CCDC

advancing structural science

What's Up

CCDC Monthly Update

21 November 2019

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advancing structural science

Today’s presenters

Pete Wood

Senior Product Manager

Dave Bardwell

Support Team Leader

Angeles Pulido

Research and Applications Scientist
Materials Science Team

Carmen Nitsche

US General Manager

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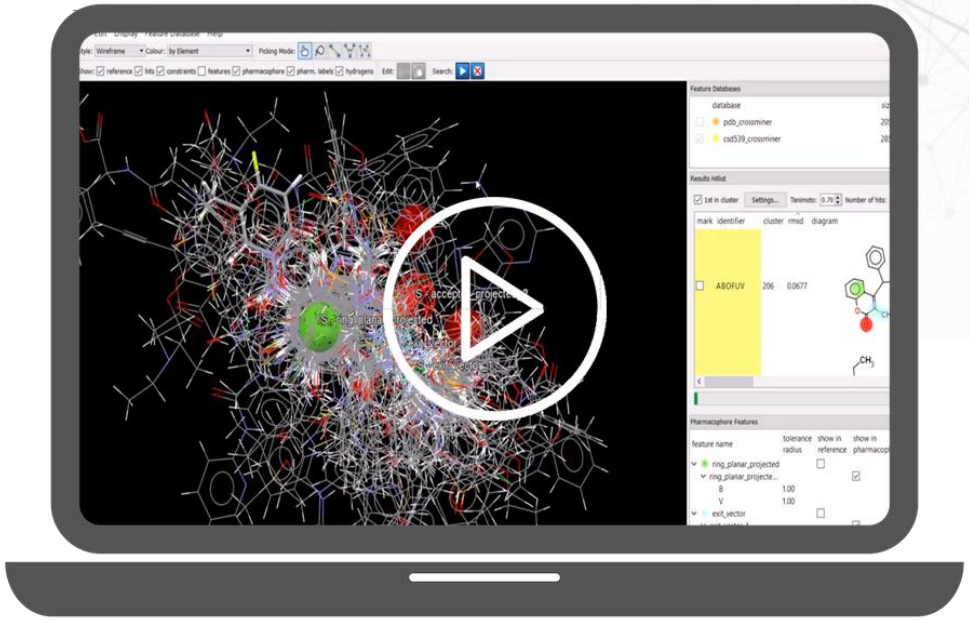
Overview

A regular update on what's happening with CCDC and an opportunity for your news/feedback and suggestions:

- Welcome & introductions
- CCDC updates, UGMs, CSP initiatives
- Coming up! Our 2020.0 CSD release
- New licensing plans and developments
- Open floor Q&A



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CCDC updates

Carmen Nitsche

US General Manager

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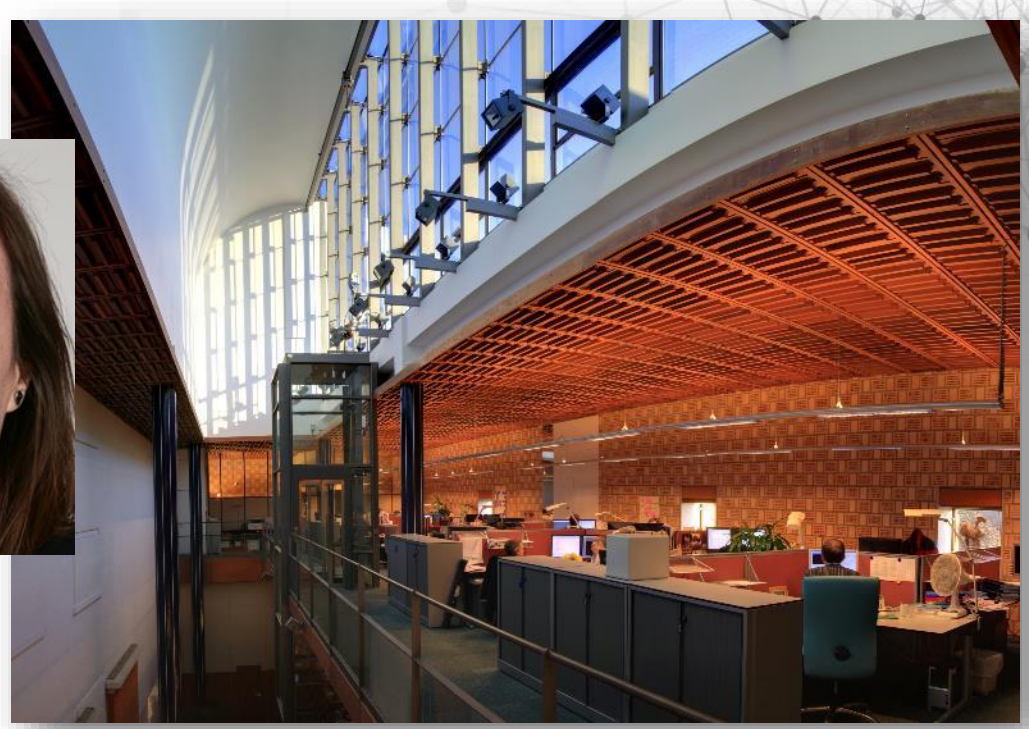
Welcome new team members

- Recently joining CCDC
  - Ana Machado – Marketing Executive



U.S. UGM in Philadelphia Oct 17th

AGENDA

- Accelerating sciences through data and machine learning
- CSD 1M Snapshot 1: Judith Currano, U. Penn
- Driving success for CCDC customers
- CSD 1M Snapshot 2: Neysa Nevins, GSK
- Product and Technology Strategy
- CSD 1M Snapshot 3: Jen Werner, Georgetown U.
- Product roadmap and future directions



