In-Depth Comparison of Polymorphic Structures Using Mercury

CCDC Virtual Workshop

14th May 2024

advancing structural science

Learning outcomes for today

- Understand the value of analysing polymorphic structures to assess their stability.
- Re-familiarise with the basics of Mercury, Mogul and Isostar.
- Understand what tools are available in the CSD-Materials suite and how they can be used to compare solid forms, including:
    - Mogul Geometry Check, Hydrogen Bond Statistics, Hydrogen Bond Propensities, Aromatics Analyser, Overlay tools and Full Interaction Maps (FIMs).
- Learn how these tools have been used in industry and what a workflow for assessing solid forms might look like.
- Gain confidence in the software used today so you can apply the techniques on your own systems/structures.

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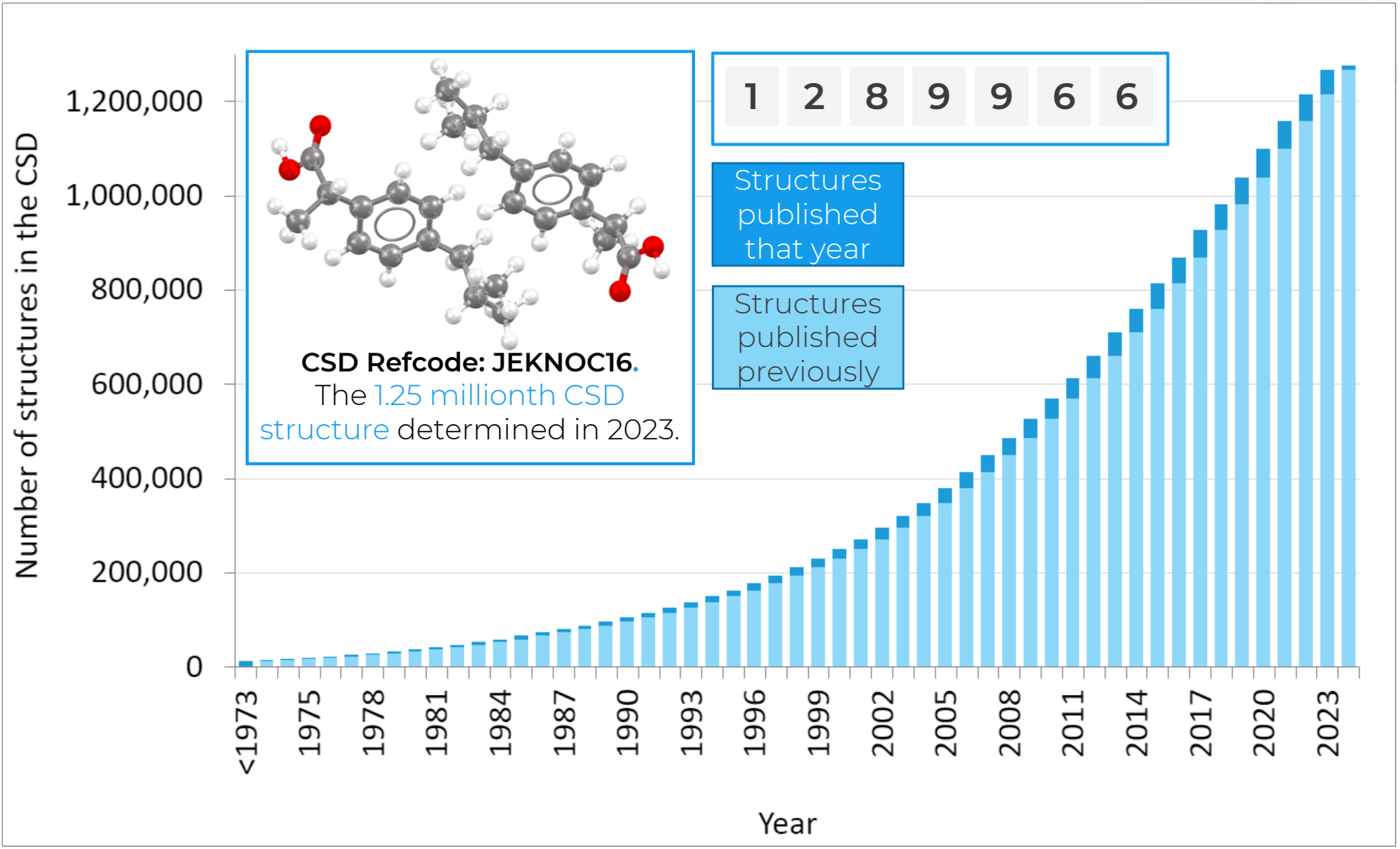
The Cambridge Structural Database



- Every published structure
  - Inc. ASAP & early view
  - *CSD Communications*
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 58 years
- A trusted CoreTrustSeal repository

Certified as Trustworthy by CoreTrustSeal

Inside the Cambridge Structural Database

The CSD is a database of all the published organic and metal-organic experimental crystal structures

Organic
45%

Metal-Organic
55%

At least one transition metal, lanthanide, actinide or any of Al, Ga, In, Tl, Ge, Sn, Pb, Sb, Bi, Po

Not Polymeric
89%

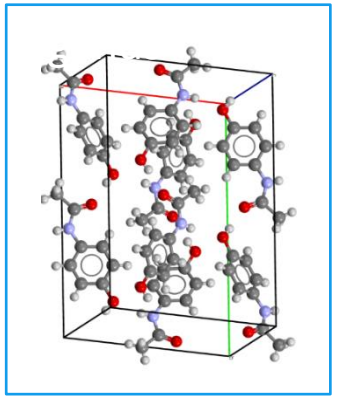
Polymeric: 11%

Single Component
58%

Multi Component
42%

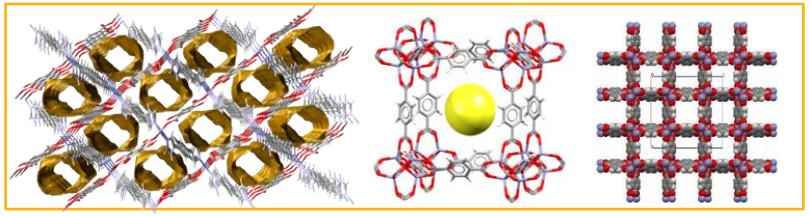
Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



