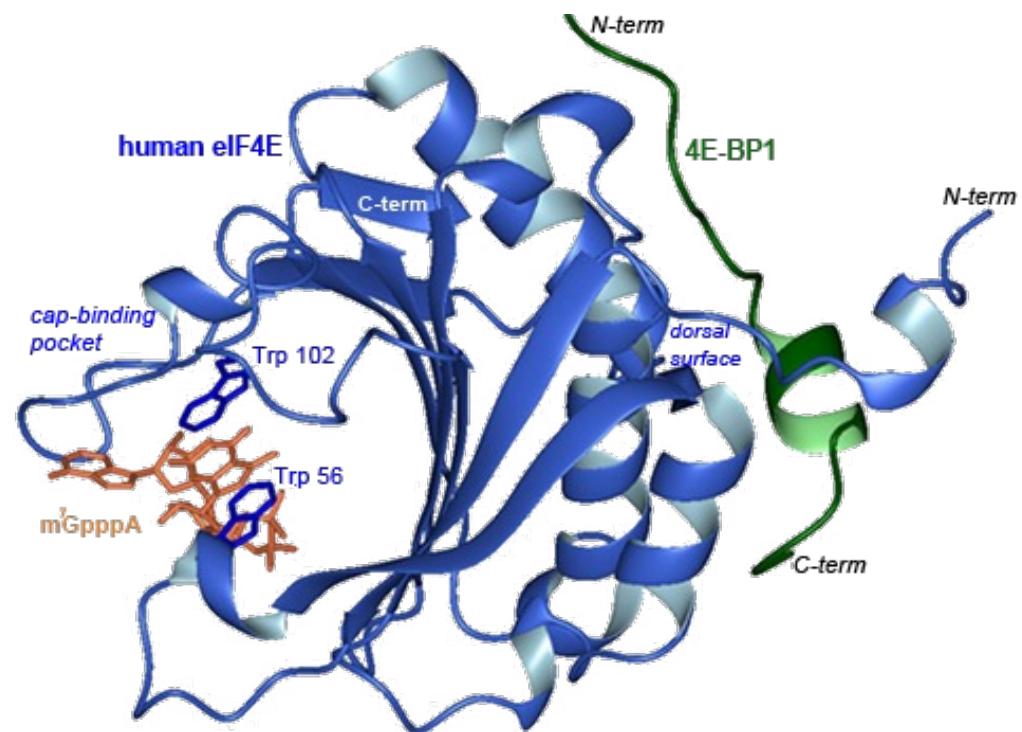
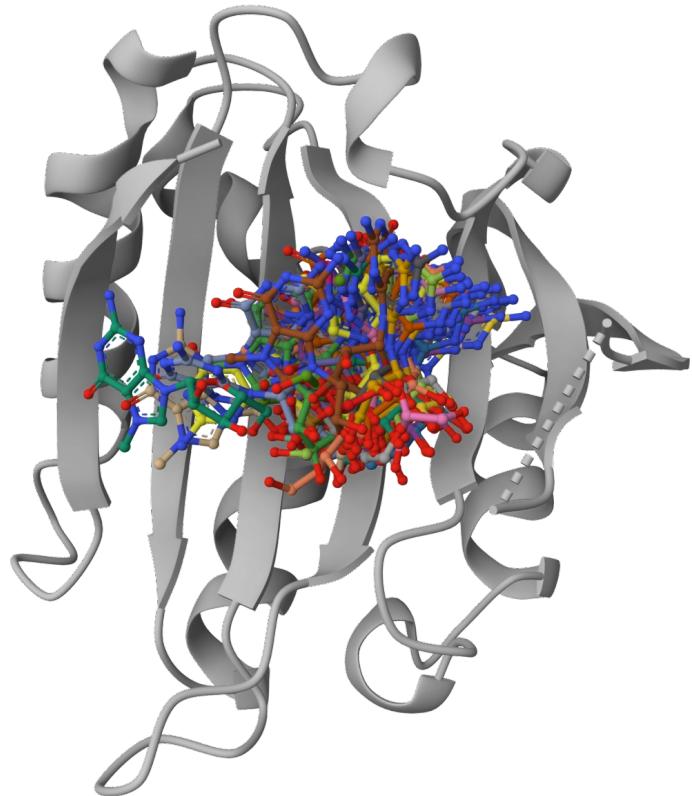
LIGANTE (5'cap)