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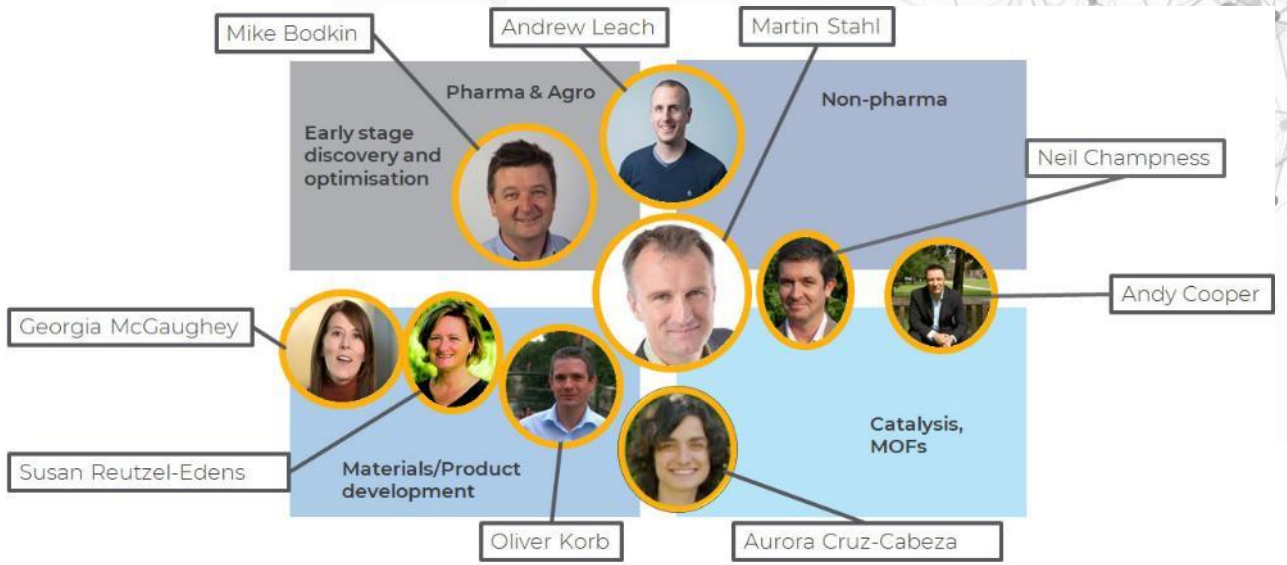
UGM highlights: Customer feedback

What are the key areas of development that you're looking for from CCDC?

- Enhance user experience
- Increase utilization
- Develop integrations
- Streamline installation
- Optimize engagement
- Develop unique areas of strength



To support customer needs, CCDC is investing to create a modern technology platform and competitive solutions driven by innovative science and a dynamic user community.

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UGM Highlights: Product Roadmap

- Major features released over 2019
  - Polyhedral Display and Polymer Expansion in Mercury
  - My Structures web interface
  - Protein-Ligand Searching and High-Throughput Docking
  - Interaction Mapping in CSD Python API
  - Hydrate Prediction and Aromatics Analyser for RPs
- Much more to come in 2019 and then 2020

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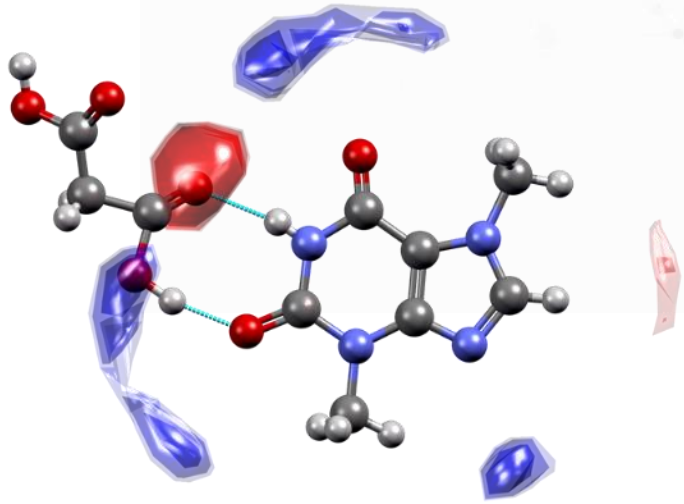
UGM Highlights: Long-Term Product Development Themes

Effective, knowledge-based applications for our user communities

- User experience
- Data management
- Visualisation
- Advanced search
- Molecular conformation
- Intermolecular interactions
- Structural property insights



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UGM Highlights: Feedback breakouts

- Discovery
  - Docking
  - Protein-Ligand Storage
  - CSD-CrossMiner
  - Solubility Prediction
  - Anything else?
- Materials
  - Solvate Prediction
  - Crystallisability Prediction
  - Co-Crystal Design
  - Aromatics Analyser
  - Anything else?
- Integrations
  - CSD Python API
  - CSD Pipeline Pilot Collection
  - CSD KNIME Nodes
  - 3rd Party Integrations
  - Anything else?

Have collated the feedback and now reviewing roadmaps and product plans to incorporate the input we received.

