

A faint, light gray network pattern of interconnected lines and nodes is visible in the background, resembling a molecular or structural diagram.

ccDC

advancing structural science

What's Up

Customer Update Webinar

23rd September 2021



Today's presenters



**Abhik
Mukhopadhyay**

Research and
Applications
Scientist



Carmen Nitsche

General Manager
CCDC Inc.



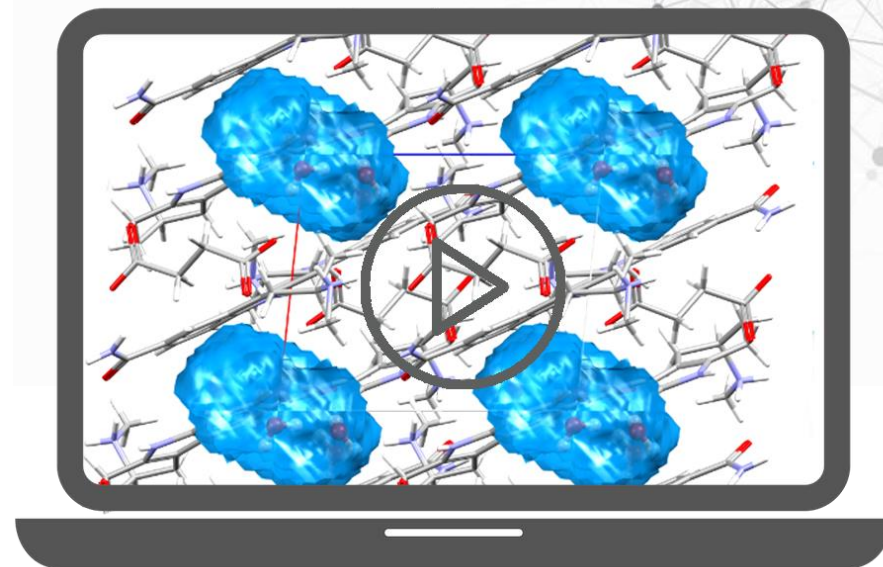
Matt Lightfoot

Principal Scientific Editor

Overview

In this webinar we will discuss:

- Latest updates and news
- SMILES to 3D structure generation
- How to enhance your CSD depositions
- Q&A: the floor is yours



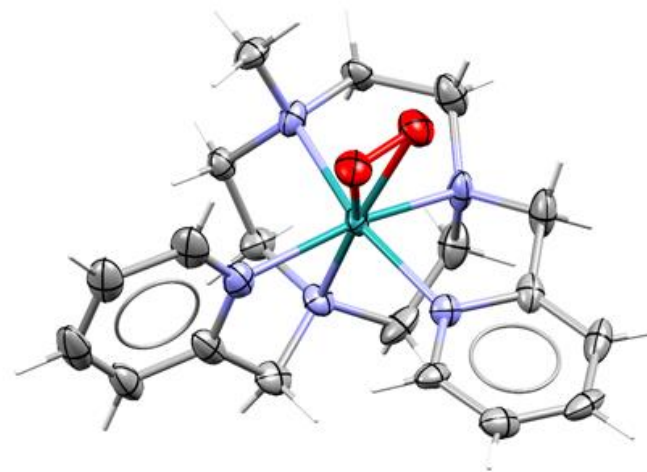
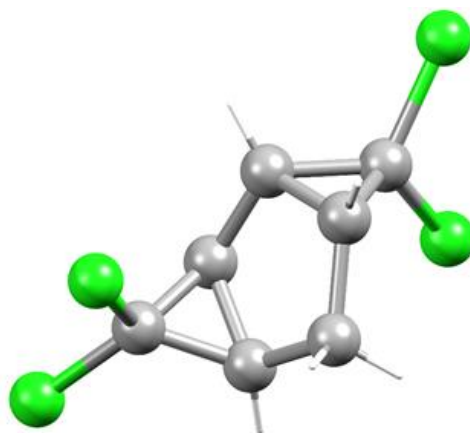
Latest updates

- 2021.2 CSD Release: September 2021

- **CSD-Discovery:** the CSD-CrossMiner is now part of the main CSD Portfolio, you can enjoy all our tools within a single installation, which improves usability and search flexibility.
- **CSD-Materials:** we have introduced a new component in Mercury, and the CSD Python API, delivering Mogul-like functionality for hydrogen bonds.
- Read more: <https://www.ccdc.cam.ac.uk/solutions/whats-new/>

Latest updates

- **CSD Sketcher v1.0: August 2021** > the first full version of CSD Sketcher, our purpose-built sketcher to enable better database searching in WebCSD.
- **CSD Data update: September 2021** > This data update brings you 16,688 new structures (17,283 new entries), including over 300 new entries generated from hardcopy data.



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

Upcoming events from CCDC



- CCDC Focus on Metal-Organic Frameworks (MOFs) Virtual Talk and Networking Event – **14th October**
- Librarian Teatime: A Focus on CSD Champions – **14th November**
 - For Chemistry Librarians in the Americas
- CCDC Virtual Workshops:
 - **2nd November** - Deposit your crystallographic data in the CSD
 - **9th November** - Learn the basics of Protein Ligand Docking using GOLD
 - **16th November** - Intermediate Mogul - Assessing molecular geometries

