How to Use the Docking Software GOLD to Perform Virtual Screening Simulations

CCDC Virtual Workshop

4th November 2025

REC

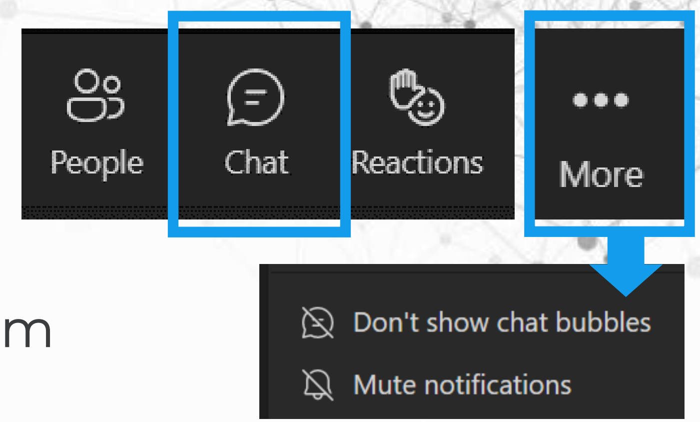
CCDC
advancing structural science

Things you need to know for today

We will make the recording available to you in the next few days

REC

- We will be recording part of today's session
  - We will **not** be recording the hands-on part
- If you have a question:
  - Type your question in the chat box
  - Use the chat box now by telling us **where you are joining from and what the weather is like there today!**
- To do the hands-on part you need:
  - Hermes and GOLD installed with an active license
  - The workshop hand-out
  - More information in the emails we sent you
- Prerequisites
  - None!



Extra tip: when someone is sharing screen, **hover on their name** in the corner of the screen to bring up the **+ and –** symbols to zoom in and out

https://info.ccdc.cam.ac.uk/2025-autumn-virtual-workshops

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Learning outcomes

- ☐ Brief overview of structure-based virtual screening.
- ☐ Basics of the Hermes interface, the CCDC's 3D visualizer for proteins.
- ☐ Cavity detection and extraction in Hermes.
- ☐ Step-by-step set-up of a virtual screening simulation in GOLD.
- ☐ Analysis of virtual screening results.
- ☐ Protein-ligand interactions insights using hotspots via Superstar.

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- *Show One:* Introduction to the CSD
- *Show One:* Virtual screening overview
- *Show One:* Case studies from Prof. Armando Albert
- *Show One:* GOLD overview and demonstration of Virtual Screening using GOLD
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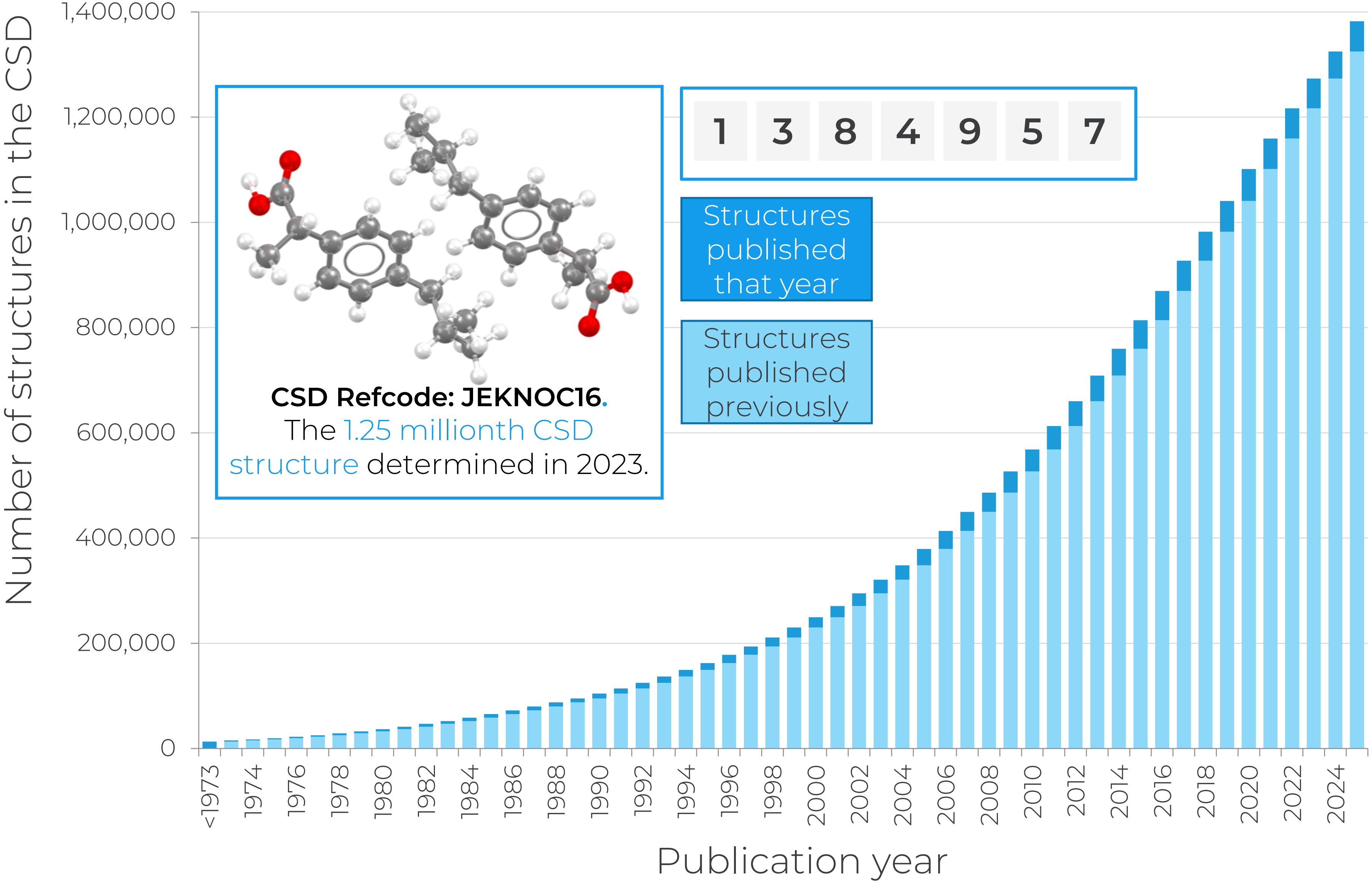
The Cambridge Structural Database

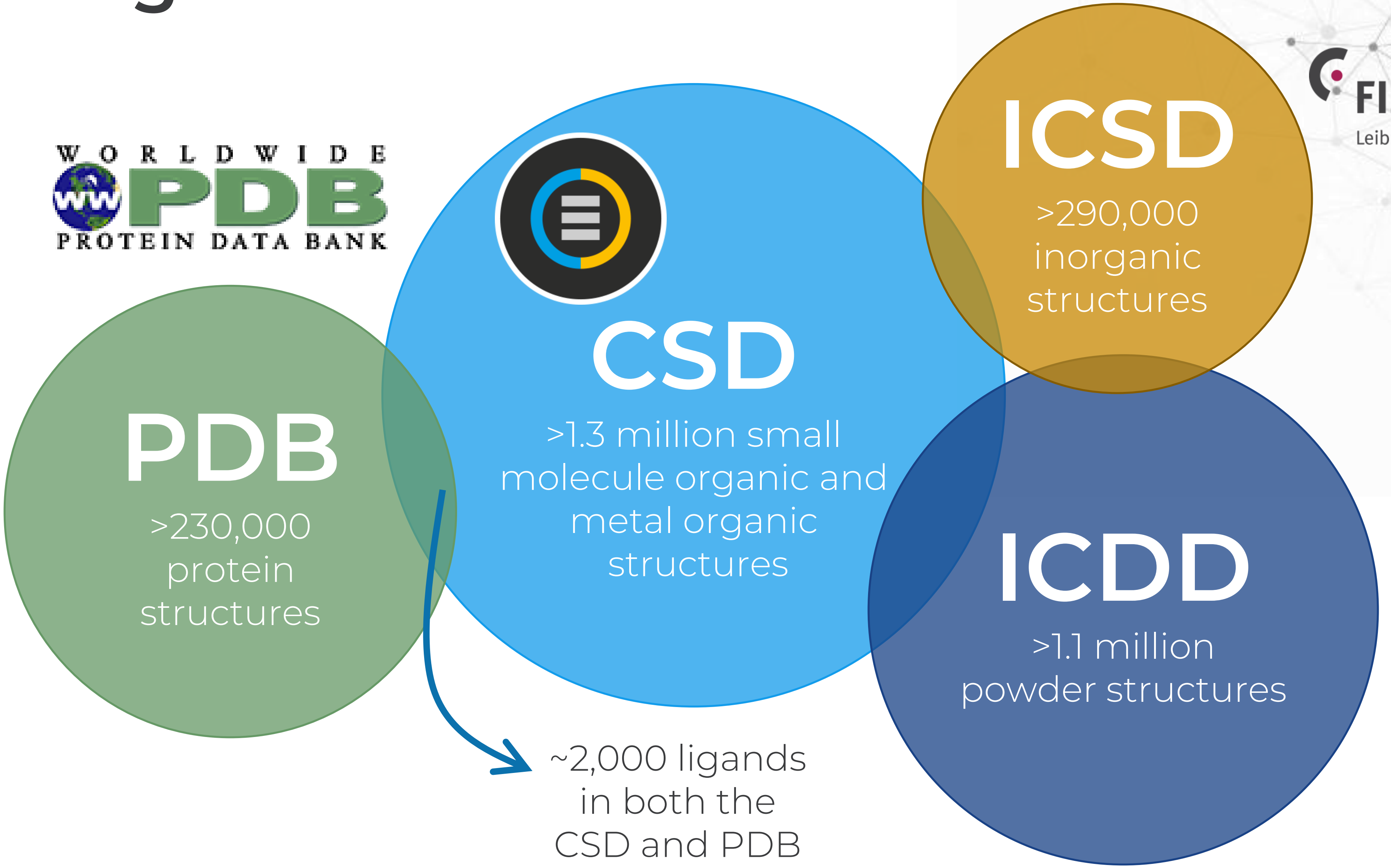


CSD Refcode: JEKNOC16.
The 1.25 millionth CSD structure determined in 2023.

- Small molecule organic and metal-organic structures
- Every published structure
  - Inc. ASAP & early view
  - *CSD Communications*
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for 60 years
- A trusted CoreTrustSeal repository

Certified as Trustworthy by CoreTrustSeal

Integrated structural databases



WORLDWIDE PDB PROTEIN DATA BANK

PDB

>230,000 protein structures

CSD

>1.3 million small molecule organic and metal organic structures

ICSD

>290,000 inorganic structures

ICDD

>1.1 million powder structures

~2,000 ligands in both the CSD and PDB

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

ICDD

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Small molecules, big impact

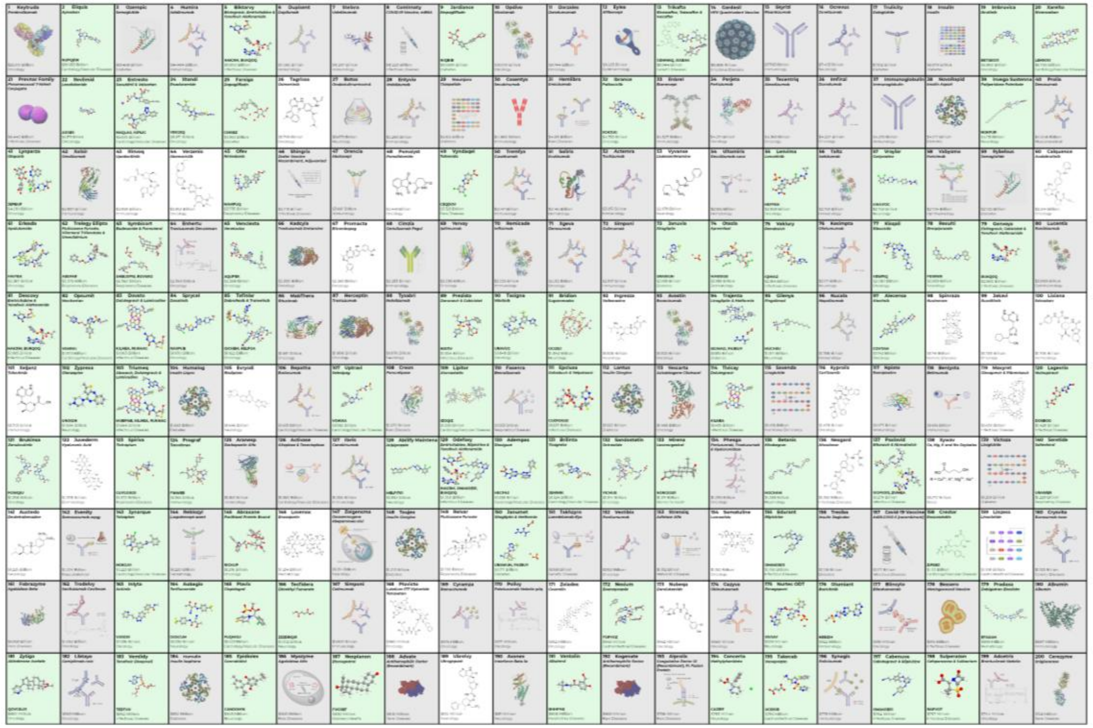
200 top drugs by retail sales in 2023

Small molecule structure in the CSD

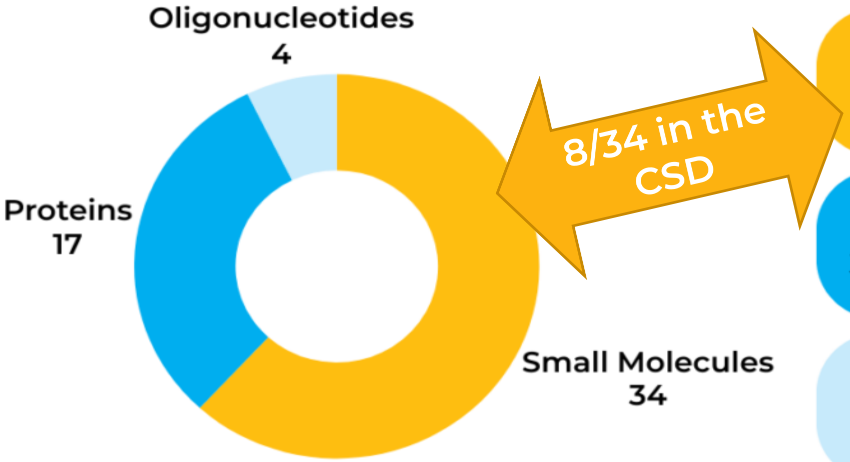
- Open-up new biological and therapeutic opportunities
- Compete against emergent modalities for rare diseases
- Are used to target RNA*

Small molecule structure CSD entry pending

Biological structure in the PDB



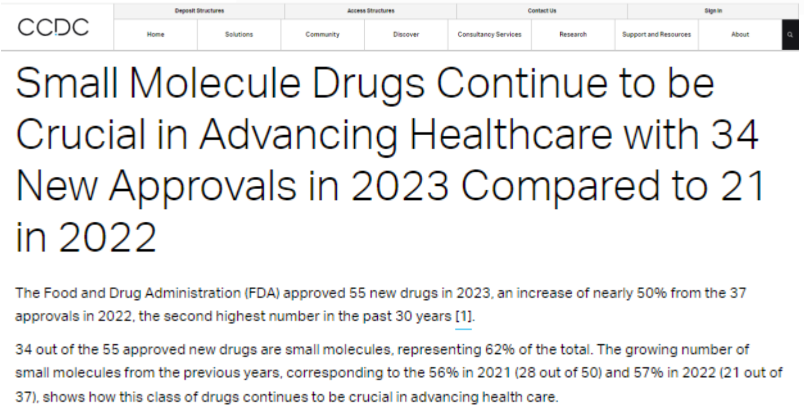
FDA novel drug approvals 2023



34 Small Molecules
31 Small molecule
2 Peptide
1 Radiolabelled

17 Proteins
8 mAb; 4 Bispecific
3 Enzyme; 1 Fusion protein
1 Hormone

4 Oligonucleotides
2 Antisense
1 siRNA
1 RNA aptamer



Small Molecule Drugs Continue to be Crucial in Advancing Healthcare with 34 New Approvals in 2023 Compared to 21 in 2022

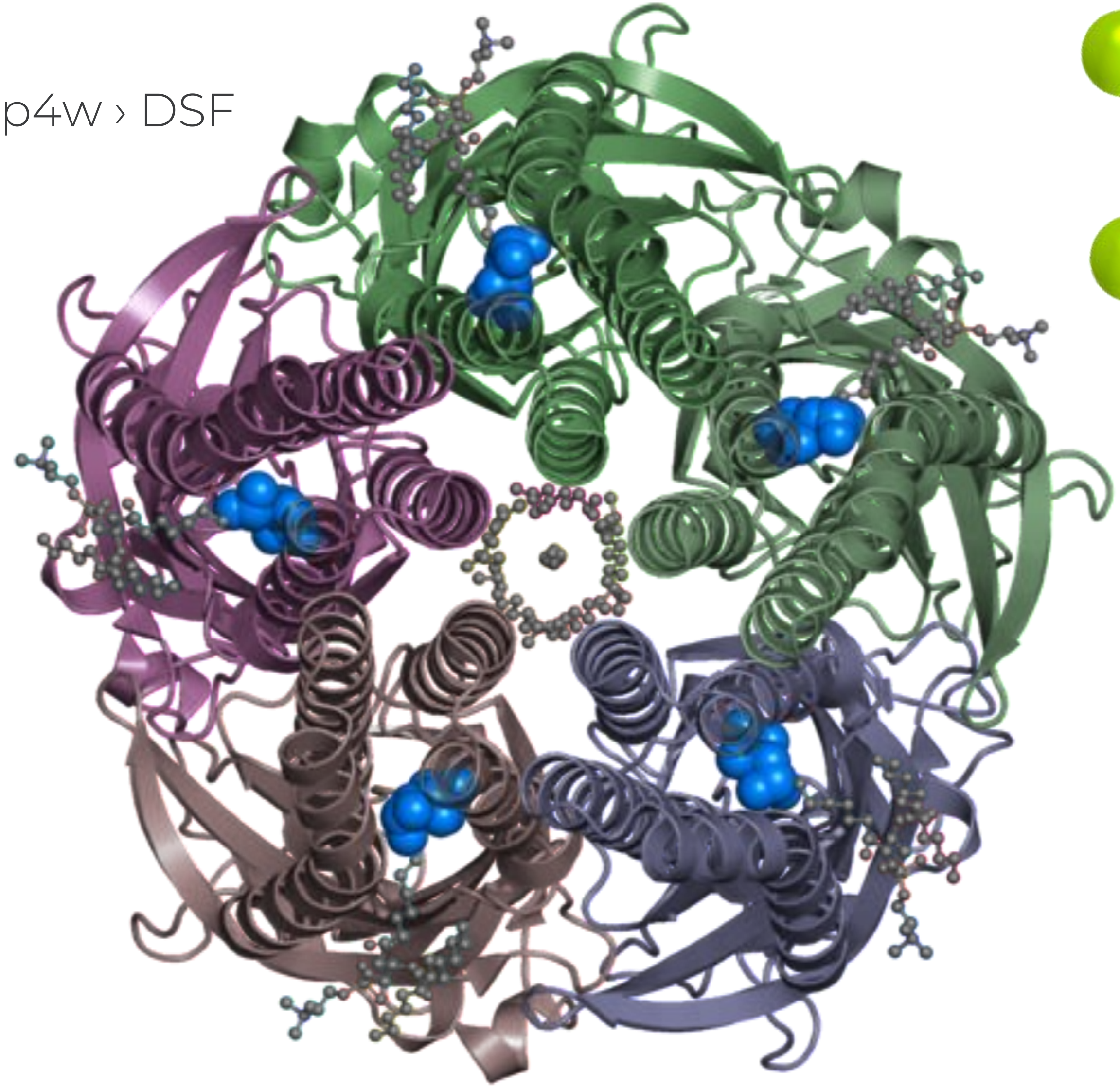
The Food and Drug Administration (FDA) approved 55 new drugs in 2023, an increase of nearly 50% from the 37 approvals in 2022, the second highest number in the past 30 years [1].

