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advancing structural science

# What's Up

## Customer Update Webinar

21st January 2021

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advancing structural science

# Today’s presenters

**David Bardwell**

Support Team Leader

**Peter Wood**

Senior Product Manager

**Abhik Mukhopadhyay**

Research and Applications Scientist

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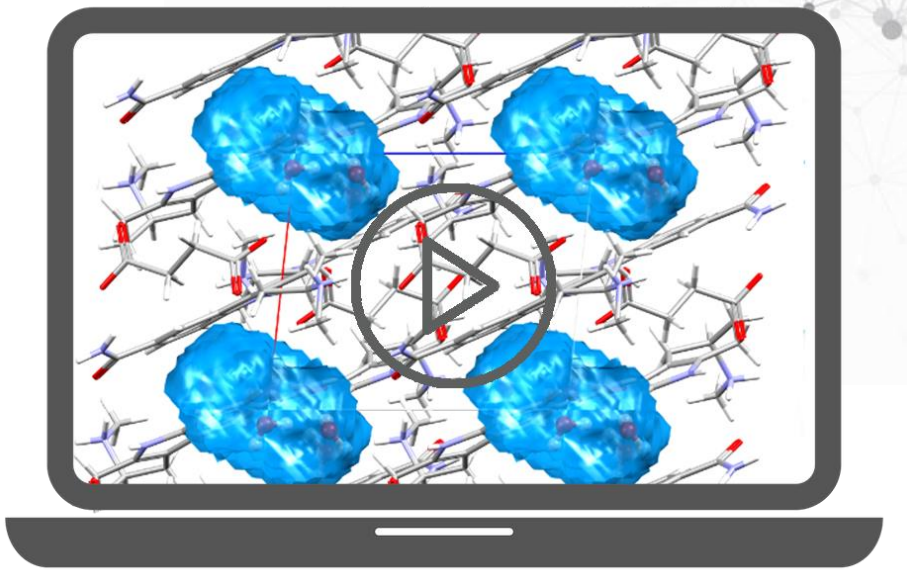
# Overview

In this webinar we will discuss:

- Latest updates and news
- IsoStar Groups: easy visualisation of intermolecular interactions
- CSD-Core: Tips and Tricks to work with Hermes
- Q&A: the floor is yours





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# Latest updates and news from CCDC >Events

- Join the **Behind the Paper** series – 22nd and 29th January
  - Register on our website now.


- CCDC **User Group Meetings 2021 – all virtual**:
  - CCDC Educators UGM – 16th and 17th March
  - CCDC Discovery Science UGM – 9th and 10th June
  - CCDC Materials Science UGM – 7th and 8th September

If you would like to present a talk in any UGM please email hello@ccdc.cam.ac.uk

Find out more at www.ccdc.cam.ac.uk

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# The CCDC team is growing…

## Recently joined CCDC

- Sofia da Fonseca – Channel Manager
- Alex Eyes – Customer Success Manager

## We're hiring!

- https://www.ccdc.cam.ac.uk/theccdcprofile/careers/
  - Research and Applications Scientist
  - Deposition Coordinator
  - Junior + Senior Software Engineers – web UI specialists
  - UX-UI Designer…. *and many more roles*.

# IsoStar

## Easy visualisation of intermolecular interactions

David Bardwell

Support Team Leader

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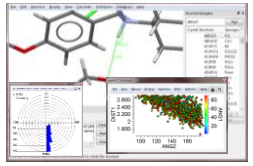
# CSD-Core overview



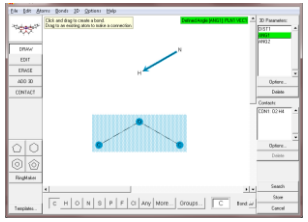
**Mercury**: Visualisation & numerical analysis



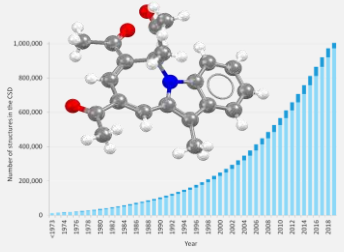
**Hermes**: Visualisation of macromolecules

**CSD Python API**: Access to data & all functionality

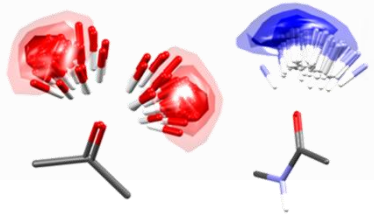
**ConQuest**: Advanced 3D searching & data generation



