

Mining Crystallographic Databases using CSD- CrossMiner

CCDC Virtual Workshop Spring 2021 – Session 2

Francesca Stanzione, Abhik Mukhopadhyay, Ilenia Giangreco,
Suzanna Ward, Ilaria Gimondi, Eva Myers

14 April 2021

Learning outcomes for today

- Familiarising yourself with CSD-CrossMiner.
- Learning how to interact with a pharmacophore query.
- Learning how to perform pharmacophore searches.
- Learning how to analyse and interact with your results.

Structural databases



PDB
>175,000
polypeptides,
nucleotides
& saccharides



CSD
>1.1 million
organic and
metal-organic

ICSD
>230,000
(no C-H and C-C
bonds)
Elements,
minerals,
metals



FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

ICDD
PDF-
4/Organics
>540,000
Includes data
derived from
CSD



CCDC

The CSD Portfolio

CSDEnterprise.

CSDMaterials.



DASH



Python API



Mercury



CSDDiscovery.



SuperStar



Python API



GOLD



CrossMiner



Mercury

CSDCore.



WebCSD



Mogul



MyStructures



ConQuest



CSD



IsoStar



Mercury



Hermes



Python API

CSDCommunity.



Mercury



enCIFer



Symmetry



Deposit



CellCheck



Educational



Access



MyStructures

Professional
Services

Research
& Knowledge
partnerships

CSD-CrossMiner

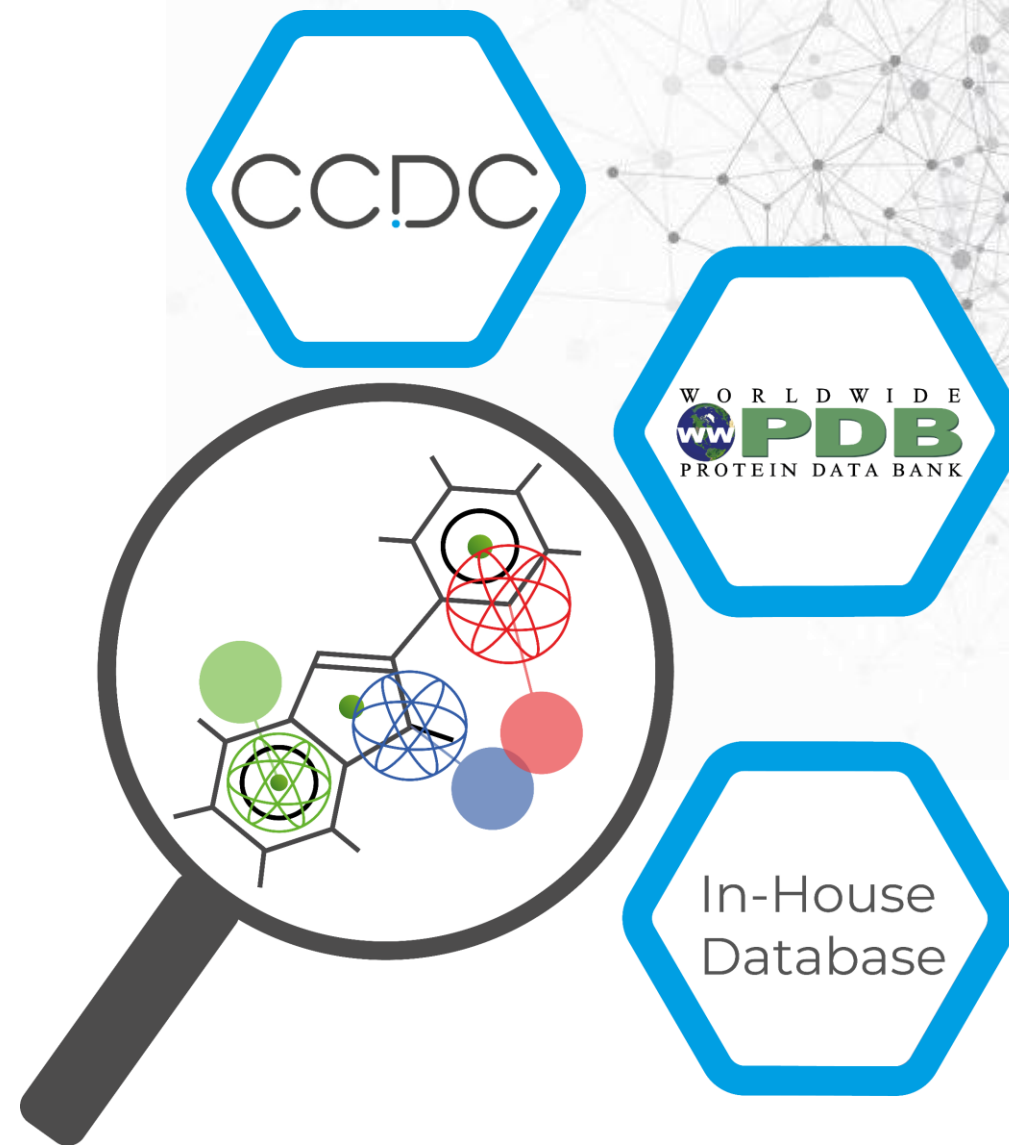


- Tool for **searching structural databases** by **pharmacophore**.
- From IUPAC: “an ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interactions
- Wikipedia: “abstract description of molecular features”



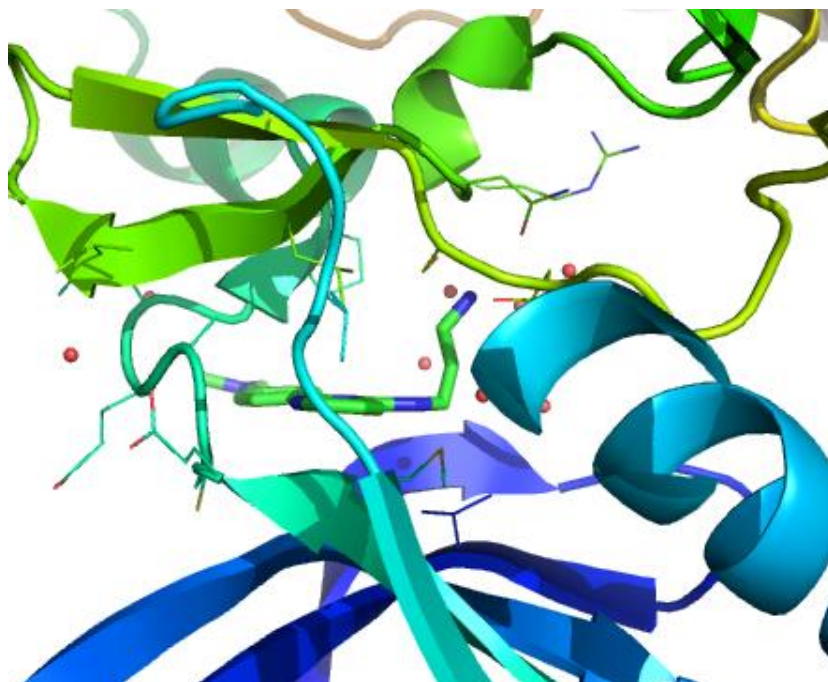
CSD-CrossMiner

- Simultaneously search the **PDB**, **CSD** and your **in-house database**.
- Designed for **speed** – modify hypotheses on the fly.
- Structures are annotated for easy **filtering** of hits



What can you do with CSD-CrossMiner?

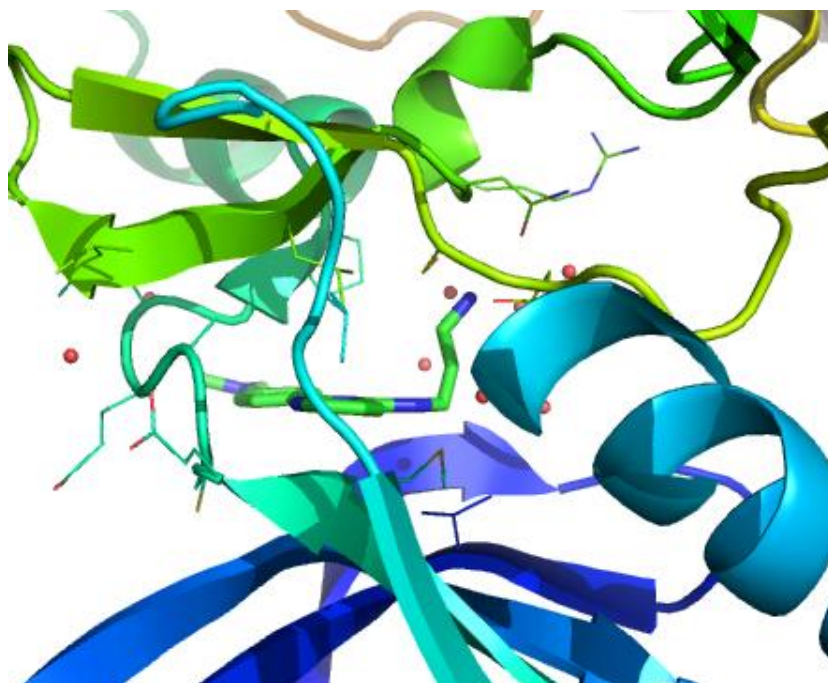
Understand protein-ligand interactions.



