CCDC

advancing structural science

# What's Up

## Customer Update Webinar

19th November 2020

CCDC

advancing structural science

# Today’s presenters

**Seth Wiggin**

Senior Scientific Editor

**Carmen Nitsche**

General Manager CCDC Inc.

**Ian Bruno**

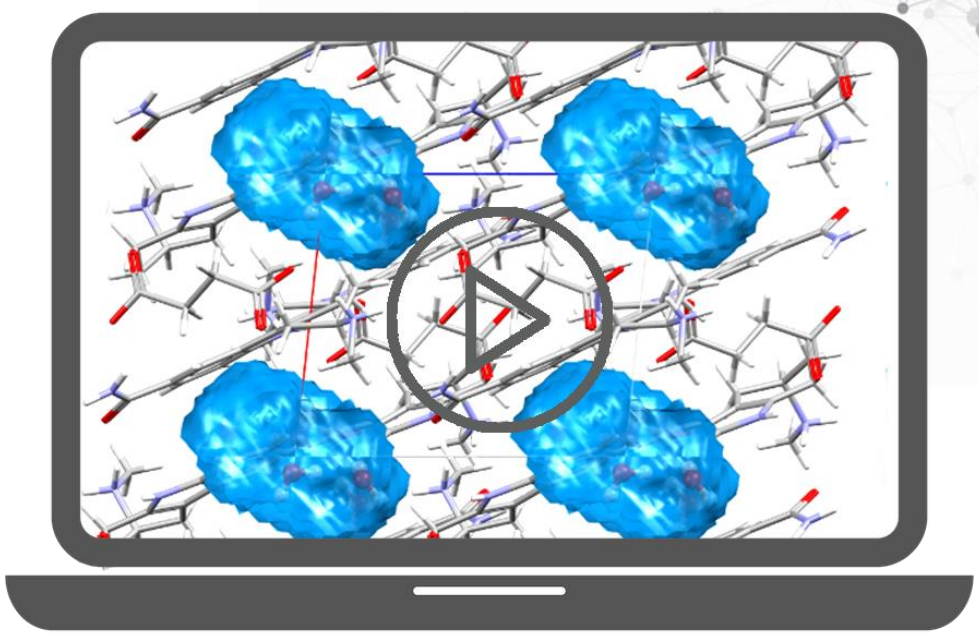
Head of Strategic Partnerships

CCDC

# Overview

In this webinar we will discuss:

- Latest updates and news
- Using the Python API in Mercury for custom reporting and analyses
- CCDC software Partnerships
- Q&A: the floor is yours





CCDC

# Latest updates and news from CCDC

- 7th Crystal Structure Prediction (CSP) Bind Test just started.

https://www.ccdc.cam.ac.uk/Community/initiatives/cspblindtests/csp-blind-test-7/

- Latest CCDC Whitepaper: **Ultra-large GOLD docking on cloud resources.** Download from our website.

https://info.ccdc.cam.ac.uk/whitepaper-ultra-large-gold-docking-on-cloud-resources


- CrystEngComm celebrates the CSD 1 million structures in a special issue.




CCDC

# Latest updates and news from CCDC >Events

- **CCDC Virtual Workshop: Aromatic Analyser**
  Live session on 24th November
  - 3 pm – 4.30 pm (GMT)

- **CCDC and BACG Crystal Conversations**
  3rd December
  - Virtual event
  - 2 pm to 4 pm (GMT)

→Register for all CCDC events here
https://www.ccdc.cam.ac.uk/News/Events

CCDC

# Using the Python API in Mercury

For custom reporting and analyses.