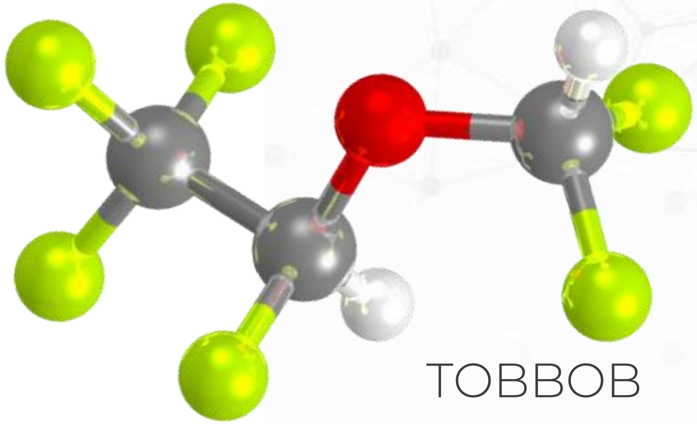
34 out of the 55 approved new drugs are small molecules, representing 62% of the total. The growing number of small molecules from the previous years, corresponding to the 56% in 2021 (28 out of 50) and 57% in 2022 (21 out of 37), shows how this class of drugs continues to be crucial in advancing health care.

Adapted from poster compiled and produced by the Njardarson Group (The University of Arizona)
**Nature Reviews Drug Discovery* 20, 85-90 (2021)

Connecting chemistry and biology

3p4w › DSF





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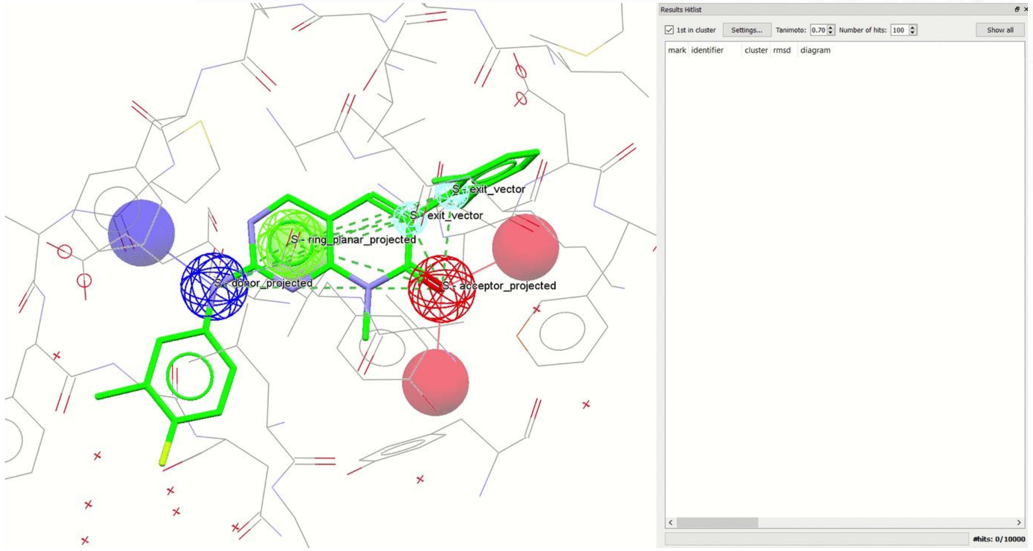


☑ 1st in cluster
Tanimoto: 0.70
Number of hits: 100

mark	identifier	cluster	rmsd	diagram

#hits: 0/10000

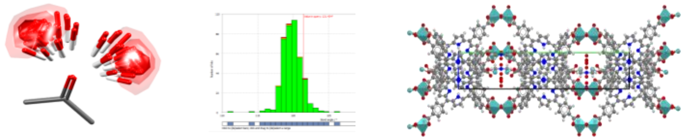
The CSD Portfolio today

CSDEnterprise.

CSDCore.

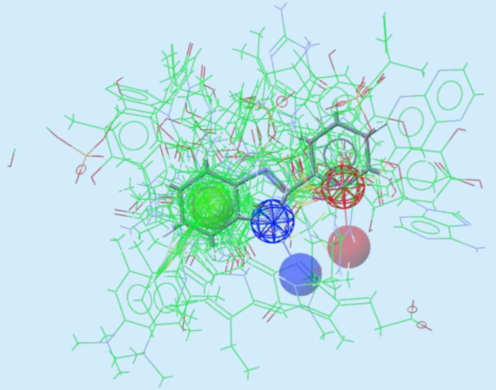
Search, visualise, analyse and communicate structural data

Insights into molecular and crystal shape and interactions



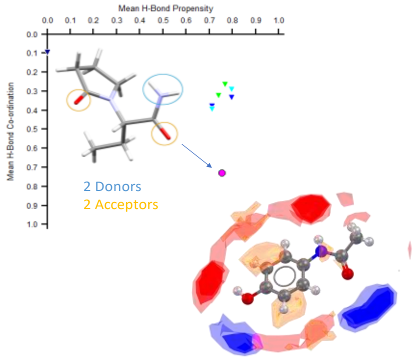
CSDDiscovery.

Design of new molecules



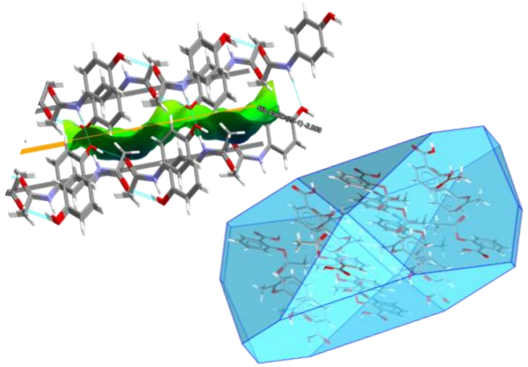
CSDMaterials.

Assessment of solid form stability and properties



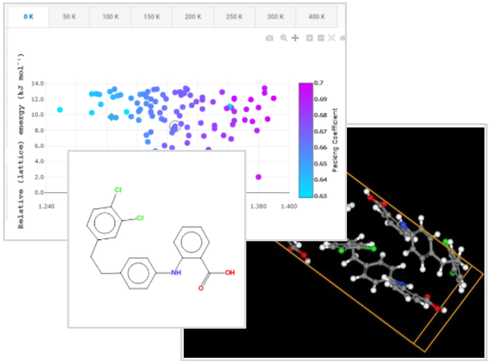
CSDParticle.

Anticipate particle properties and behaviour



CSDTheory.

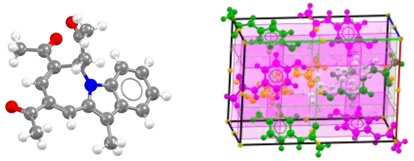
Insights from predicted structure landscapes



CSDCommunity.

Deposit, publish, access and visualise structural data

Free functionality to share and learn from structures



Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists ♦ Functional Materials Scientists ♦ Educators ♦ Industry and Academia

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CSDEnterprise.

CSDCore.

Exploring structures and interactions

CSD
ConQuest
WebCSD
Mercury
Hermes
Mogul
Isostar
CSD-Editor
CSD Python API

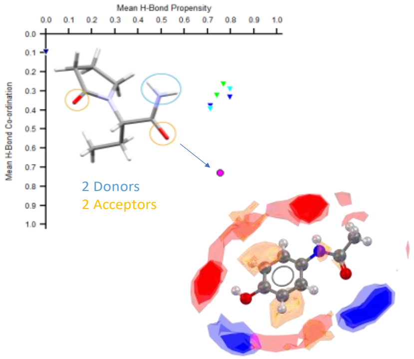
CSDDiscovery.

Design of new molecules

GOLD
Mercury
CrossMiner
SuperStar
API

CSDMaterials.

Assessment of solid form stability and properties



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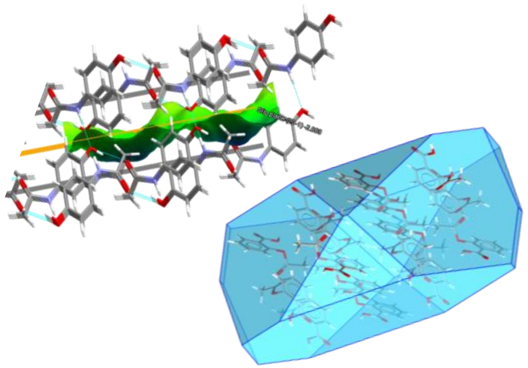

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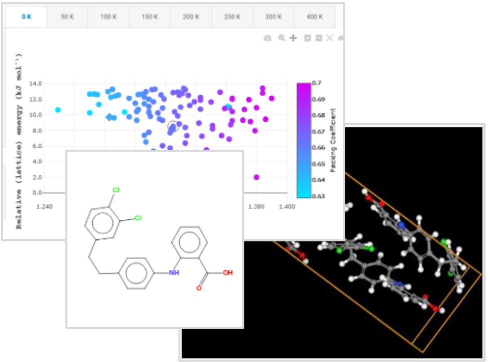

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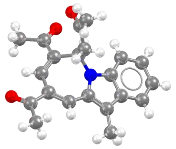

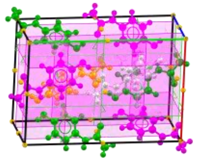

Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists ♦ Functional Materials Scientists ♦ Educators ♦ Industry and Academia

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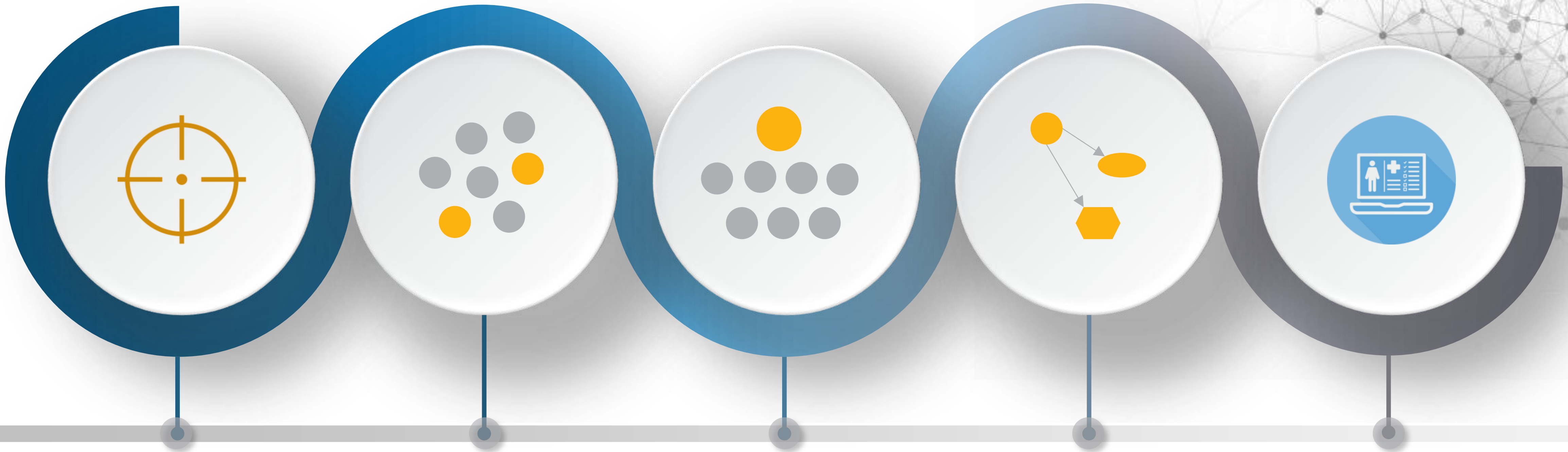
Drug Discovery Pipeline



Target selection

Hit-identification

Structure- based virtual screening.

Hit to lead

Assess how changes affect binding.
Optimize compound geometry.
Predict binding of small molecules to active pockets in proteins.

Lead optimisation

Check the impact of changes with docking pose prediction.
Understand how changes affect conformations.

Drug development

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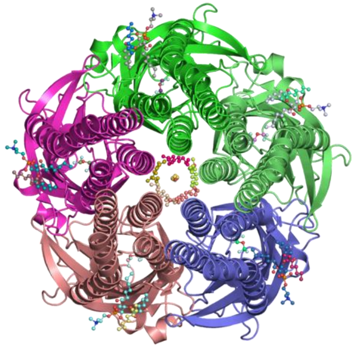
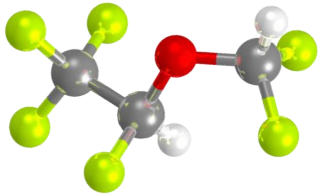
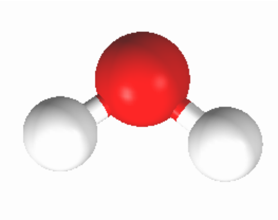
Proteins and ligands – the basics



Proteins are large biomolecules and macromolecules made up of one or more long chains of amino acids.



Ligands are small molecules that bind to the protein and can change the protein function.



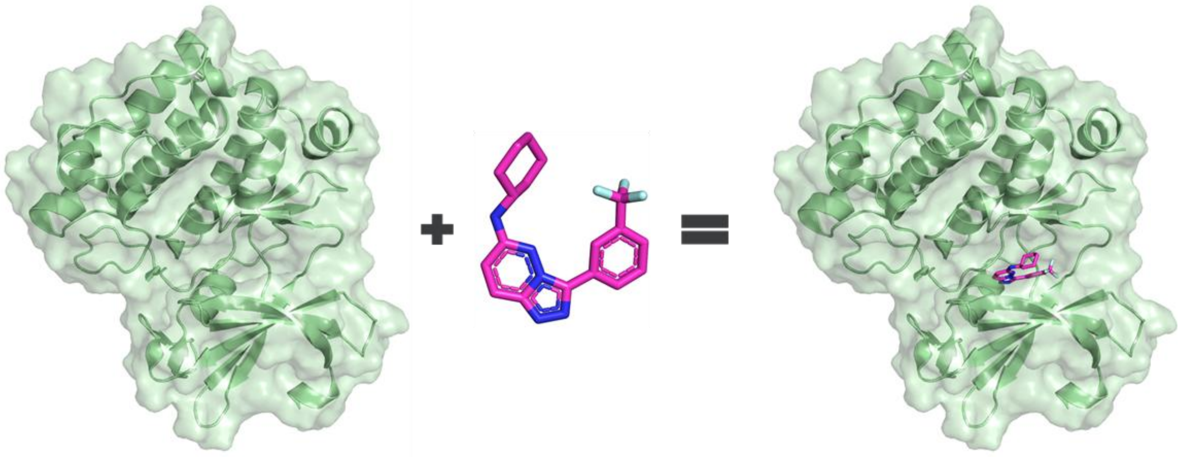
Functional waters are found in the binding site of a protein and mediate the interactions between the ligand and the protein.

Docking and its importance

- Docking is a **computational technique** for the exploration of the possible binding modes of a substrate (ligand) to a given receptor, enzyme or other binding site.

  Glossary of Terms Used In Computational Drug Design, *Pure&Appl. Chem.*,Vol. 69, No. 5, pp. 1137-1152, 1997

- An efficient strategy to identify bioactive conformations.
- To identify possible compounds that binds to specific target of interest.
- Quick screen library of compounds.
- Many docking programs have been developed and applied in drug discovery.



Protein Ligand Protein-Ligand Complex

Other useful terminology

- Ensemble - A group of things or people acting or taken together as a whole.