Cambridge Structural Database



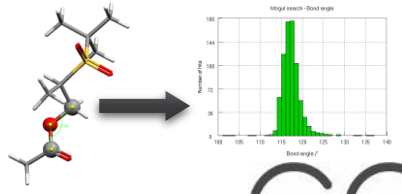
**IsoStar**: Intermolecular interaction analysis



**WebCSD**: Online search & entry level interface


CSD-Editor: Create in-house database

**Mogul**: Molecular geometry analysis



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# What is IsoStar?

- IsoStar uses the wealth of interaction information in the CSD to show the 3D characteristics of interactions between functional group pairs
- Provides a pre-calculated library of intermolecular interactions from both the CSD and the PDB
- Allows easy exploration of the intermolecular interaction distribution for functional groups of interest
- Shows the most likely interaction geometry based on experimental evidence

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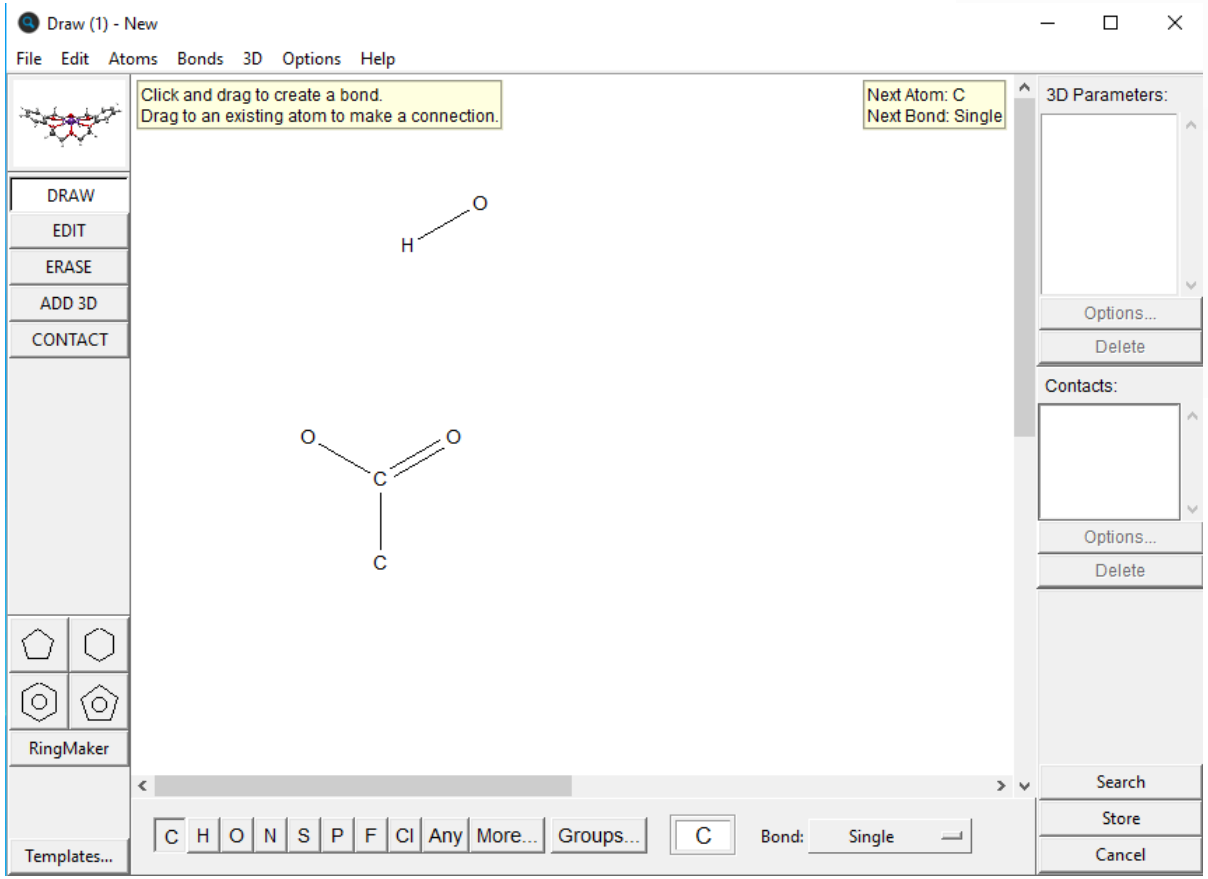
# What is IsoStar?