Register at www.ccdc.cam.ac.uk/News/Events

CCDC will be attending

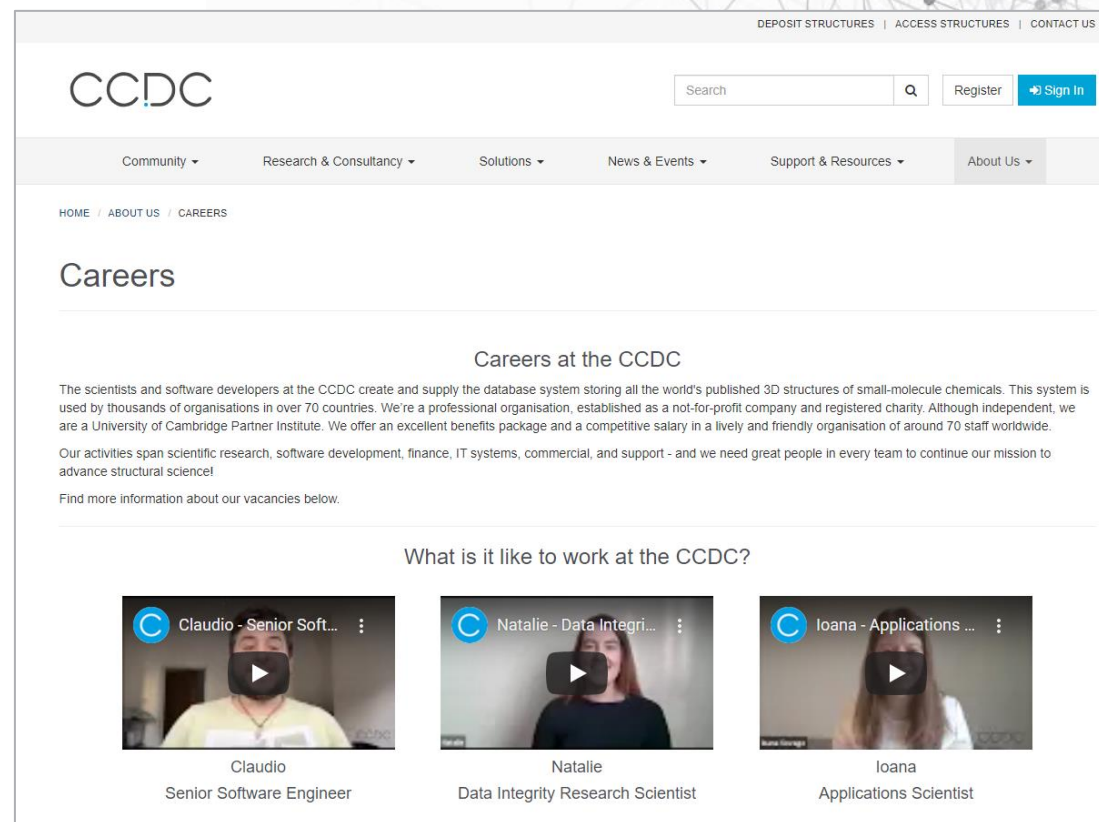


- 4th RSC-BMCS/ RSC-CICAG Artificial Intelligence in Chemistry – 27th to 28th September
- Chem-Bio Informatics Society Annual Meeting 2021 – 26th October to 28th October
- Pan-African Crystallographic Conference – 15th November to 19 November

Register at www.ccdc.cam.ac.uk/News/Events

The CCDC team is growing...

- Currently hiring for roles including:
 - Software engineers
 - Product Manager
 - Business Transformation Project Manager
 - Sales Executive, US



Find out more and apply at: www.ccdc.cam.ac.uk/theccdcprofile/careers/

CSD Software

SMILES to 3D structure generation

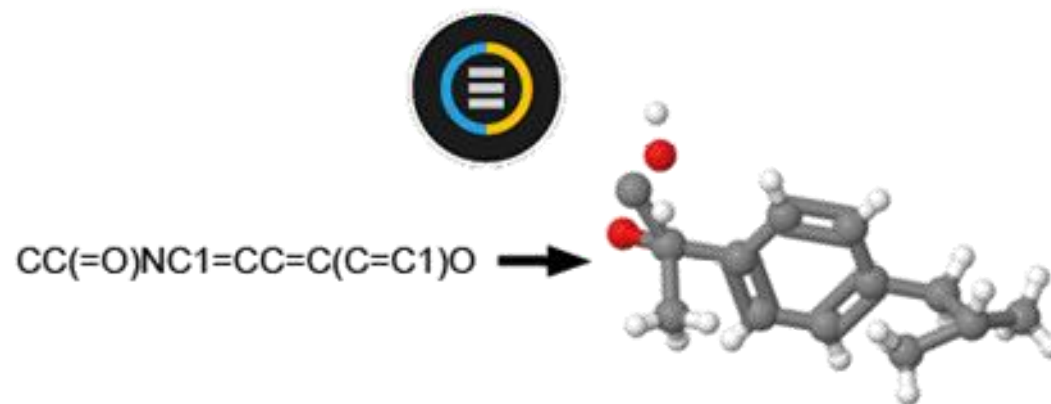


Abhik Mukhopadhyay

Research and Applications Scientist

What is it?

- Improvement to the Ligand Preparation workflow in the CSD Python API.
- CCDC Molecule objects can now be created from SMILES strings.
- This improvement will allow to:
 - Use SMILES as a molecule input format to the CSD Python API for the first time.
 - Take a SMILES string and generate a molecule with 3D atom coordinates.
- Generating molecular information from SMILES comes with a CSD-Core license.
- In addition, generating 3D coordinates of the molecule comes with a CSD-Discovery or CSD-Materials licence.



CCDC

Background

- It was not possible before to generate 3D coordinates from SMILES string using CSD Python API.
- Absence of this feature was a bottleneck situation in CADD workflow.
- Addition of this feature will now allow computational chemists to generate 3D coordinates from SMILES string as part of the ligand preparation workflow of any CADD project, e.g. virtual screening.



Why would you use, what are the benefits?

- Users can read SMILES string using CSD Python API and perform other tasks.
- It will be to now easy to incorporate CSD Python API in ligand preparation steps of any CADD workflow.
- Generate 3D coordinates from SMILES using CSD conformer generator that uses CSD knowledgebase.