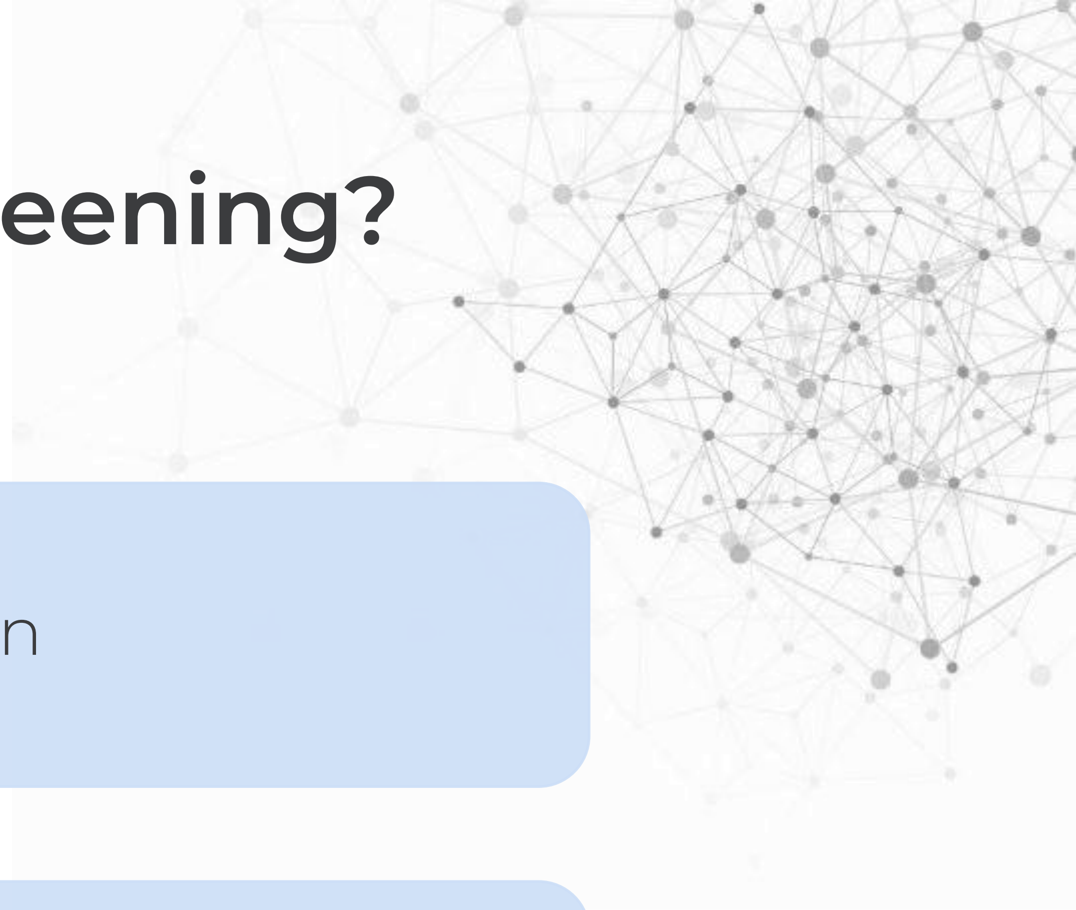
- Ensemble Docking - Aims to address the issue of protein flexibility by adding multiple protein structures into a single Genetic Algorithm (GA) run.

Glossary of Terms Used In Computational Drug Design, *Pure&Appl. Chem.*,Vol. 69, No. 5, pp. 1137-1152, 1997

- Pharmacophore – "Ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interaction with a specific biological target structure and to trigger (or block) its biological response".

C.G.Wermuth, C.R.Ganellin, P.Lindberg, L.A. Mitscher (1998). "Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998)"

What is *in silico* virtual screening?



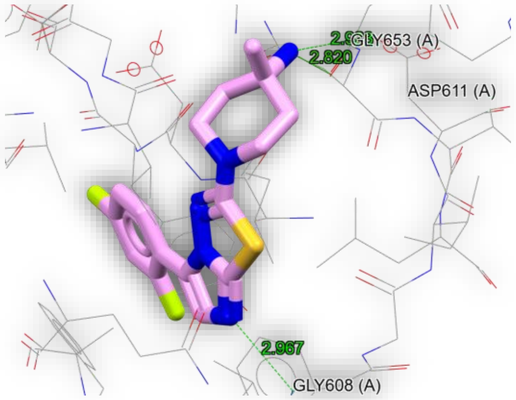
Commonly used computational method to search libraries of small molecules

- Hit identification
- Lead optimization
- Scaffold hopping

Why perform virtual screening rather than HTS?

- To reduce research time
- To reduce chemical waste
- To reduce cost

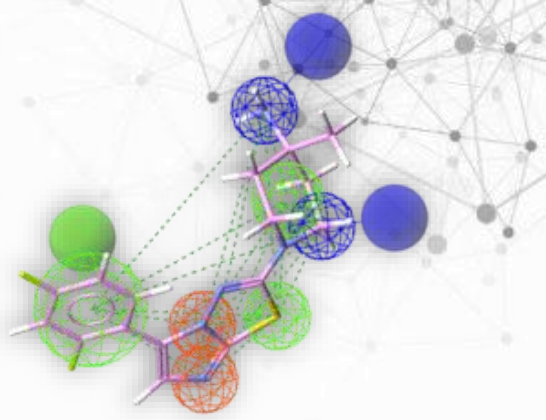
In silico virtual screening approaches



In silico Virtual screening

Structure-based drug design

Ligand-based drug design



AI-based methods

Ultra large libraries

Fragment-based drug design

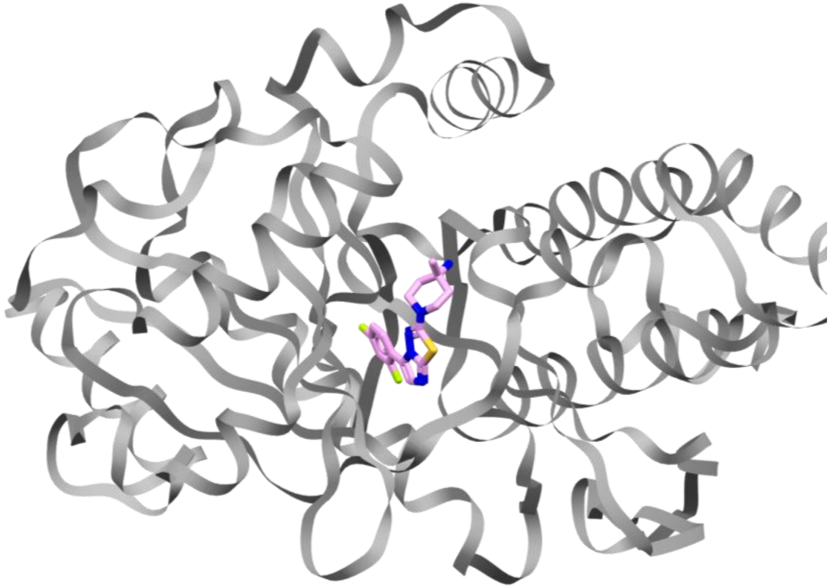
In silico virtual screening approaches

Target-focused libraries

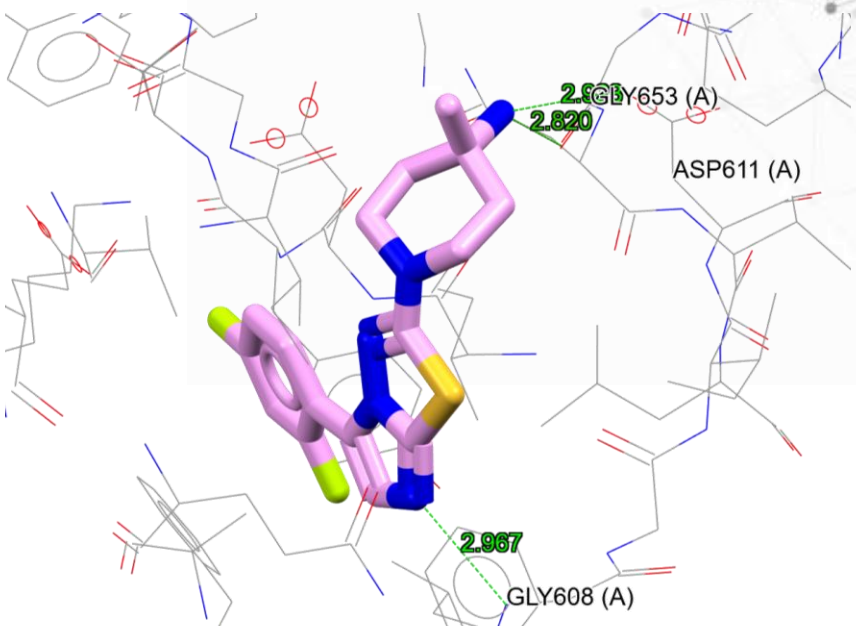
- High quality screening collections
- Fewer compounds to be screened to obtain potential hit candidates
- Reduce costs (computational and financial resources)
- Focused libraries can be selected from a larger, more diverse collections using computational methods (such as *in silico* docking or similarity calculations)
- Selection of a suitable scaffold / core with one or two attachment points for functional groups /side chains
- Look at synthetic accessibility

Structure-Based Drug Design (SBDD)

Receptor selection and preparation



Binding site identification

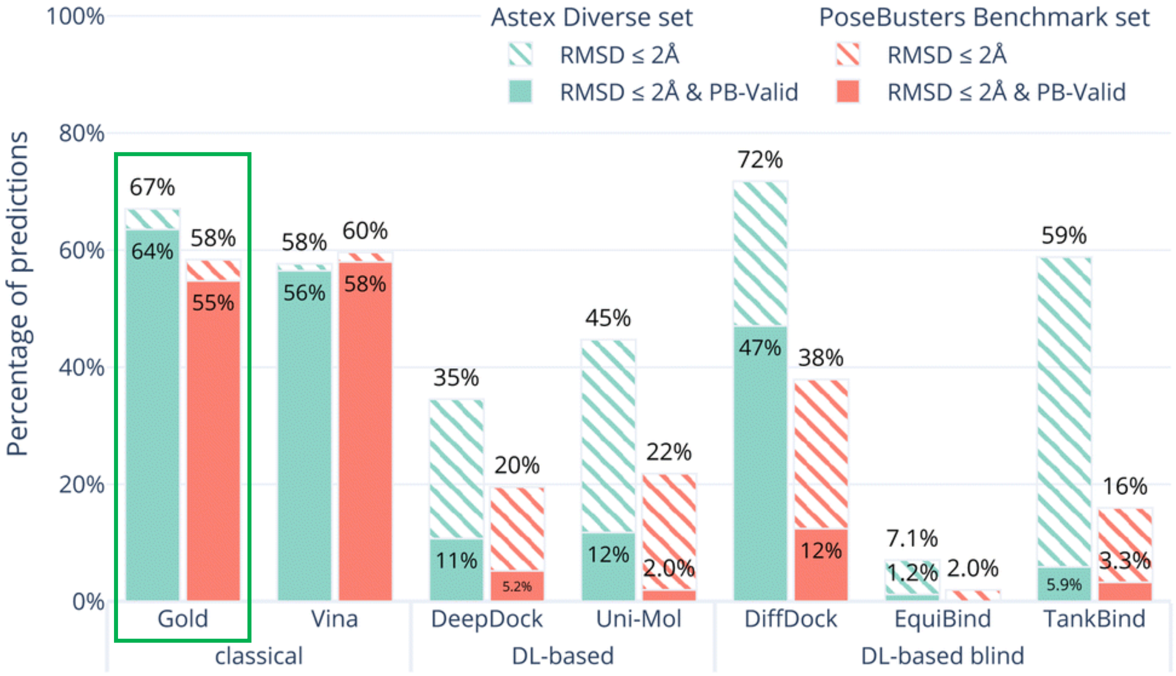


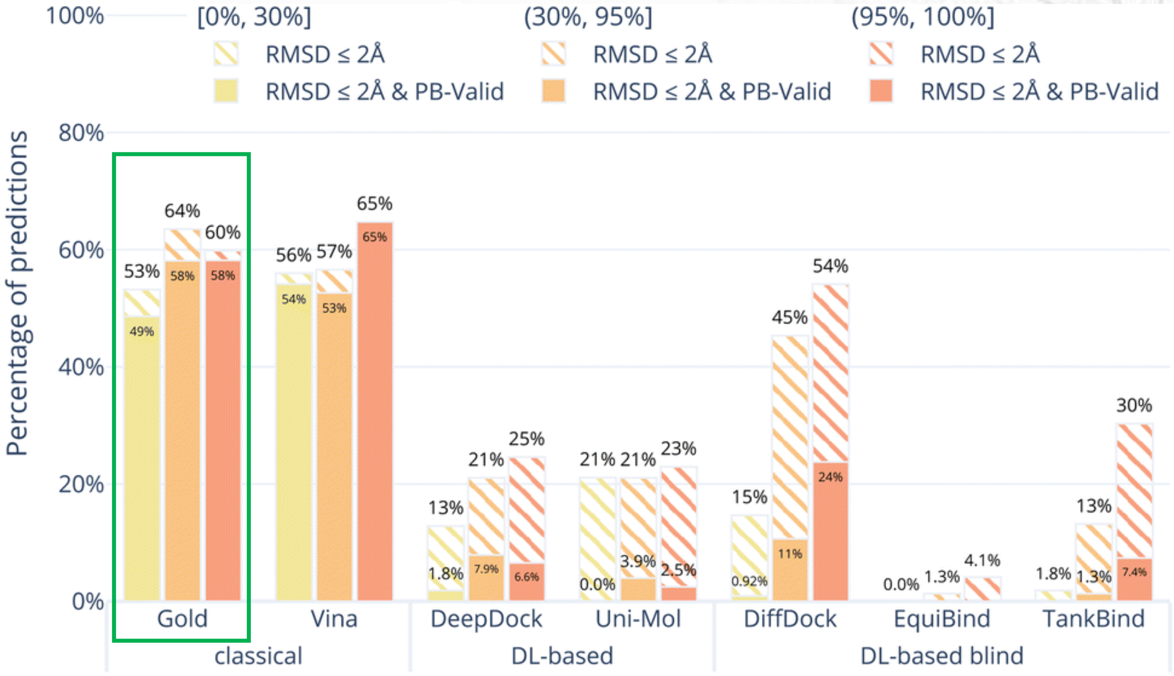
Additional notes: literature research, UNIPROT, PDB searching for similar structures, alignment / superimposition with other co-crystal structures

AI- vs Physically-based docking methods in 2025

PoseBusters: AI-based docking methods fail to generate physically valid poses or generalise to novel sequences [1]

No DeepLearning-based (DL-based) docking method yet outperforms standard docking methods when both physical plausibility and binding mode RMSD is taken into account.





[1] Martin Buttenshoen et al. *Chem. Sci.*, **2024**, 15, 3130-3139

Agenda

Please add your questions for Prof. Albert in the chat and he will answer either in writing or verbally during the hands-on part.

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- *Show One: Case studies from Prof. Armando Albert*
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Prof. Armando Albert

Instituto de Química Física "Blas Cabrera“, Consejo Superior de Investigaciones Científicas

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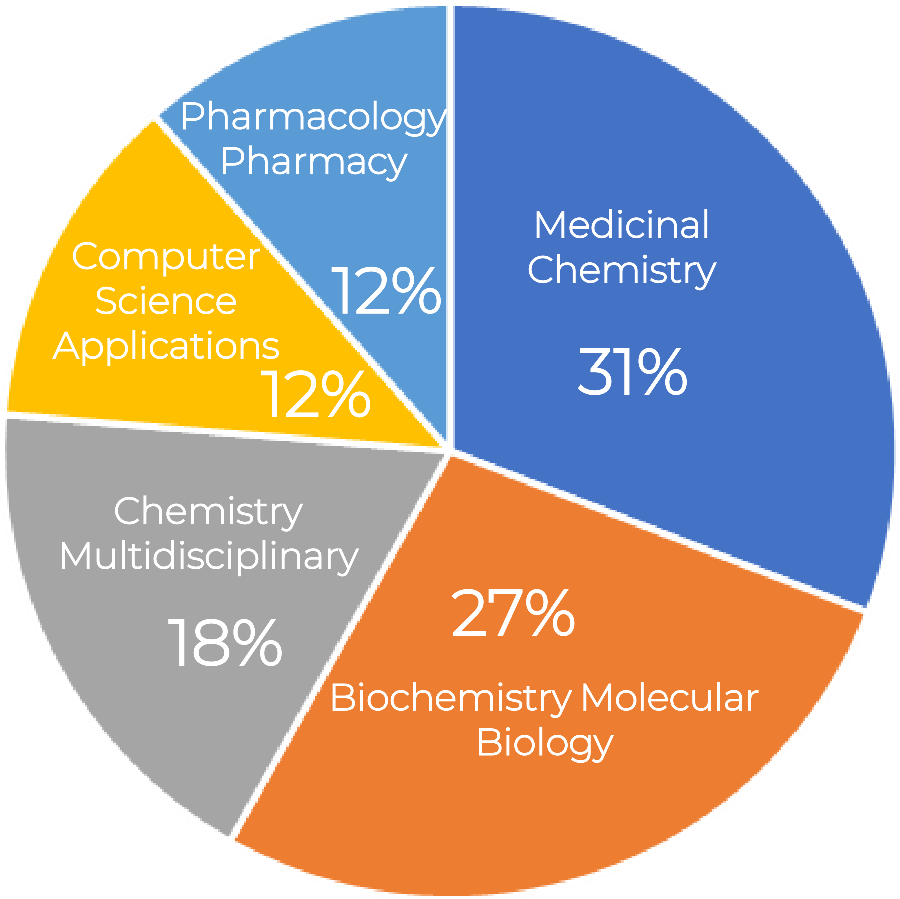
GOLD: Protein-Ligand Docking Software