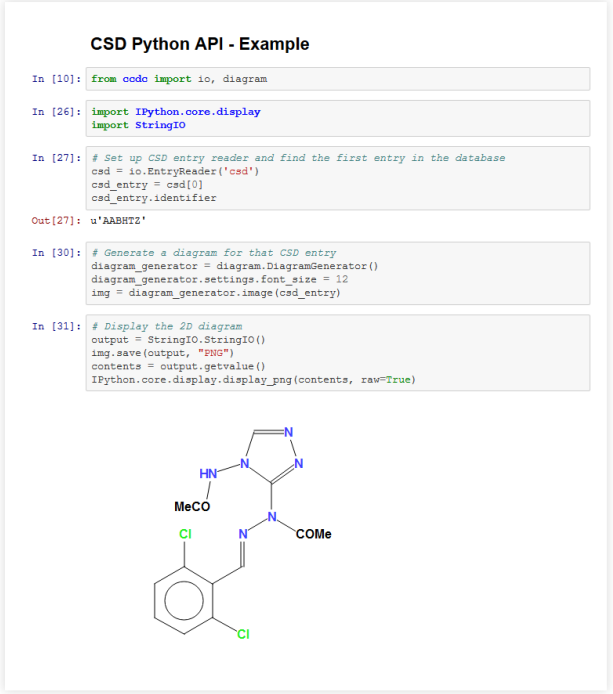
Seth Wiggin

Senior Scientific Editor

CCDC

# What is the CSD Python API?

- The **CSD Python API** (Application Programming Interface) enables you to use many capabilities of the CSD-System without being bound by graphical (or command line) interfaces
- You can readily create CSD-driven analyses and workflows, tailor them to your needs and then publish them to your own menu in Mercury for **specialist analysis** and **easier communication**



**CSD Python API - Example**

```
In [10]: from ccdc import io, diagram

In [26]: import IPython.core.display
         import StringIO

In [27]: # Set up CSD entry reader and find the first entry in the database
         csd = io.EntryReader('csd')
         csd_entry = csd[0]
         csd_entry.identifier
Out[27]: u'AABHTZ'

In [30]: # Generate a diagram for that CSD entry
         diagram_generator = diagram.DiagramGenerator()
         diagram_generator.settings.font_size = 12
         img = diagram_generator.image(csd_entry)

In [31]: # Display the 2D diagram
         output = StringIO.StringIO()
         img.save(output, "PNG")
         contents = output.getvalue()
         IPython.core.display.display_png(contents, raw=True)
```



python™

CCDC

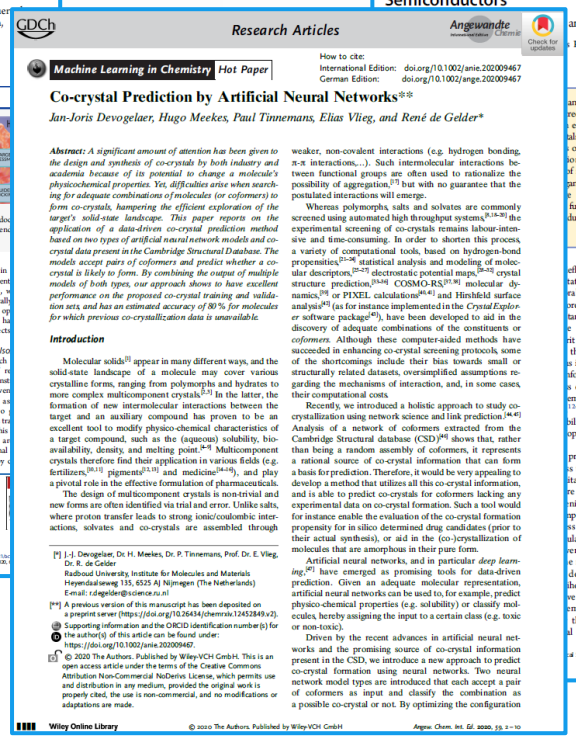
**Functions** include:

- Full search capabilities
- Geometry analysis
- Interaction analysis
- Descriptor calculation
- 2D diagram generation

1.

Hotspots API: A Python Package for the Detection of Small Molecule Binding Hotspots and Application to Structure-Based Drug Design

2.



Co-crystal Prediction by Artificial Neural Networks

3.