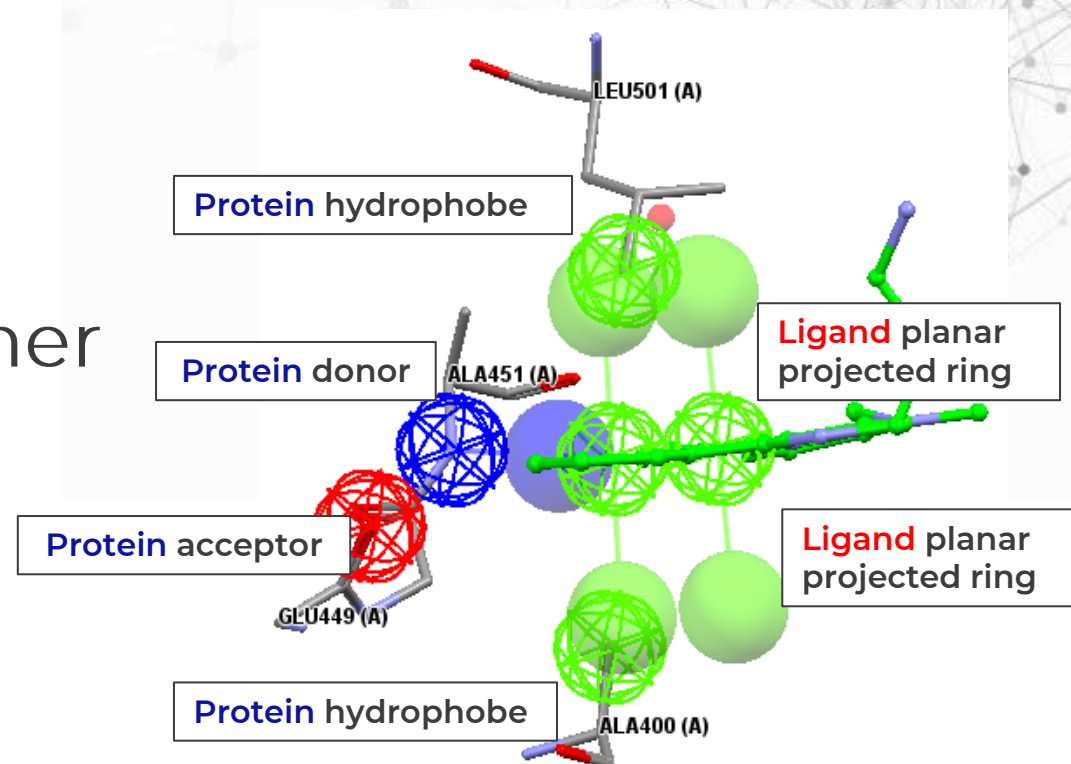
CSD-CrossMiner



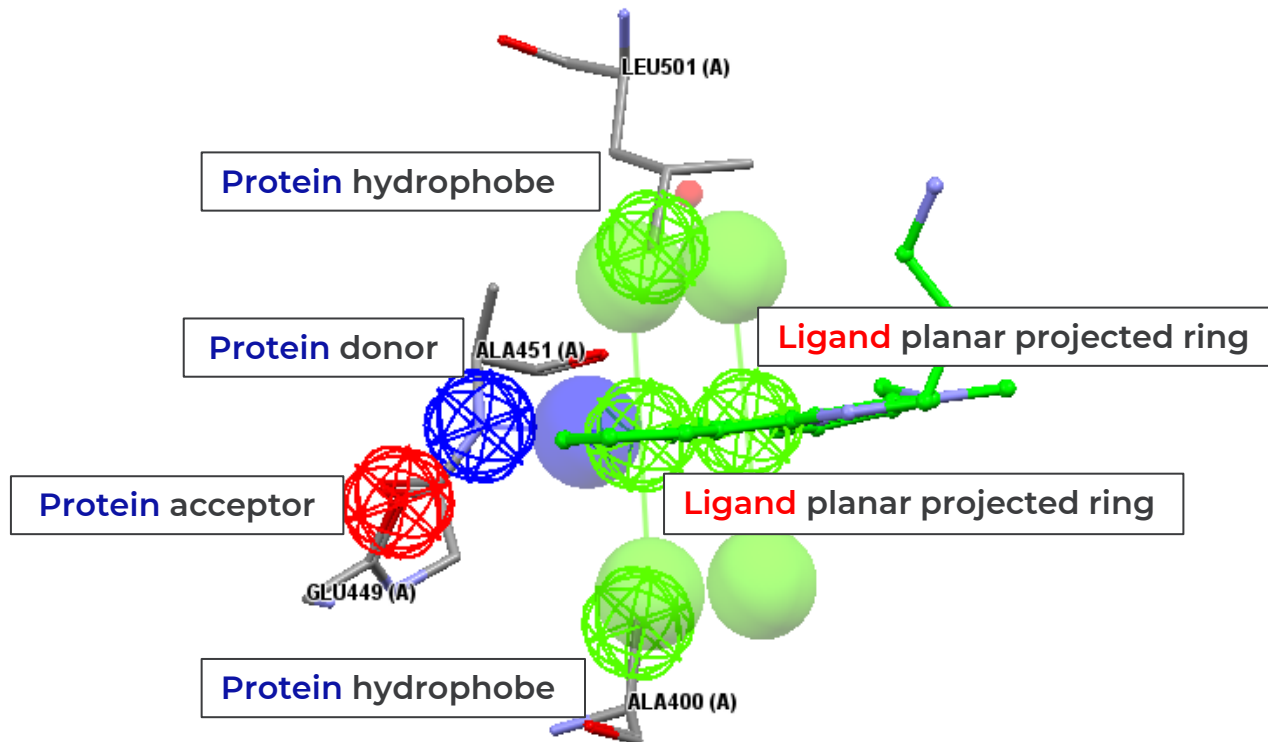
Understand protein-ligand interactions.



CSD-CrossMiner

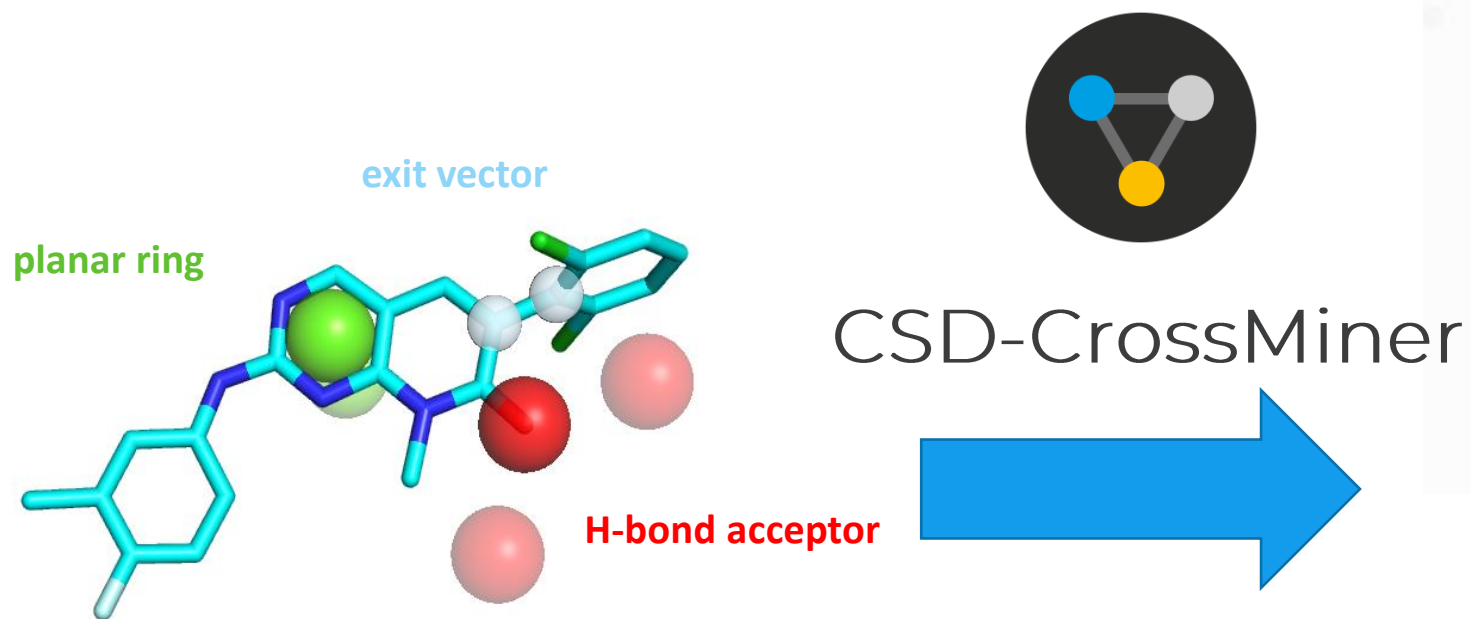


Understand protein-ligand interactions.



- Determine **common protein binding sites** in PDB structures
- Determine **structural motifs** that bind in **similar environments**
- Shed light into **cross-pharmacology** between protein targets

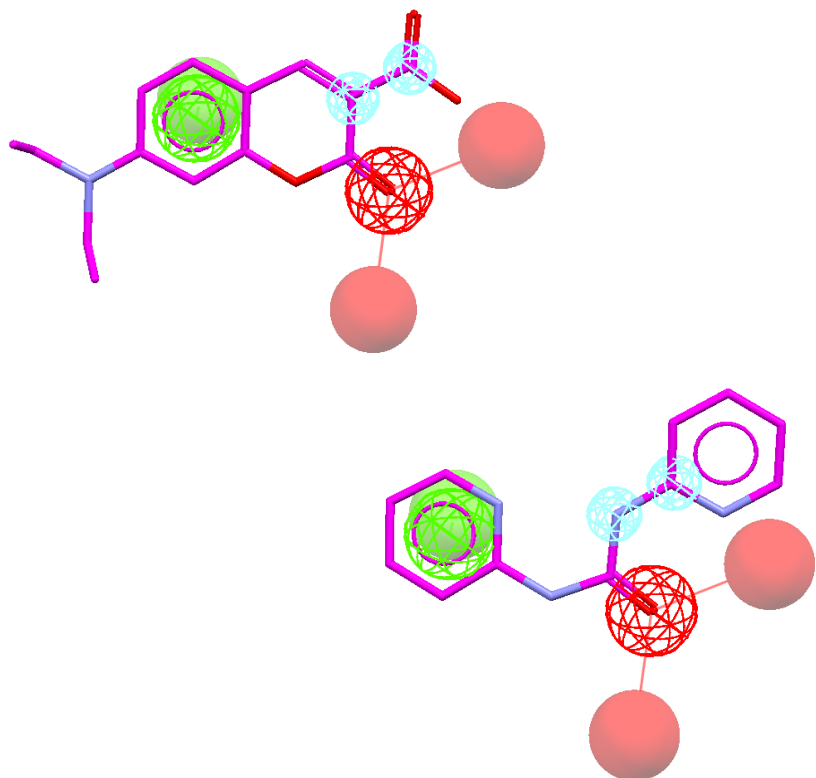
Generate new ideas.



Generate new ideas.



Generate new ideas.