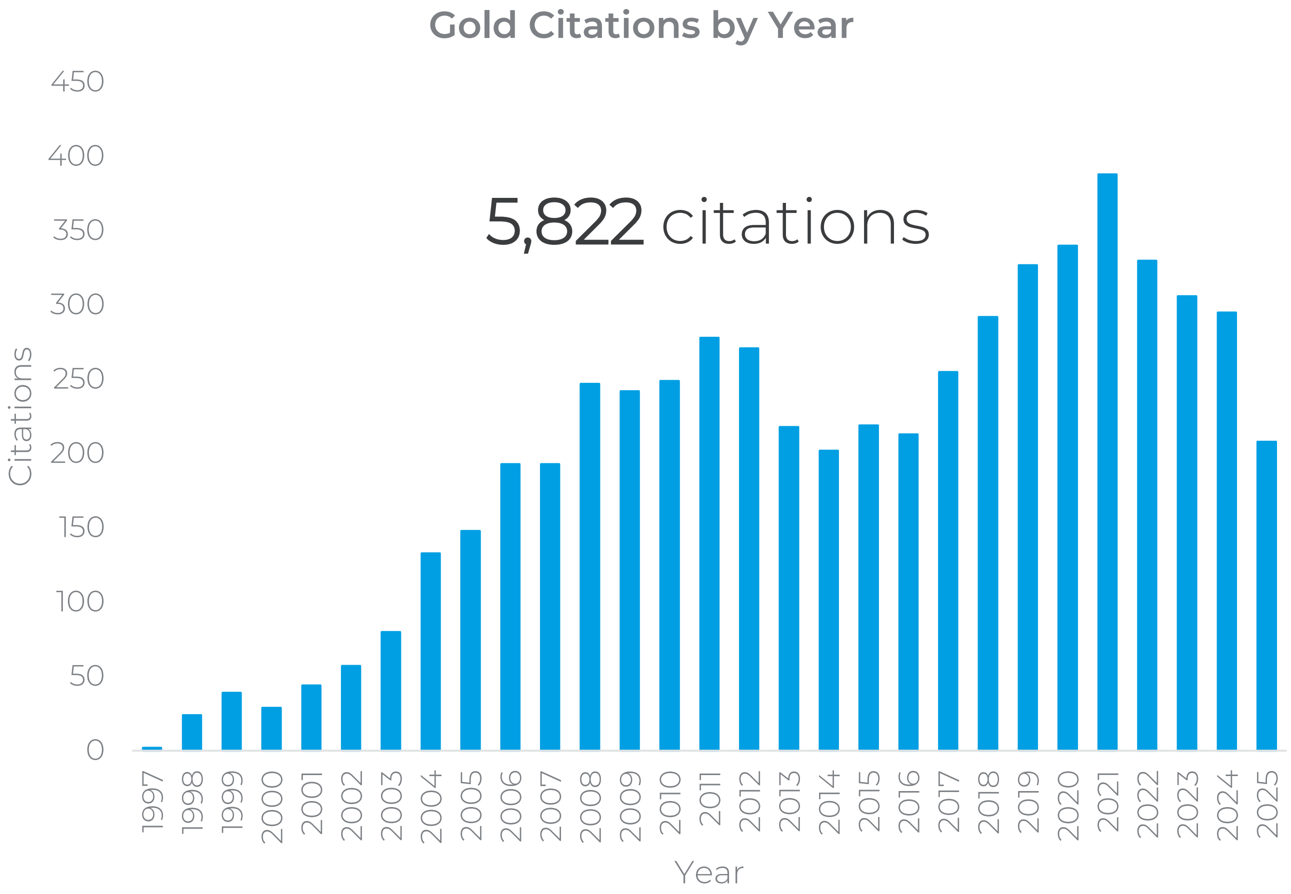
- **GOLD (Genetic Optimisation for Ligand Docking)** is a genetic algorithm for docking flexible ligands into protein binding sites.
- **GOLD** has proven success in virtual screening, lead optimisation, and identifying the correct binding mode of active molecules.
- Relied on by researchers in academia and industry worldwide.

- Reliable
- Flexible
- Configurable

GOLD docking in research

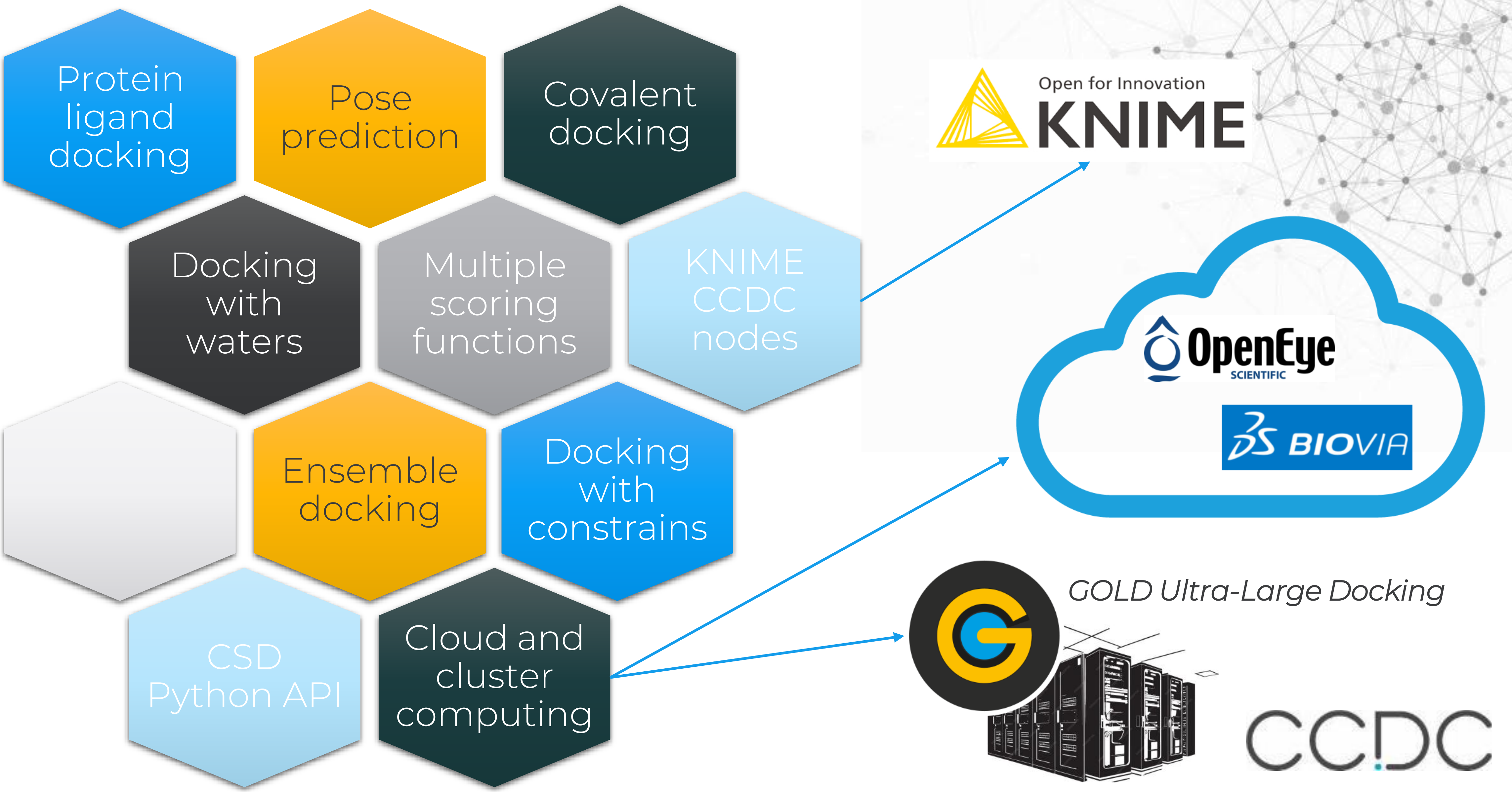
Top 5 citation categories





Development and validation of a genetic algorithm for flexible docking, *J. Mol. Biol.*, Vol. 267, pp. 727-748., 1997.
DOI: https://doi.org/10.1006/jmbi.1996.0897

GOLD: All in one molecular docking package



Protein ligand docking

Pose prediction

Covalent docking

Docking with waters

Multiple scoring functions

KNIME CCDC nodes

Ensemble docking

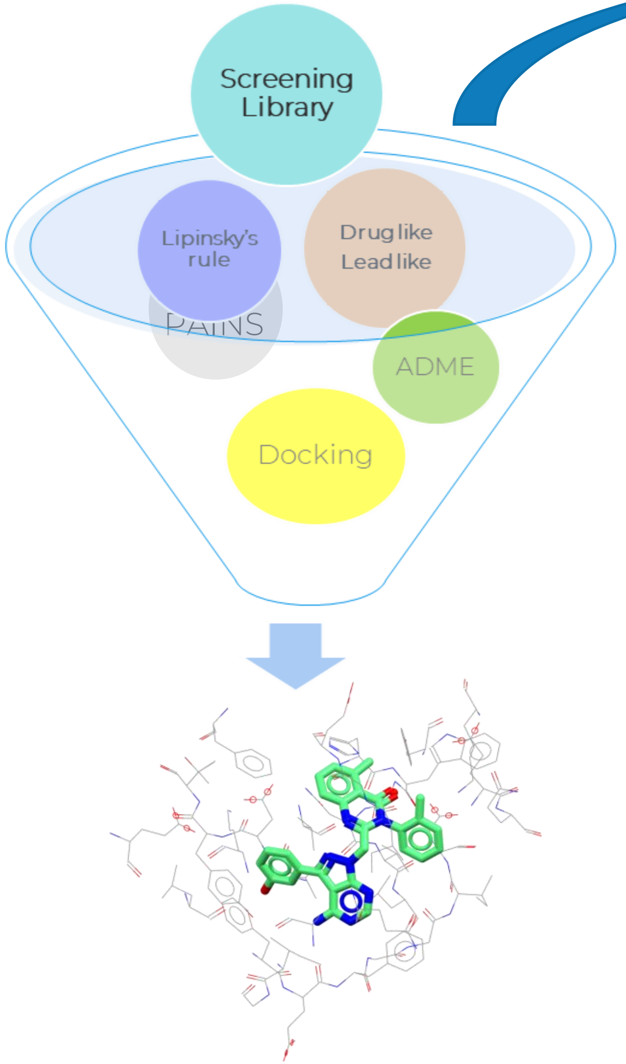
Docking with constrains

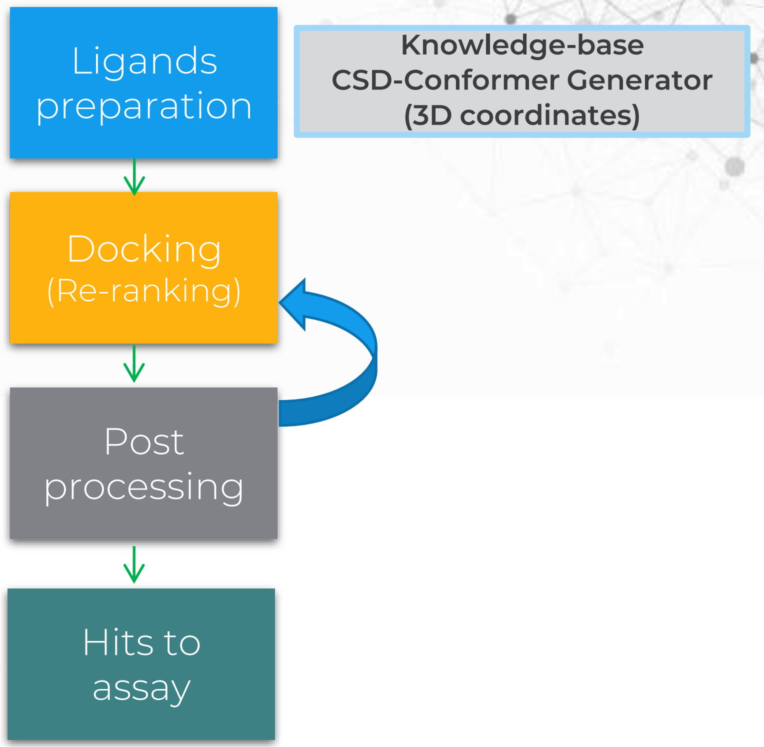
CSD Python API

Cloud and cluster computing

GOLD Ultra-Large Docking

SBDD virtual screening using GOLD





Input files SDF, MOL2 — **Ligands preparation** — Knowledge-base CSD-Conformer Generator (3D coordinates)

GOLD setting — **Docking (Re-ranking)**

Docking solutions analysis — **Post processing**

Selected ligands are tested in validated biological assay — **Hits to assay**

SBDD = Structure-Based Drug Design

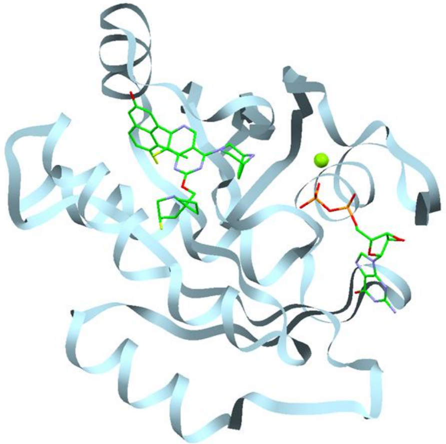
Using GOLD for *in silico* virtual screening

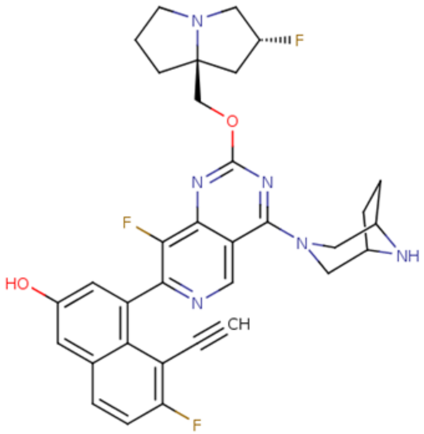
Today we will be using:

KRAS Hydrolase (GPTase) enzyme (X-ray structure, PDB 7RPZ)

Ligand MRTX-1133 [4-(4-[(1R,5S)-3,8-diazabicyclo[3.2.1]octan-3-yl]-8-fluoro-2-{[(2R,4R,7aS)-2-fluorotetrahydro-1H-pyrrolizin-7a(5H)-yl]methoxy}pyrido[4,3-d]pyrimidin-7-yl)-5-ethynyl-6-fluoronaphthalen-2-ol]

Target-focused curated from ChEMBL https://www.ebi.ac.uk/chembl/





We will use the KRAS inhibitors library for performing structure-based virtual screening, identify potential new protein-ligands interactions, insight to design novel potential inhibitors.

For the hands-on part we prepared the files for you.

Steps in GOLD docking

Target selection

- Co-crystal structure of protein-ligand complex from PDB

Protein preparation

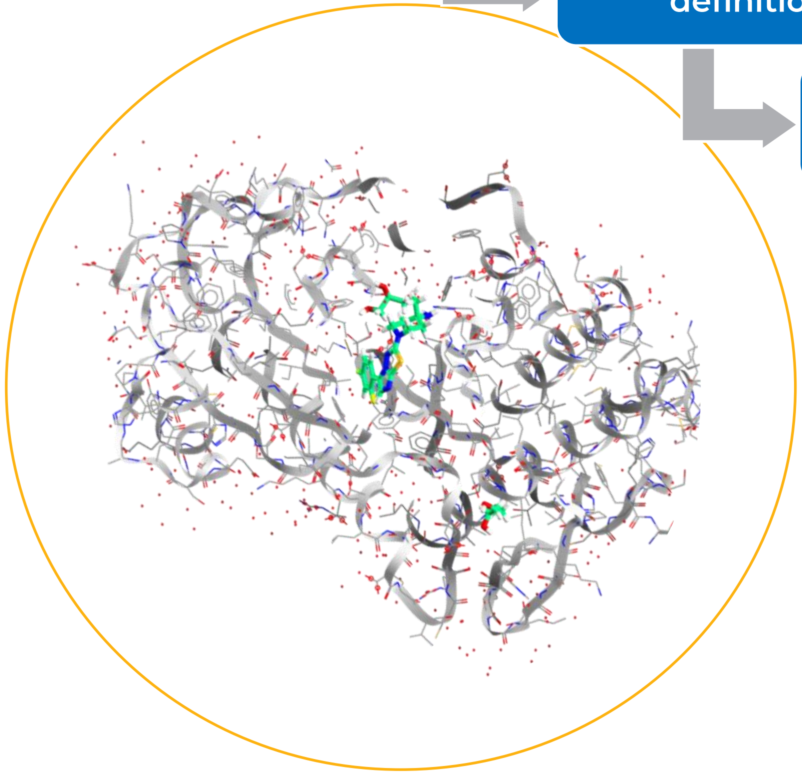
Binding site definition

Ligand(s) selection for docking

Scoring function selection

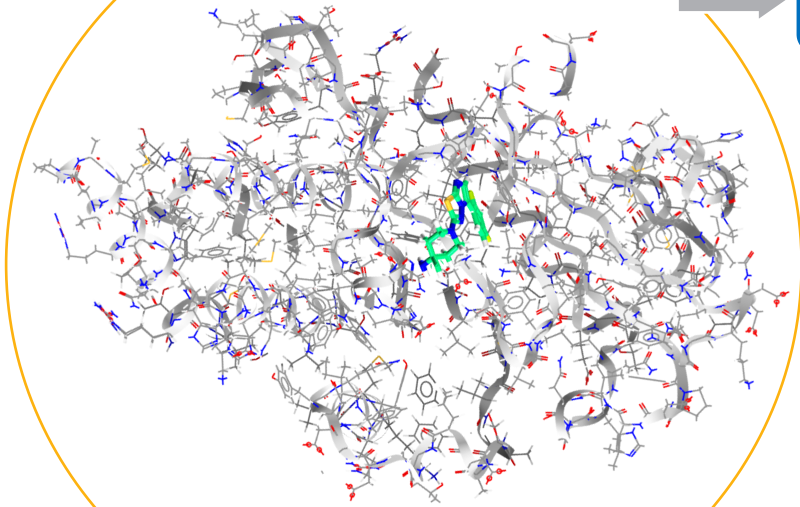
Setup and running the docking calculation