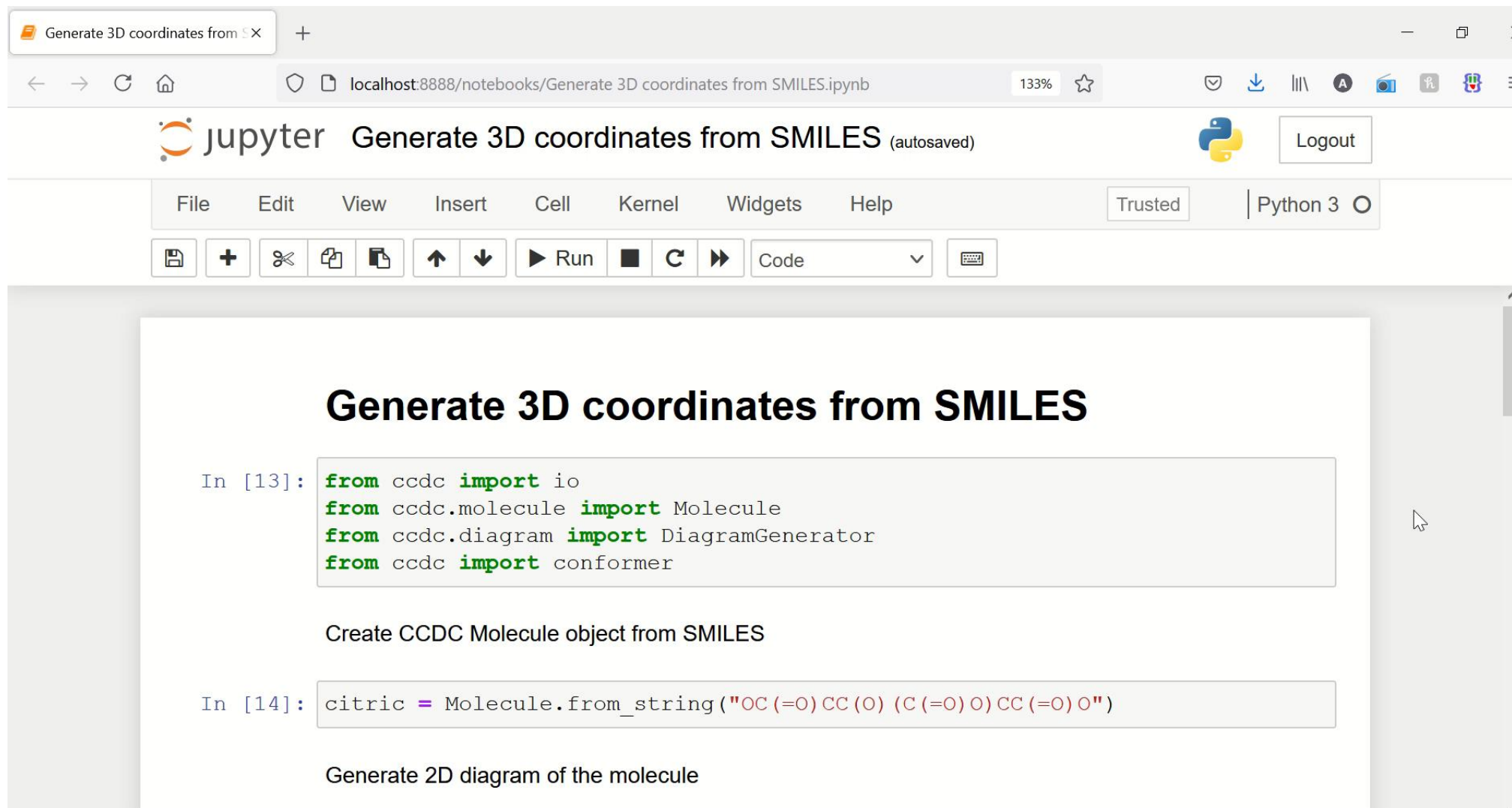
Overview of functionality

- Will allow reading molecule SMILES in CSD Python API.
- Users can generate 3D coordinates from SMILES using CSD conformer generator.
- Conformer Generator functionality will now accept molecules and atoms without coordinates as a starting point for Conformer Generation.
- Key features:
 - Molecules can be read from SMILES strings, with stereochemistry information preserved.
 - 3D conformers can be generated from such molecules and any other molecule without initial 3D coordinates.
 - SMILES strings with stereochemistry information can be generated from molecules.

How does CSD SMILES to 3D structure work?

- The tool uses the CSD Conformer Generator – uses knowledge from the 1 million+ experimentally derived structures, to predict and generate appropriate conformers - so bond lengths and angles are based on known data.
- The 3D coordinate generator is an iterative, atom-template based process, guided by stereochemistry information and ring positioning heuristics, with continuous optimisation based on CSD geometry distributions.

Demo



The screenshot shows a Jupyter Notebook titled "Generate 3D coordinates from SMILES (autosaved)" running on a local server at localhost:8888. The notebook has a menu bar with File, Edit, View, Insert, Cell, Kernel, Widgets, and Help. Below the menu is a toolbar with icons for saving, adding cells, deleting, copying, pasting, and running code. The main content area displays two code cells. The first cell, labeled "In [13]:", contains Python code to import necessary modules from the ccdc package. The second cell, labeled "In [14]:", contains code to create a CCDC Molecule object from a SMILES string and generate a 2D diagram of the molecule.

Generate 3D coordinates from SMILES

```
In [13]: from ccdc import io
from ccdc.molecule import Molecule
from ccdc.diagram import DiagramGenerator
from ccdc import conformer
```

Create CCDC Molecule object from SMILES

```
In [14]: citric = Molecule.from_string("OC(=O)CC(O)(C(=O)O)CC(=O)O")
```

Generate 2D diagram of the molecule

Summary

- The process generates a CSD Python API Molecule file from the SMILES string, which could then be saved as a mol2 file.
- This feature is currently available through the CSD Python API.
- Users can control stereochemistry of a molecule during ligand preparation:
 - By using stereochemistry markers on the SMILES input to generate isomeric structures.