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Events update

RSFD Summit, CSP WG & Blind Test

Angeles Pulido
Research and Applications Scientist
Materials Science Team

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Events: CSP activities & initiatives

- Rational Solid Form Design (RSFD) Summit
  - 21st & 22nd October – Cambridge (MA) US
- CSP Working Group (WG) kick-off meeting
  - 6th November – Cambridge, UK
- CSP Blind Test VII – estimated launch end 2020
  - Coming soon…

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Rational Solid Form Design Summit

Bridging the gap between the latest technology advancements and pharmaceutical research

- Organized by XtalPi and sponsored by CCDC
- 100+ attendees: academia & industry
- 20+ scientific talks, focus areas:
  - *In Silico* Solid State
  - Advancing CSP
  - CSP Industrial Applications
  - AI and Machine Learning
- 2 Panel discussions

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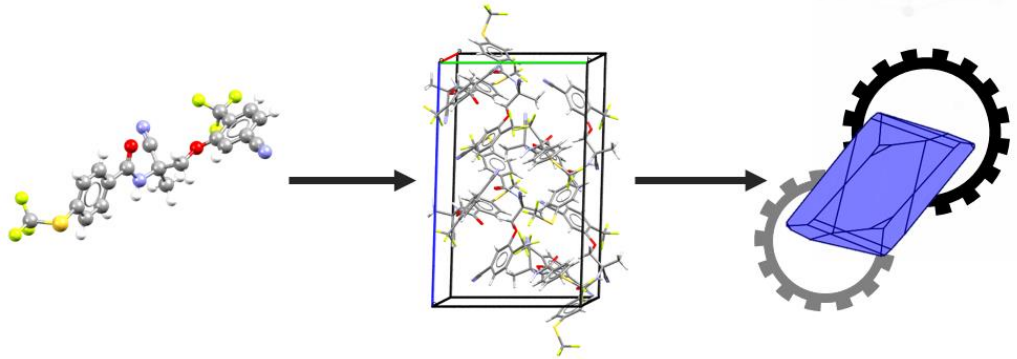
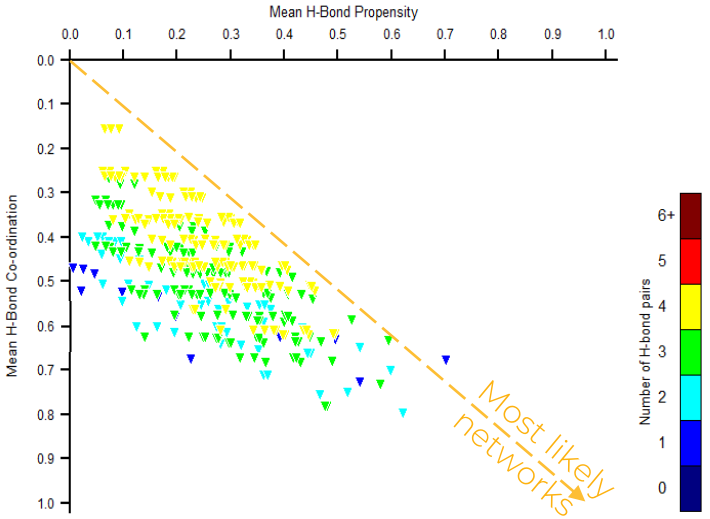
Digital Design – from Molecules to Products with Solid Form Informatics (Pete Wood)



Molecule **Form** **Properties**

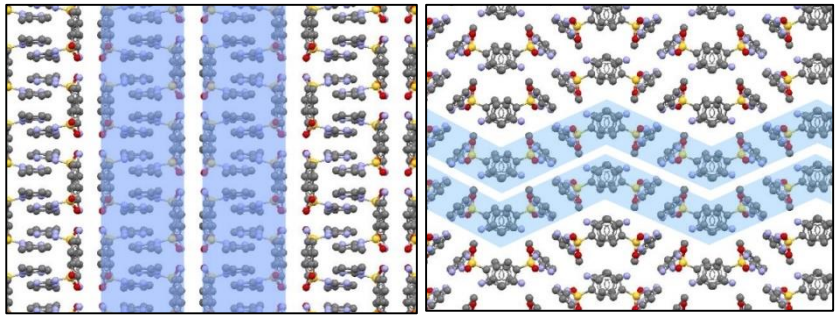
Hydrogen bond networks



Hydrogen bond propensity

Mechanical properties

Form-I Form-II



SLFNMA01/02

M. J. Bryant *et al.*, *CrystEngComm* (2018), **20**, 2698-2704

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Rational Solid Form Design Summit

- *In Silico* Solid-State Panel Discussion
  - Jürgen Harter – CEO, CCDC (panellist)
- CSP Panel Discussion
- Key topics:
  - Relevance of CSP in pharmaceutical pipelines
  - Where we would like to be in 5-10 years
    - Gaps and challenges to be addressed
    - How to best tackle the common challenges