Analysis of the results and visualisation

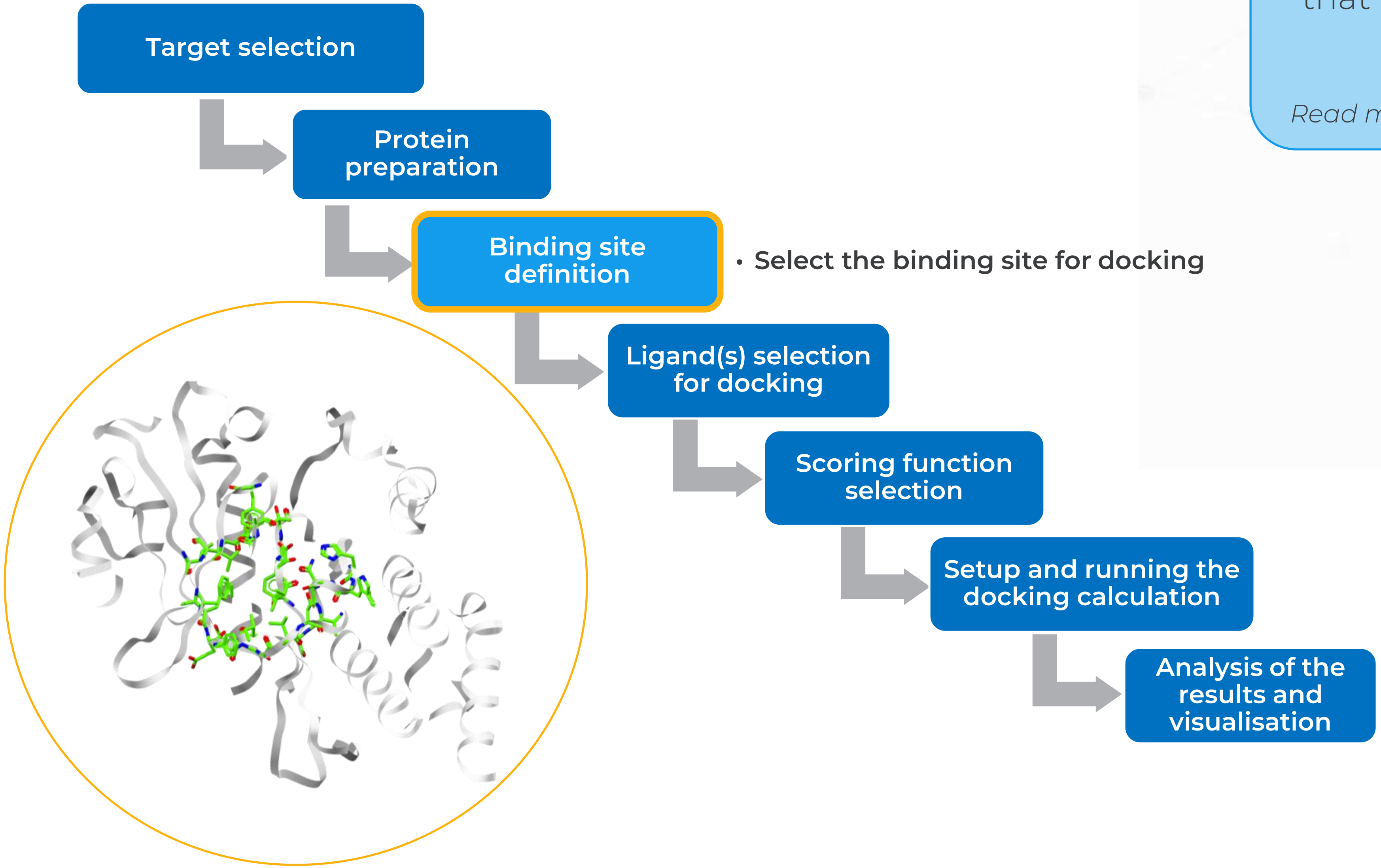


Steps in GOLD docking

1. Target selection
2. **Protein preparation**
   - Add hydrogens
   - Remove water/additives
   - Extract ligand
3. Binding site definition
4. Ligand(s) selection for docking
5. Scoring function selection
6. Setup and running the docking calculation
7. Analysis of the results and visualisation



Steps in GOLD docking



Target selection

Protein preparation

Binding site definition

- Select the binding site for docking

Ligand(s) selection for docking

Scoring function selection

Setup and running the docking calculation

Analysis of the results and visualisation

Binding site: a region on a macromolecule such as a protein that binds to another molecule with specificity

Read more in the Glossary in the handout .

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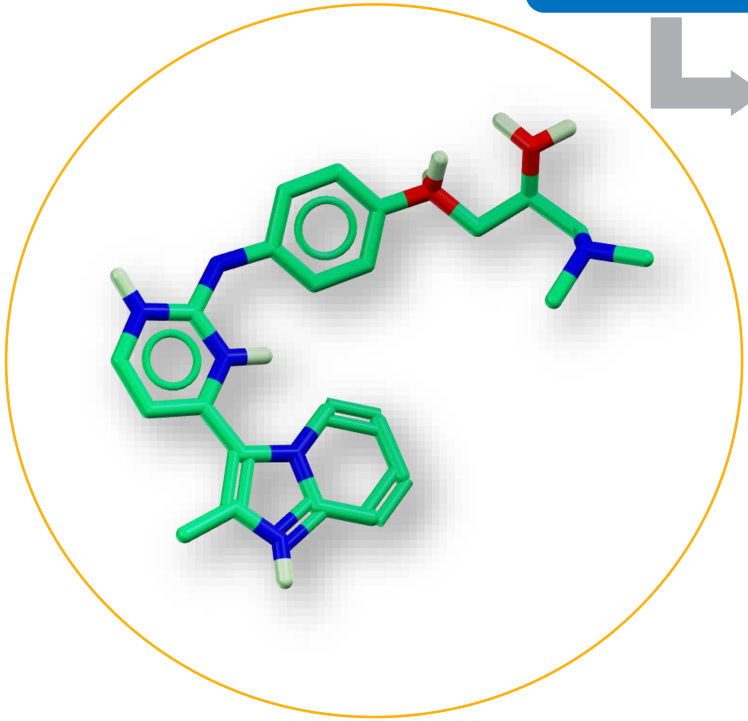
Steps in GOLD docking

- Target selection
- Protein preparation
- Binding site definition
- **Ligand(s) selection for docking**
  - SDF, MOL2 (Ligand prepared for the demo)
- Scoring function selection
- Setup and running the docking calculation
- Analysis of the results and visualisation



Steps in GOLD docking

1. Target selection
2. Protein preparation
3. Binding site definition
4. Ligand(s) selection for docking
5. Scoring function selection
   - Optionally rescoring
6. Setup and running the docking calculation
7. Analysis of the results and visualisation

Scoring functions: mathematical functions used to approximately predict the binding affinity between two molecules after they have been docked.

Read more in the Glossary in the handout .

Scoring functions in GOLD

- ChemPLP
- GoldScore
- ChemScore
- ASP (Astex Statistical Potential)

Learn more in the FAQ

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Steps in GOLD docking

Target selection

Protein preparation

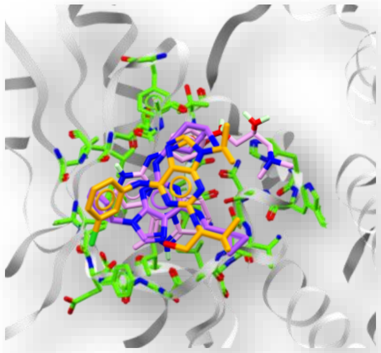
Binding site definition

Ligand(s) selection for docking

Scoring function selection

Setup and running the docking calculation

Analysis of the results and visualisation



Steps in GOLD docking

Target selection

Protein preparation

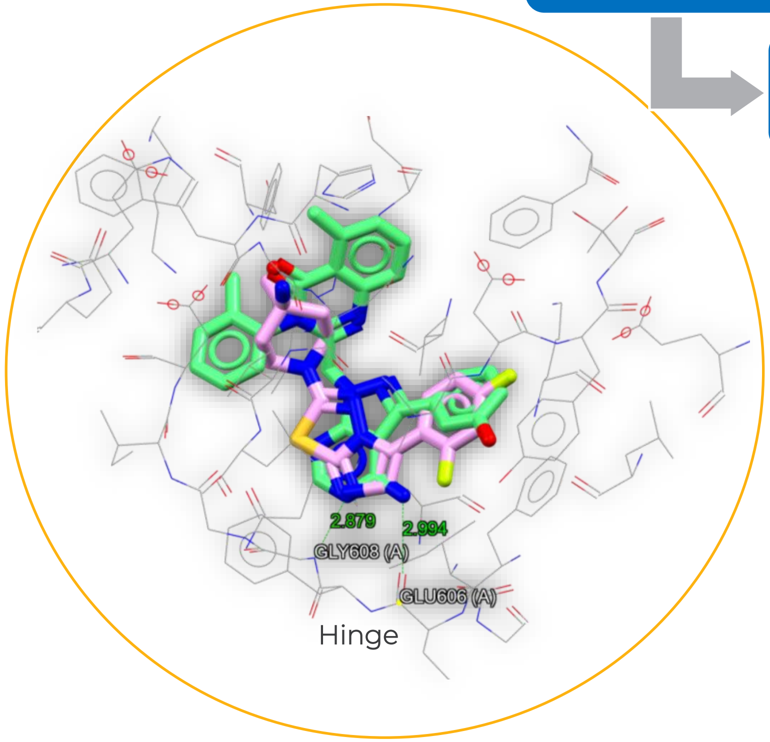
Binding site definition

Ligand(s) selection for docking

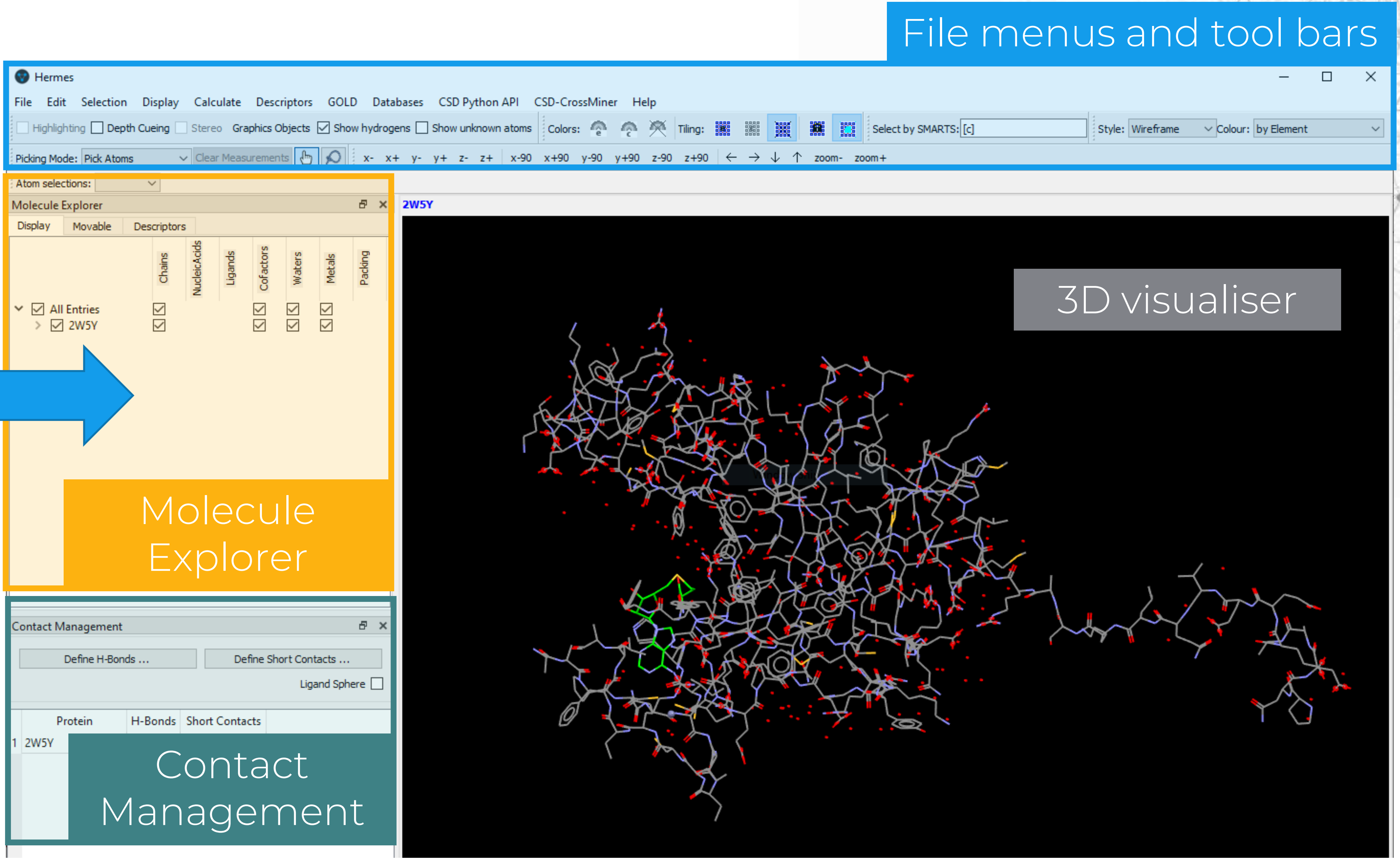
Scoring function selection

Setup and running the docking calculation

Analysis of the results and visualisation



Before docking: Hermes Interface



File menus and tool bars

3D visualiser

Molecule Explorer

Contact Management

Picking Mode: Pick Atoms

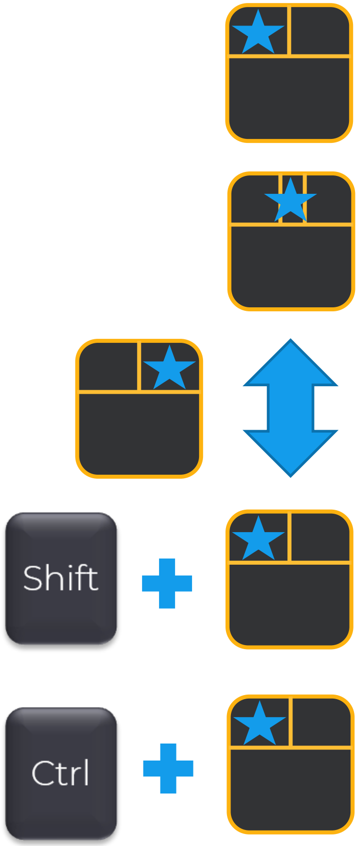
Select by SMARTS: [c]

Style: Wireframe

Colour: by Element

Protein	H-Bonds	Short Contacts
1 2W5Y		

Navigation basics



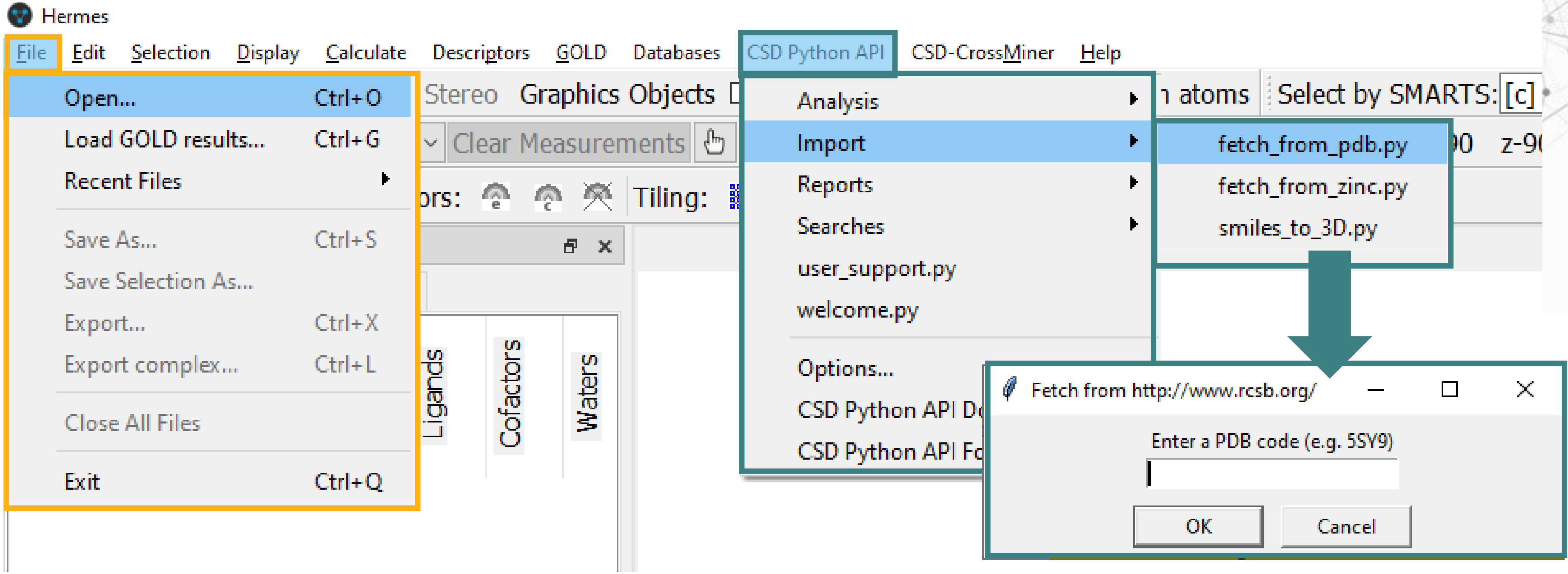
- Left mouse button and move – rotate molecules
- Middle Mouse wheel – move molecules up and down
- Right mouse button and move up and down – zoom in and out of molecules
- Shift + Left mouse button and move - rotate in the plane molecules
- Ctrl + Left mouse button and move - translate molecules

Did you know?
The basic navigation features in **Hermes** are the same in **Mercury** - our small molecule visualisation software.
So… if you are an expert in one you are an expert in both!