CSD Community

How to enhance your CSD depositions



Matt Lightfoot

Principal Scientific Editor

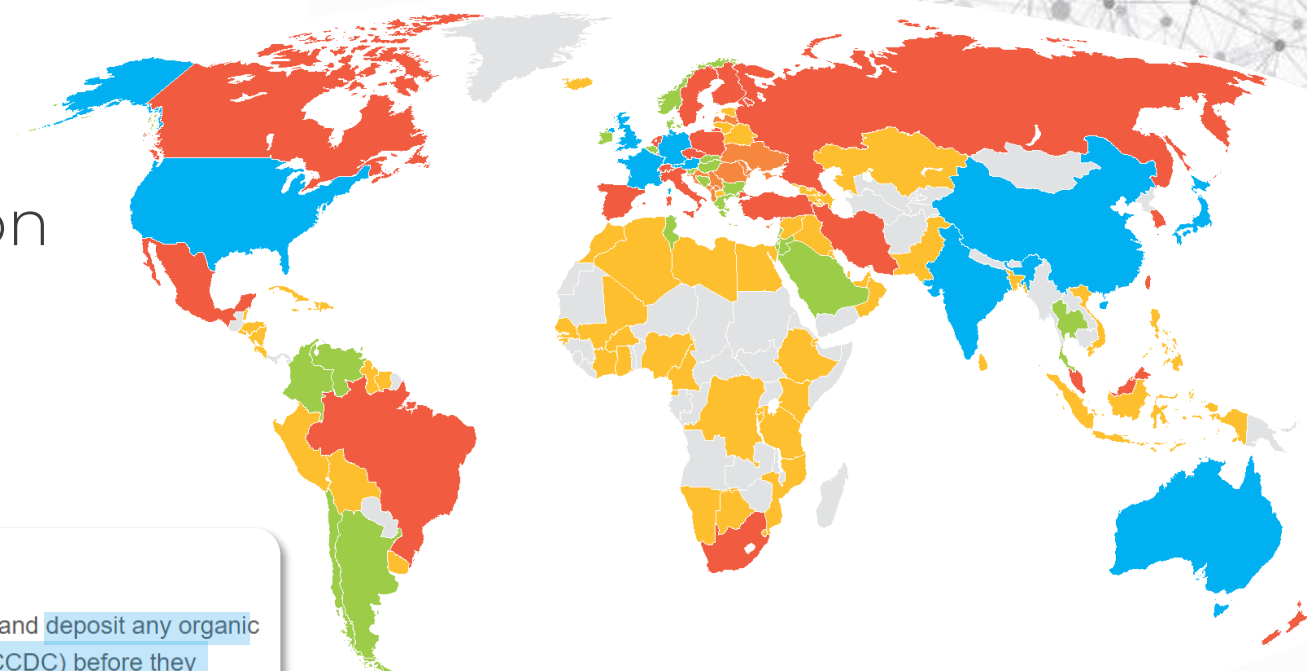
Deposition

- Data deposited pre-publication
 - Enables links to data sets at the point of publication
 - Tailored deposition service

Small molecule single crystal data

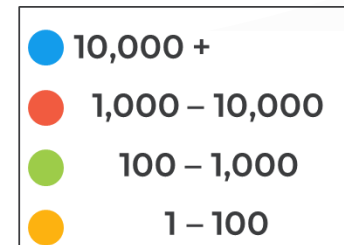
Authors should present their crystal data in a CIF (Crystallographic Information File) format and deposit any organic or organometallic structural information with the [Cambridge Crystallographic Data Centre \(CCDC\)](#) before they submit their manuscript to us. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and organometallic compounds will be entered into the Cambridge Structural Database. Authors are encouraged to deposit inorganic crystal structures with the [ICSD](#), hosted by FIZ Karlsruhe.

During submission of a manuscript to the Royal Society of Chemistry using our online submission system, authors will be asked to provide CCDC reference numbers; CIFs should not be submitted with the manuscript (these should have already been deposited with the CCDC/ICSD, see above). Any revised CIFs obtained subsequently should be deposited directly with the CCDC before the revised manuscript is submitted to us. CCDC or ICSD numbers should be included in the manuscript prior to submission.



Countries contributing data

Analysis based on sampling of email addresses



>30% of depositions from China

www.ccdc.cam.ac.uk/deposit

When should you deposit data?

- **Pre-publication** – when you have finished a structure is when you know most about the dataset
- Enables you to **check and correct data** prior to inclusion in a manuscript
- Deposited data is stored **privately** at the CCDC prior to publication
- Most publishers require data to be deposited **before manuscript submission**
 - Enables publishers and referees secure access to the data during the peer review process
 - Enables links to the data to be added at the point of publication

What data can you deposit with us?



PDB
>>175,000
polypeptides,
nucleotides
& saccharides



CSD
>1.1 million
structures
organic and
metal-organic

ICSD

240,000
(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

Ways to enhance your data during deposition

- The importance of including structures factors
- Data validation and integrity checks and adding responses
- How you can enhance the metadata in your depositions

Structure factors

Structure factors: what

The CCDC and FIZ Karlsruhe strongly encourage the inclusion of structure factor data in the IUCr's Crystallographic Structure Database (ICSD), in line with recommendations from the IUCr's Commission on Structure Factor Data.

What are structure factors?

Structure factors are created from experimental crystallographic data. For detailed information, see the IUCr's Commission on Structure Factor Data.

Currently, there are two types of information that CCDC and FIZ Karlsruhe encourage to be included in the CIF file: structure factor intensities (.hkl). They can also be appended to the CIF file as structure factor amplitudes (.mtz).

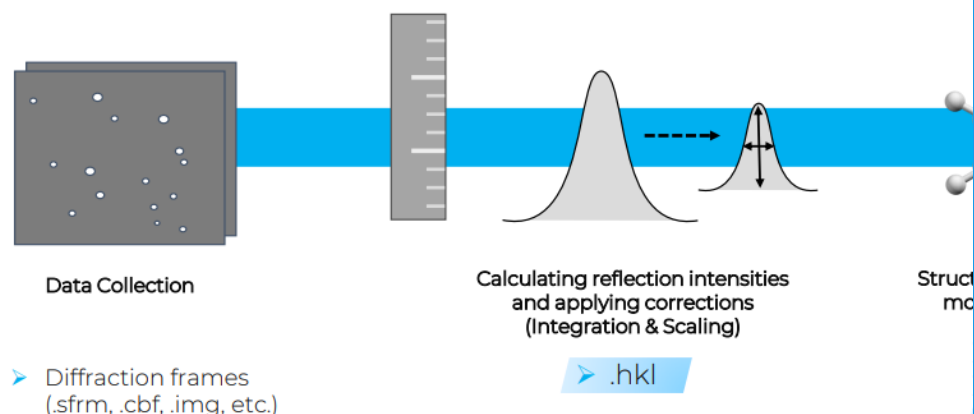
- The **.hkl** file contains the intensity and standard uncertainty values: h , k and l - to identify the reflection. This information is used to calculate the structure factors.
- The **.fcf** file contains the structure factors, which can be recreated using the .hkl and .res file. This last one contains constraints that have been applied). The .fcf file is used for refinement.