- IsoStar data is presented as a set of 3D scatterplots
- Each scatterplot represents the non-bonded intermolecular interactions between a *central* group and a *contact* group
- Each interaction presented in the scatterplot is a hit located via a search of the data in the CSD or PDB
- The central group of each hit is superimposed so that the relative position of each contact group can be examined

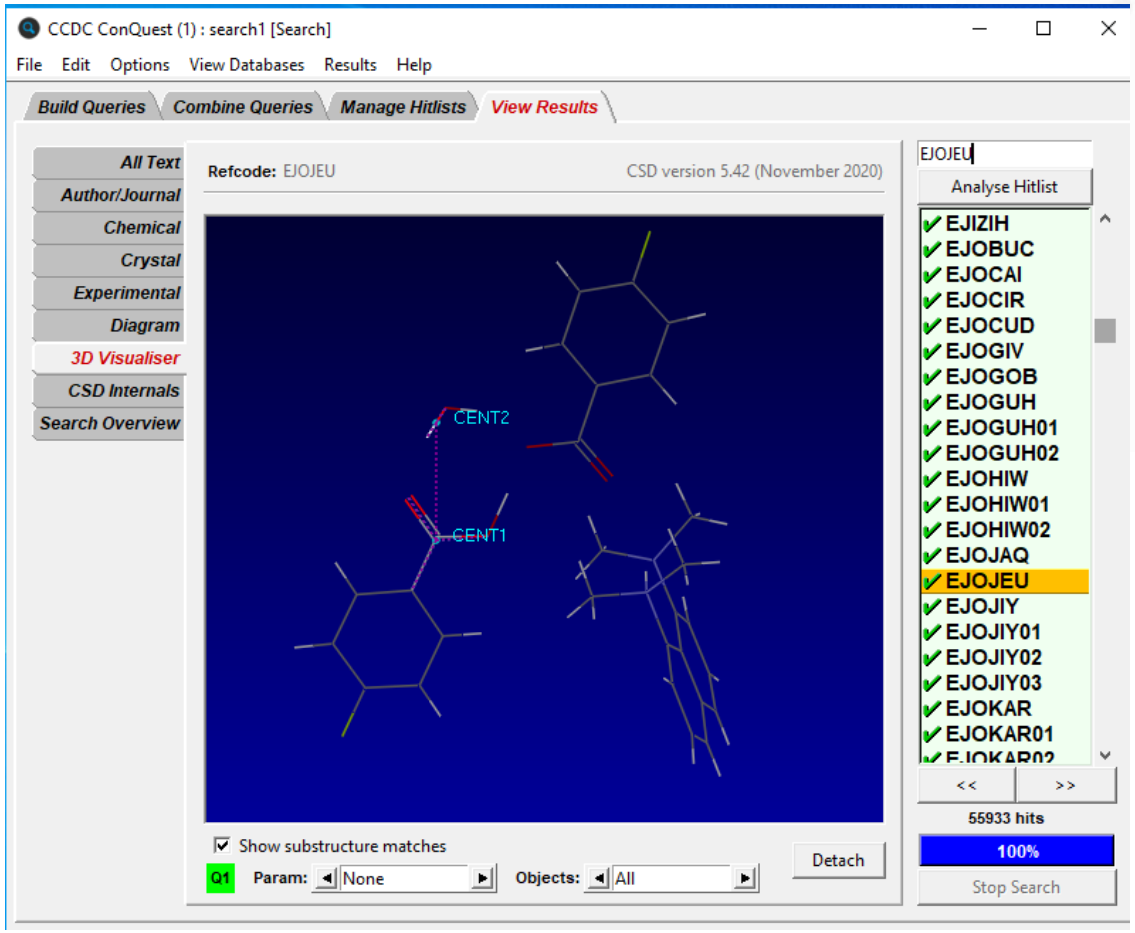
# IsoStar Scatterplots

- At their heart, all scatterplots are derived from a search for intermolecular interactions