Virtual Screening for High Carrier Mobility in Organic Semiconductors


1. https://doi.org/10.1021/acs.jcim.9b00996
2. https://doi.org/10.1002/anie.202009467
3. https://doi.org/10.1021/acs.jpclett.6b01657


CCDC

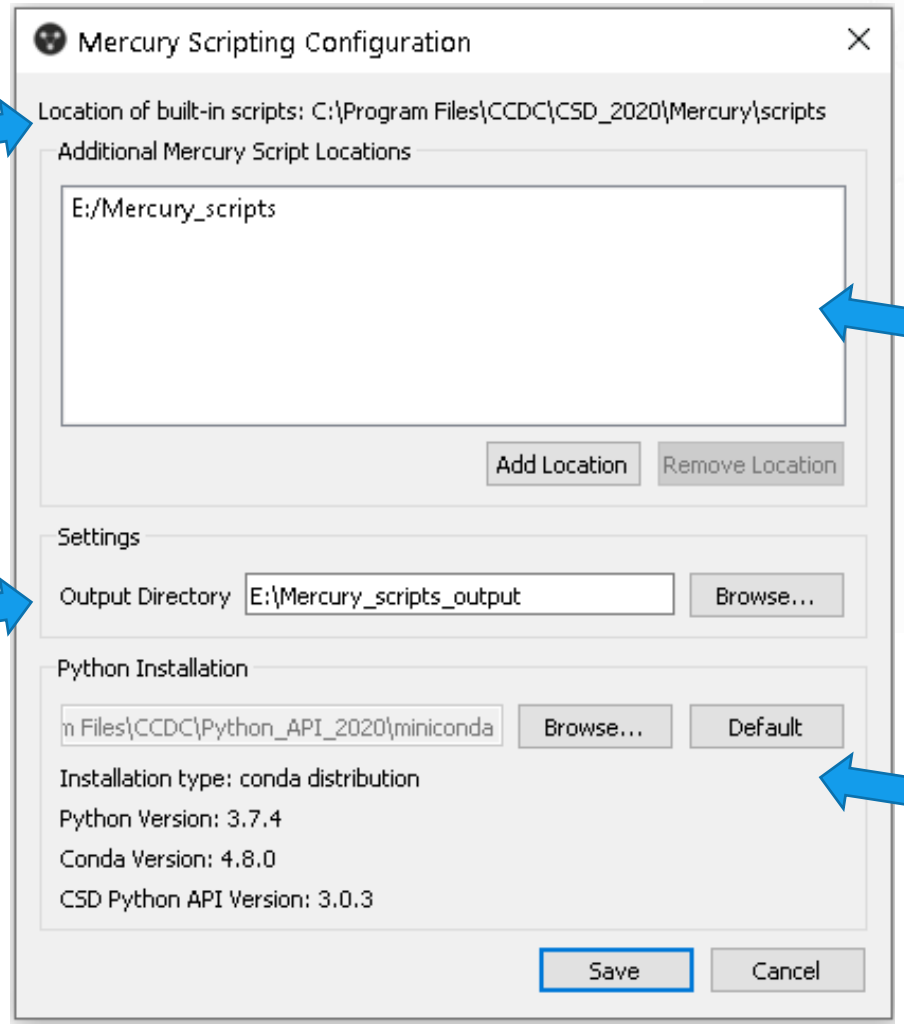
# Benefits of scripting workflows

- Automating reporting and analyses **saves time**
- Results will be **consistent** and **predictable**
- Having a scripted workflow makes it easy to **share knowledge** with colleagues