These files provide more information about the crystal structure, as part of the publications standard.

Why is it important to share structure factor data?

- It's good data practice - by sharing the data used to create the structure, then it is already stored, especially if you move the data to another repository.
- CheckCIF (the IUCr's CIF checking service) can do checks on the .res in the CIF allows such checks to be performed.
- Several journals require the deposition of structure factor data.

A number of different files are created at each stage of a crystallographic experiment – here we have listed some of the main ones. Files may have different names/some may be combined in different crystallographic software.



If the diffraction frames have been deposited in another repository, the DOI can be associated with your dataset during deposition under "Raw Data DOI"

Files for CCDC deposition:

- **Mandatory**
- **Recommended**

If no structure factor data has been uploaded, you should:

- Go back and upload a new dataset which includes structure factors
- Most refinement software now embeds this into a CIF
- If it is historic data and no structure factor data is available, you need to add a comment before proceeding.

Data validation and integrity checks



- IUCr's [checkCIF](#) service is embedded into deposition
- Alerts provide potential errors, unusual findings and suggestions for improvement
 - All alerts should be [checked](#)
 - Depositors decide to [improve](#) their model/dataset or add a [comment](#) to provide information about the reason for the alert
 - Comments are embedded into the CIF and [available](#) during peer-review and to CSD users after publication
- checkCIF ultimately helps to [improve the quality of data](#) published and provides users of the data [more information about potential issues](#) in the datasets

● **Alert level A**
[PLAT183 ALERT 1 A](#) Missing _cell_measur
[PLAT184 ALERT 1 A](#) Missing _cell_measur
[PLAT185 ALERT 1 A](#) Missing _cell_measur

● **Alert level**
[PLAT029 ALERT](#)

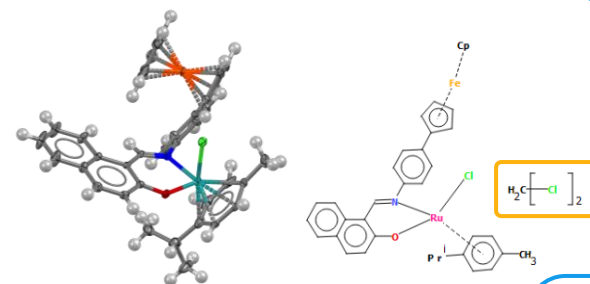
● **Alert level**
[ABSMU01 ALERT](#)

Alerts are hyperlinked to more information about the alert and what action should be taken

The image shows a screenshot of the CCDC FIZ Karlsruhe website. On the left, there's a search bar with "Simple Search" and "Structure Search" tabs. Below it, a query "Your query was: Identifier(s): Zoybia" is shown. A table of results follows, with columns "Database Identifier" and "Deposition Number". The first result is "ZOYBIA" with deposition number "1022107". On the right, a "Download deposited CIF" dialog box is open. It has three radio button options: "Deposited CIF(s)" (selected), "Deposited CIF(s) without structure factor data", and "Deposited file(s) with any available structure factor data and checkCIF reports included". Below these is a "User Details" section with a text area and a "We ask you provide your name, email address and affiliation before downloading data to allow us to better understand usage patterns so that we can maintain and improve the free services we provide. For more information see our Privacy Policy. Alternatively, click opt-out if you do not want to provide this information." message.

Enhancing key metadata

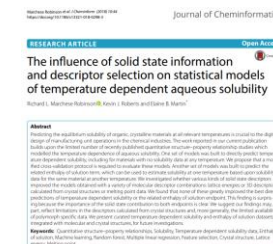
- Depositors are asked to **check** and **enhance** key meta-data
- Helps to improve the quality of key information
- Helps to ensure data is **correctly curated and represented** in the CSD
- Helps to improve the **availability** of data
- Ultimately improves the **discoverability** and **re-use** of datasets and enables scientists worldwide to **learn more from the data**



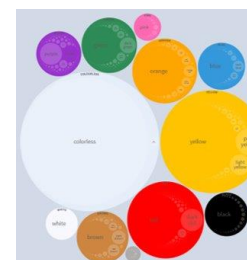
CSD BAGNEG Example of SQUEEZED data being represented correctly




>170K
melting
points in
the CSD



Additional metadata being used
to help predict solubilities






EDGE ARTICLE

[Check for updates](#)

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View Article Online
[DOI: 10.1039/C9SC01437A](#)



A data-driven perspective on the colours of metal-organic frameworks†

David M. P. Johnson^a, Christopher L. R. Luximon^a, Mohamed Arfan^a, Christopher Lacey^a, Lucy Perry^a and Bernd Strohriegl^b

ROYAL SOCIETY OF CHEMISTRY

Colour is at the core of chemistry and has been fascinating humans since ancient times. It is a key design parameter of pharmaceuticals, pigments of natural dyes and other useful compounds. In chemistry, a **synthetic** hueless compound, the product of a rational design, is often called a **Chaldranite**. It is this, the design of synthetic materials and chemical transformations of natural materials, that we focus on in this article. We present a **data-driven** perspective on the colours of metal-organic frameworks (MOFs) and their derivatives. We present a **data-driven** perspective on the colours of metal-organic frameworks (MOFs) and their derivatives. We present a **data-driven** perspective on the colours of metal-organic frameworks (MOFs) and their derivatives.

ROYAL SOCIETY OF CHEMISTRY

Received 24th October 2019
Accepted 11th November 2019

DOI: 10.1039/C9SC01437A

ROYAL SOCIETY OF CHEMISTRY

Example of using CSD data to assess the colours of Metal-Organic Frameworks

Raw data DOIs

Associated DOIs

Raw data DOI ?