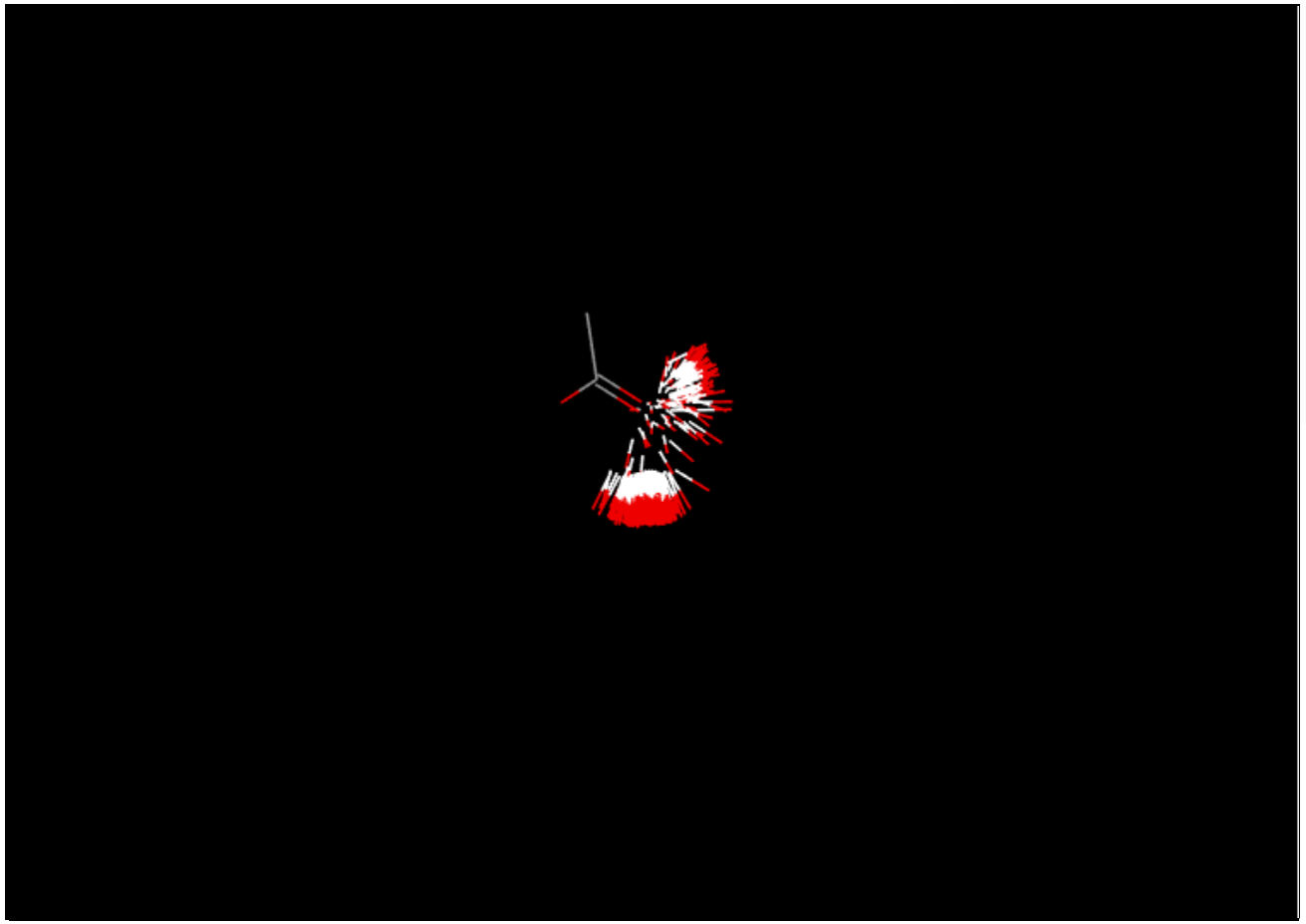
# IsoStar Scatterplots

- This results in a lot of hits for all interactions of this type



# IsoStar Scatterplots

- All of these interactions can be plotted together, with the central groups all superimposed



# How to access IsoStar?

- IsoStar is a *client-server* application
  - The *server* hosts the interface for all available scatterplots
  - The *client* allows you to view and manipulate each scatterplot
- The IsoStar server is available via isostar.ccdc.cam.ac.uk
  - A version that you can install and make available on your own local network is also available
- The IsoStar client is a part of the CSD Software portfolio and is installed together with ConQuest, Mercury, Mogul etc.