CCDC

# CSD Python API Mercury interface

Mercury contains built-in scripts offering a range of search and analysis



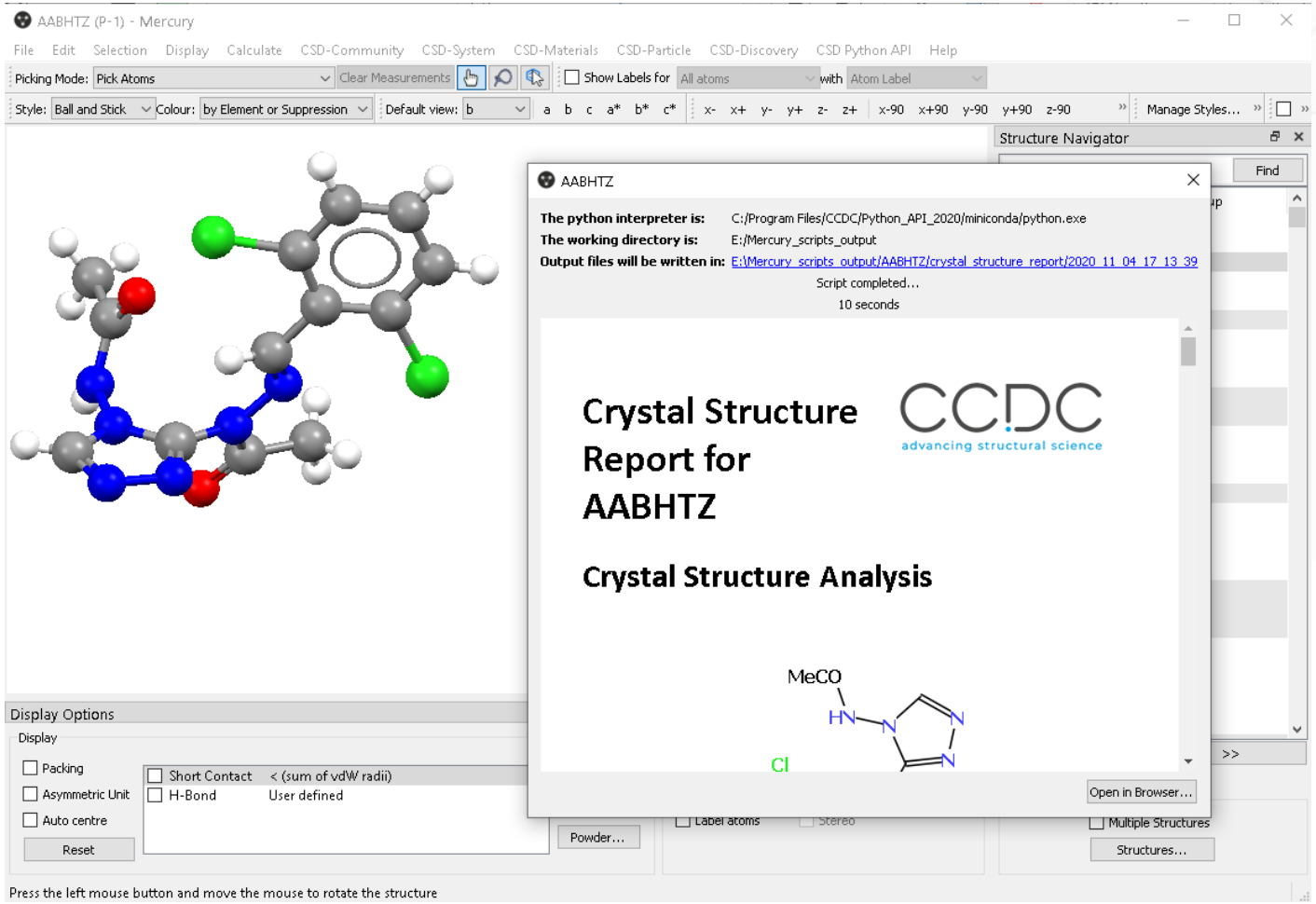

Additional script locations can be added for custom scripts from a variety of sources

The script output can be written to any specified location

The Python installation used by Mercury is configurable

CCDC

# Mercury Demo




CCDC

# Conclusions

- Using Mercury's CSD Python API interface allows easy access to the API's functionality for reports and analysis
- Automating workflows via Python scripting saves time and effort
- It is simple to customize scripts for your own **specialist analysis** and **communication needs**
- Thank you for your attention

CCDC

# CCDC Software Partnerships

## Past, present and future plans.

Ian Bruno

Head of Strategic Partnerships

CCDC

# CCDC Partnerships

## Structure Solution

Rigaku oxford diffraction
BRUKER
Malvern Panalytical a spectris company
Crystals
OlexSys
Phenix
GΦL Global Phasing Limited

## Data Publication

ACS Chemistry for Life®
IUCr
ROYAL SOCIETY OF CHEMISTRY
WILEY
Taylor & Francis Group an informa business
ELSEVIER
SPRINGER NATURE
DE GRUYTER
Hindawi
DataCite