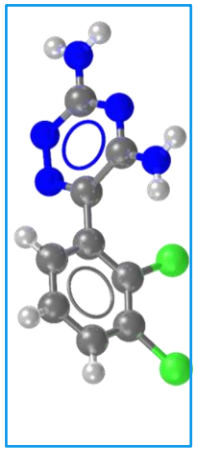
Metal-Organic

- Metal Organic Frameworks
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding



Additional data

- 13,478 polymorph families
- 174,987 melting points
- 1,075,904 crystal colours
- 951,746 crystal shapes
- 30,275 bioactivity details
- 13,641 natural source data
- > 350,000 oxidation states

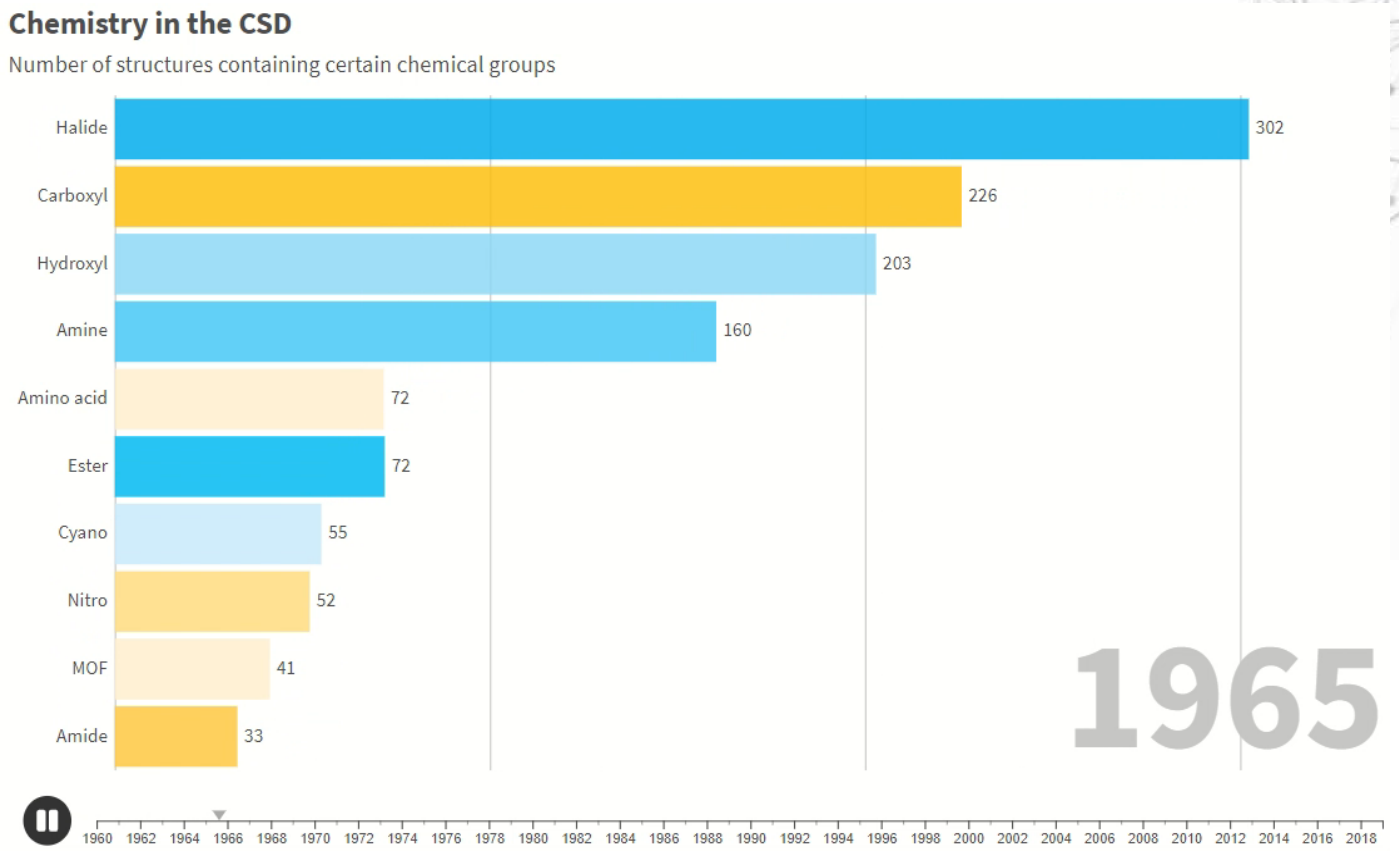


Links and subsets

- DrugBank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticide PDB

Exploring the CSD

- > 1 million structures
  - > 94M 3D coordinates
- > 28 million bond lengths
  - > 2M unique distributions
- > 40 million valence angles
  - > 3M unique distributions
- > 14 million torsion angles
  - > 800K unique distributions
- > 2 million rings
  - > 400K unique distributions
- > 2 million hydrogen bonds
  - >30 million Isostar contacts