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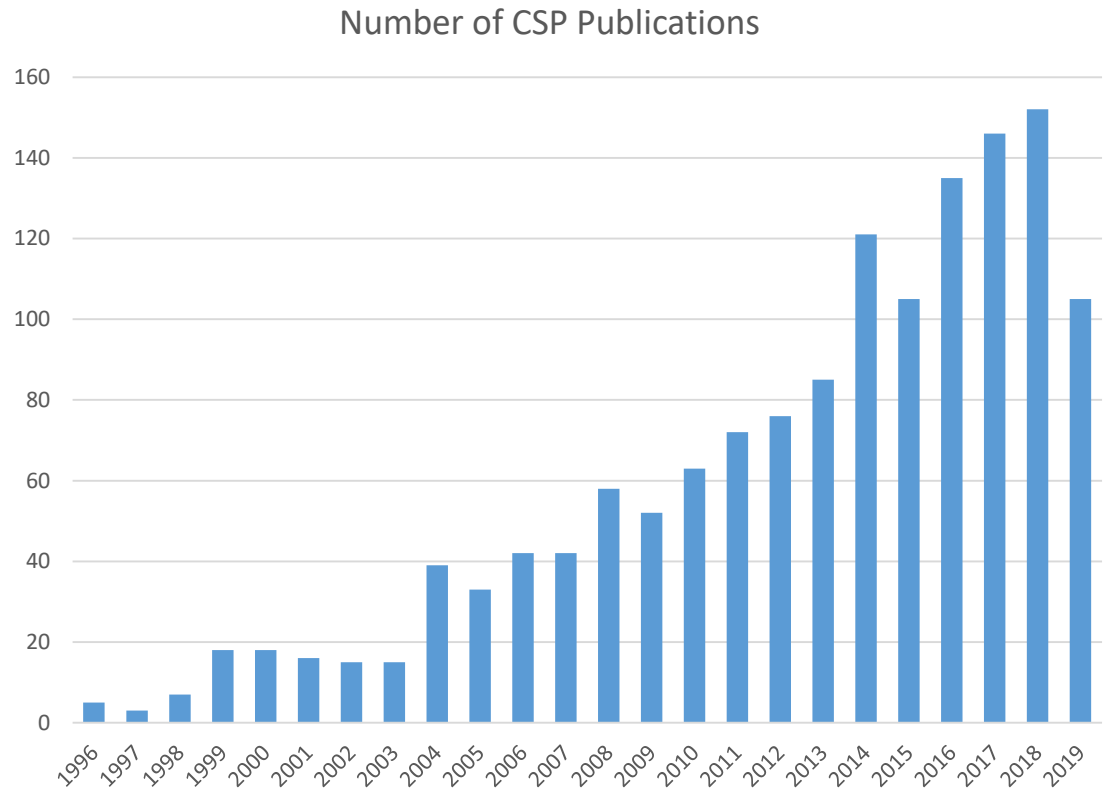
CSP Working Group (WG) Initiative

The rise of Crystal Structure Prediction



Web of Science topic search for “Crystal Structure Prediction”

The challenge – To store, view, retrieve and navigate these structures alongside experimental data in order to gain insights that complement or reinforce what has been observed experimentally

CSP WG formation:
Inspired by Crystal Form Consortium (Cambridge, UK, April 2019)

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CSP WG Kick-off meeting

Hosted:

- CCDC, Cambridge, UK (6th Nov 2019)

Attendees:

- 40+ (on site & remotely)

Participants:

- 15 Industry partners
- 11 Academic partners
- 3 CSP providers

Discussions on the day:

- Scientific impact and value proposition
- Key deliverables and expectations
- Participation and wider engagement
- Framework of the working group

Conclusion:

- Strong appetite, from the community, for creation of a CSP WG led by CCDC

Next steps:

- Creation of value proposition and definition of deliverables - CCDC (Q4 2019)

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Towards Seventh CSP Blind Test

CrossMark

feature articles

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‡ Present Address: Department of Chemistry, London Centre for Nanotechnology, University College London, 20 Gordon Street, London WC1H 0AJ, England.
§ Retired.

Keywords: crystal structure prediction; polymorphism; lattice energies; Cambridge Structural Database

Supporting information: this article has supporting information at journals.iucr.org/b

Report on the sixth blind test of organic crystal structure prediction methods

Anthony M. Reilly,[a]* Richard I. Cooper,[b] Claire S. Adjiman,[c] Saswata Bhattacharya,[d] A. Daniel Boese,[e] Jan Gerit Brandenburg,[f]‡ Peter J. Bygrave,[g] Rita Bylsma,[h] Josh E. Campbell,[g] Roberto Car,[i] David H. Case,[g] Renu Chadha,[j] Jason C. Cole,[a] Katherine Cosburn,[k,l] Herma M. Cuppen,[h] Farren Curtis,[k,m] Graeme M. Day,[g] Robert A. DiStasio Jr,[i,n] Alexander Dzyabchenko,[o] Bouke P. van Eijck,[p]§ Dennis M. Elking,[q] Joost A. van den Ende,[h] Julio C. Facelli,[r,s] Marta B. Ferraro,[t] Laszlo Fusti-Molnar,[q] Christina-Anna Gatsiou,[c] Thomas S. Gee,[g] René de Gelder,[h] Luca M. Ghiringhelli,[d] Hitoshi Goto,[u,v] Stefan Grimme,[f] Rui Guo,[w] Detlef W. M. Hofmann,[x,y] Johannes Hoja,[d] Rebecca K. Hylton,[w] Luca Iuzzolino,[w] Wojciech Jankiewicz,[z] Daniël T. de Jong,[h] John Kendrick,[aa] Niek J. J. de Klerk,[h] Hsin-Yu Ko,[i] Liudmila N. Kuleshova,[y] Xiayue Li,[k,bb] Sanjaya Lohani,[k] Frank J. J. Leusen,[aa] Albert M. Lund,[q,cc] Jian Lv,[dd] Yanming Ma,[dd] Noa Marom,[k,ee] Artëm E. Masunov,[ff,gg,hh,ii] Patrick McCabe,[a] David P. McMahon,[g] Hugo Meekes,[h] Michael P. Metz,[jj] Alston J. Misquitta,[kk] Sharmarke Mohamed,[ll] Bartomeu Monserrat,[mm,nn] Richard J. Needs,[mm] Marcus A. Neumann,[oo] Jonas Nyman,[g] Shigeaki Obata,[u] Harald Oberhofer,[pp] Artem R. Oganov,[qq,rr,ss,tt] Anita M. Orendt,[r] Gabriel I. Pagola,[t] Constantinos C. Pantelides,[c] Chris J. Pickard,[uu,vv] Rafal Podeszwa,[z] Louise S. Price,[w] Sarah L. Price,[w] Angeles Pulido,[g] Murray G. Read,[a] Karsten Reuter,[pp] Elia Schneider,[ww] Christoph Schober,[pp] Gregory P. Shields,[a] Pawanpreet Singh,[j] Isaac J. Sugden,[c] Krzysztof Szalewicz,[jj] Christopher R. Taylor,[g] Alexandre Tkatchenko,[d,xx] Mark E. Tuckerman,[ww,yy,zz] Francesca Vacarro,[k,aaa] Manolis Vasileiadis,[c] Alvaro Vazquez-Mayagoitia,[bb] Leslie Vogt,[ww] Yanchao Wang,[dd] Rona E. Watson,[w] Gilles A. de Wijs,[h] Jack Yang,[g] Qiang Zhu[qq] and Colin R. Groom[a]