<https://pubchem.ncbi.nlm.nih.gov/compound/N7-Methylguanosine>

<https://www.rcsb.org/ligand/G7M>



PREDIÇÃO VS. MODELOS EXPERIMENTAIS



ENSITRELVIR x SARS-CoV-2 MAIN PROTEASE (MPRO)

Article Contents

- Abstract
- METHODS
- RESULTS
- DISCUSSION
- Supplementary Data
- Notes
- References
- Author notes
- Supplementary data

JOURNAL ARTICLE CORRECTED PROOF

Ensitrelvir for the Treatment of Nonhospitalized Adults with COVID-19: Results from the SCORPIO-HR, Phase 3, Randomized, Double-blind, Placebo-controlled Trial

Anne F Luetkemeyer , Kara W Chew, Stuart Lacey, Michael D Hughes, Linda J Harrison, Eric S Daar, Joseph Eron, Courtney V Fletcher, Alexander L Greninger, Diane Hessinger ...

Show more

Author Notes

Clinical Infectious Diseases, ciaf029, <https://doi.org/10.1093/cid/ciaf029>

Published: 17 February 2025 Article history ▾

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Abstract

Background

Ensitrelvir, a severe acute respiratory syndrome coronavirus-2 main protease inhibitor, has demonstrated clinical and virologic efficacy in previous studies.



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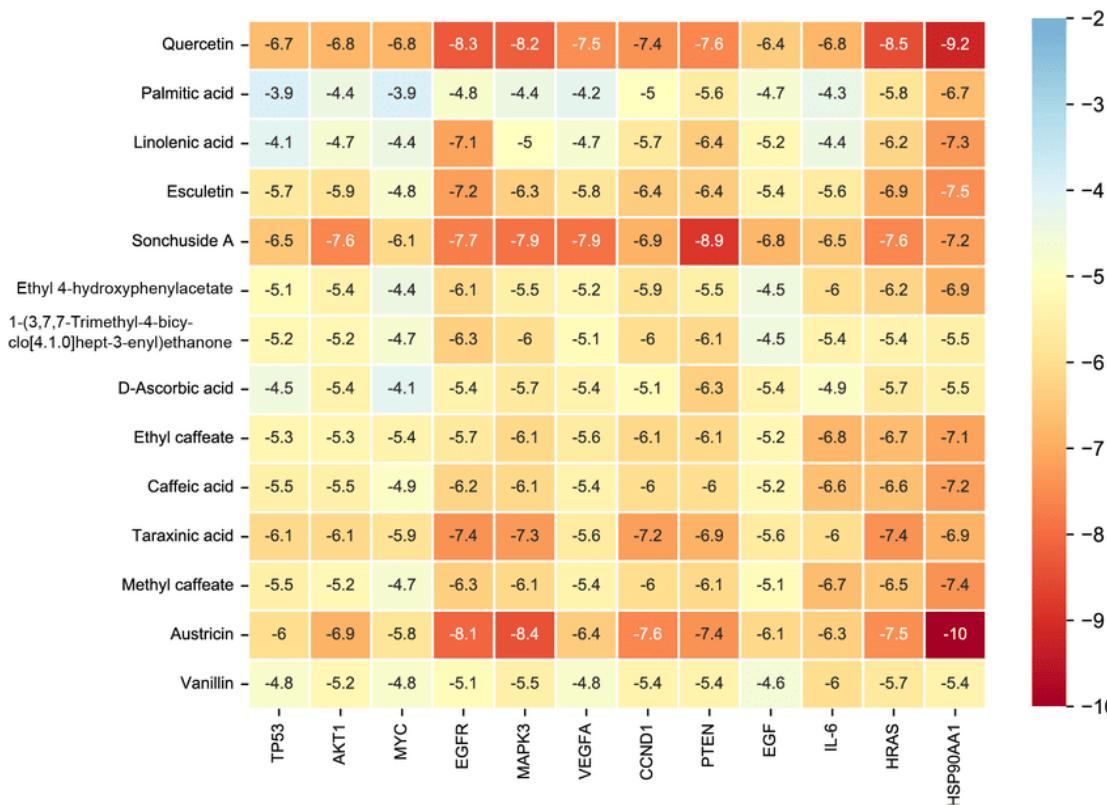
See also