Images and graphics created using the CSD Python API and Flourish

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A wealth of data in the CSD

>42% Multiple component structures

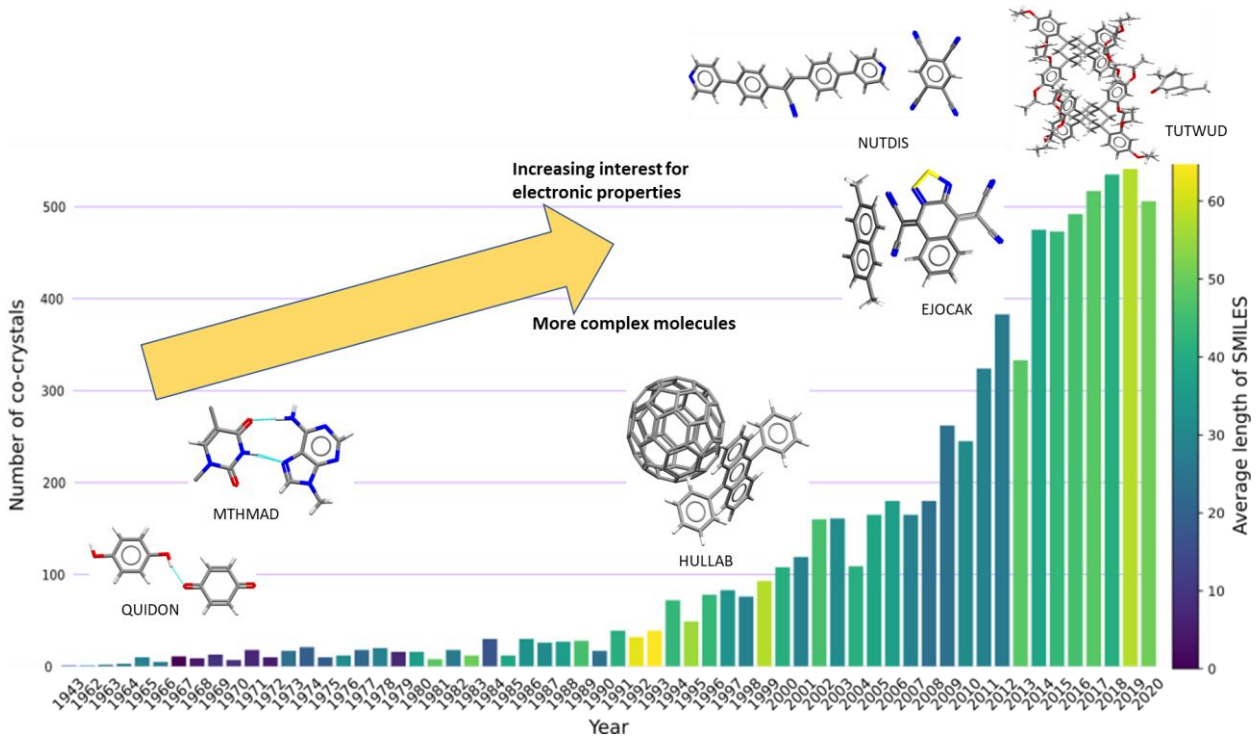
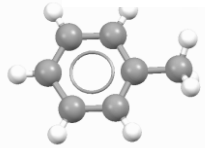
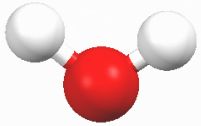


Chart showing the number of co-crystals in the CSD by year and colour coded by the average SMILES length. Image created by Katerina Vriza*, a CCDC sponsored PhD student.

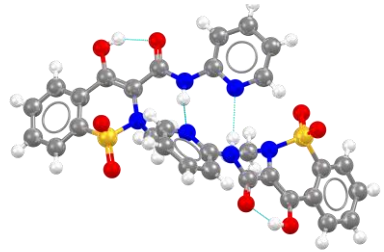


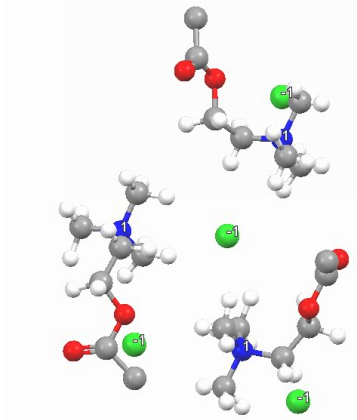
Solvates
>270K

Hydrates
>150K

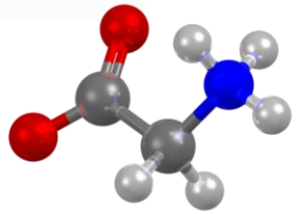


Polymorphs
>13K polymorphic families





Salts
>300K



Refcode families
>1 Million

*Katerina Vriza, University of Liverpool, PhD on Data driven discovery of functional molecular co-crystal