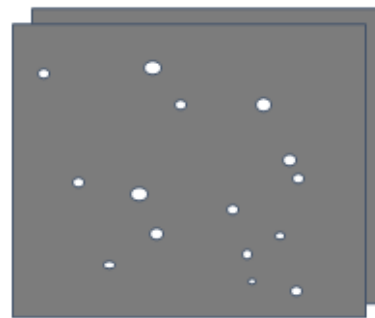
Data fields

Compound name ?

Bis(acetonitrile- λ N)-{(2R_p,2''R_p)-1,1''-[1,2-ethanediylbis(nit

Synonyms/other names ?

Crystal colour ?

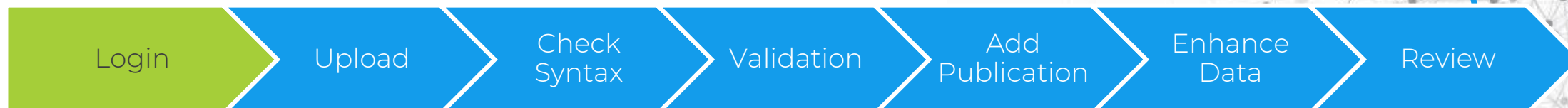


Raw data DOIs are for data created during data collection

- Diffraction frames e.g. .sfrm, .cbf, .img, etc

- We do not accept **diffraction frame data** during deposition
- But you can choose to upload your diffraction frames in another repository or institution repository
 - If you do publish your diffraction frames you should add the DOI to “Raw data DOI”
- Raw data DOI should **not** include the DOI of associated articles

Deposition



CIF deposition and validation service

[Click here to continue to the deposition process without signing in.](#)

If you have not registered for a CCDC account before you can register using the button below. To find out more about CCDC accounts and what you are able to do once you have logged in, please see our [support page](#).

Sign in with your CCDC account

Username or Email

ward@ccdc.cam.ac.uk

Password

.....

☐ Remember me?

Sign In

Register

[Forgotten Username or Password](#)

Register

Sign In

If you don't want an account on our website you can click here

Why register?

- Simplifies deposition
- Gives you access to see, edit and share your data
- Enables you to link your CSD licence to use WebCSD

Deposition Numbers - Message (HTML)

File Message Insert Options Format Text Review Help Tell me what you want to do

Send From deposit_reply@ccdc.cam.ac.uk To... Depositor Cc...

Subject Deposition Numbers

Dear Depositor,

Thank you for depositing your crystal structure(s) at the Cambridge Crystallographic Data Centre. The data have been assigned to the following deposition numbers.

CCDC XXXXXXXX-XXXXXXY

Summary of Data CCDC XXXXXXXX

Formula: C_x H_y O_z
Unit Cell Parameters: a XXXX b XXXX c XXXX Space Group

Summary of Data CCDC XXXXXXXY

CrossRef | CAS | Web of Science® Times Cited: 16 | 'ejournals@cambridge-find full text'

17 CCDC 1543805 (16) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from [The Cambridge Crystallographic Data Centre](#).

McKervey, A. R. Maguire, S. M. Tuladhar and M. Fiona Twohig, *J. Chem. Soc.* 1047–1054 DOI: [10.1039/P19900001047](https://doi.org/10.1039/P19900001047); (b) H. Duddeck, *J. Chem. Soc.*, 1055–1063 DOI: [10.1039/P19900001055](https://doi.org/10.1039/P19900001055); (c) P. Panne and J. M. Fox, *J. Am. Chem. Soc.* 112, 1000–1001 (1990).
[External Links](#)

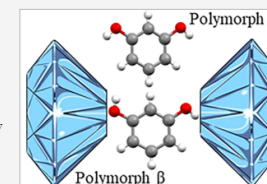
Footnote

† Electronic supplementary information (ESI) available: Experimental procedures and spectroscopic data. For ESI and crystallographic data in CIF or other electronic format see DOI: [10.1039/b815536](https://doi.org/10.1039/b815536)

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Abstract

Polymer α of resorcinol, at ambient pressure transform to β GS K when it transforms to polymer β , is exceptionally resistant to high pressure. The crystals of polymer α can be compressed to over 4 GPa without transforming to the β phase. We have performed high-pressure recrystallization of resorcinol aqueous and methanol solutions, and they yielded polymer α below 0.5 GPa and polymer β above this pressure. Our single-crystal X-ray diffraction studies on resorcinol polymers in a diamond-anvil cell reveal the structural origins of the phase transition. The high pressure changes the angular dimensions of bistable hydrogen bonds OH...O, which destabilizes the H-atoms and the structure of polymer α above 0.5 GPa, consistent with the calorimetric and NMR results. The high-temperature, high-pressure polymer β achieves the more dense packing through the changed conformation of one of the hydroxyl groups and the considerable twisting of the hydrogen bonds necessary for the formation of additional C—H...O bonds. The large temperature and pressure hysteresis of the polymorphs α and β are connected with the different topologies of their O—H...O networks.



Synopsis

The pressure- and temperature-dependent transition between resorcinol polymorphs α and β has been rationalized in terms of transforming H-bonds and their networks.

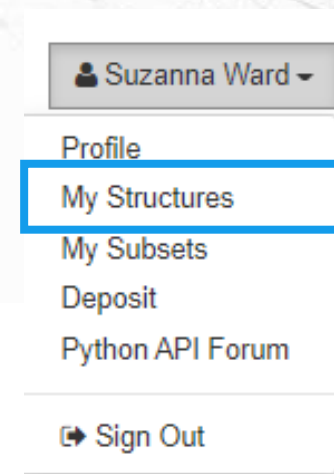
Introduction

Resorcinol, an intermediate often used in chemical practice and a pharmaceutical agent, was one of the first organic compounds for which the phenomenon of polymorphism was described and the first organic compound for which the structures of both polymorphs were determined in 1938 by Robertson and Ubbelohde.^[1,2] Until today, the resorcinol crystals belong to the best known examples of polymorphs.^[3]

[illegible]

What happens to your data after deposition?