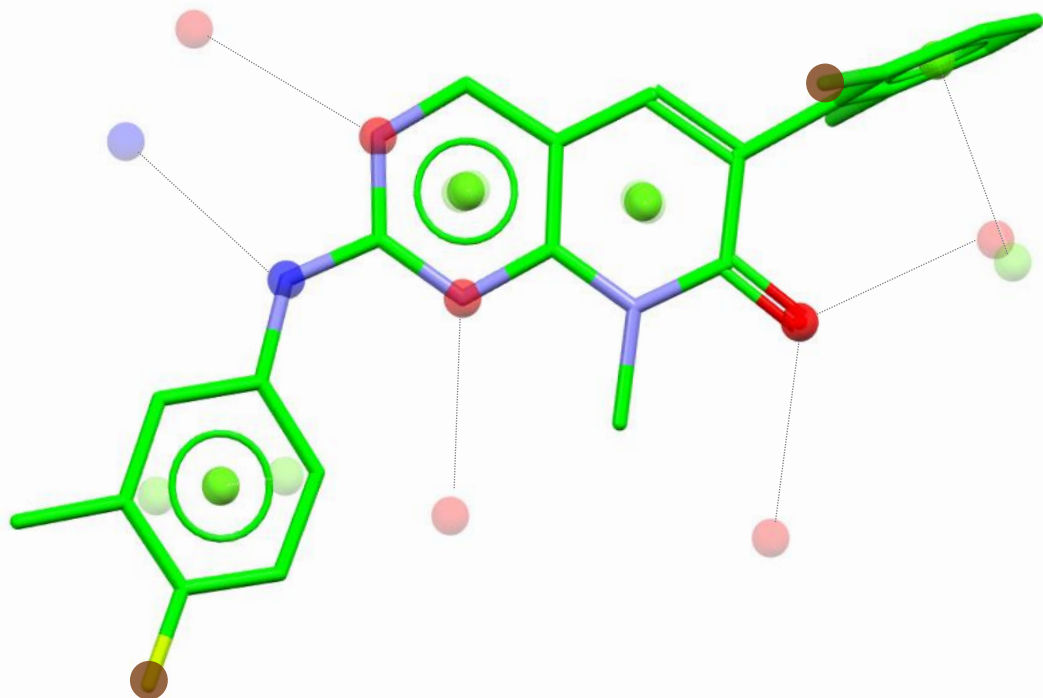
- Design novel motifs that mimic established ligands
- Scaffold-hopping: retrieve a diversity of ligand topologies that can be used as scaffolds
- Look at chemistries that interact with unexplored parts of the binding site.

How does it work?



Look at the features.

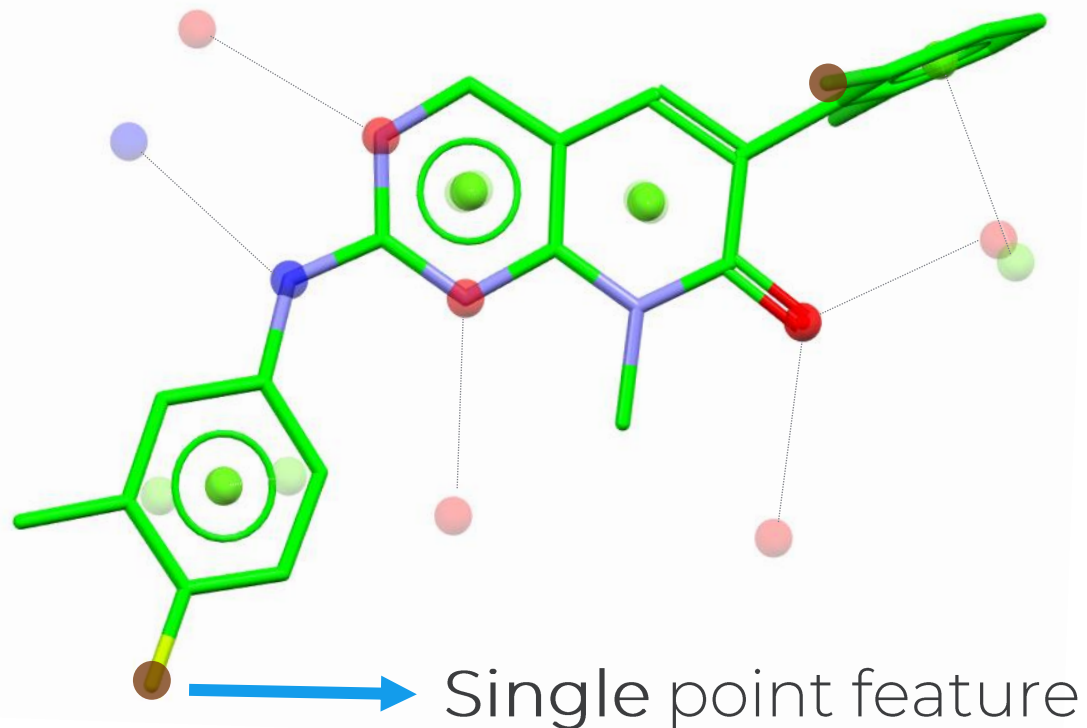
Donor Planar ring
Acceptor Halogen



- Molecules **annotated** with steric and electronic features.
- Based on **SMARTS patterns** – user editable.

Look at the features.

Donor Planar ring
Acceptor Halogen

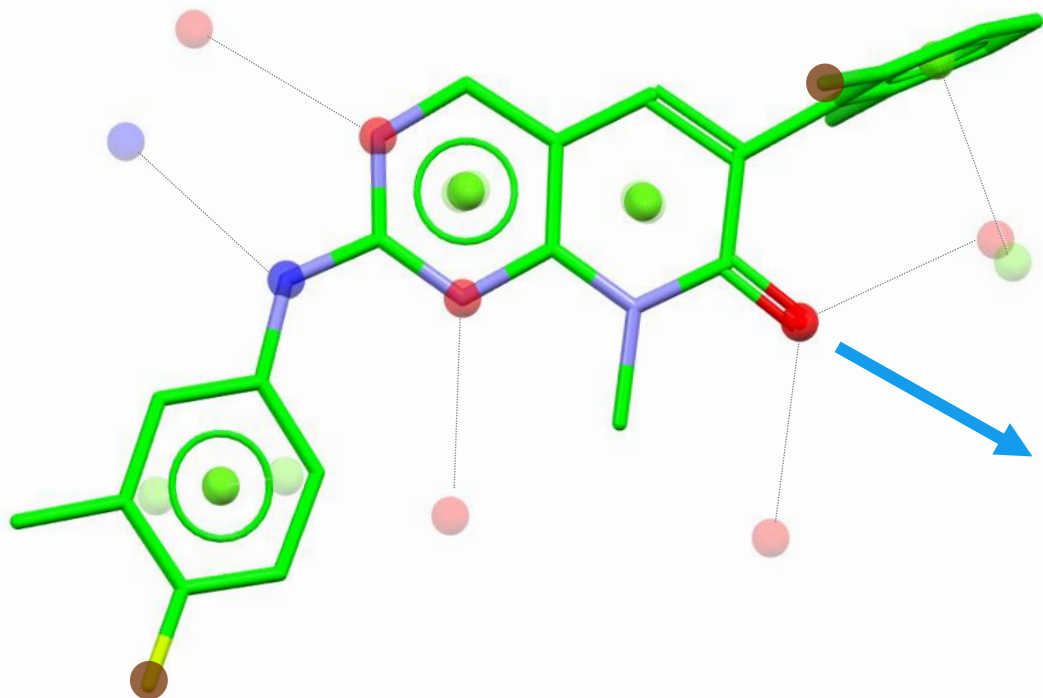


- Molecules **annotated** with steric and electronic features.
- Based on **SMARTS patterns** – user editable.

Look at the features.

Donor Planar ring
Acceptor Halogen

- Molecules **annotated** with steric and electronic features.
- Based on **SMARTS patterns** – user editable.

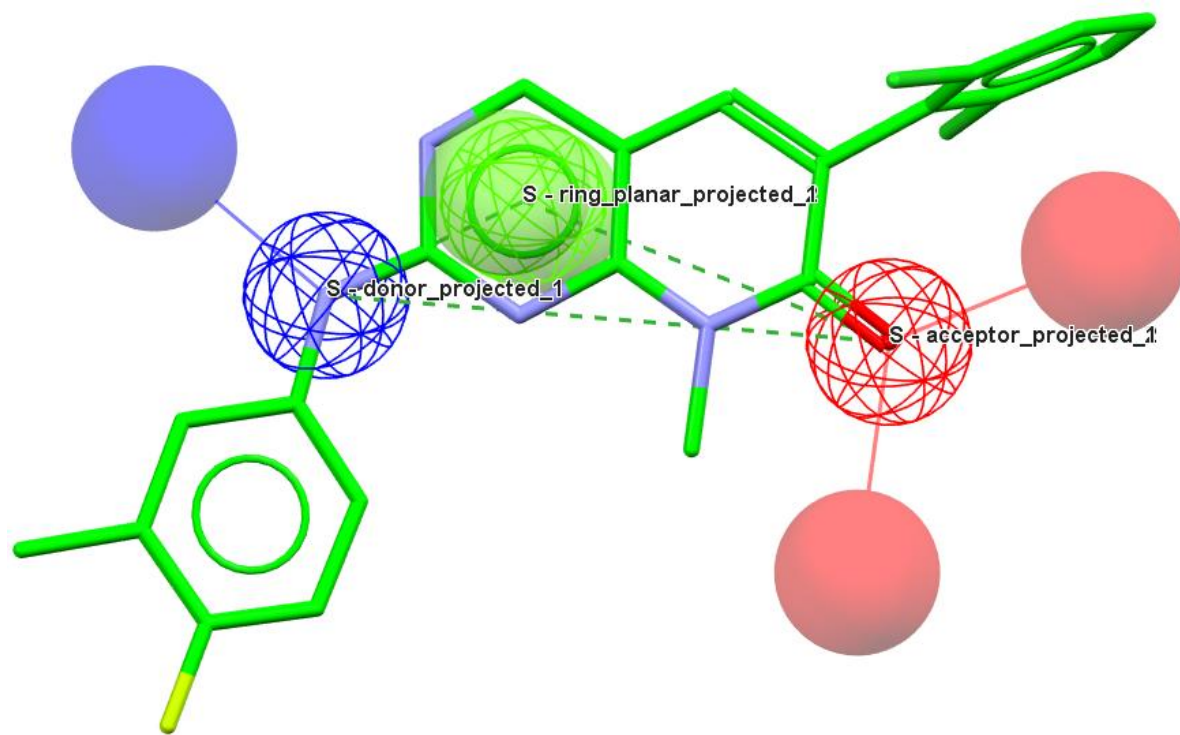


Directional two
point feature

Build the pharmacophore query.