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Small molecules, big impact

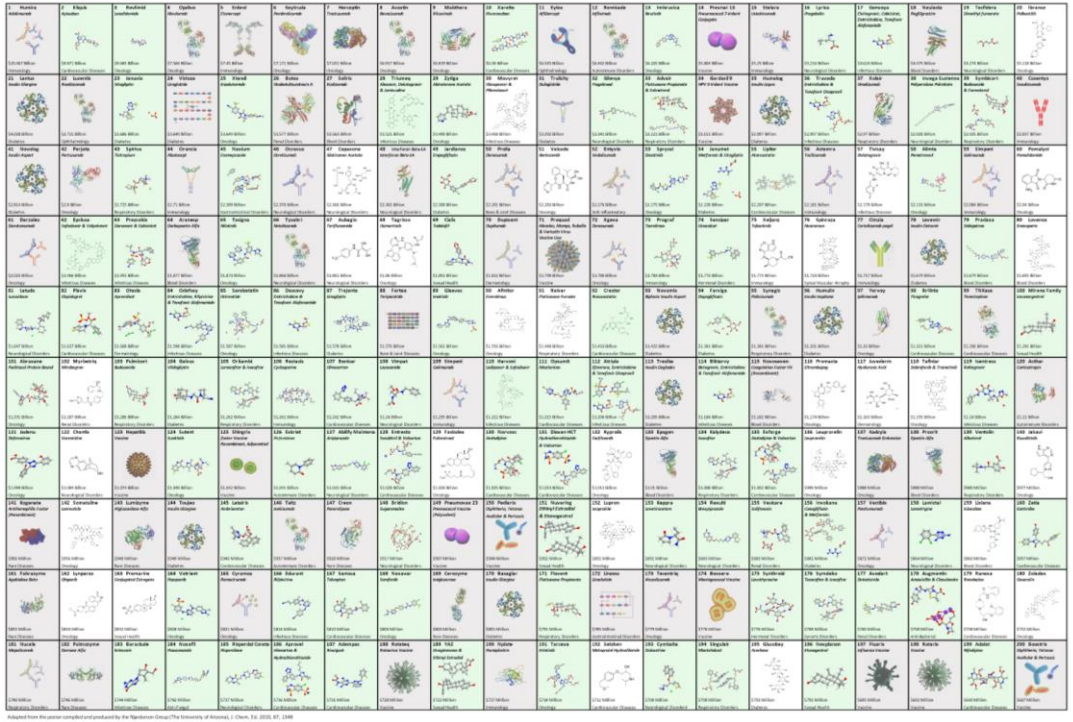
200 top drugs by retail sales in 2000

Small molecule structure in the CSD

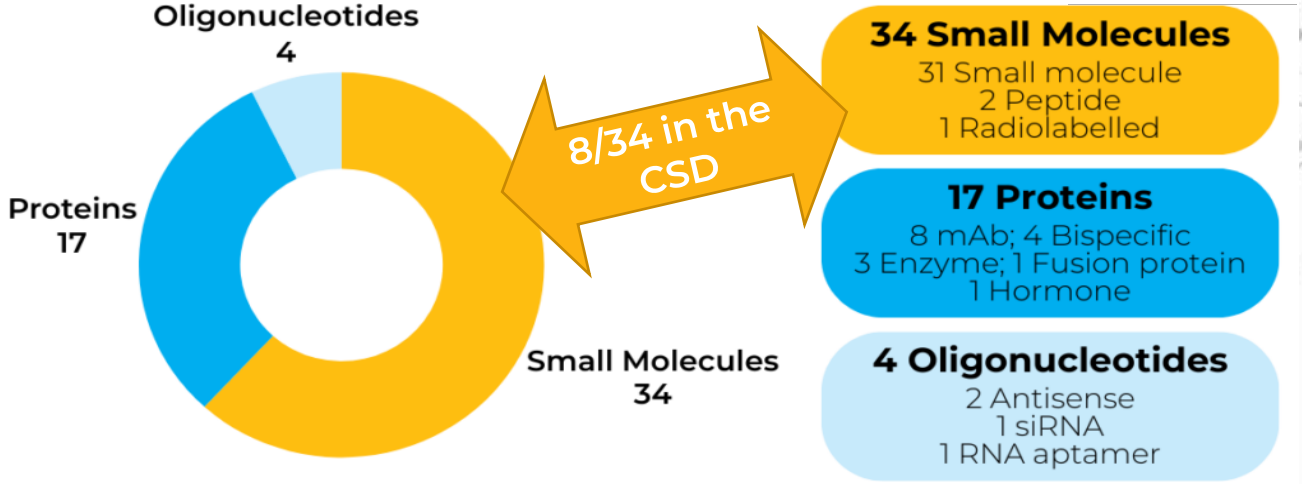
- Open-up new biological and therapeutic opportunities
- Compete against emergent modalities for rare diseases
- Are used to target RNA*

Small molecule structure CSD entry pending

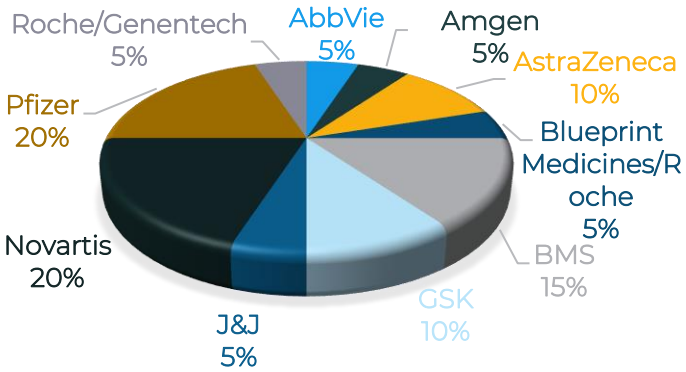
Biological structure in the PDB



FDA novel drug approvals 2023



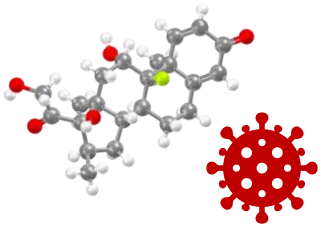
Missing FDA drugs 2020-23



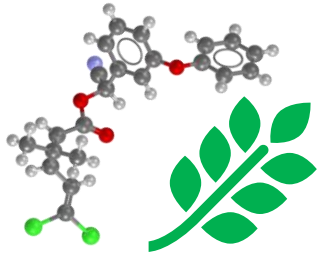
How can we help you to increase the amount of industrial data shared through the CSD?

Adapted from poster compiled and produced by the Njardarson Group (The University of Arizona)
Nature Reviews Drug Discovery **20**, 85-90 (2021)

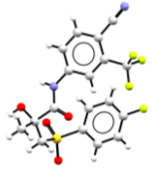
COVID-19



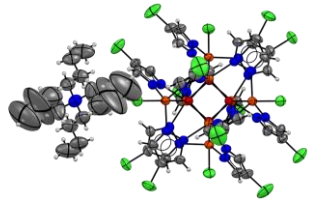
Pesticides



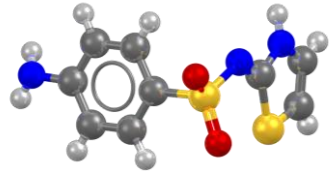
Drugs



ADPs



Best representative

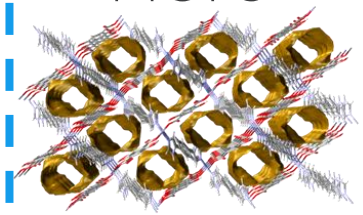


Teaching

MOF Dimensionality

- 1D
- 2D
- 3D

MOFs



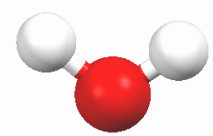
CSD Subsets

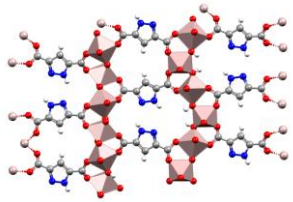
Groups of structures that may be more difficult to find in CSD from searching alone