CSP Blind Tests (1998-2016)
organized by CCDC

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Upcoming 2019 events

- AsCA: Dec 18-20, Singapore
  - CSD 1 million evening reception – Wednesday 18th December
    - Visit us at booth A08 to pick up your ticket

AsCA 2019 SINGAPORE

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2020 Events

- BioIT *World Conference and Expo (April 21-23)*
- CCDC UGM *Boston (April 24)*
- BCA UK *Leeds University (April 6-9)*
- EU UGM *Cambridge (June)*
- ACA Summer School *Purdue University(May 31-June 6)*
- ACA San Diego *(July 31-August 7)*
- CCDC UGM *San Diego–\ (August 13)*
- American Chemical Society Meeting *San Francisco (August 16-20)*
- IUCr *Prague (August 22-30)*

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Coming soon! 2020.0 CSD release

Pete Wood

Senior Product Manager

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2020.0 CSD Release

- The 2020.0 CSD release includes exciting new software functionality as well as the latest CSD **Data Update**

- For all CSD licensed users, we are upgrading our CSD Python API to be **Python 3.7** enabled by default
- For CSD-Discovery users we are pleased to be launching significant optimisations to GOLD to enable **Ultra-Large Docking**
- For CSD-Materials users we have introduced a new **H-Bond Coordination Quick-View** component allowing fast assessment of the H-bonding in a structure based on coordination likelihood information
- For Research Partners, we are launching a **CSD Pipeline Pilot Component Collection**, which will become available to other CSD licensed users later on in 2020
- This release further streamlines our entirely opt-in **Product Telemetry** system
- We are also rolling out a new **Licensing** system across our entire suite!

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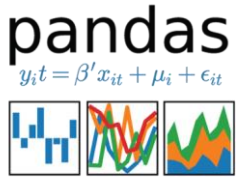
Py3 CSD Python API

AVAILABLE NOW

- Early in 2019 optional Python 3 packages were provided
- With the 2020.0 CSD release Python 3.7 becomes the default version for all CSD applications
- The CSD Python API will be Python 3 enabled straightaway at the point of installation
  - Easy integration with other key scientific Python packages



- pip and conda packages for Python 2.7 still available on request

https://downloads.ccdc.cam.ac.uk/documentation/API/

https://www.ccdc.cam.ac.uk/forum/csd_python_api/

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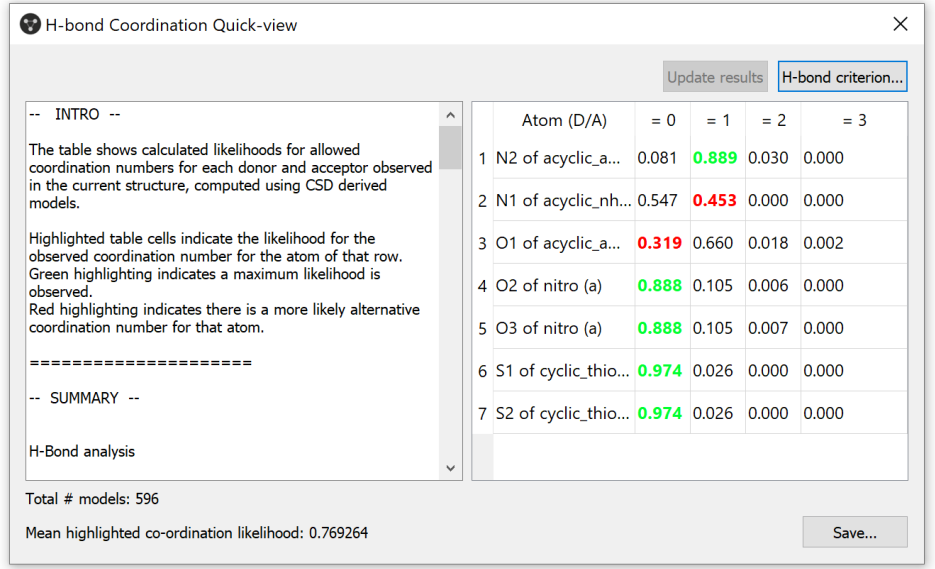
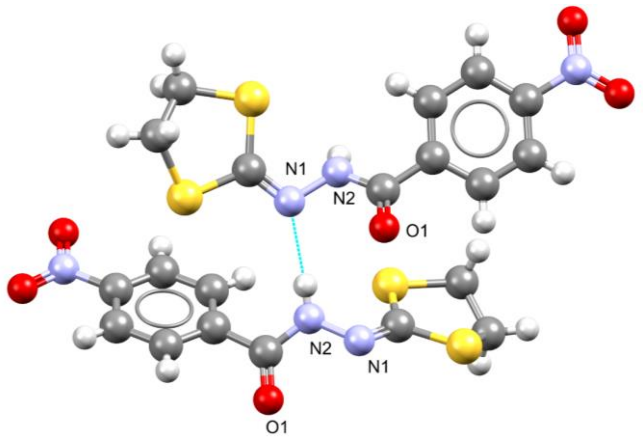
H-Bond Coordination Quick-View