COMMENTARY

<https://build.nvidia.com/mit/difffdock>

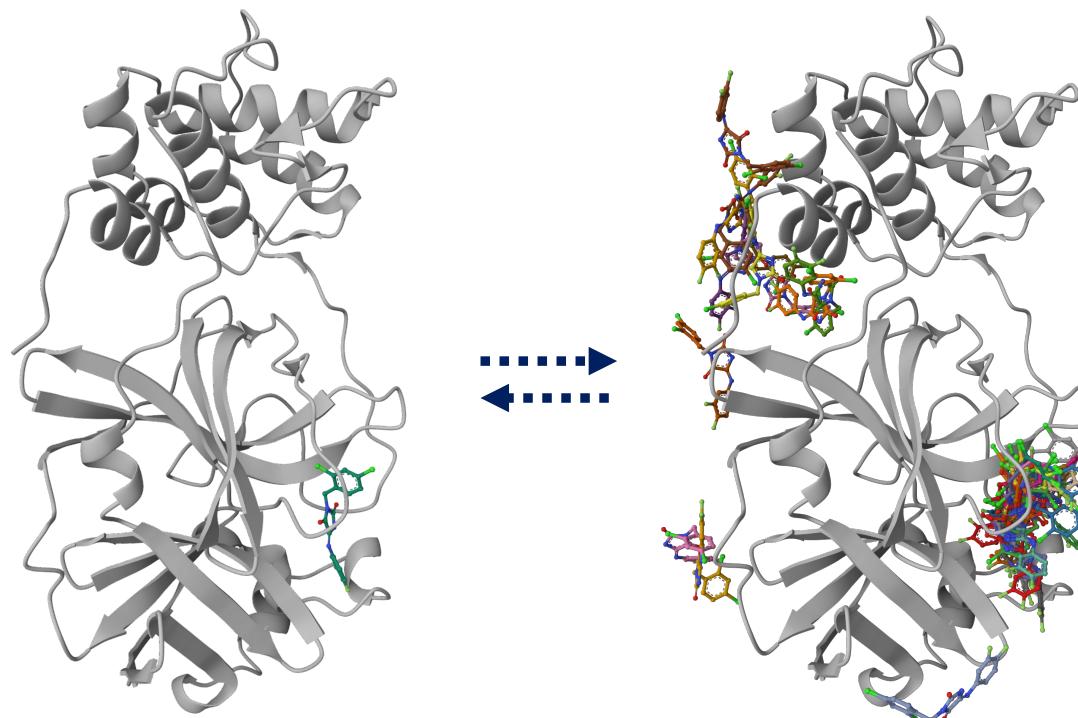
SELECIONANDO OS MELHORES PARES

Os resultados do docking devem ser analisados para identificar a melhor conformação. Parâmetros como energia de ligação, Root Mean Square Deviation (RMSD) e interações específicas são considerados.