## Data Linking

ICSD
ICDD International Centre for Diffraction Data
WORLDWIDE PDB PROTEIN DATA BANK
PubChem
ChemSpider The free chemical database
PPDB
DRUGBANK
ChEMBL
Clarivate Analytics
InChITRUST

## Software Integrations

BIOVIA
Chemical Computing Group
SCHRÖDINGER.
WAVEFUNCTION
BioSolveIT
Open for Innovation KNIME
optibrium
cresset

CCDC

# CCDC Software Partnerships

## Structure Solution

Rigaku oxford diffraction
BRUKER
Malvern Panalytical a spectris company
Crystals
OlexSys
Phenix
GΦL Global Phasing Limited

## Data Publication

ACS Chemistry for Life®
IUCr
ROYAL SOCIETY OF CHEMISTRY
WILEY
ELSEVIER
Taylor & Francis Group an informa business
SPRINGER NATURE
DE GRUYTER
Hindawi
DataCite

## Data Linking

ICSD
ICDD
WORLDWIDE PDB PROTEIN DATA BANK
PubChem
ChemSpider The free chemical database
PPDB
DRUGBANK
ChEMBL
Clarivate Analytics
InChITRUST

## Software Integrations

BIOVIA
Chemical Computing Group
SCHRÖDINGER.
WAVEFUNCTION
BioSolveIT
Open for Innovation KNIME
optibrium
cresset

CCDC

# General Priorities for Software Partnerships

- Make CSD data and functionality more readily accessible to chemists across an organisation
- Make it possible to combine CSD data and functionality with other scientific methods
- Make it easier for CSD-based data functionality to be used in custom workflows
- Enable the use of CSD data to help with structure solution and refinement in chemistry and biology

CCDC

# Current Integrations

## Protein-Ligand Docking

- Discovery Studio
- MOE
- StarDrop
- GOLD

## CSD Searching

- Spartan
- Materials Studio
- ConQuest

*Materials Studio also interfaces to Motif Searching in CSD-Materials*

## Ideas Generation

- MOE CSD Linker Database
- Spark CSD Fragment Database
- ReCore CSD Index

*CSD-based libraries for third party systems available to download at https://www.ccdc.cam.ac.uk/support-and-resources/downloads/*

## Workflow Environments

- CCDC Pipeline Pilot Collection
- CCDC KNIME Components

CCDC

# Current Integrations

## Geometry Analysis

| | | |
|---|---|---|
| SCHRÖDINGER. | Maestro | *Validation of molecular geometries* |
| Chemical Computing Group | MOE | |
| GΦL Global Phasing Limited | Grade | *Optimisation of ligand geometries in proteins* |
| Phenix | Phenix | |
| Crystals | Crystals | *Restraints for structure refinement based on experimental data* |
| Mogul | | |

## Structure Solution

| | | |
|---|---|---|
| Rigaku oxford diffraction | Rigaku / Oxford Diffraction | |
| BRUKER | Bruker | *Reduced cell searching using CellCheckCSD* |
| Malvern Panalytical | HighScore | *CSD-based Search/Match database available for download* |
| OlexSys | Olex$^2$ | *Direct link to CCDC Deposition Services* |