- Quick assessment of the likelihood of H-bond behaviour based on coordination numbers in the observed structure
- Green highlighting indicates that the observed outcome is optimal based on CSD-derived likelihoods
- Red highlighting indicates there is a more optimal coordination outcome for that donor or acceptor based on CSD data
- Released to CSD-Materials users in Mercury in the 2020.0 CSD Release



	Atom (D/A)	= 0	= 1	= 2	= 3
1	N2 of acyclic_a...	0.081	**0.889**	0.030	0.000
2	N1 of acyclic_nh...	0.547	**0.453**	0.000	0.000
3	O1 of acyclic_a...	**0.319**	0.660	0.018	0.002
4	O2 of nitro (a)	**0.888**	0.105	0.006	0.000
5	O3 of nitro (a)	**0.888**	0.105	0.007	0.000
6	S1 of cyclic_thio...	**0.974**	0.026	0.000	0.000
7	S2 of cyclic_thio...	**0.974**	0.026	0.000	0.000



CSD refcode: DEDMUX02

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Ultra-Large Docking

- We have further optimised GOLD for use in ultra-large docking projects including libraries of hundreds of millions of compounds
- Docking using GOLD can now be performed with optimised I/O settings to streamline use
- Specialised Docker containers have been developed for deployment of GOLD in ultra large docking projects
- Released to CSD-Discovery users in GOLD in the 2020.0 CSD Release

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CSD Pipeline Pilot Collection

- We are launching our first CSD Pipeline Pilot components, allowing workflow access to CSD data and features
- The CSD PP Component Collection includes components for CSD data access, searching, conformer generation and virtual screening as well as viewer nodes
- This is released to Research Partners alongside the 2020.0 CSD Release
- The collection will become available to other users beyond the Research Partners in a later release during 2020

BIOVIA

PIPELINE PILOT

FINIAconsulting
informatic solutions

python™

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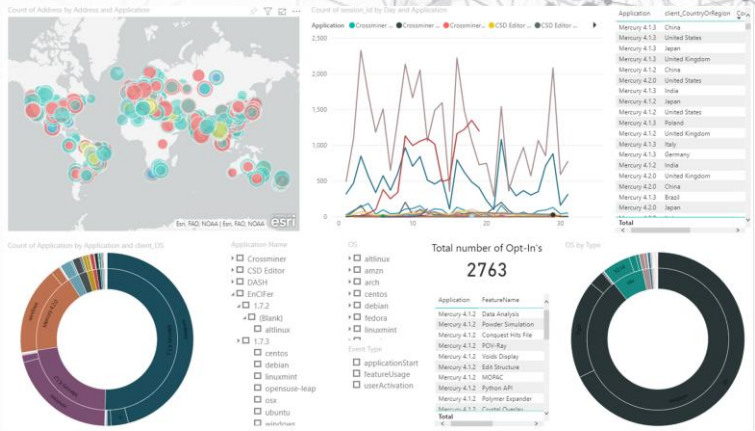
Product Telemetry

- We'd like to track some basic, anonymous diagnostic data on which CSD components are most used (Product Telemetry)
- This is entirely **opt-in**, either at point of installation, or first use after installation
- It doesn't affect speed, security or usability
- Telemetry info is anonymous – we don't track user names, IPs, site codes or what the user is doing
- Focusses on better understanding of usage across the CCDC portfolio
- Helps us make better data-driven decisions on how best to help you




```
{
  "eventName":"applicationStart",
  "telemetryVersion":"1.0",
  "applicationName":"Mercury",
  "applicationVersion":"4.1.2",
  "sessionID":"{2b3e6224-7f90-4a67-9778-
54bd38a008e4}",
  "timestamp":"2019-04-10T07:52:26Z",
  "operatingSystem":"CentOS",
  "operatingSystemVersion":"6.10",
  "cpuArchitecture":"x86_64"
}
```


https://www.ccdc.cam.ac.uk/telemetry/

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Licensing

Development and plans

Dave Bardwell

Support Team Leader

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Why do we need a new licensing system?

- Current system is very old – over 20 years!
- The existing system has been stretched as far as it will go
  - Maximum number of products reached
  - Tied to specific licensing years
  - Unable to specify duration of licence
- Does not meet the needs of CCDC for delivering the new products and services we have planned for you

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What benefits does the new system bring?

- Modern, secure, regularly updated third-party licensing system
  - Lets CCDC play to our strengths and concentrate on bringing you improved scientific software and data
- Allows both online and offline activation
- Highly flexible – allows us to expand licensing to meet our needs in future years
- Will allow you to use any software release as long as you have a valid licence
- Lets us create licences that last any time period we choose

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What's the best thing about licensing?