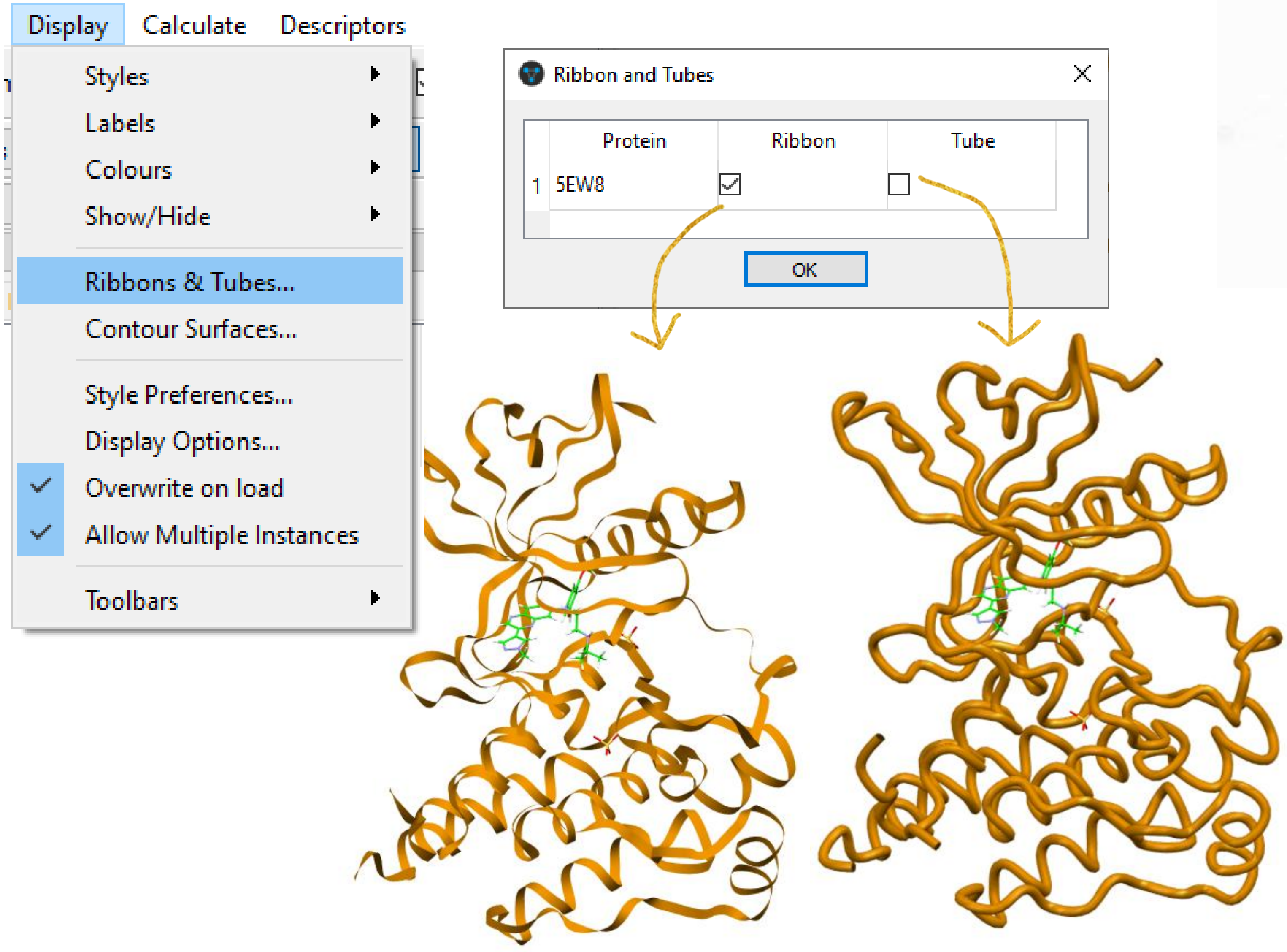
Loading structures into Hermes

From a file: File > Open

From a DB or SMILES: CSD Python API > Import

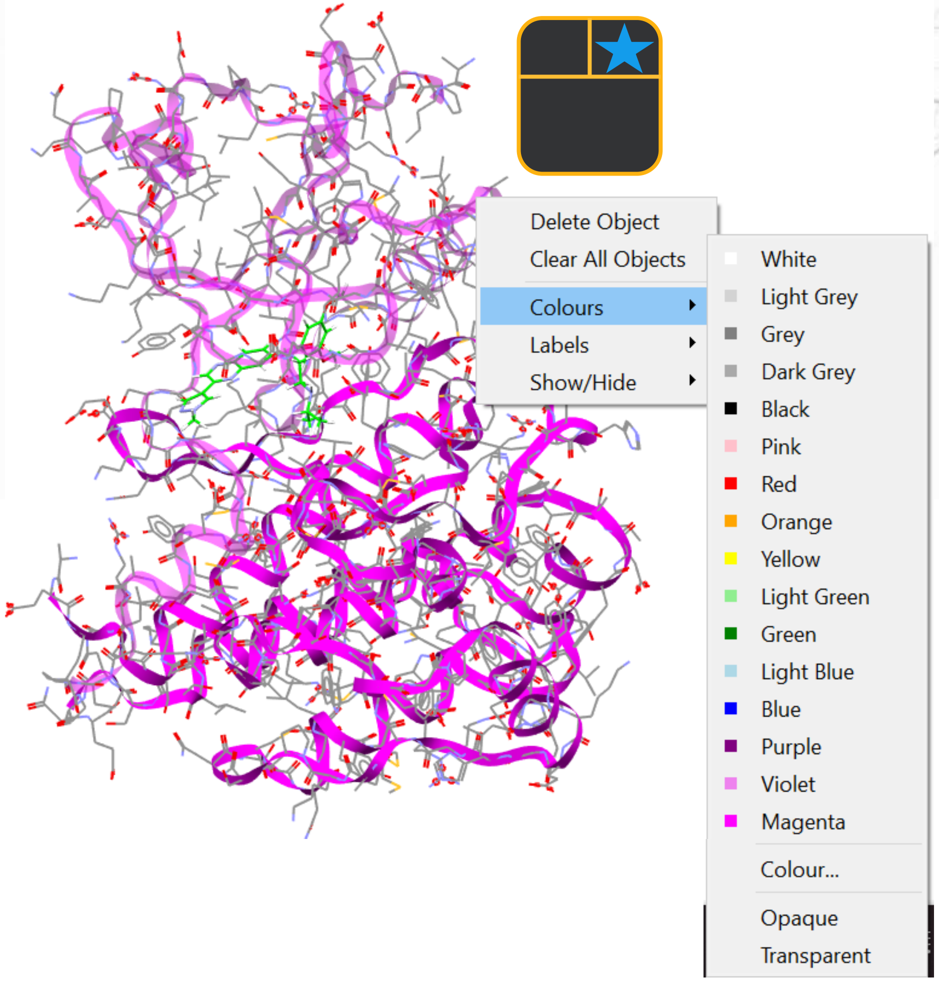


Ribbon & Tubes options

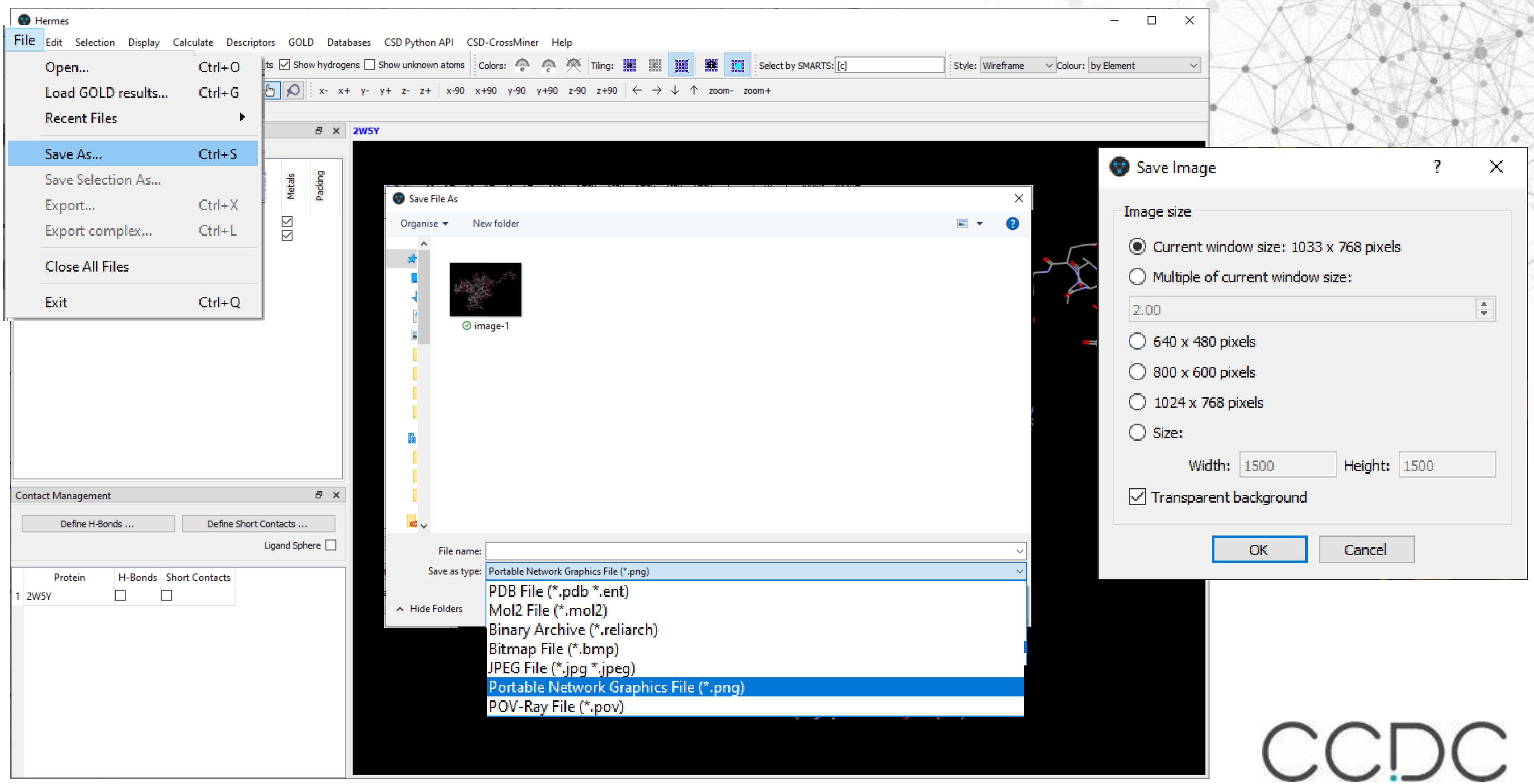


	Protein	Ribbon	Tube
1	5EW8	☑	☐

Colours and transparency



Creating high-resolution images



☑ Show hydrogens ☐ Show unknown atoms

Select by SMARTS: [c]

Style: Wireframe

Colour: by Element

Protein	H-Bonds	Short Contacts
1 2W5Y	☐	☐

Save File As

File name:

Save as type: Portable Network Graphics File (*.png)

- PDB File (*.pdb *.ent)
- Mol2 File (*.mol2)
- Binary Archive (*.reliarch)
- Bitmap File (*.bmp)
- JPEG File (*.jpg *.jpeg)
- Portable Network Graphics File (*.png)
- POV-Ray File (*.pov)

Save Image

Image size

● Current window size: 1033 x 768 pixels

○ Multiple of current window size:

2.00

○ 640 x 480 pixels

○ 800 x 600 pixels

○ 1024 x 768 pixels

○ Size:

Width: 1500 Height: 1500

☑ Transparent background

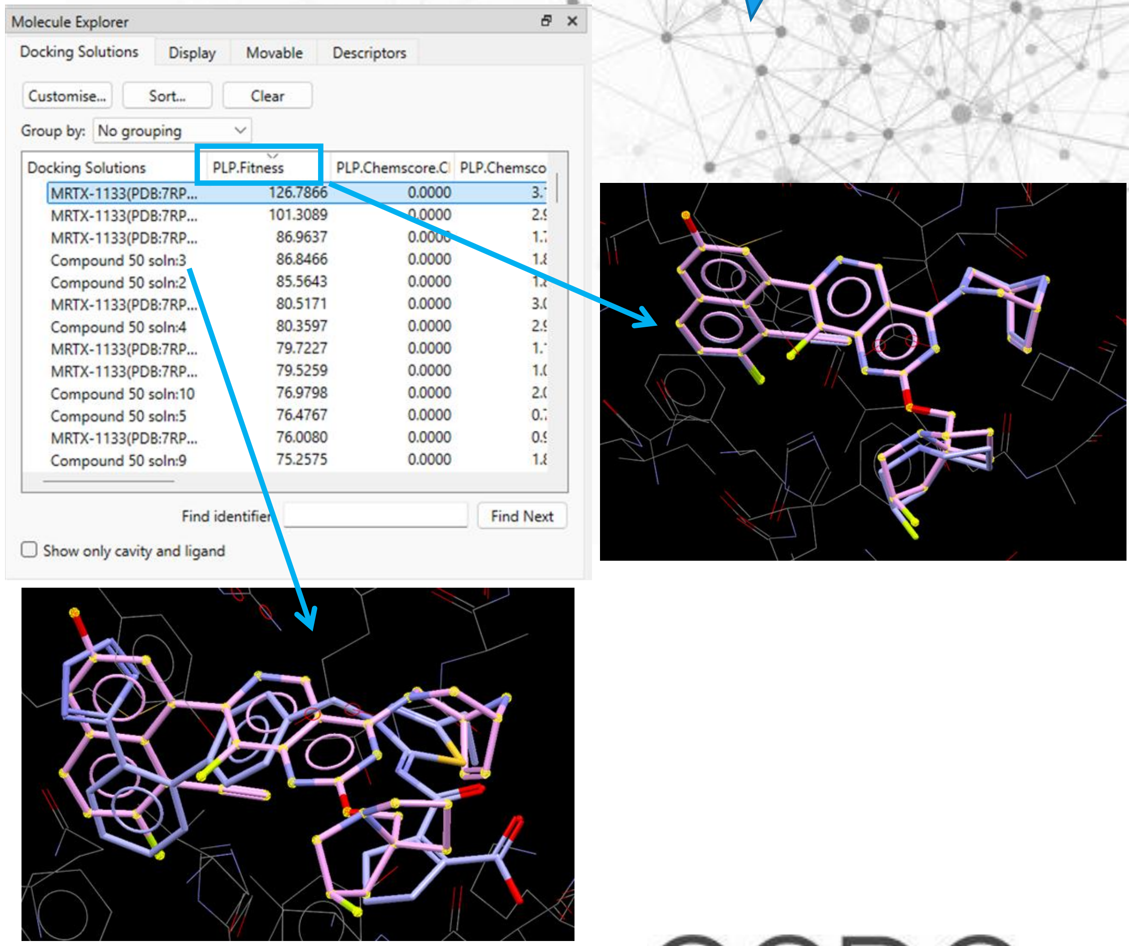
We are recording today's session and will make the recording available to you in the next few days

Demonstration

Approaches to virtual screening using target-focused libraries

In this demonstration we will:

- Navigate the interface.
- Import a protein-ligand complex from the PDB.
- Set up GOLD virtual screening.
- Run GOLD.
- Visualise and inspect the docking solutions.



Group by: No grouping

Docking Solutions	PLP.Fitness	PLP.Chemscore.C	PLP.Chemsco
MRTX-1133(PDB:7RP...	126.7866	0.0000	3.
MRTX-1133(PDB:7RP...	101.3089	0.0000	2.
MRTX-1133(PDB:7RP...	86.9637	0.0000	1.
Compound 50 soln:3	86.8466	0.0000	1.
Compound 50 soln:2	85.5643	0.0000	1.
MRTX-1133(PDB:7RP...	80.5171	0.0000	3.
Compound 50 soln:4	80.3597	0.0000	2.
MRTX-1133(PDB:7RP...	79.7227	0.0000	1.
MRTX-1133(PDB:7RP...	79.5259	0.0000	1.
Compound 50 soln:10	76.9798	0.0000	2.
Compound 50 soln:5	76.4767	0.0000	0.
MRTX-1133(PDB:7RP...	76.0080	0.0000	0.
Compound 50 soln:9	75.2575	0.0000	1.