- Easy access to the most relevant structures
- Benefit from our in-house and external expertise
- Convenient starting point for analysis using CSD or 3rd party tools
- A basis for your research and crystal engineering

Added in 2022

Hydrates

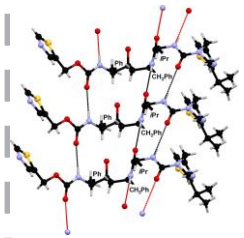


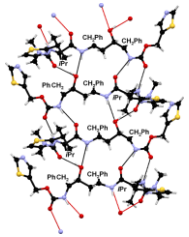


Electron Diffraction

High Pressure

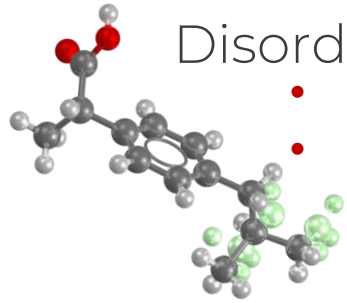
Polymorphs

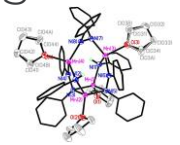




Disorder

- Minimal
- Significant





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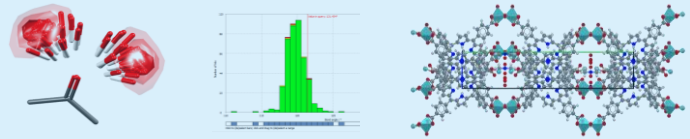
The CSD Portfolio today

CSDCore.

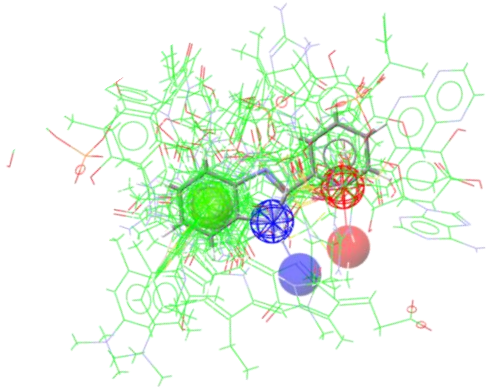
Search, visualise, analyse and communicate structural data

Insights into molecular and crystal shape and interactions



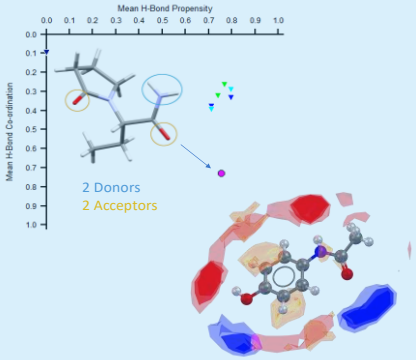
CSDDiscovery.

Design of new molecules



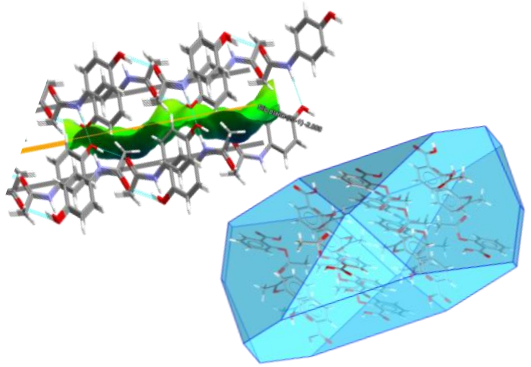
CSDMaterials.

Assessment of solid form stability and properties



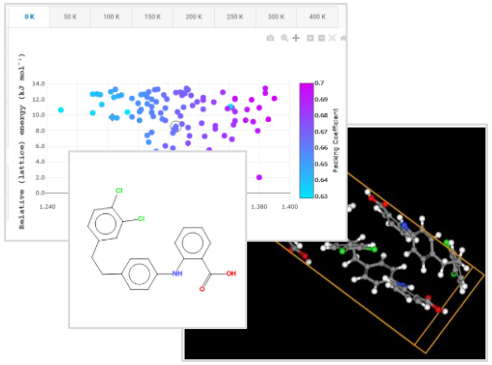
CSDParticle.

Anticipate particle properties and behaviour



CSDTheory.

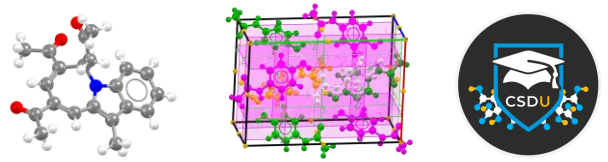
Insights from predicted structure landscapes



CSDCommunity.