Donor
Acceptor

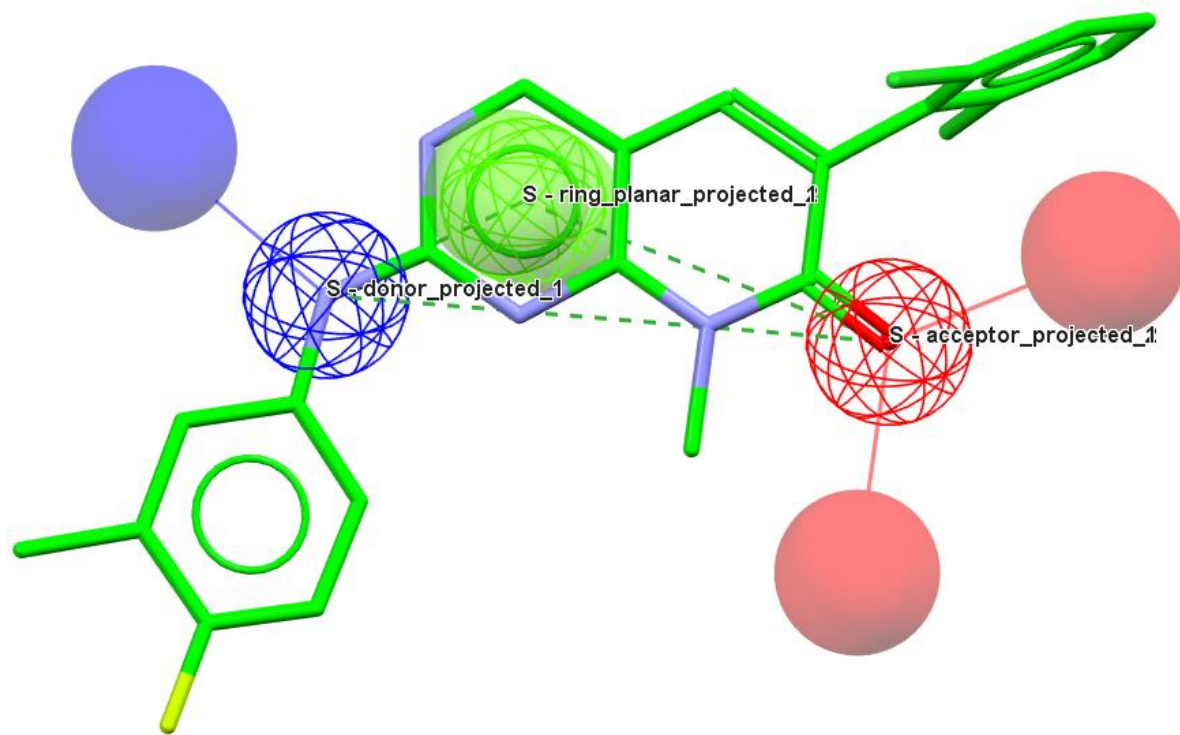
Planar ring



Build the pharmacophore query.

Donor
Acceptor

Planar ring



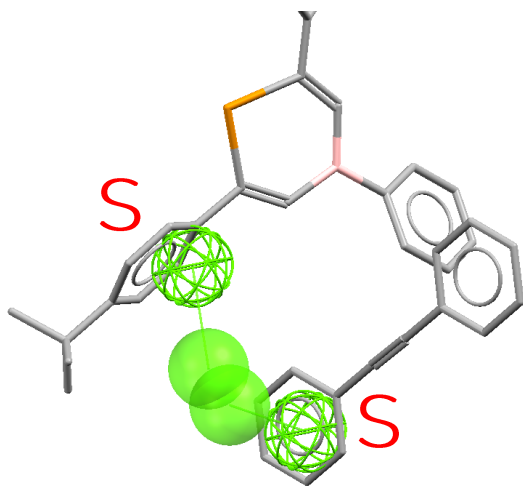
- Tolerance sphere around each feature.
- Radius reflects the uncertainty of position.

Build the pharmacophore query.

- Customise the query – define the **nature** of the point.

Build the pharmacophore query.

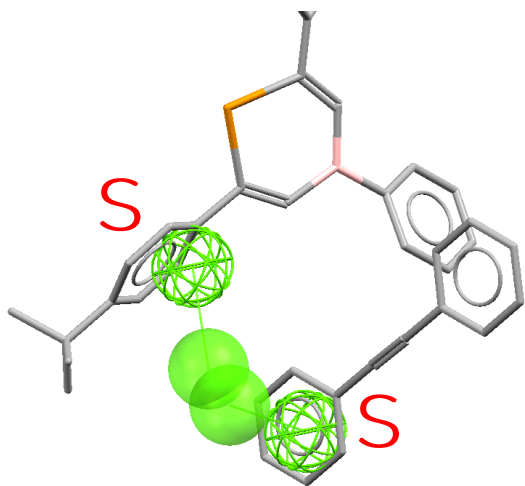
- Customise the query – define the **nature** of the point.



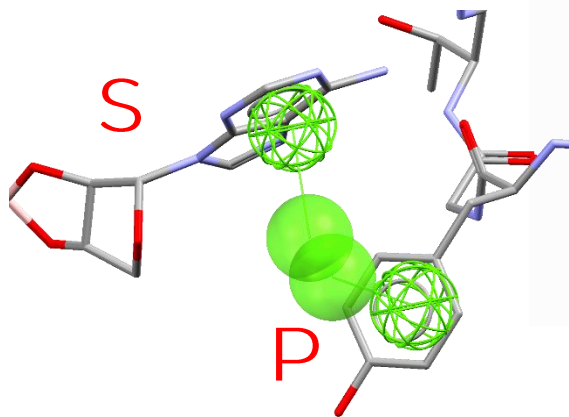
Small molecule (**S**)

Build the pharmacophore query.

- Customise the query – define the **nature** of the point.



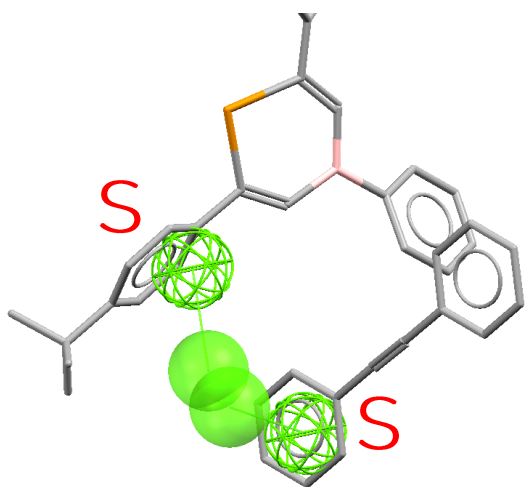
Small molecule (**S**)



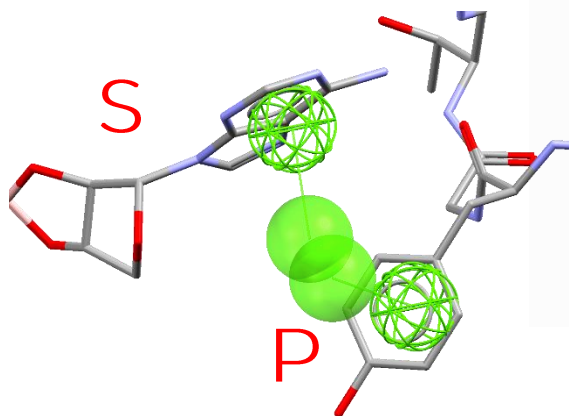
Protein (**P**)

Build the pharmacophore query.

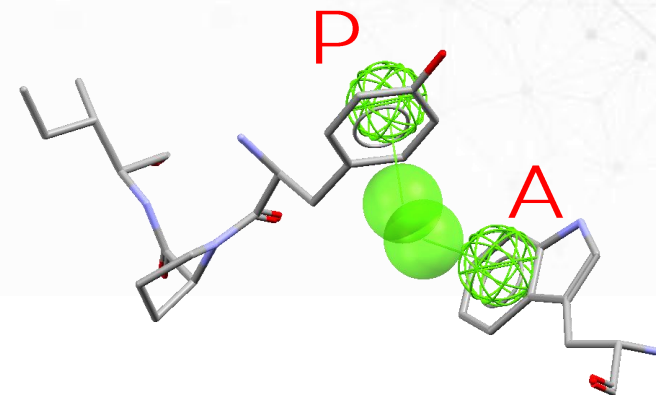
- Customise the query – define the **nature** of the point.



Small molecule (**S**)



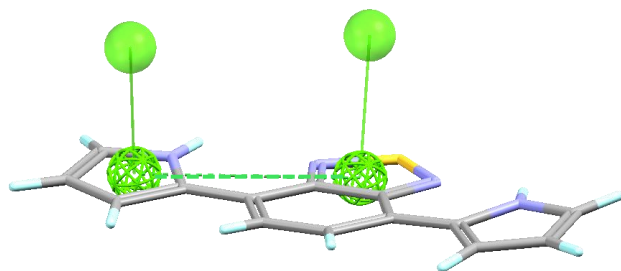
Protein (**P**)



Any molecule (**A**)

Build the pharmacophore query.

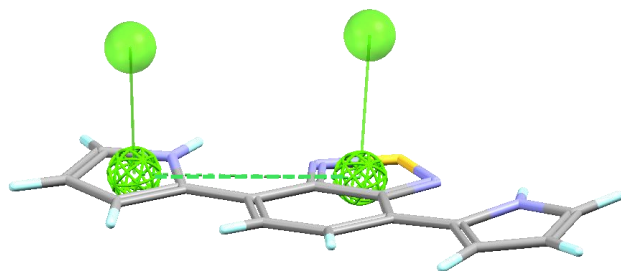
- Customise the query – define the **nature** of the point.