(not noticing it's there)

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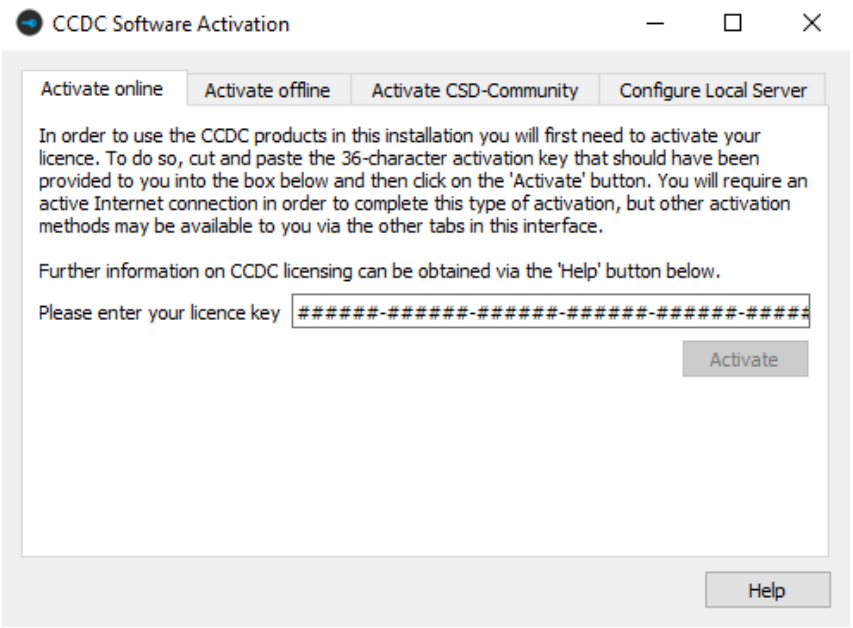
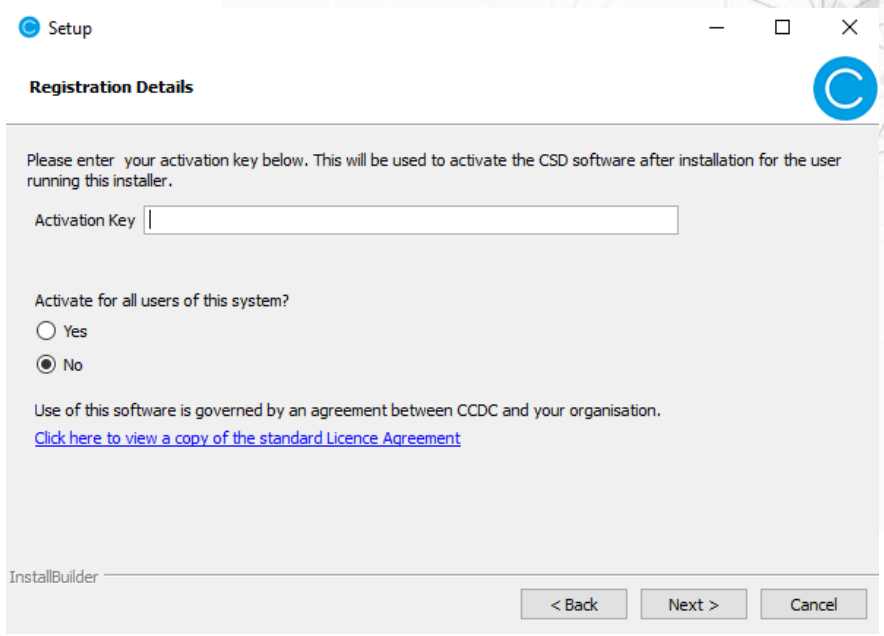
How does it work?

- Activation, either in the installer:





- Or afterwards, with an activation tool

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How does it work?

- Connects to a licensing server in the cloud
  - An offline route is also possible
- Once activated, does not require an internet connection again
  - Allows offline use, or taking an install on a laptop to a conference etc.
- But if you do have a connection, it will make use of it
  - Updates your licence automatically from the CCDC licence server
  - So if you extend your licence by another year, you won't need to re-activate – it will just be picked up automatically