Deposit, publish, access and visualise structural data

Free functionality to share and learn from structures



Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists ♦ Functional Materials Scientists ♦ Educators ♦ Industry and Academia

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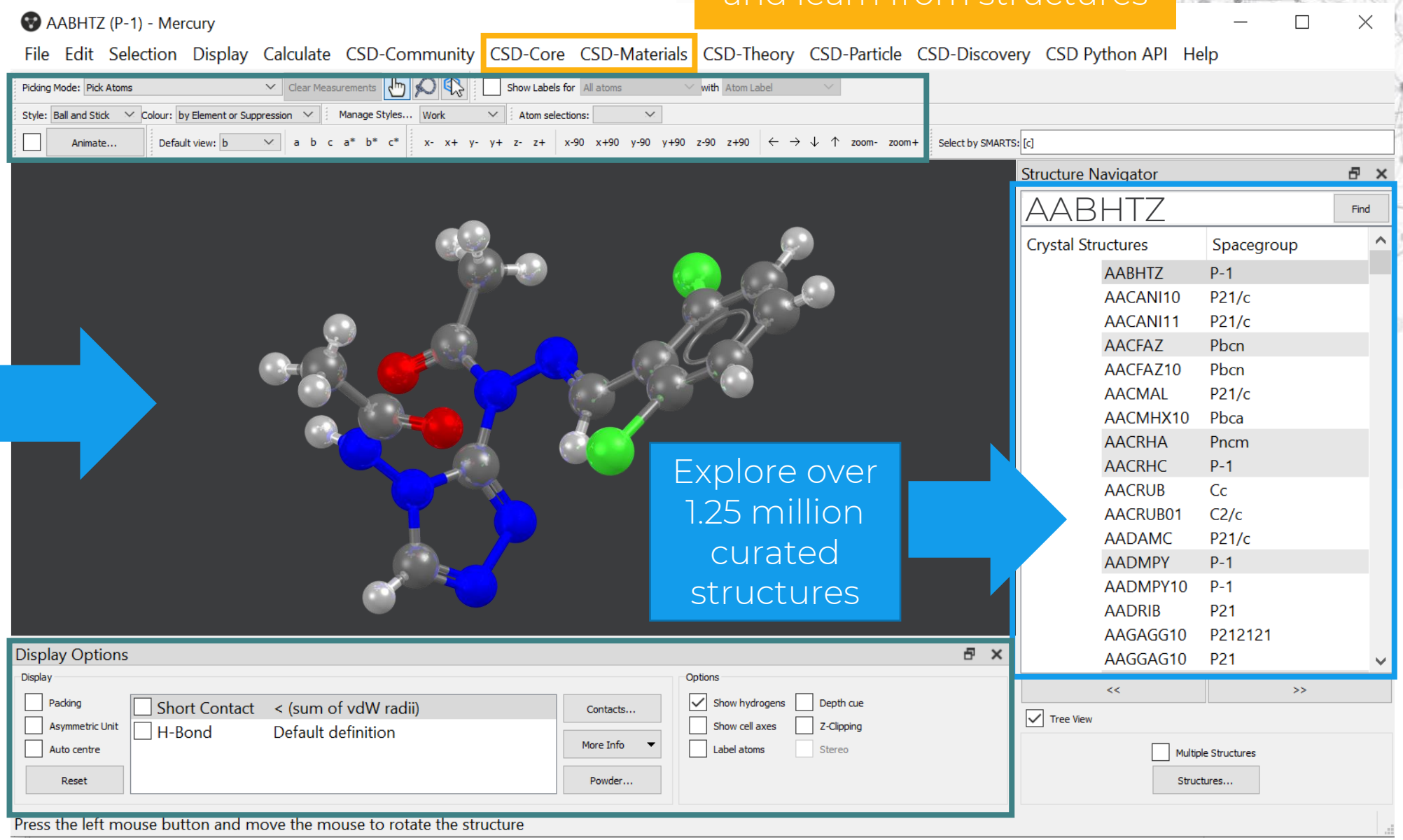
Mercury Overview

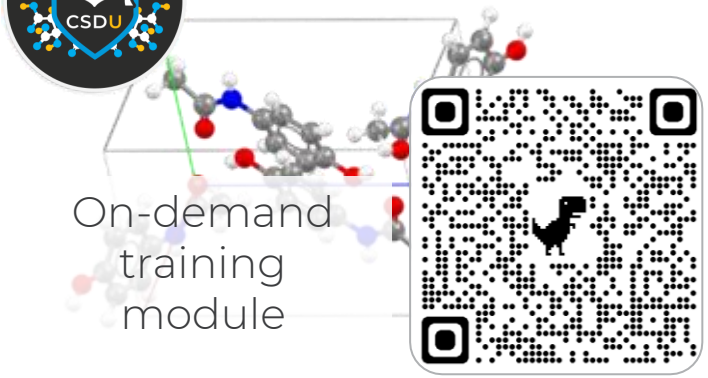
More advanced functionality to analyse and learn from structures



Display options to visualise and navigate structures

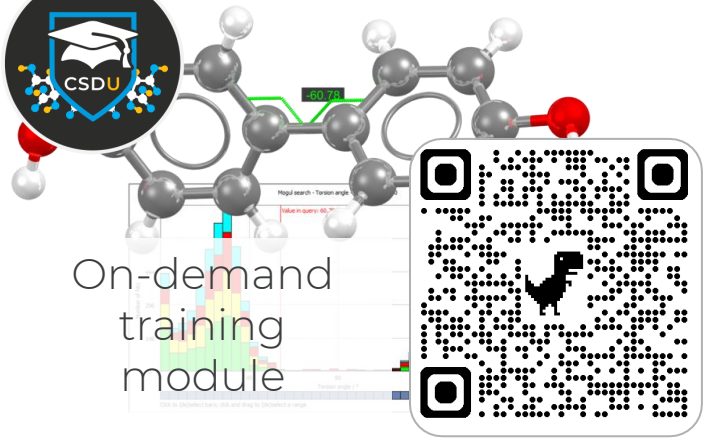
Previous training on Mercury and some of the tools we will use today