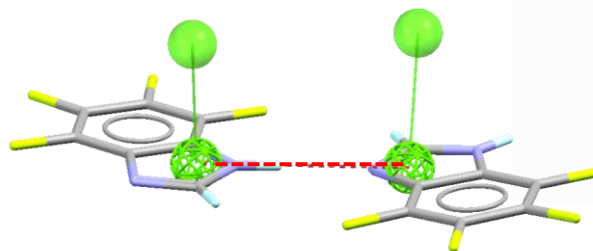
Intra-molecular
constraint

Build the pharmacophore query.

- Customise the query – define the **nature** of the point.



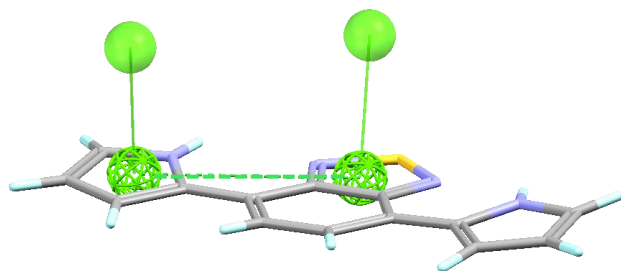
Intra-molecular
constraint



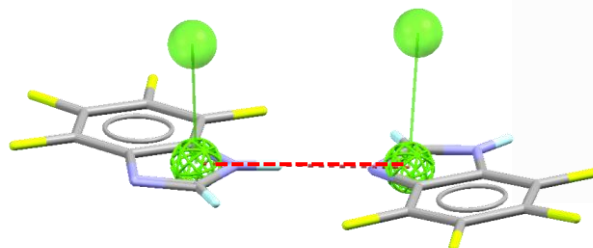
Inter-molecular
constraint

Build the pharmacophore query.

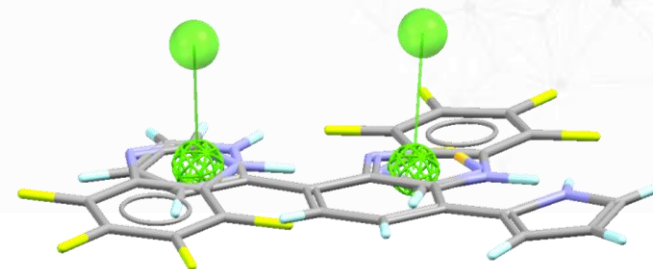
- Customise the query – define the **nature** of the point.



Intra-molecular
constraint



Inter-molecular
constraint



No constraint

Run the search

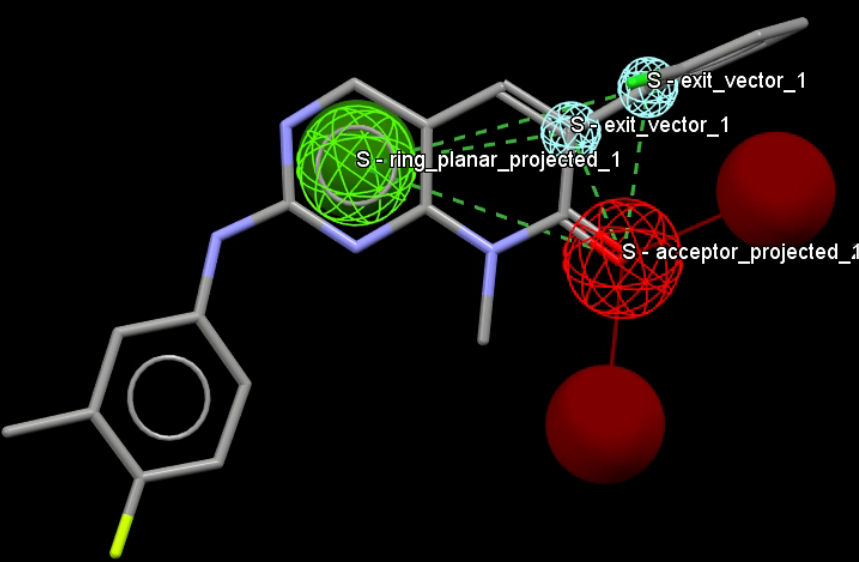
37

2HZ1 - CSD-CrossMiner

File Edit Display Feature Database Help

Style: Wireframe Colour: by Element Picking Mode:

Show: ☒ reference ☒ hits ☒ constraints ☐ features ☒ pharmacophore ☒ pharm. labels ☐ hydrogens Edit: Search:



Feature Databases

database	size
<input checked="" type="checkbox"/> pdb_crossminer	326877
<input checked="" type="checkbox"/> nucleic_acid_crossminer	6041
<input checked="" type="checkbox"/> csd542_crossminer	428847

Results Hitlist

☒ 1st in cluster Settings... Tanimoto: 0.70 Number of hits: 100 Show all

mark	identifier	cluster	rmsd	diagram	chain	deposition
------	------------	---------	------	---------	-------	------------

#hits: 0/10000

Show One: CSD-CrossMiner Interface

38

The screenshot displays the CSD-CrossMiner software interface. The main window shows a 3D molecular model with several labeled features: P-acceptor_projected_1, P-acceptor_projected_2, S-heavy_atom_1, S-heavy_atom_2, P-donor_projected_1, and P-hydrophobe_1. The interface includes a menu bar (File, Edit, Display, Feature Database, Help) and a toolbar with various icons. A 'Show' section on the left lists checkboxes for reference, hits, constraints, features, pharmacophore, pharm. labels, and hydrogens. A 'Search' button is also present.

Overlaid on the main window are three smaller windows:

- Feature Databases:** A table listing databases and their sizes.
- Results Hitlist:** A table showing search results with columns for mark, identifier, cluster, rmsd, diagram, chain, deposition_date, and ec_number.
- Pharmacophore Features:** A table listing pharmacophore features with columns for feature name, tolerance radius, show in reference, and show in pharmacophore.

Blue arrows point to specific elements in the overlaid windows: one points to the 'pdb_crossminer' entry in the Feature Databases window, another points to the 'Results Hitlist' window, and a third points to the 'Pharmacophore Features' window.

database	size
<input checked="" type="checkbox"/> pdb_crossminer	326877
<input checked="" type="checkbox"/> nucleic_acid_crossminer	6041
<input checked="" type="checkbox"/> csd542_crossminer	428847

mark	identifier	cluster	rmsd	diagram	chain	deposition_date	ec_number
------	------------	---------	------	---------	-------	-----------------	-----------

feature name	tolerance radius	show in reference	show in pharmacophore
All		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom		<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe		<input type="checkbox"/>	<input type="checkbox"/>
ring		<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar		<input type="checkbox"/>	<input type="checkbox"/>

The 3D window basics



- Left mouse button and move – rotate structures / pharmacophores

- Middle Mouse wheel – move structures / pharmacophores up and down



- Right mouse button and move up and down – zoom in and out of structures / pharmacophores



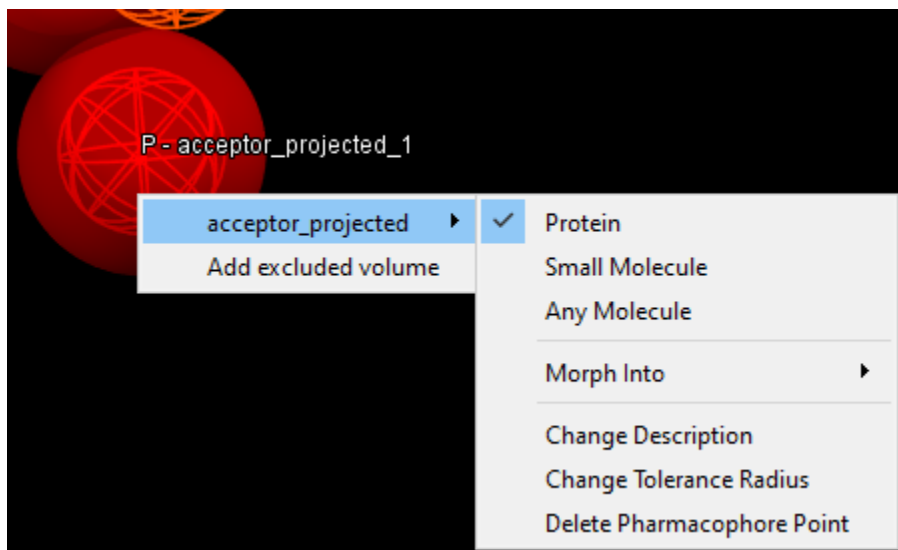
- Shift + Left mouse button and move - rotate in the plane structures / pharmacophores



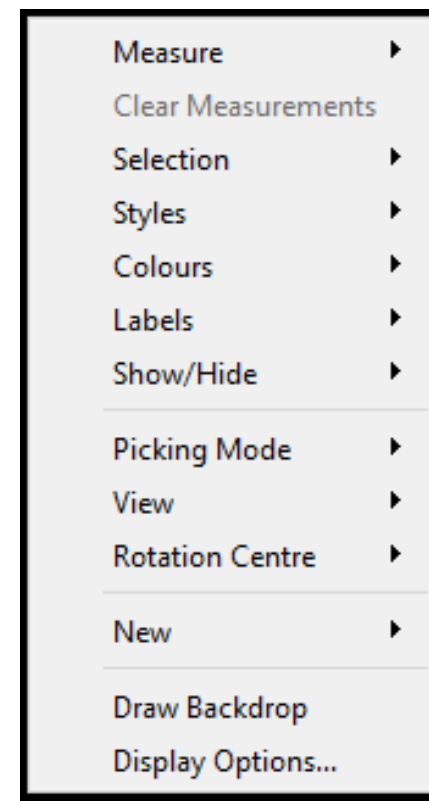
- Ctrl + Left mouse button and move - translate structures / pharmacophores

The 3D window basics – Right Click

On a feature
(Pharmacophore context menu)



Away from a feature
(3D view menu)