VISUALIZAÇÃO AS INTERAÇÕES MOLECULARES

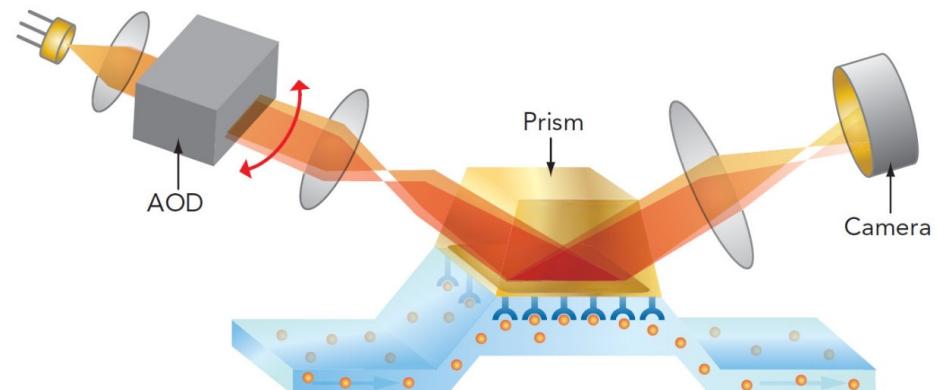
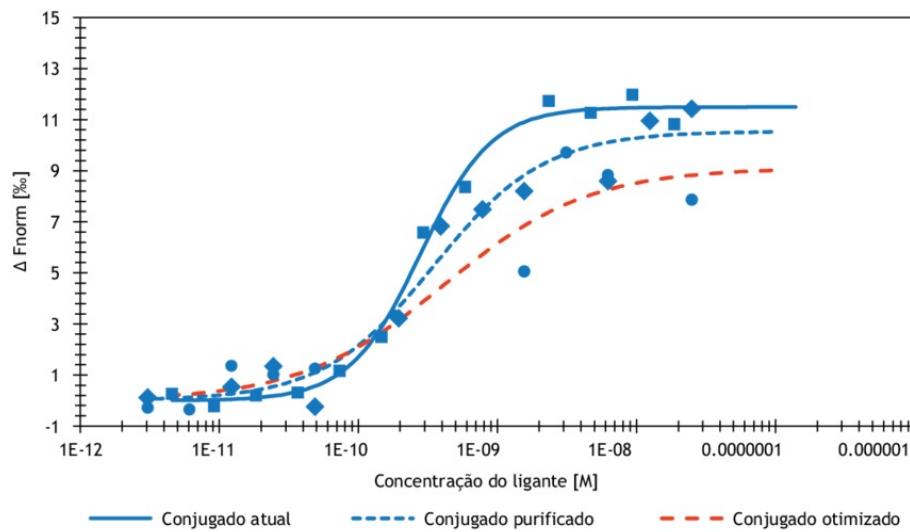
Ferramentas como **PyMOL**, **Chimera** e **VMD** permitem visualizar as interações moleculares e identificar padrões como ligações de hidrogênio, contatos hidrofóbicos e interações iônicas. Comparar múltiplas conformações ajuda a entender a estabilidade do complexo formado, comparando com dados experimentais (caso disponíveis).



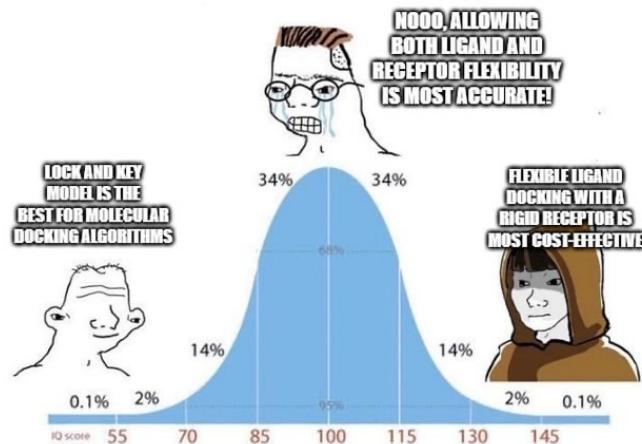
QUAIS AS PROXIMAS ETAPAS APÓS O DOCKING?

Após a realização do docking, os próximos passos incluem:

- **Refinamento das estruturas:** Usando simulações de dinâmica molecular para validar a estabilidade do complexo.
- **Ensaios experimentais:** Validar as interações previstas por meio de experimentos laboratoriais (ex: termoforese em microescala, ressonância plasmônica de superfície, etc)
- **Otimização molecular:** Modificação química dos ligantes para melhorar a afinidade e seletividade.



THAT'S ALL, FOLKS!



E QUALQUER DÚVIDA,
É SÓ MANDAR UM E-MAIL OU MENSAGEM

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 <https://github.com/madsondeluna>