Mercury Visualisation 101



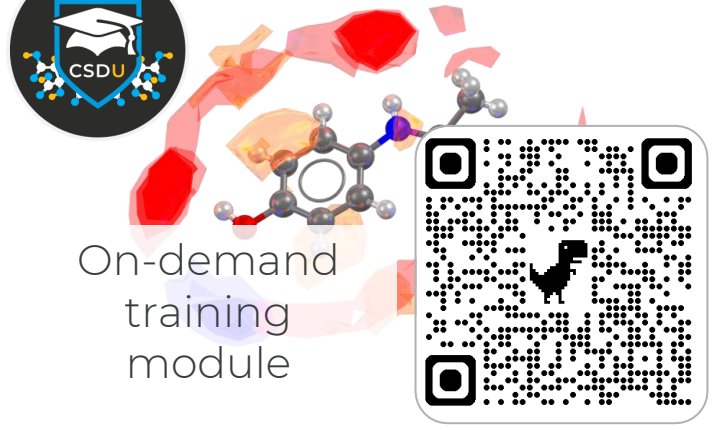
On-demand training module

Mogul Analysis 101

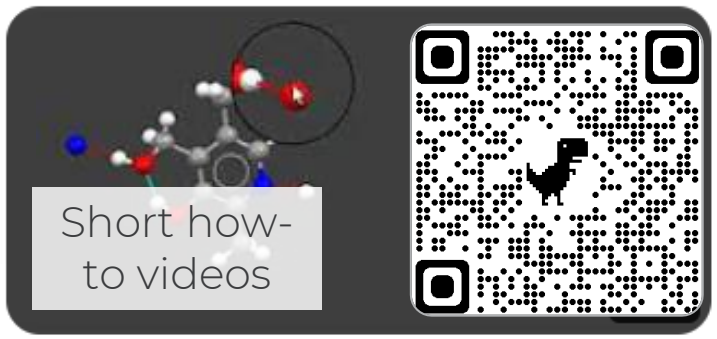


On-demand training module

Full Interaction Maps



On-demand training module



Short how-to videos

How to define and visualize hydrogen bonds in Mercury - video...

Self-guided exercises

See all resources on our website and on our YouTube channel!

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Comparing polymorphs

- It can be useful to compare polymorphs and to contextualise them against the structures of the Cambridge Structural Database
  - Quickly visualise differences in conformations and crystal packing.
  - Quickly understand which features of the structure are “unusual” and which may have an impact on the relative stability of the forms.
  - We will briefly cover a number of tools that we use regularly when looking at polymorphs.

Molecular conformation

Intermolecular interaction and packing

Aromatic interaction

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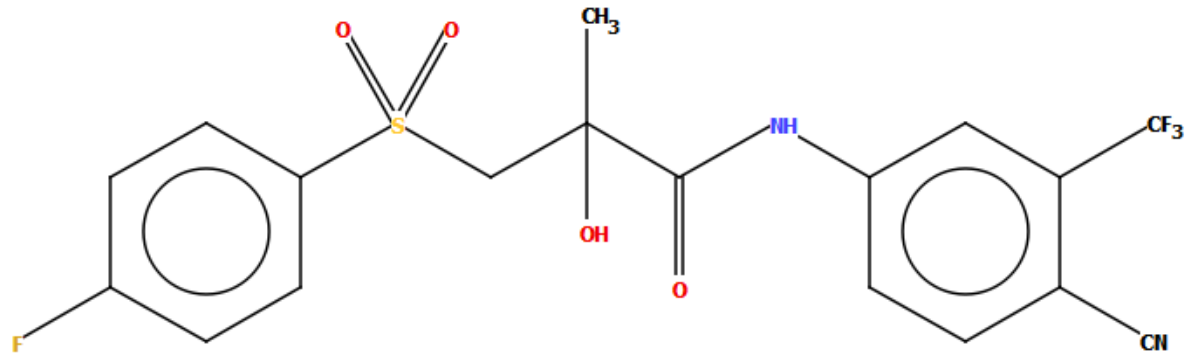
Bicalutamide

- Antiandrogen medication to treat prostate cancer
- Biopharmaceutical classification: Type II – low water solubility, high permeability
- High pka of 12 – poorly soluble in physiological media



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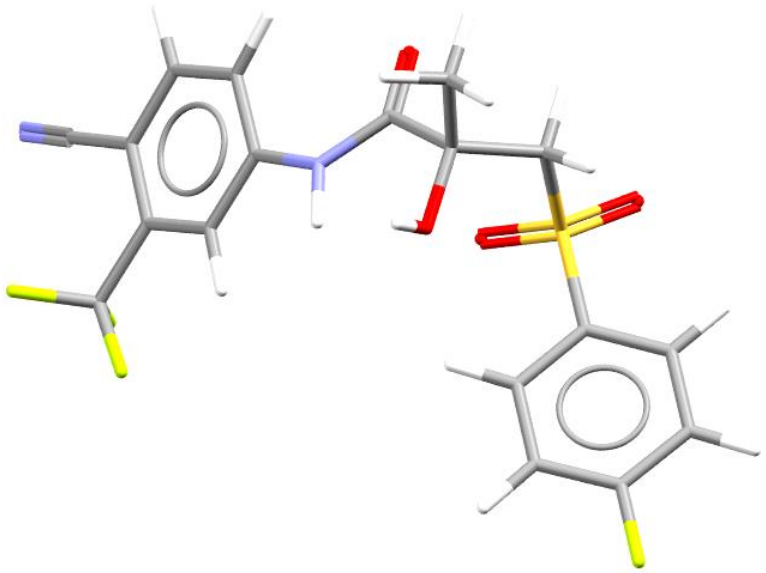
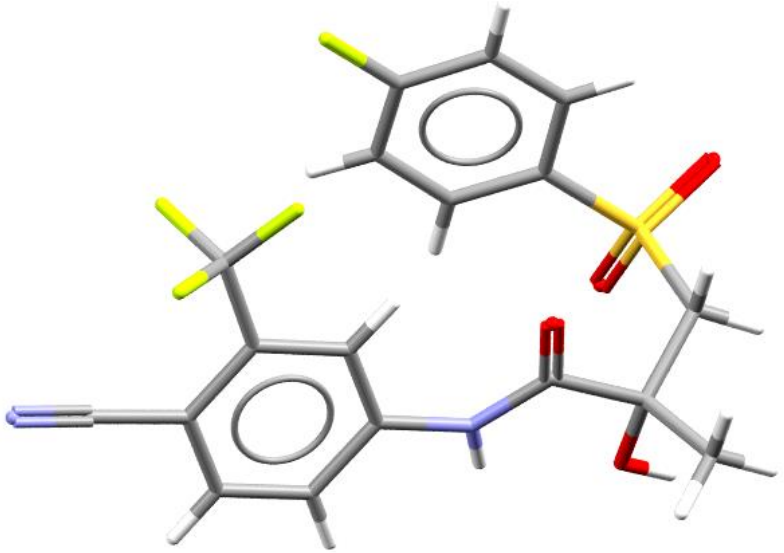
Two polymorphs