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# Live Demo

CCDC IsoStar 2020.3

Home | Ligand Terminal | Ligand Acyclic Links | Ligand Ring Systems | Ligand Solvates | Protein Plots | Custom Plots | Help

Home

Ligand
*Terminal*
C,H only
N,C,H only
O,C,H only
N,O,C,H only
Si-containing
P-containing
S-containing
Se-containing
Halo-containing

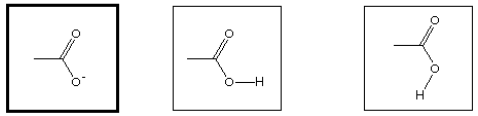
*Acyclic links*
C,H only
N,C,H only
O,C,H only
N,O,C,H only
P-containing
S-containing
Se-containing

*Ring systems*
Phenyls
C,H only
N,C,H only
O,C,H only
N,O,C,H only
S-containing
Nucleic acid bases

*Solvates, etc.*
Inorganic
Organic

Protein
Terminal
Links
Ring systems

Custom Plots



charged carboxylic acid uncharged carboxylic acid; cis uncharged carboxylic acid; trans

## charged carboxylic acid

(PDB scatterplots for all the above groups are identical, because the groups are indistinguishable in protein crystal structures; More Information)

General| C,H only| N-H| O-H| Other N or O| Sulfur| Halo/halide| Alkali Metal| Amino acid

| General | | | | |
|---|---|---|---|---|
| Links to statistical data | Links to theoretical energy data | | | |
| ***Contact Group*** | ***CSD*** | ***PDB*** | ***Stats*** | ***Theory*** |
| any C,N,O,S or H | 9995 | 9937 | | |
| any polar X-H (X= N,O or S) | 4997 | 9995 | | |

* This search has not been done.

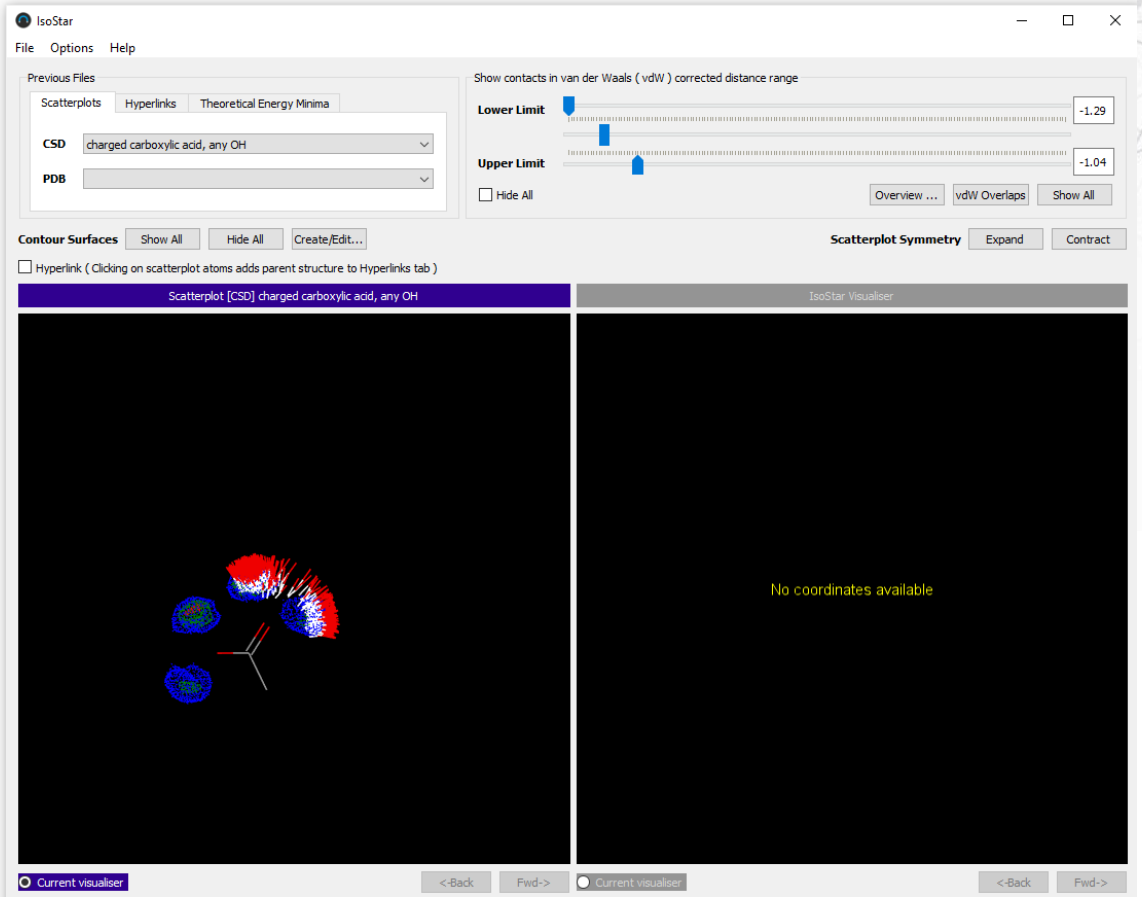
General| C,H only| N-H| O-H| Other N or O| Sulfur| Halo/halide| Alkali Metal| Amino acid