Find identifier

☐ Show only cavity and ligand

Agenda

- *Show One:* Introduction to the CSD
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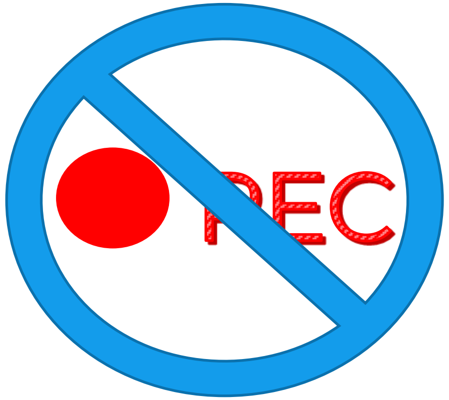
Try One

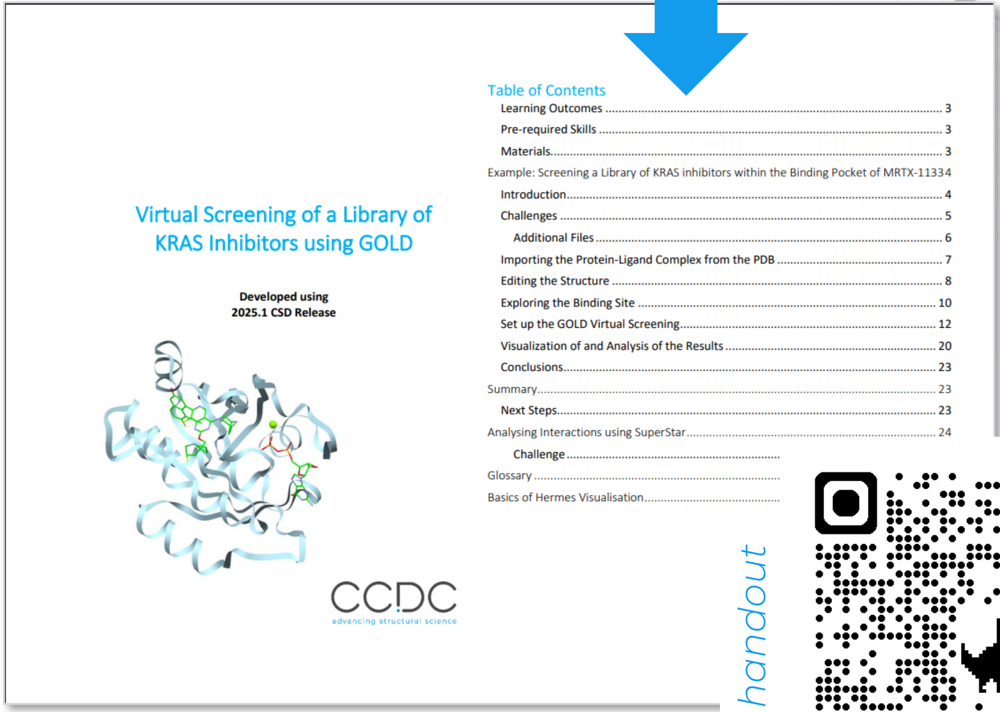


It’s your turn!

- Try the Case Study from the handout.
- Your tutors are here to help you!
- To ask questions during this time type a message in the chat box.

link to webpage

How to Use the Docking Software GOLD to Perform Virtual Screening Simulations



Virtual Screening of a Library of KRAS Inhibitors using GOLD

Developed using
2025.1 CSD Release

CCDC
advancing structural science

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link to handout

Agenda

REC

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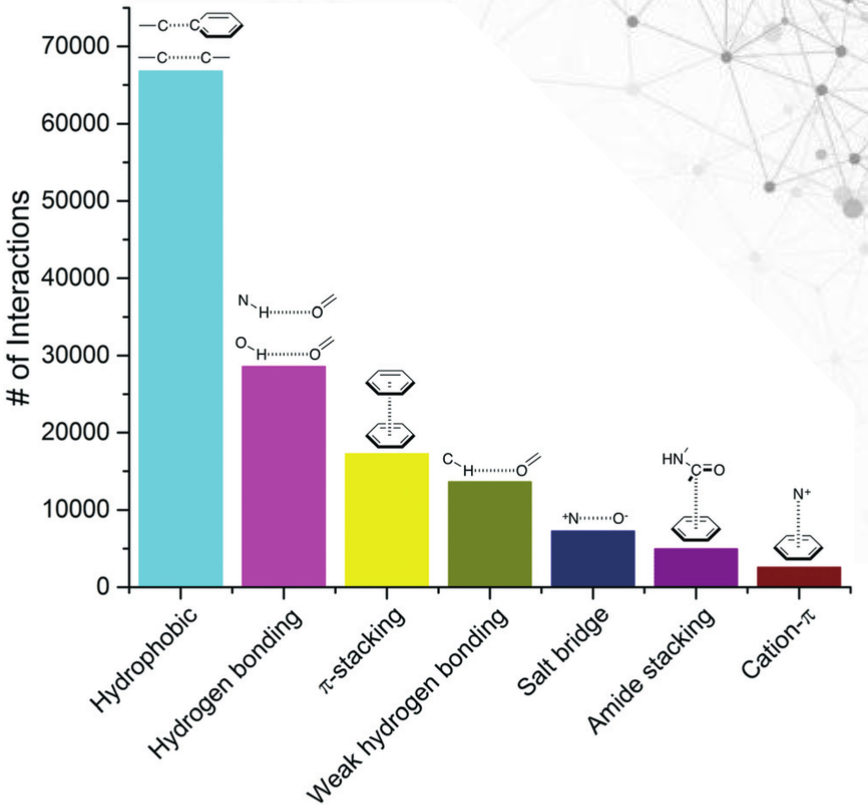
Explore More: More advanced uses

- Not enough time to explore everything you can do within a virtual-screening process
- But here are a selection of more advanced tips and tricks on using data driven approaches as well as some additional case studies

The session has resumed recording

Data driven approaches: non-covalent interactions

- Critical driving force for the structure, stability, and function of proteins.
- Important for drug discovery as their interplay is responsible for binding affinity within proteins and ligands.



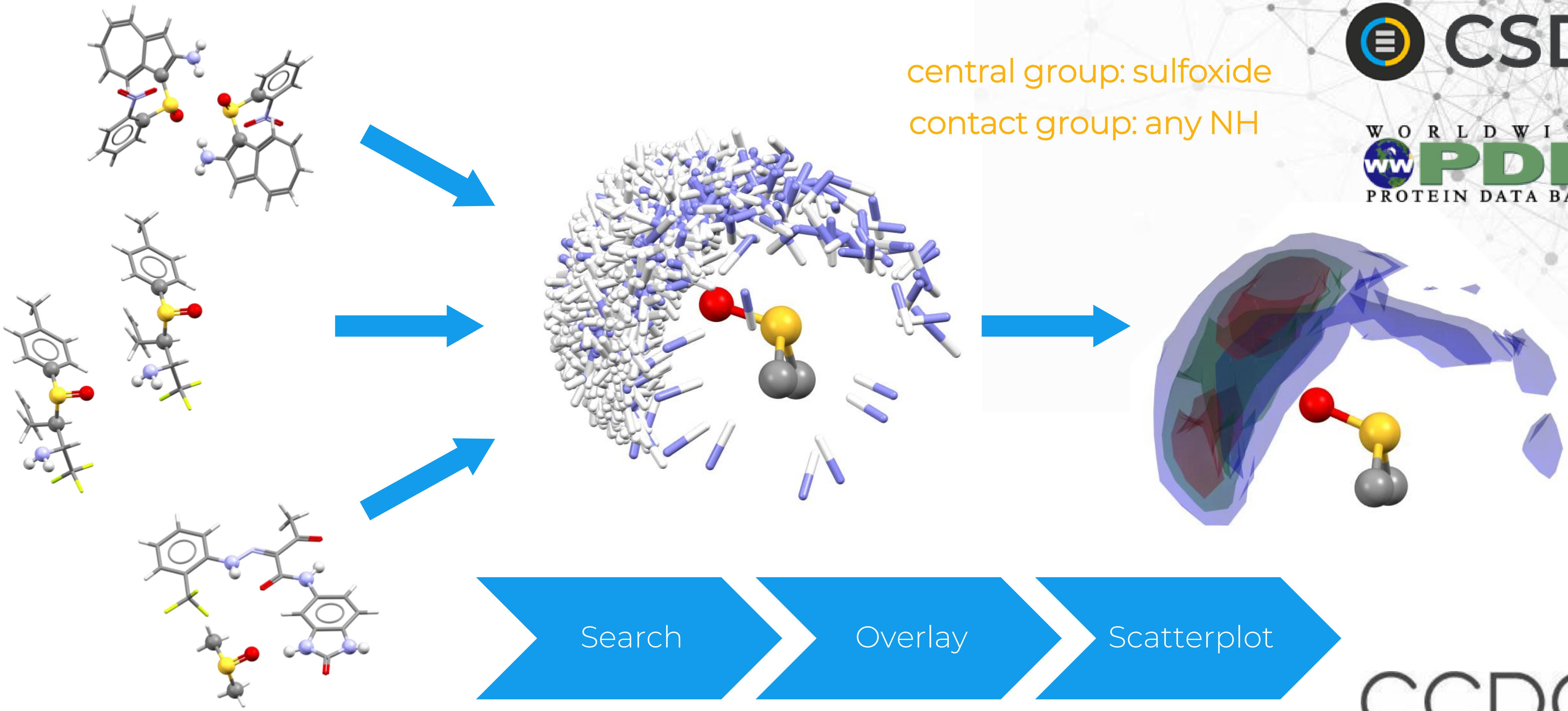
Most common non-covalent interactions observed in protein–ligands extracted from the PDB

Freitas & Schapira. *Med. Chem. Commun.*, 2017, 8, 1970–1981.

IsoStar: An interactions knowledge base

CSD

WORLDWIDE PDB PROTEIN DATA BANK



central group: sulfoxide

contact group: any NH

Search

Overlay

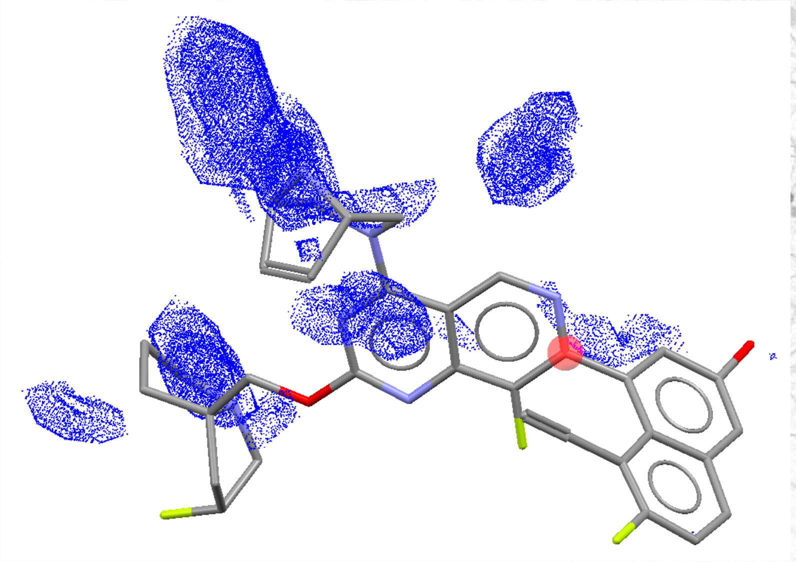
Scatterplot

CCDC

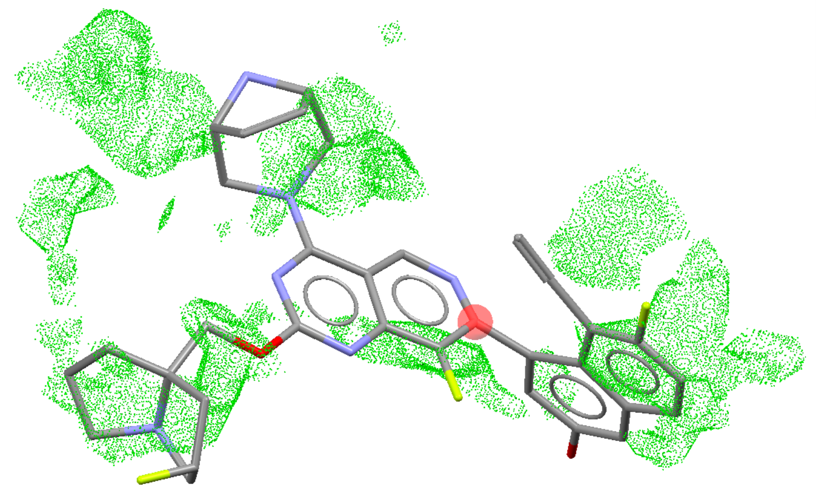
SuperStar

- Provides the interaction preferences for all or selected cavities in protein.
- Interaction preferences visualised simply in 3D based on validated experimental structural knowledge (i.e. CSD or PDB data from IsoStar).
- Contour plots using probes, hotspots as peaks in contours.
- Accessed through Hermes (protein visualiser).

H-bond donor propensity map (NH-probe)

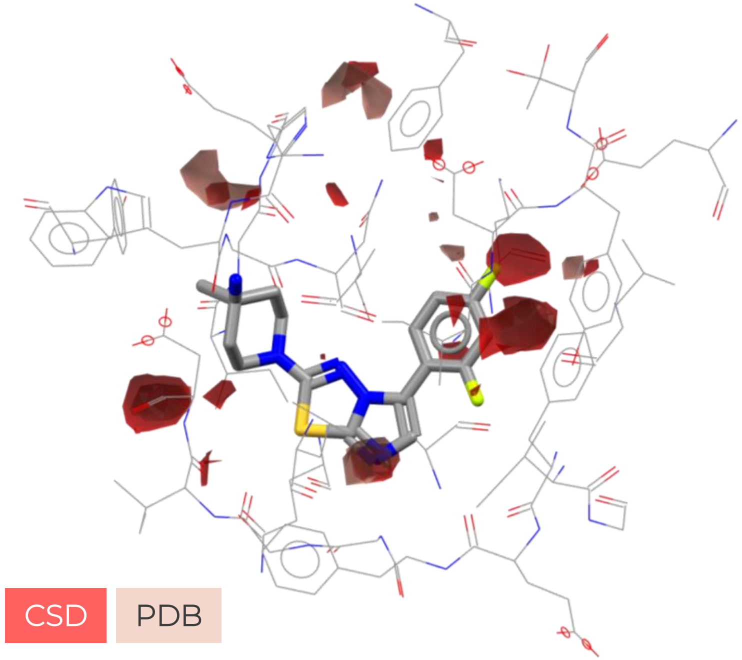


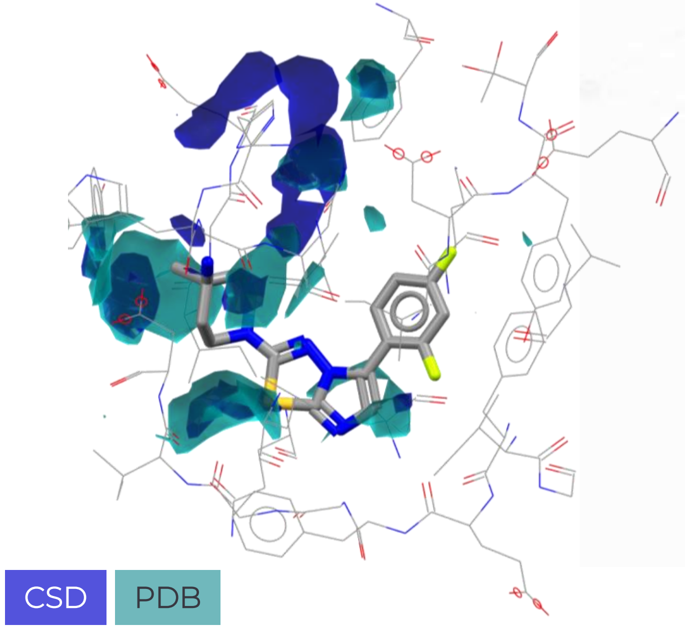
Hydrophobic propensity map (CH-aliphatic probe

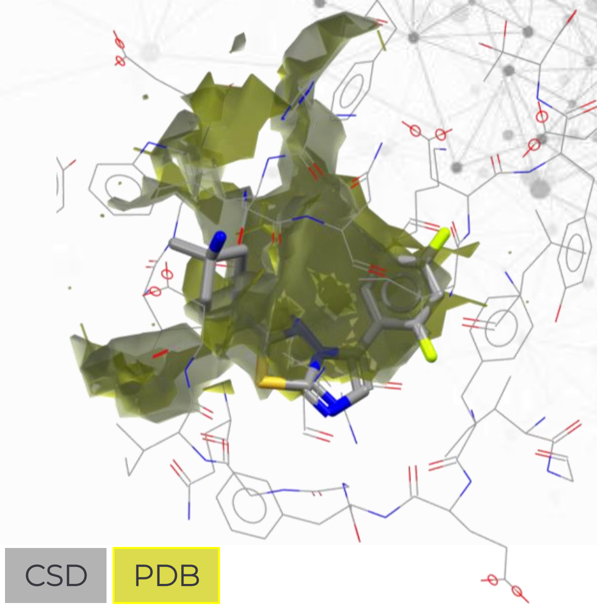


SuperStar: A knowledge-based approach for identifying interaction sites in proteins.
Verdonk M. L., *et al. J. Mol. Biol.* (1999) 289, 1093-1108.

Superstar: a Knowledge-based method







- Estimates the probability of an interaction:
  - Between a protein and a small functional group (probe).
  - Based on how often the interaction has been observed in the knowledge-based library of intermolecular interactions.
- Druggable target

Applications:

- Identify potential binding hot-spots in proteins and ligands.
- Validation of docking poses.
- Identify structural waters.