Show One: CSD-CrossMiner Menus

41

The screenshot displays the CSD-CrossMiner application window. The 'File' menu is open, showing options such as 'Load Reference...', 'Close Reference', 'Load Feature Database...', 'Close Feature Database', 'Save Feature Database...', 'Export Identifiers', 'Load Pharmacophore...', 'Save Pharmacophore', 'Save PyMOL Pharmacophore', 'Close Pharmacophore', 'Save Marked Hits', 'Save Visible Hits', 'Save All Hits', 'Save as Image...', 'Export POVRay file...', 'Create Structure Database', and 'Exit'. The main window area shows a 3D molecular model with several pharmacophore features highlighted: 'P-acceptor_projected_1' (red), 'S-heavy_atom_1' (orange), 'S-heavy_atom_2' (orange), 'P-hydrophobe_1' (green), and 'P-donor_projected_1' (blue). The 'Feature Databases' panel on the right lists 'pdb_crossminer' (326877), 'nucleic_acid_crossminer' (6041), and 'csd542_crossminer' (428847). The 'Results Hitlist' panel shows search parameters: '1st in cluster' checked, 'Settings...' button, 'Tanimoto: 0.70', 'Number of hits: 100', and a 'Show all' button. The 'Pharmacophore Features' panel lists various features with checkboxes for 'show in reference' and 'show in pharmacophore'.

feature name	tolerance radius	show in reference	show in pharmacophore
All		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom		<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe		<input type="checkbox"/>	<input type="checkbox"/>
ring		<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar		<input type="checkbox"/>	<input type="checkbox"/>
ring_planar_projected		<input type="checkbox"/>	<input type="checkbox"/>
purine		<input type="checkbox"/>	<input type="checkbox"/>
pyrimidine		<input type="checkbox"/>	<input type="checkbox"/>
adenine		<input type="checkbox"/>	<input type="checkbox"/>
cytosine		<input type="checkbox"/>	<input type="checkbox"/>
guanine		<input type="checkbox"/>	<input type="checkbox"/>

Show One: CSD-CrossMiner Menus

42

The screenshot displays the CSD-CrossMiner application window. The 'File' menu is open, showing options like 'Undo: Not Available', 'Redo: Not Available', 'Deprotonate Reference', 'Protonate Reference', 'Options', 'Load Pharmacophore...', 'Save Pharmacophore', 'Save PyMOL Pharmacophore', 'Close Pharmacophore', 'Save Marked Hits', 'Save Visible Hits', 'Save All Hits', 'Save as Image...', 'Export POV-Ray file...', 'Create Structure Database', and 'Exit'. The main workspace shows a 3D molecular model with several pharmacophore features highlighted: 'P-acceptor_projected_1' (red), 'S-heavy_atom_1' (orange), 'S-heavy_atom_2' (orange), 'P-hydrophobe_1' (green), and 'P-donor_projected_1' (blue). The 'Feature Databases' panel lists 'pdb_crossminer' (326877), 'nucleic_acid_crossminer' (6041), and 'csd542_crossminer' (428847). The 'Results Hitlist' panel shows search parameters: '1st in cluster' checked, 'Tanimoto: 0.70', 'Number of hits: 100', and '#hits: 0/10000'. The 'Pharmacophore Features' panel lists various features with checkboxes for 'show in reference' and 'show in pharmacophore'.

feature name	tolerance radius	show in reference	show in pharmacophore
All		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom		<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe		<input type="checkbox"/>	<input type="checkbox"/>
ring		<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar		<input type="checkbox"/>	<input type="checkbox"/>
ring_planar_projected		<input type="checkbox"/>	<input type="checkbox"/>
purine		<input type="checkbox"/>	<input type="checkbox"/>
pyrimidine		<input type="checkbox"/>	<input type="checkbox"/>
adenine		<input type="checkbox"/>	<input type="checkbox"/>
cytosine		<input type="checkbox"/>	<input type="checkbox"/>
guanine		<input type="checkbox"/>	<input type="checkbox"/>

Show One: CSD-CrossMiner Menus

43

The screenshot displays the CSD-CrossMiner application window. The 'Display' menu is open, showing options for visualization styles (Wireframe, Stick, Ball and Stick, Spacefill, Ellipsoid), settings (Stick settings..., Ball and Stick settings..., Spacefill settings..., Ellipsoid settings..., Measurement settings...), element colors (Element colours..., Symmetry Equivalence colours...), and drawing options (Draw Backdrop, Display Options..., Toolbars). The main window shows a 3D molecular model with several spheres labeled: 'P-acceptor_projected_1', 'S-heavy_atom_1', 'S-heavy_atom_2', and 'P-hydrophobe_1'. The 'Feature Databases' panel lists 'pdb_crossminer' (326877), 'nucleic_acid_crossminer' (6041), and 'csd542_crossminer' (428847). The 'Results Hitlist' panel shows search parameters: '1st in cluster' checked, 'Tanimoto: 0.70', and 'Number of hits: 100'. The 'Pharmacophore Features' panel lists features like 'acceptor', 'acceptor_projected', 'donor_ch_projected', 'donor_projected', 'heavy_atom', 'hydrophobe', 'ring', 'ring_non_planar', 'ring_planar_projected', 'purine', 'pyrimidine', 'adenine', 'cytosine', and 'guanine', each with checkboxes for 'tolerance radius', 'show in reference', and 'show in pharmacophore'.

File Edit Display Feature Database Help

Wireframe
Stick
Ball and Stick
Spacefill
Ellipsoid
Stick settings...
Ball and Stick settings...
Spacefill settings...
Ellipsoid settings...
Measurement settings...
Element colours...
Symmetry Equivalence colours...
Draw Backdrop
Display Options...
Toolbars

Ctrl+Q

Feature Databases

database	size
<input checked="" type="checkbox"/> pdb_crossminer	326877
<input checked="" type="checkbox"/> nucleic_acid_crossminer	6041
<input checked="" type="checkbox"/> csd542_crossminer	428847

Results Hitlist

☒ 1st in cluster Settings... Tanimoto: 0.70 Number of hits: 100 Show all

mark	identifier	cluster	rmsd	diagram	chain	deposition_date	ec_number	is_covalent	molecule
------	------------	---------	------	---------	-------	-----------------	-----------	-------------	----------

#hits: 0/10000

Pharmacophore Features

feature name	tolerance radius	show in reference	show in pharmacophore
All	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring_planar_projected	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
purine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
pyrimidine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
adenine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
cytosine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
guanine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Show One: CSD-CrossMiner Menus

44

The screenshot displays the CSD-CrossMiner application window. The 'Display' menu is open, showing options for wireframe, stick, ball-and-stick, spacefill, and ellipsoid models, as well as settings for element colors, symmetry, and toolbars. The main window shows a 3D molecular model with several features highlighted: 'P-acceptor_projected_1' (red), 'S-heavy_atom_1' (orange), 'S-heavy_atom_2' (orange), and 'P-hydrophobe_1' (green). The 'Feature Databases' panel lists 'pdb_crossminer', 'nucleic_acid_crossminer', and 'csd542_crossminer'. The 'Results Hitlist' panel shows search parameters and a table of results. The 'Pharmacophore Features' panel lists various features with checkboxes for tolerance, reference, and pharmacophore inclusion.

Feature Databases

database	size
<input checked="" type="checkbox"/> pdb_crossminer	326877
<input checked="" type="checkbox"/> nucleic_acid_crossminer	6041
<input checked="" type="checkbox"/> csd542_crossminer	428847

Results Hitlist

☒ 1st in cluster Settings... Tanimoto: 0.70 Number of hits: 100 Show all

mark	identifier	cluster	rmsd	diagram	chain	deposition_date	ec_number	is_covalent	molecule
------	------------	---------	------	---------	-------	-----------------	-----------	-------------	----------

#hits: 0/10000

Pharmacophore Features

feature name	tolerance radius	show in reference	show in pharmacophore
All		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom		<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe		<input type="checkbox"/>	<input type="checkbox"/>
ring		<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar		<input type="checkbox"/>	<input type="checkbox"/>
ring_planar_projected		<input type="checkbox"/>	<input type="checkbox"/>
purine		<input type="checkbox"/>	<input type="checkbox"/>
pyrimidine		<input type="checkbox"/>	<input type="checkbox"/>
adenine		<input type="checkbox"/>	<input type="checkbox"/>
cytosine		<input type="checkbox"/>	<input type="checkbox"/>
guanine		<input type="checkbox"/>	<input type="checkbox"/>

Show One: CSD-CrossMiner Interface

The screenshot displays the CSD-CrossMiner software interface. At the top, there are dropdown menus for 'Style' (set to Wireframe) and 'Colour' (set to by Element). Below these are checkboxes for 'Show' and 'features'. A 'Picking Mode' section contains icons for normal selection, lasso selection, and distance/angle measurement. A 'Feature Databases' section includes 'Search' buttons with play and stop icons. A 'Pharmacophore Features' panel at the bottom lists various features with checkboxes for 'tolerance radius', 'show in reference', and 'show in pharmacophore'. The main workspace shows a molecular structure with highlighted pharmacophore features: 'P-donor_projected_1' (blue sphere), 'S-heavy_atom_1' (orange sphere), 'S-heavy_atom_2' (orange sphere), and 'P-hydrophobe_1' (green sphere). Blue callout boxes provide instructions: 'Edit Pharmacophore Features (Off - On)' points to the 'Edit' buttons; 'Start, Pause, Stop the search' points to the search controls; and 'Change Picking Mode, choosing between normal, lasso selection, measure distances, measure angles, and measure torsions' points to the picking mode icons.