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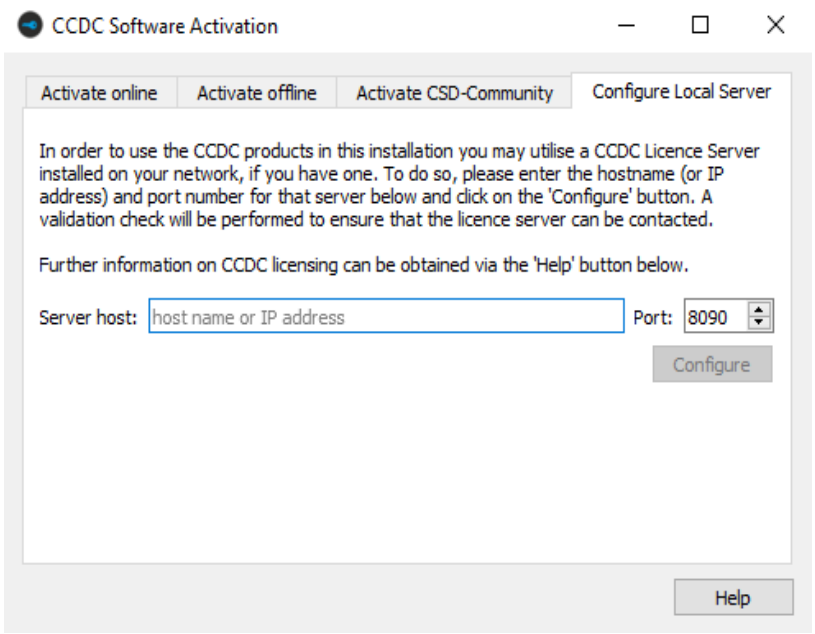
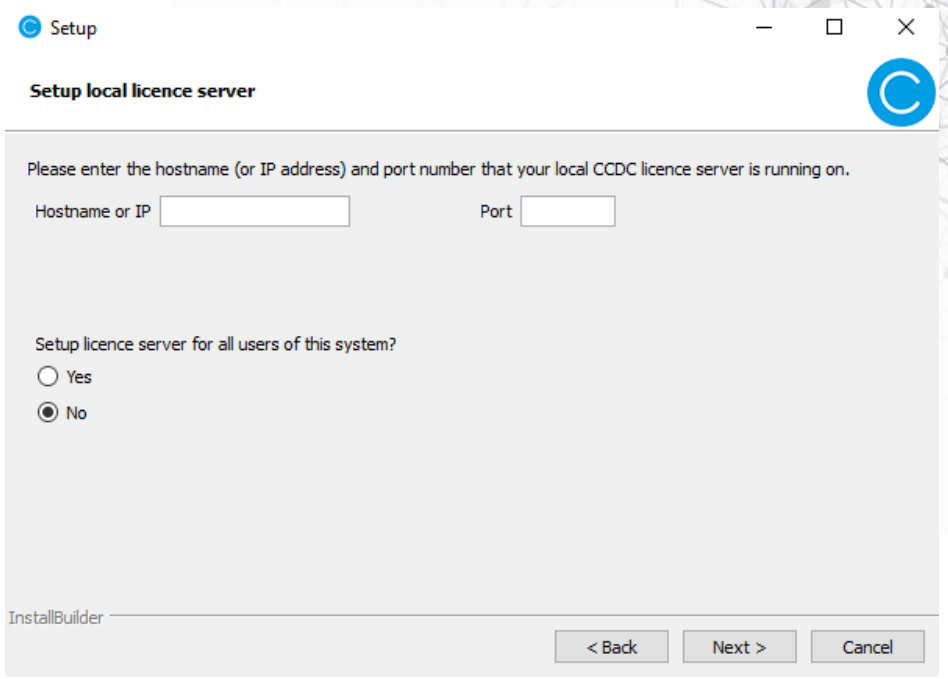
Or you can set up your own local licence server….

- Then select to use that in the installer:





- Or afterwards, with the activation tool

How does that work?

- Download a lightweight licence server and activate it
  - Available for Windows, Linux and MacOS
- Run that licence server on any system on your network
  - Can be run as a service or daemon
- All CCDC software can be told to look for that local licence server instead of needing to activate individually
  - Removes any need to communicate outside your network
  - Allows easy deployment that requires no end-user set up or knowledge of licensing

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What do these changes mean for me?

- If you used to register individual installs, almost no change
  - Just use the activation code instead of the old site/confirmation codes
- IP-based licence keys are no more
  - Plan to set up installs to auto-activate or use a local licence server
- The 3 month grace period for licences is no more
  - Licences now expire when your subscription ends
  - But renewing will automatically update your existing licence if you are online

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Future improvements

- View and manage your licences on an online portal
  - See what activations have been made with your licence and where
  - Deactivate current licences in order to move them elsewhere
- Self-purchasing
  - Renew and upgrade via an online portal

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Q&A

The floor is yours

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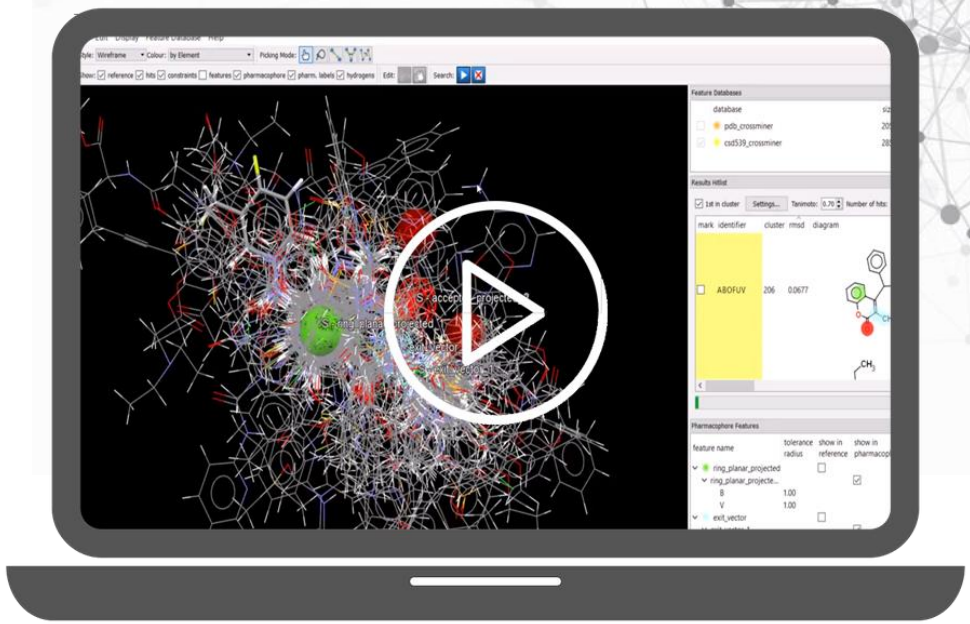
Next What's Up Webinar

- Next webinar: January 2020 – date tbc!
- Send us your ideas and news

  hello@ccdc.cam.ac.uk



Thank you

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