| C,H only | | | | |
|---|---|---|---|---|
| Links to statistical data | Links to theoretical energy data | | | |
| ***Contact Group*** | ***CSD*** | ***PDB*** | ***Stats*** | ***Theory*** |
| any alkyl C-H | 4997 | 9938 | | |
| methylene | 1999 | 2734 | | |
| methyl | 1999 | 1625 | | |
| any aromatic C-H | 4997 | 2781 | | |
| substituted aromatic carbon | 2498 | 102 | | |
| phenyl | 1427 | 745 | | |

* This search has not been done.

General| C,H only| N-H| O-H| Other N or O| Sulfur| Halo/halide| Alkali Metal| Amino acid

| N-H | | | | |
|---|---|---|---|---|
| Links to statistical data | Links to theoretical energy data | | | |
| ***Contact Group*** | ***CSD*** | ***PDB*** | ***Stats*** | ***Theory*** |
| any NH | 4997 | 8574 | | |

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# CSD-Core

## Tips and Tricks to work with Hermes

Abhik **Mukhopadhyay**

Research and Applications Scientist

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# CSD-Core overview



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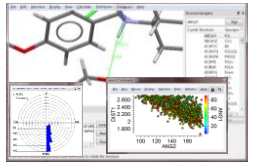

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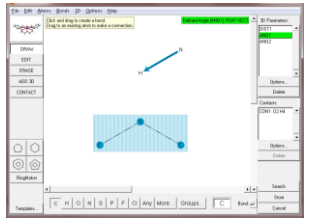

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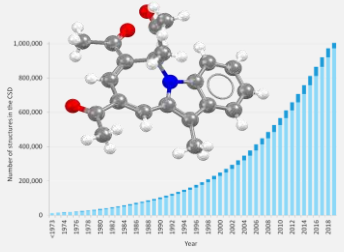

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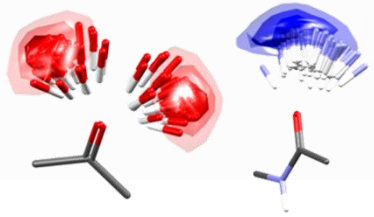

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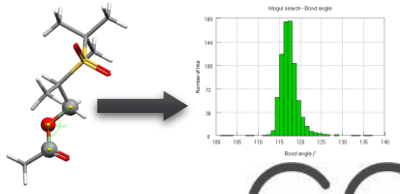

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# What is Hermes?

- The Hermes visualiser is a program for visualising protein structures in three dimensions.
- Hermes can be used for display and editing of protein and small molecule structures.
- Hermes also hosts interfaces to CSD discovery tools like GOLD, Mogul, SuperStar, the CSD Ligand Overlay, and descriptors for GOLD docking poses.

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# Why would you use, what are the benefits?

- To visualise and analyse biological macromolecules (protein and nucleic acids)
- Hermes can read and write different coordinate file formats (PDB, mol2 etc)
- Allows user to share and present their research (publication quality image and session sharing)
- A visualiser that users from different domain can use.

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# Tips

- A range of 3D visualisation options,
  - wireframe, capped stick, ball and stick, and space fill
  - colours, labelling schemes, and the ability to hide and then re-display atoms, residues, ligands, water molecules, etc.
- Read in protein and ligand structures from external files
  - .pdb and .mol2
- Load and visualise contoured surfaces.
- Superimposition of protein structure
  - least squares overlay
  - sequence alignment.
- Measure and display distances, angles and torsion angles.
- Edit ligand and cofactor
- Prepare publication quality displays and save them.