- It is [stored privately until published](#) in an associated scientific article or you decide to publish directly through the CSD or ICSD
- If you have registered on our website you can access your data at any time using our [My Structures](#) service
 - Enables you to view and retrieve datasets
 - Enables you to edit and update datasets
 - Enables you to share your datasets with co-workers
 - Enables you to create your own institutional database
 - Enables you to publish your data directly through the CSD/ICSD
- If you have not published your data [after one year](#), we will [email](#) you to ask if you would like to publish it



My Structures – view, edit, retrieve, share

My Structures

Search by Deposition Number



Clear Filters

Save Settings

Reset Settings

Suzanna Ward

Profile

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Deposit

Python API Forum

Sign Out

After depositing structures they may take a few minutes to appear in the table. If you are still unable to see your structures after you have received your Deposition Numbers please contact deposit@ccdc.cam.ac.uk

To change the displayed columns or filter results you should click on the down arrow of the relevant column heading. To order the results by a particular column click on the column heading you wish to order your results by.

You can select which structures are displayed by using the dropdown box below. Different subsets can be created using the 'Add to Subset' button and you can view or export these subsets.

All structures

Default Data View

My Downloads

Associate More Structures

Add to Subset

Share Structures

<input type="checkbox"/>		Deposition ...	Datablock	Deposited On	Deposited By	Refcode	Formula	Embargoed...	Status
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<input type="checkbox"/>	Details		data_5_93GPa	28/04/2021			C7 H7 N1 O2	28/02/2022 ?	Unpublished
<input type="checkbox"/>	Details	1584792	data_tBu10kbar	09/11/2017			C11 H15 N1 O2	29/11/2019 ?	Unpublished
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<input type="checkbox"/>	Details	825800	data_2007may0...	06/06/2011	ward@ccdc.cam...	EPAHOT	C8 H5 N1 O3		Published in the CSD

Curating the data into the CSD and ICSD

After publication your data is enhanced and curated

- Every entry undergoes both automated and manual processes
- Enhanced and curated by experts at CCDC
- Ensuring accessibility, discoverability and re-usability of the data

```
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_chemical_name_systematic ?
_chemical_name_common ?
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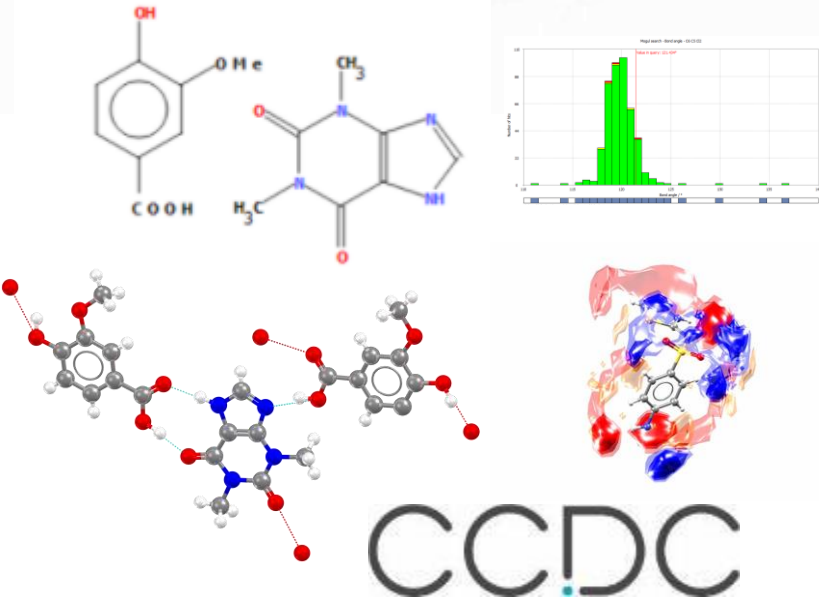
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  'x, -y, -z'
  'x, -y+1/2, z-1/2'

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_cell_length_c 13.3746(8)
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_cell_angle_beta 90.572(2)
_cell_angle_gamma 90.00
_cell_volume 2378.0(2)
_cell_formula_units_Z 4
_cell_measurement_Temperature 173(2)
_cell_measurement_reflns_used 29773
_cell_measurement_theta_min 1.81
_cell_measurement_theta_max 28.33
```



Author(s)	A. Jacobs, F.M.A. Noa
Reference	CrystEngComm (2015), 17, 98
Publication DOI	10.1039/C4CE01795A
Deposition	CCDC 1022107
Formula	2(C ₈ H ₈ O ₄), C ₇ H ₈ N ₄ O ₂
Compound	bis(4-Hydroxy-3-methoxybenzoic acid) 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
Synonym	bis(Vanillic acid) theophylline
Spacegroup	Name: P21/c Number: 14
Cell	a: 11.274(4) b: 15.771(1) c: 13.375(4) alpha: 90.00 beta: 90.57(1) gamma: 90.00 Volume: 2377.967
Reduced Cell	a: 11.274 b: 13.375 c: 15.771 alpha: 90.00 beta: 90.00 gamma: 90.57 Volume: 2377.967
Molecular Volume	594.492
Chemical Units	2
Z, Z'	Z: 4.0 Z': 1.0
R-Factor (%)	4.7
Disorder	C7A, O4A and C9A, O5A disordered over two sites with occupancies 0.812/0.188.
Temperature (K)	173
Density	CCDC: 1.443 Author: 1.44
Intensity Meas	diffractometer
Average Sigma (C-C)	0.001-0.005Å
Colour	colorless
Habit	rectangle
Recryst. Solvent	water



Where to find more guidance

The CCDC CIF Deposition Guidelines

This page is designed to help you deposit your data, check your CIFs and provide you more information as you go through our deposition process. Click on the boxes below to navigate to the section of interest.

Basic
guidelines

Required
CIF fields

Authorship
guidelines

Checking
CIFs

Correcting
CIFs

Useful
resources

Structure
Factors

Translated
guidelines

Basic Guidelines

When preparing your CIF (What is a CIF?) for deposition please include as much information as possible and check it carefully. This is especially true for [CSD Communications](#) where there is no paper to describe the chemistry and experimental details leading to your structure.