Style: Wireframe Colour: by Element Picking Mode: [normal] [lasso] [distance] [angle] [torsion]

Show: [checked] re [checked] features [checked]

Search: [play] [stop] [X]

Search: [pause] [stop] [X]

Edit: intra [hand icon]

Edit: intra [hand icon]

Change Picking Mode, choosing between normal, lasso selection, measure distances, measure angles, and measure torsions

Edit Pharmacophore Features (Off - On)

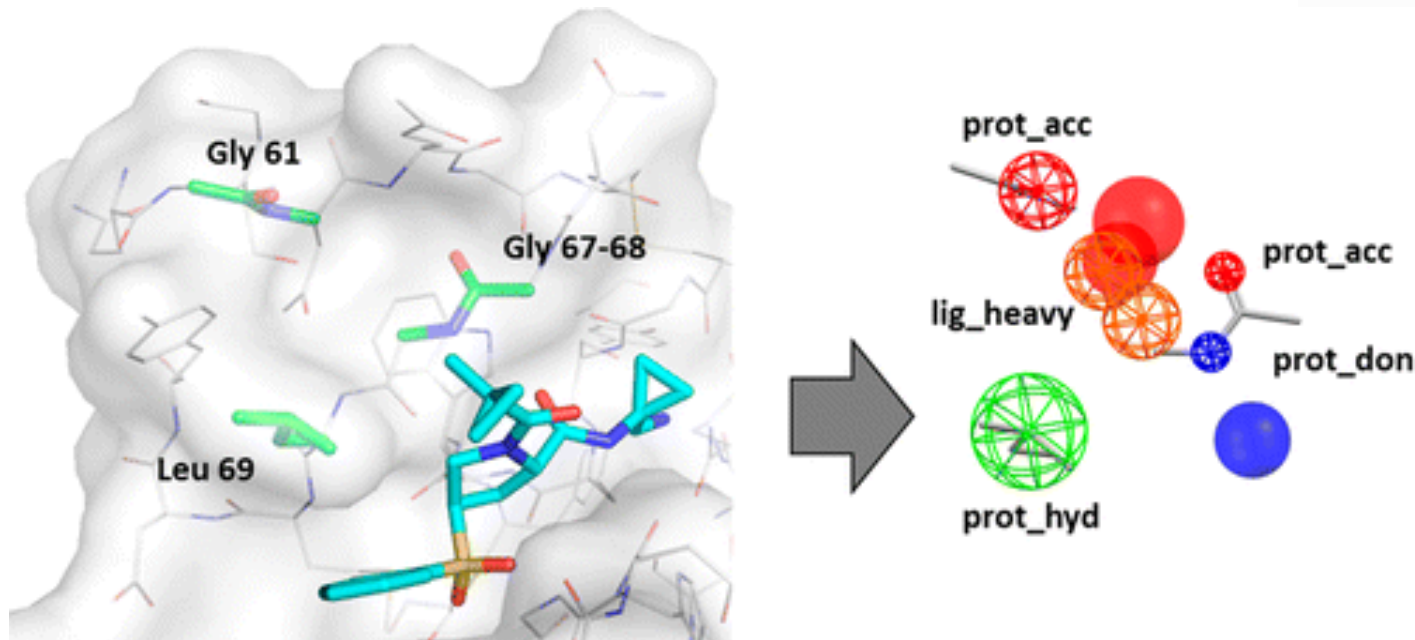
Start, Pause, Stop the search

Pharmacophore Features

feature name	tolerance radius	show in reference	show in pharmacophore
All	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
acceptor_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_ch_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
donor_projected	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
heavy_atom	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
hydrophobe	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring_non_planar	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ring_planar_projected	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
purine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
pyrimidine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
adenine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
cytosine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
guanine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
thymine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Show One: CSD-CrossMiner Demo

- Cathepsin L in complex with a nitrile inhibitor



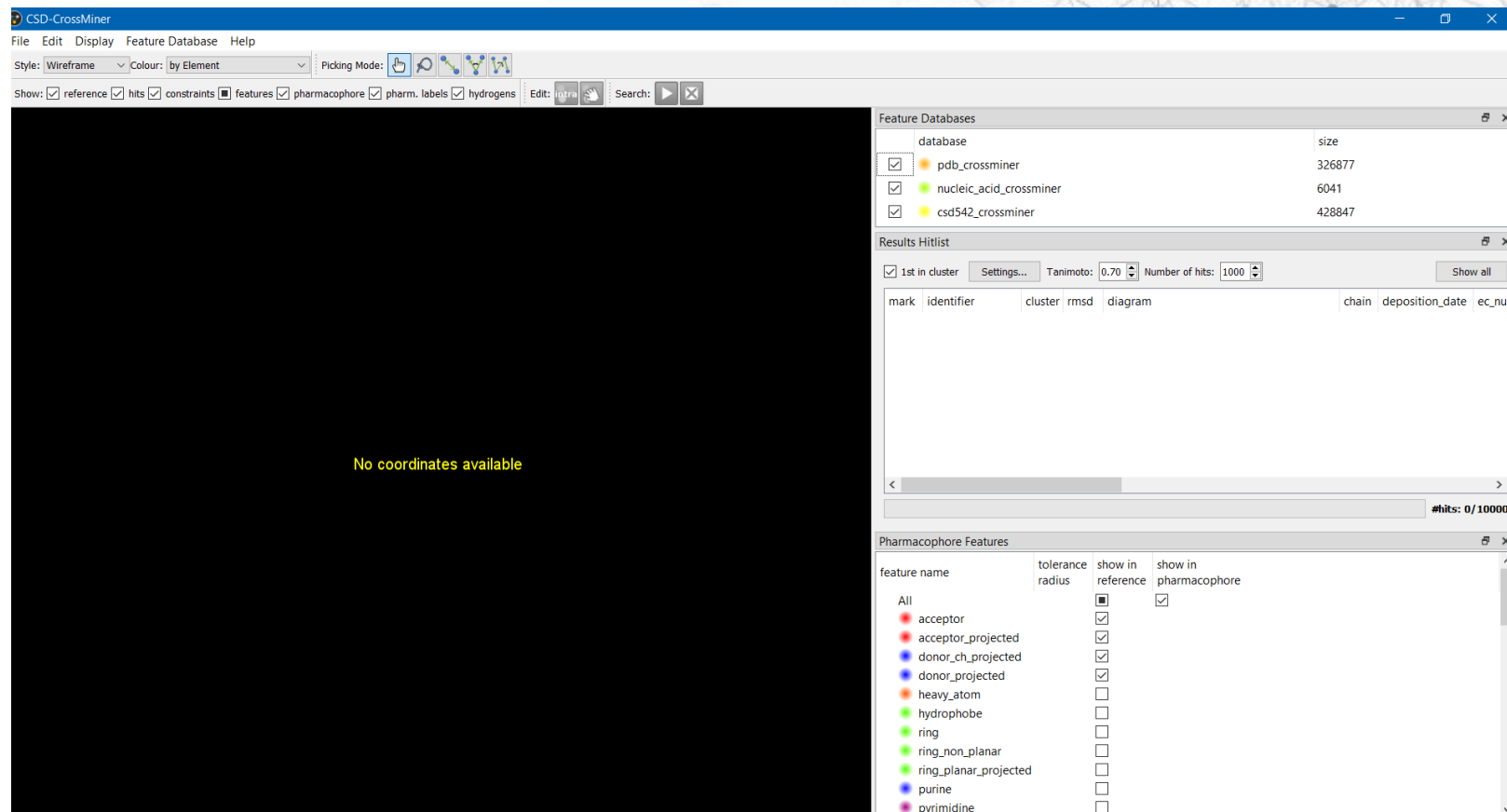
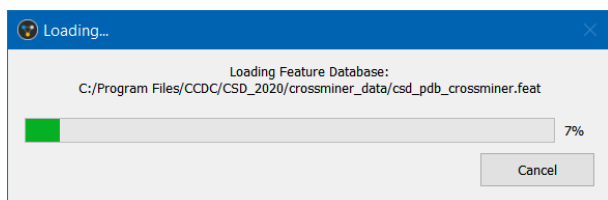
2XU1 PDB code