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# Tricks

- How to prepare protein or small molecule structures
- How to show protein structures in ribbon
- How to analyse binding sites in protein ligand structures

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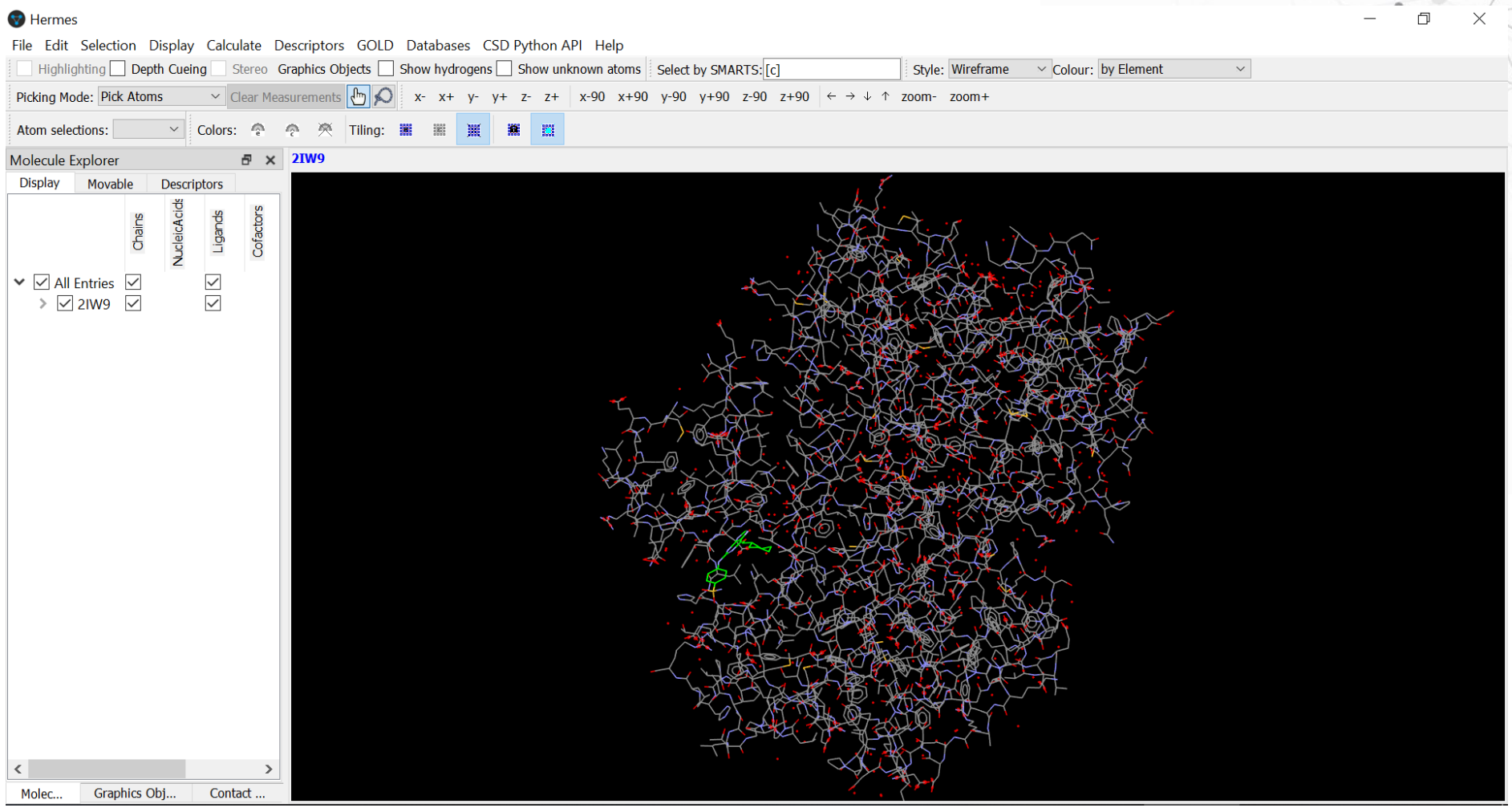
# Live Demo

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# Summary

- Hermes, a macromolecular structure visualiser, is now available for CSD-Core users.
- We have shown how to visualise, edit and analyse structures in Hermes.
- Please do let us know your feedback on Hermes and if you have any feature requests.