If we are unable to validate your structure from the information you have provided we may contact you. If we cannot resolve the issue, unfortunately, we may not be able to add your structure to the [CSD](#).

In this section

The CCDC CIF Deposition Guidelines.pdf

Structure factors: what are they and why share them?

The Benefits of Data Sharing

Related Topics

Deposit a Structure

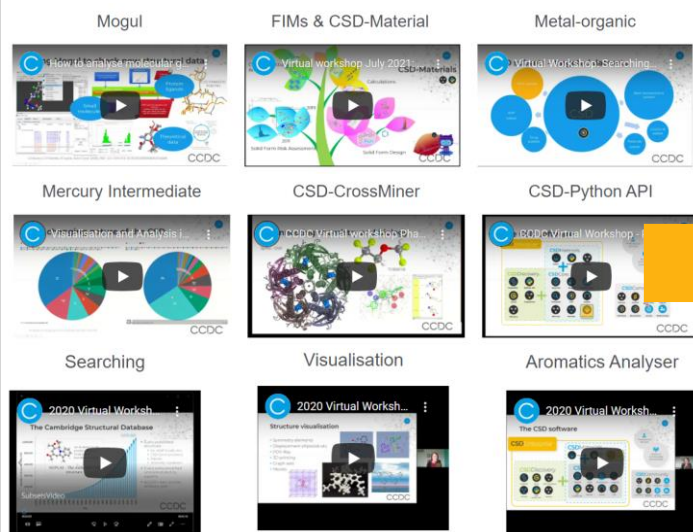
Structure Deposition Information

Correcting CIFs

CSD Communications

Keen to learn more about CSD deposition?

CCDC Virtual Workshops



Next series Nov 2021

November 2021 series

Session 1 – Depositing data into the CSD

- 2nd November
- 90 min interactive session
- Expert tutors on hand to help
- Spaces limited so [register now!](#)



Show
one

...



Try
one

...

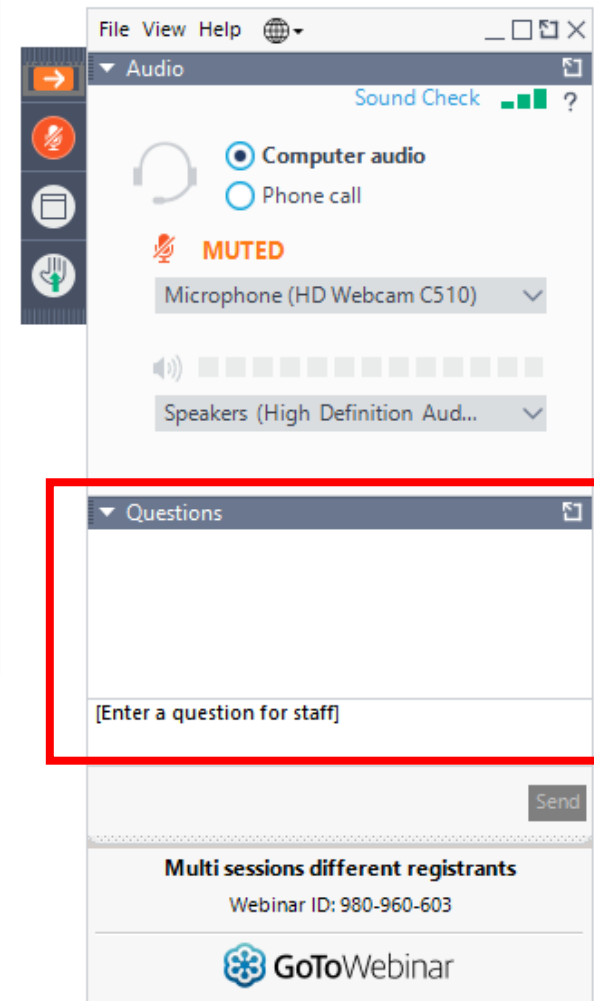


Explore
more



Q&A

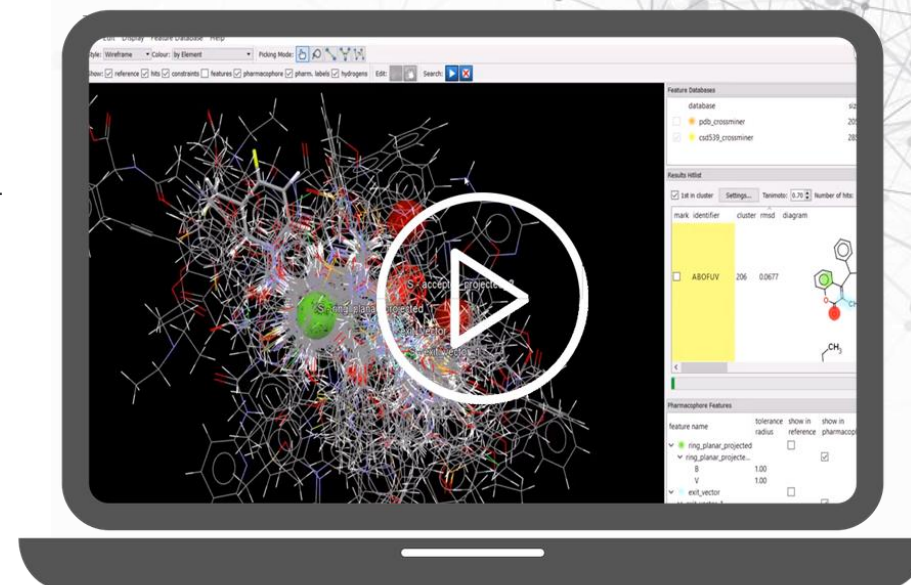
- Type your questions in the box as shown



Next What's Up Webinar

- Next webinar: **November 18th**
 - CSD-CrossMiner: new features from 2021.2 release
 - DASH: what has changed?
- Follow us on social media
- Send us your ideas and news

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Thank you

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