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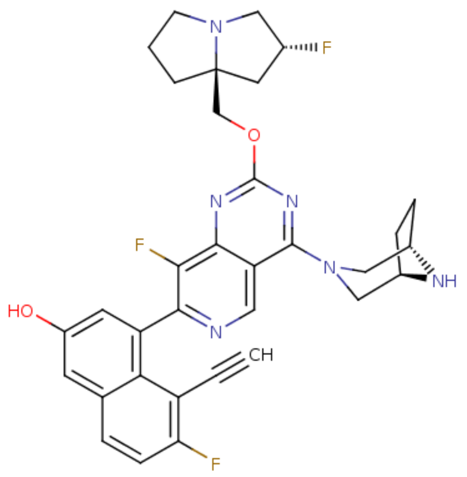
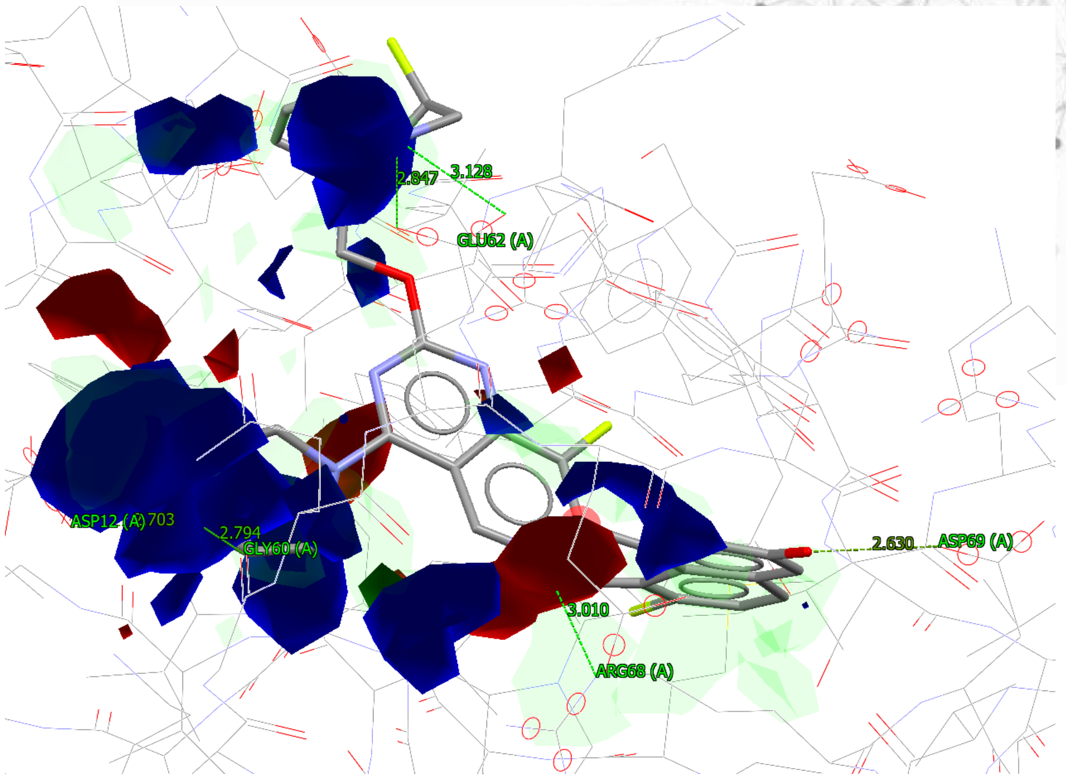
SuperStar application





Validation of docking poses

Binding mode of MRTX-1133 validated by showing good match of:

- H-bond donor interactions between amino groups in MRTX-1133 and residues ASP12, GLY60, and GLU62.
- H-bond acceptor interactions between N with ARG68 and Hydroxyl group with ASP69

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What we have learnt

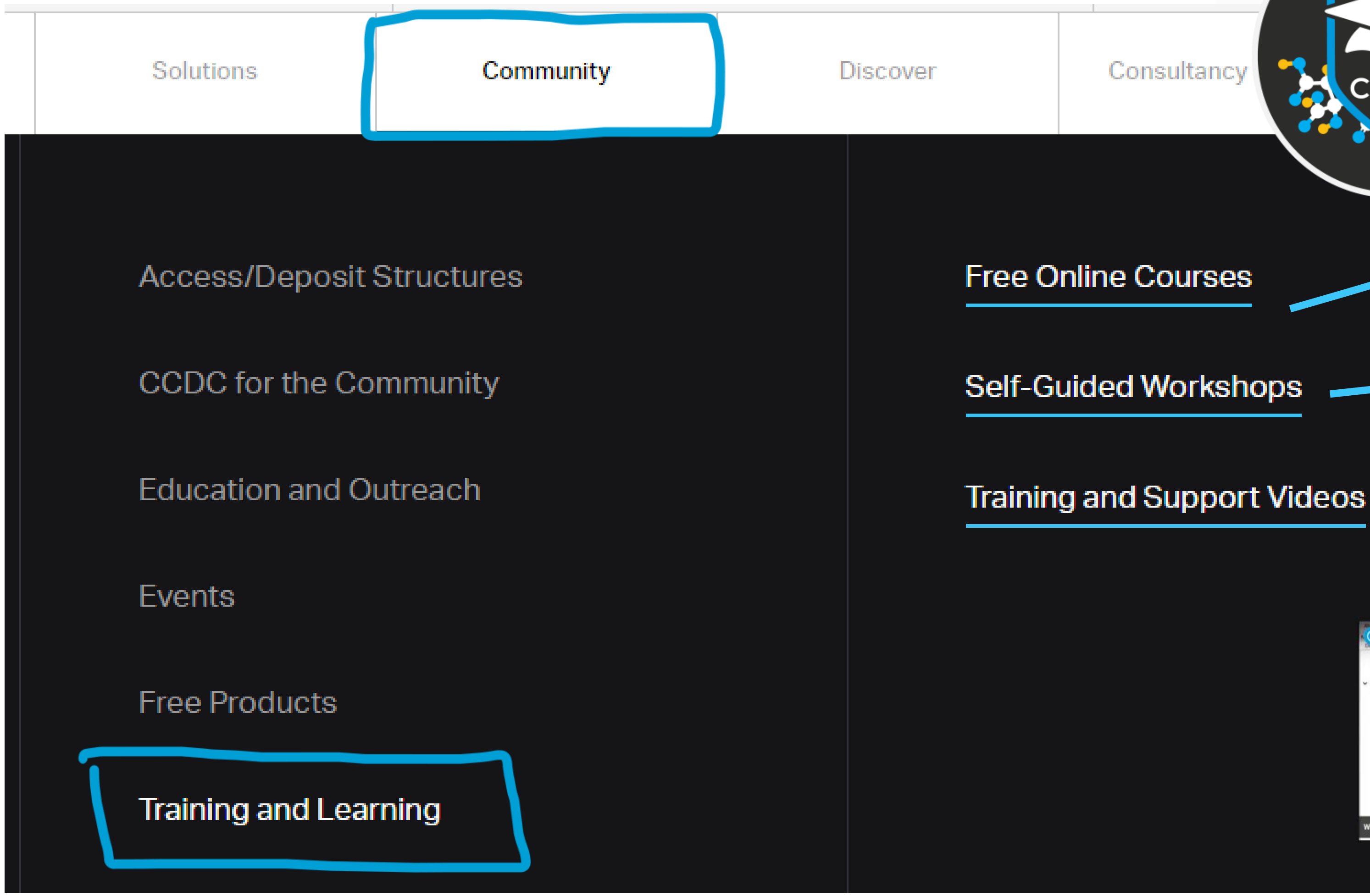
- ✓Brief overview of structure-based virtual screening.
- ✓Basics of the Hermes interface, the CCDC's 3D visualizer for proteins.
- ✓Cavity detection and extraction in Hermes.
- ✓Step-by-step set-up of a virtual screening simulation in GOLD.
- ✓Analysis of virtual screening results.
- ✓Protein-ligand interactions insights using hotspots via Superstar.

We will make the recording available to you in the next few days.

CCDC

Want to explore more?

On-demand training resources



Solutions

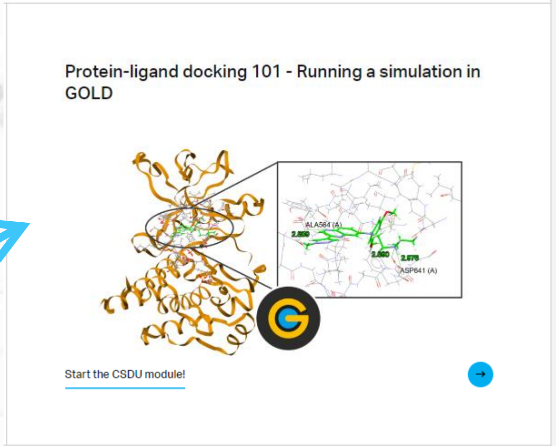
Community

Discover

Consultancy

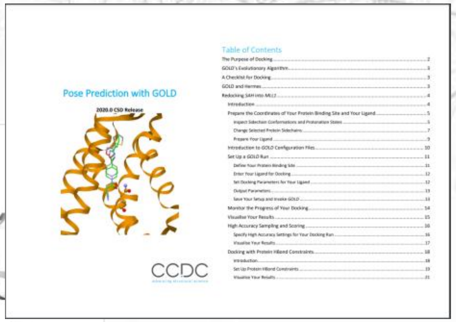
- Access/Deposit Structures
- CCDC for the Community
- Education and Outreach
- Events
- Free Products
- Training and Learning

- Free Online Courses
- Self-Guided Workshops
- Training and Support Videos



Protein-ligand docking 101 - Running a simulation in GOLD

Start the CSDU module!



Pose Prediction with GOLD

2020.0 CSD Release

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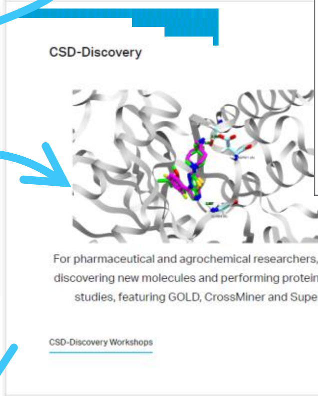
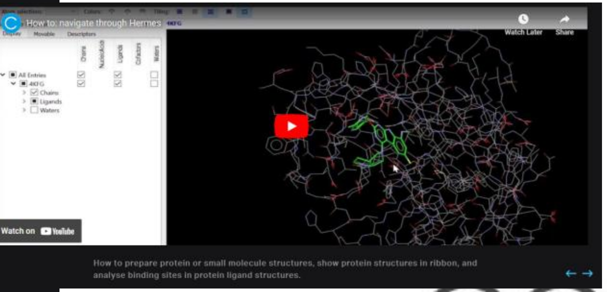


CSD-Discovery

For pharmaceutical and agrochemical researchers, tools for discovering new molecules and performing protein docking studies, featuring GOLD, CrossMiner and SuperStar

CSD-Discovery Workshops

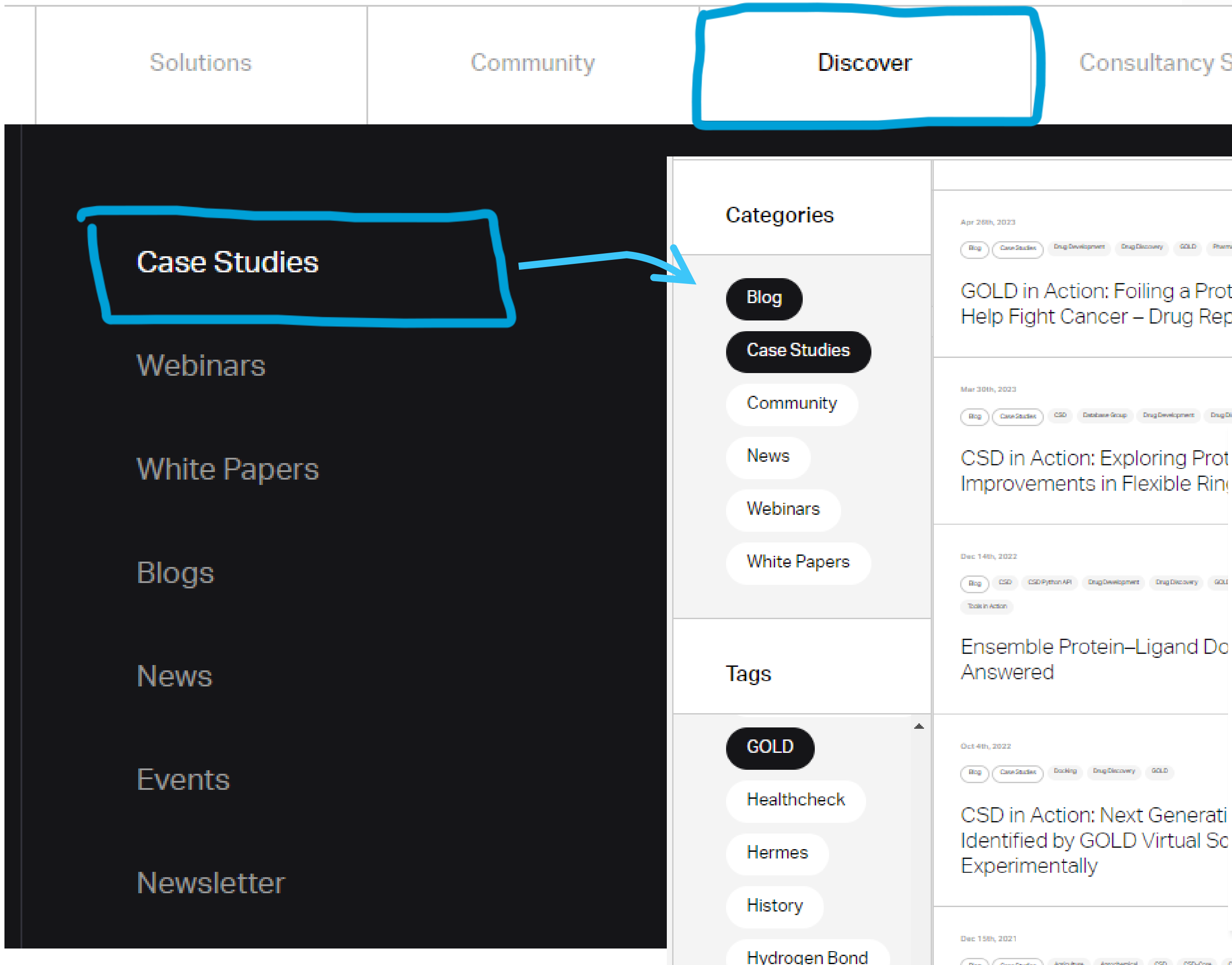


How to: navigate through Hermes

How to prepare protein or small molecule structures, show protein structures in ribbon, and analyse binding sites in protein ligand structures.

Want to explore more?

Case Studies



Apr 26th, 2023

GOLD in Action: Foiling a Protein–Protein Interaction to Help Fight Cancer – Drug Repurposing using GOLD

Mar 30th, 2023

CSD in Action: Exploring Prot
Improvements in Flexible Rin

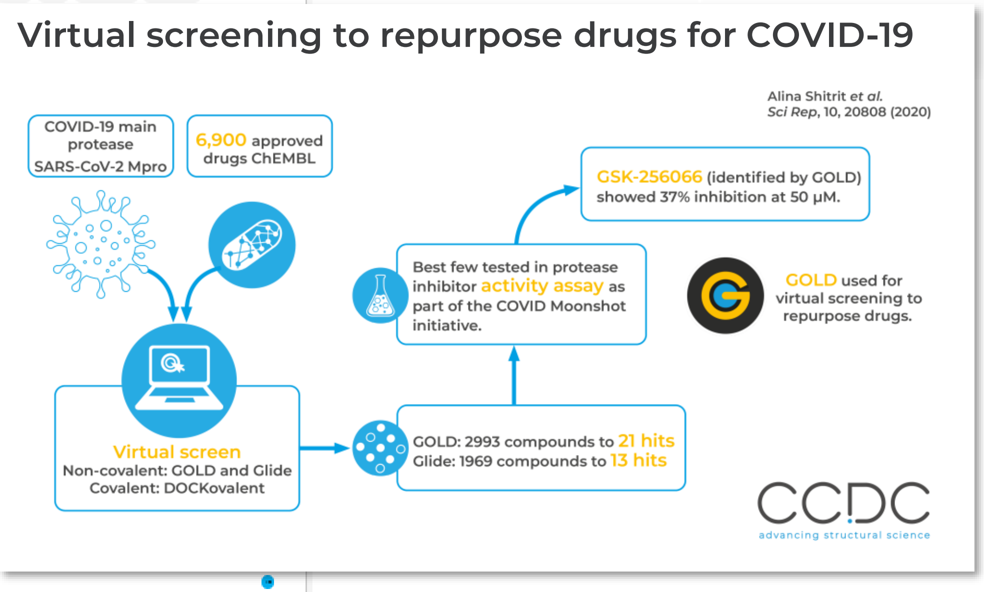
Dec 14th, 2022

Ensemble Protein–Ligand Do
Answered

Oct 4th, 2022

CSD in Action: Next Generati
Identified by GOLD Virtual Sc
Experimentally

Dec 15th, 2021



Virtual screening to repurpose drugs for COVID-19

Alina Shitrit *et al.*
Sci Rep, 10, 20808 (2020)

COVID-19 main protease SARS-CoV-2 Mpro

6,900 approved drugs ChEMBL

Virtual screen
Non-covalent: GOLD and Glide
Covalent: DOCKovalent

GOLD: 2993 compounds to 21 hits
Glide: 1969 compounds to 13 hits

Best few tested in protease inhibitor activity assay as part of the COVID Moonshot initiative.

GSK-256066 (identified by GOLD) showed 37% inhibition at 50 µM.

GOLD used for virtual screening to repurpose drugs.

How to cite the tools seen today

- **GOLD**
  Development and Validation of a Genetic Algorithm for Flexible Docking
  G. Jones, P. Willett, R. C. Glen, A. R. Leach and R. Taylor, J. Mol. Biol., 267, 727-748, 1997
  DOI: 10.1006/jmbi.1996.0897
- **SuperStar**
  Combined use of physiochemical data and small-molecule crystallographic contact propensities to predict interactions in protein binding sites
  J. W. M. Nissink, R. Taylor, Org. Biomol. Chem., 2, 3238-3249, 2004
  DOI: 10.1039/B405205F
- **CSD**
  The Cambridge Structural Database
  C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, *Acta Cryst.* (2016). B72, 171-179
  DOI: 10.1107/S2052520616003954

More reference papers for GOLD

More reference papers for CSD Software

CCDC

Want to explore more?

CCDC Webinars

- **13th November** - Using general purpose **force fields** in solid form studies
- **20th November, Panel** – **Frontiers in MOFs**: Creating Real-World Solutions with MOFs

Check our Events online for more virtual and in person events.

Using General Purpose Force Fields in Solid Form Studies

Lily Hunnisett
Computational Solid-State Scientist, CCDC

Thursday, 13th November
15:00 (GMT)/ 10:00 (EST)

Frontiers in
MOFs

Creating Real-World Solutions with MOFs

Panel discussion with experts from academia and industry.

20th November, 3pm GMT