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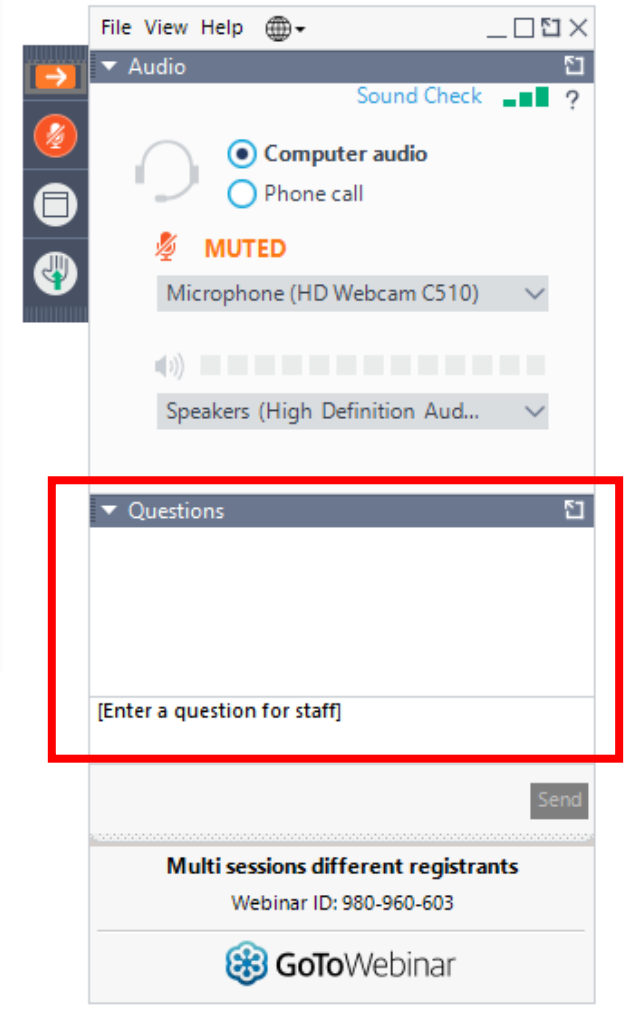
# Q&A

- Type your questions in the box as shown

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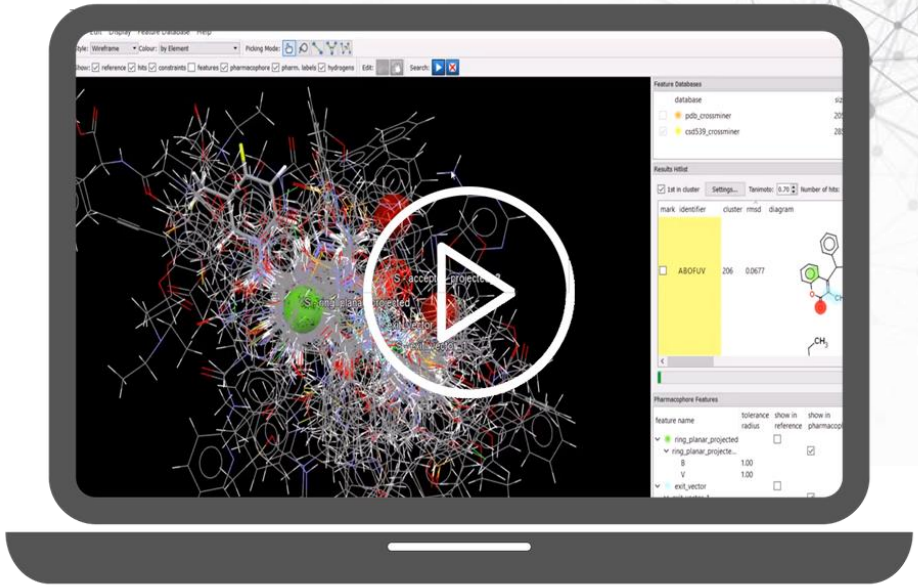
# Next What's Up Webinar

- Next webinar: **March 18th**
- Follow us on social media
- Send us your ideas and news

  hello@ccdc.cam.ac.uk



# Thank you

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