Show One: CSD-CrossMiner Demo

47

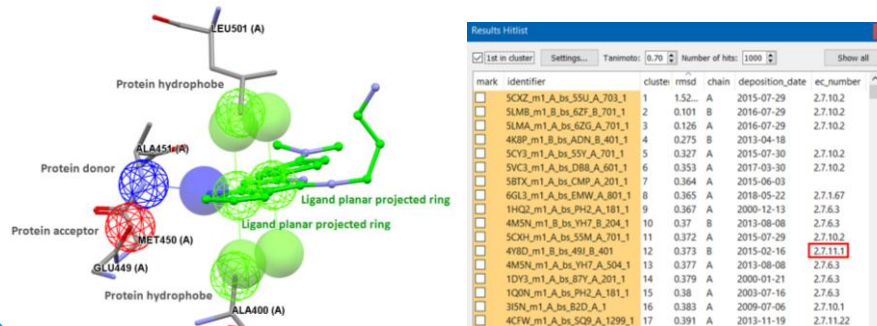


1. By default the provided *csd_pdb_crossminer.featt* feature database will be loaded

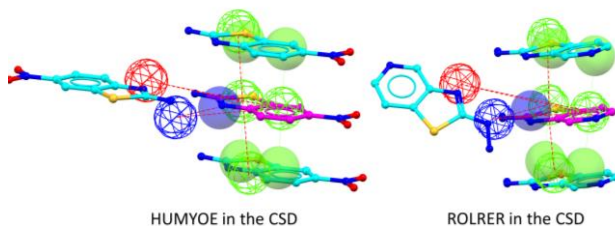


What else can you explore in CSD-CrossMiner? 62

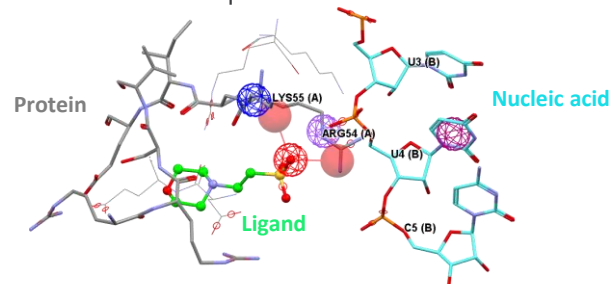
Identify common protein-ligand pattern



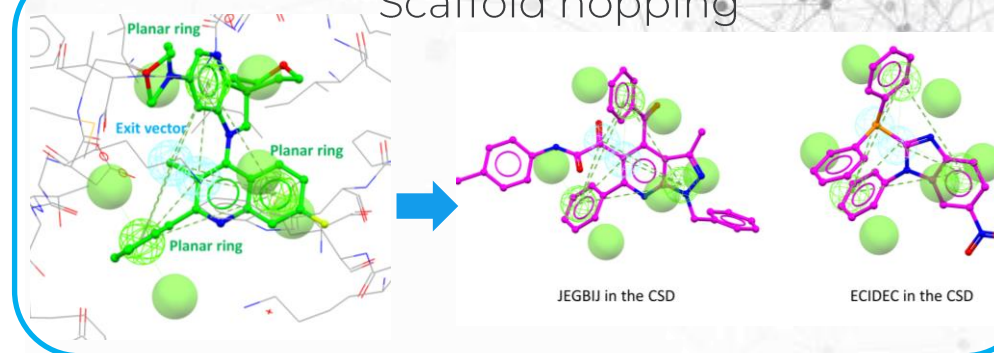
Mine co-crystals



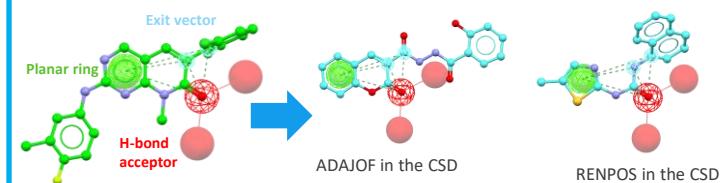
Identify nucleic-acids-protein pattern



Scaffold hopping



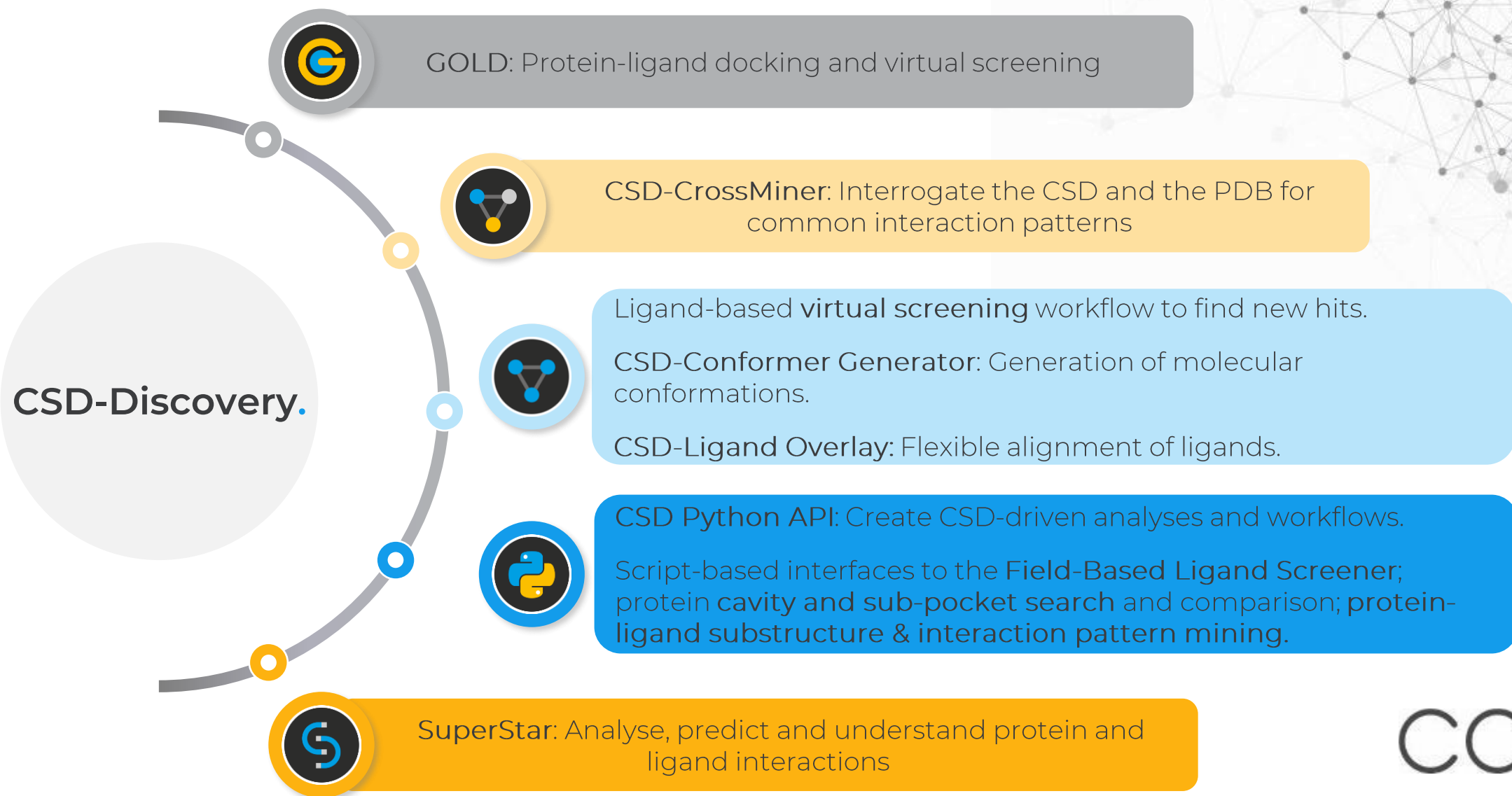
Find bioisosters



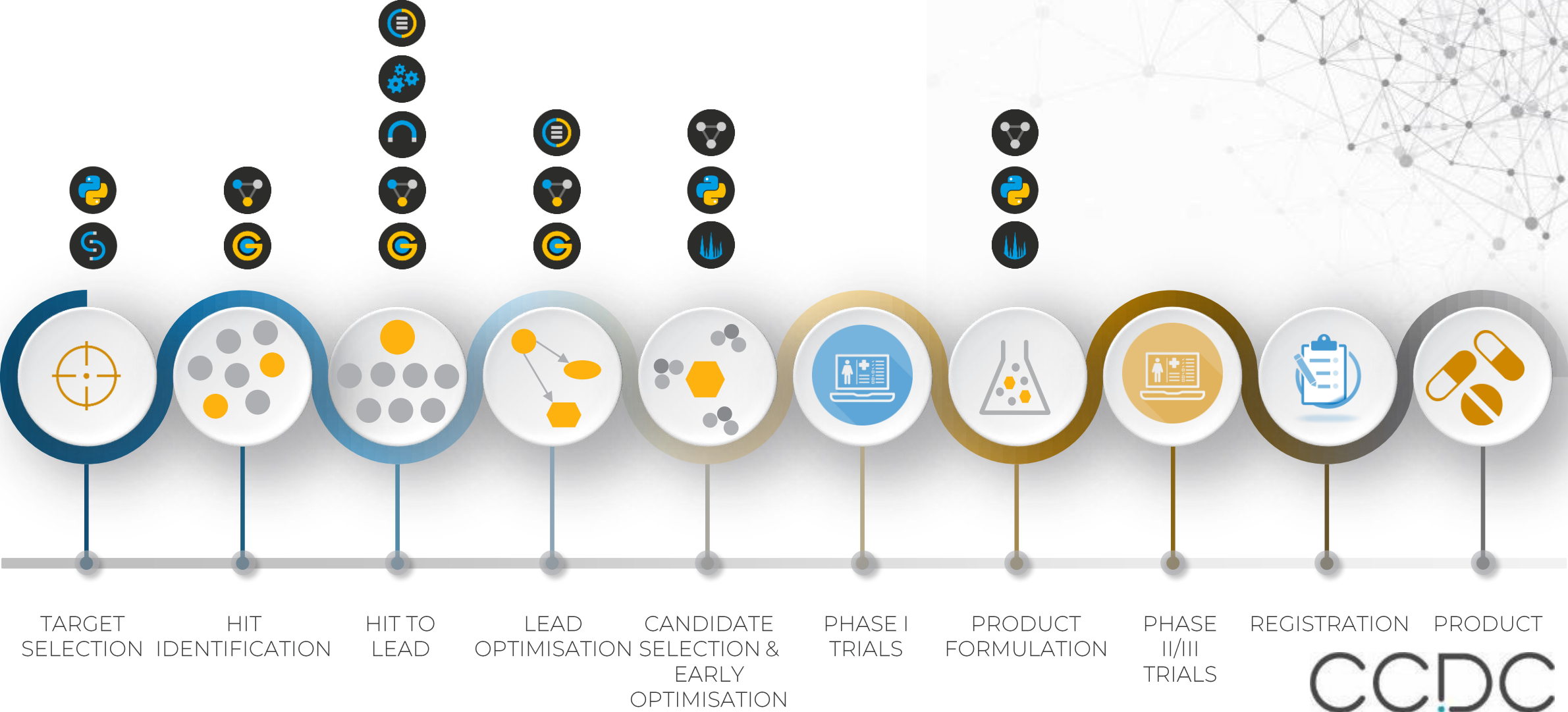
...and more!

CCDC

CSD-Discovery overview

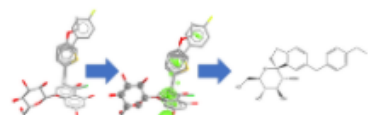


Drug Discovery Pipeline



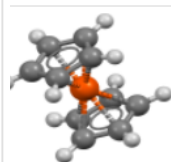
Want to explore more?

Training and Educational Resources

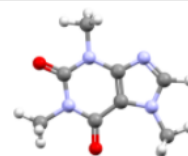


CSD-Discovery

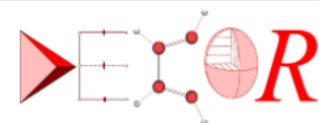
For pharmaceutical and agrochemical researchers, tools for discovering new molecules and performing protein docking studies.



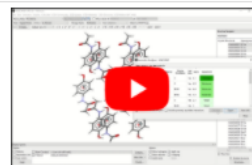
Information on the Teaching Subset



Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography



Watch software training and support videos



Explore the Periodic Table through Crystal Structures



Access fun science activities for kids through the CCDC Home learning page

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials in chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore. Our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials are part of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of these, over one million entries are available for free through our Access Structures portal.

For anyone looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and want to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.

To stay up to date with the latest news from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter [here](#).

Register for E&O newsletter

Self-guided workshops

<https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/>

Download a series of self-guided workshop materials for CCDC tools and features

YouTube and LabTube channels links from <https://www.ccdc.cam.ac.uk/Community/educationalresources/ccdc-videos/>

CCDC

Want to explore more?

CCDC Virtual Workshops:

- 21st Apr - [Programmatic search and analysis using the CSD Python API](#)

How did it go today?

Let us know and help us improve filling in this short survey:

<https://www.surveymonkey.co.uk/r/SLMYVC3>

- Follow [#CSDTopTipTuesday](#) for weekly tips on using our software
- [What's Up](#) Webinars
 - Next one is 20th May
 - Featuring our Ligand Overlay tool
- [Discovery Science Meeting](#)
 - 9th – 10th June 2021
 - Registration and call for abstracts now open



CCDC