CCDC

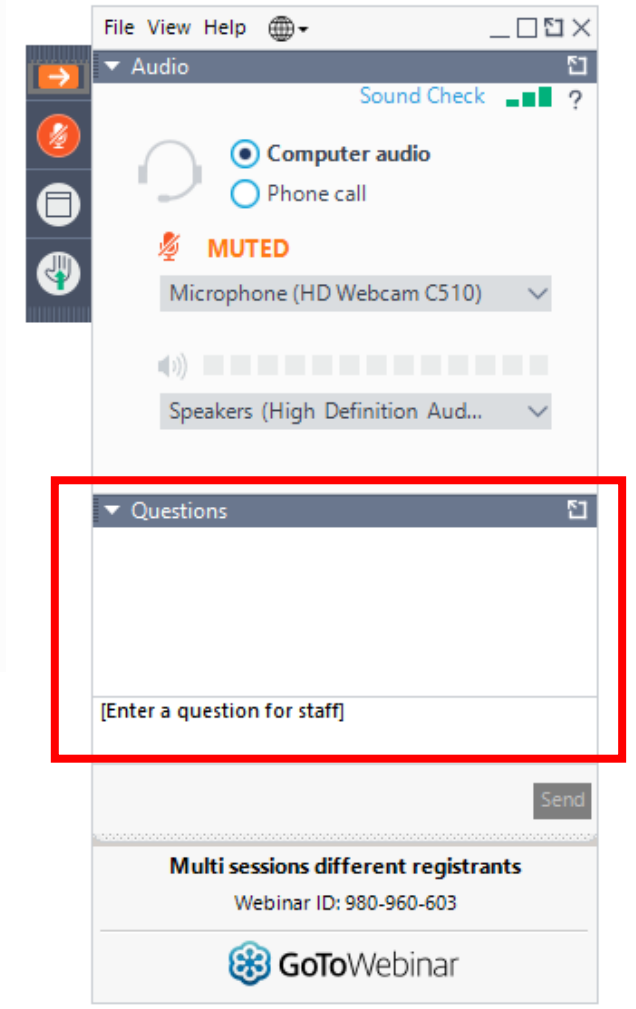
# Current Priorities

- Move existing integrations to use the CSD Python API
  - Current integrations use command line options to CCDC software – the CSD Python API offers greater flexibility and extensibility
- Extend to other CCDC functionality
  - Interest has been expressed in the ability to access Full Interaction Maps from within other packages – we are discussing this with the relevant partners
- Improve existing integrations
  - Refreshing existing interfaces to GOLD to accommodate new functionality – we would be interested in your feedback on options you would like to see exposed

CCDC

# Q&A

- Type your questions in the box as shown

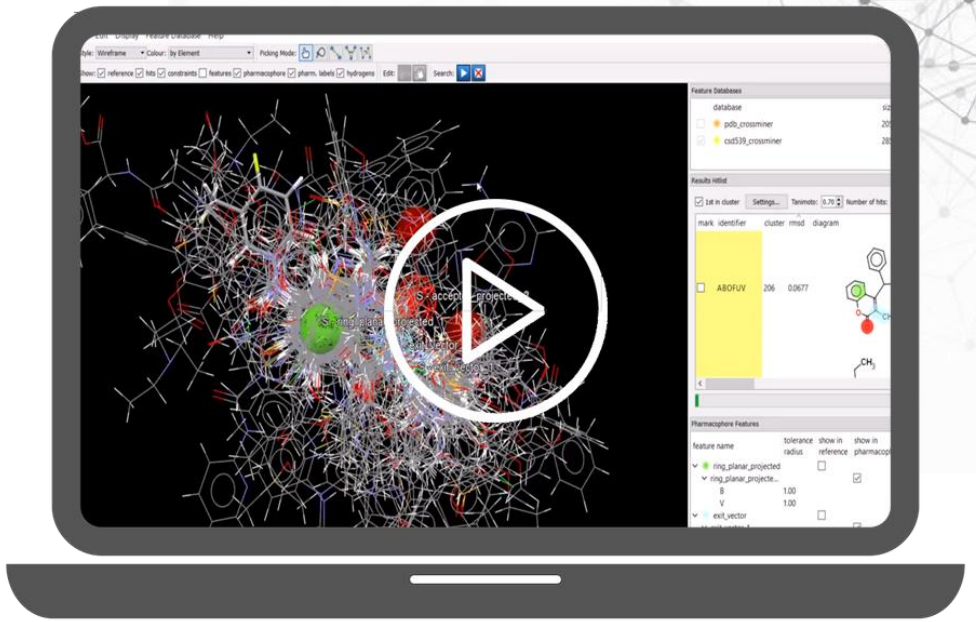



CCDC

# Next What's Up Webinar

- Next webinar: January 21st
- Follow us on social media
- Send us your ideas and news

  hello@ccdc.cam.ac.uk



# Thank you

hello@ccdc.cam.ac.uk

The Cambridge Crystallographic Data Centre
12 Union Road, Cambridge CB2 1EZ, United Kingdom
Registered Charity No. 800579