- JAYCES03, Form I



$P2_1/c$

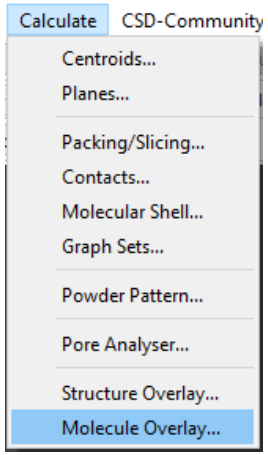
JAYCES02, Form II

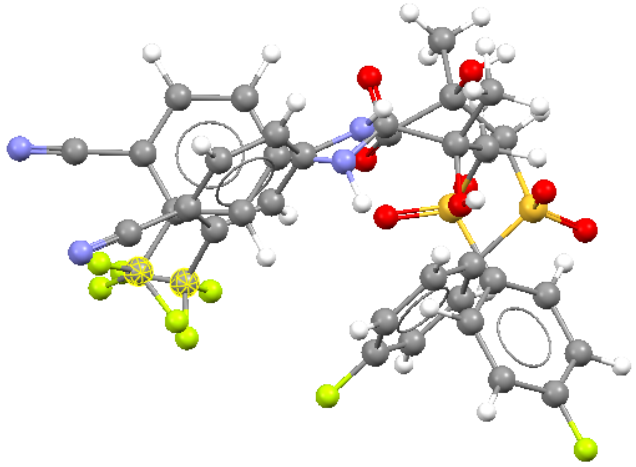


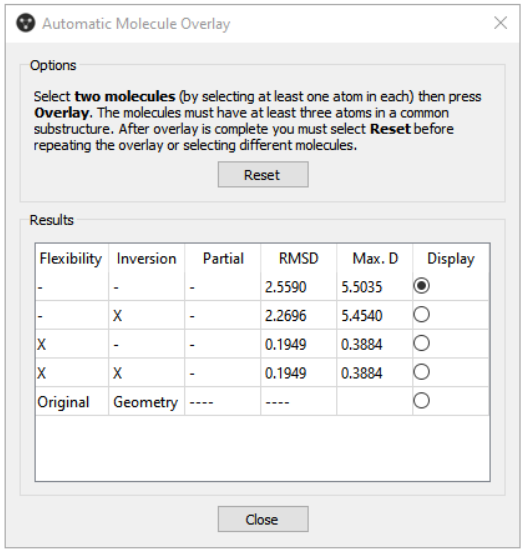
P-1

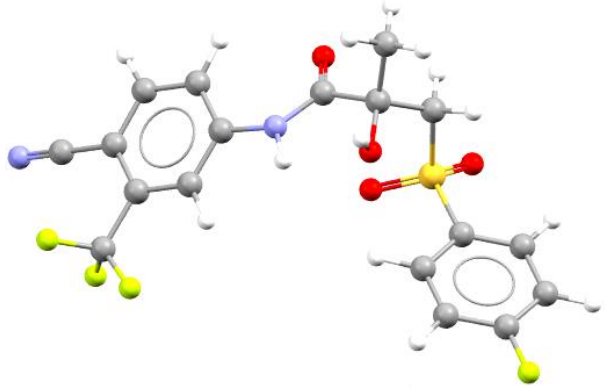
Molecular conformation

- Molecule Overlay (Calculate Menu)

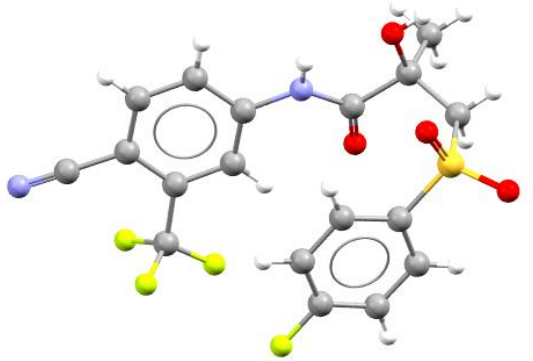








JAYCES03



JAYCES02

Very different conformations!

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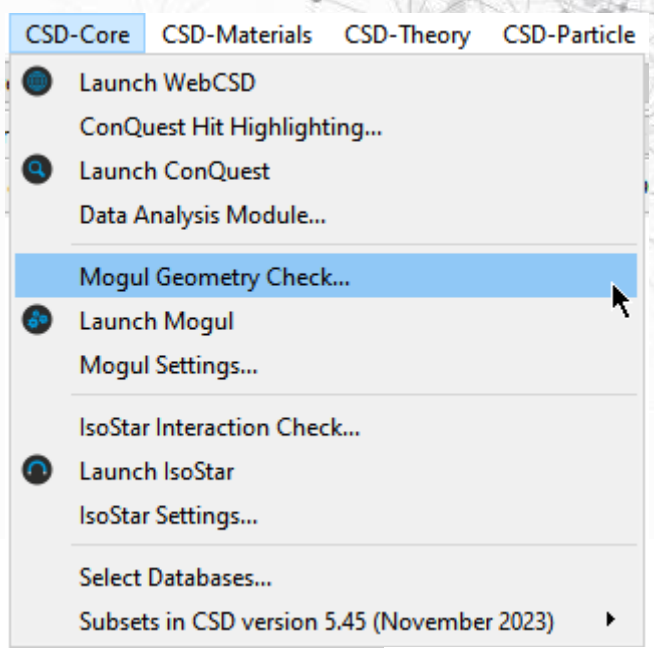
Molecular conformation

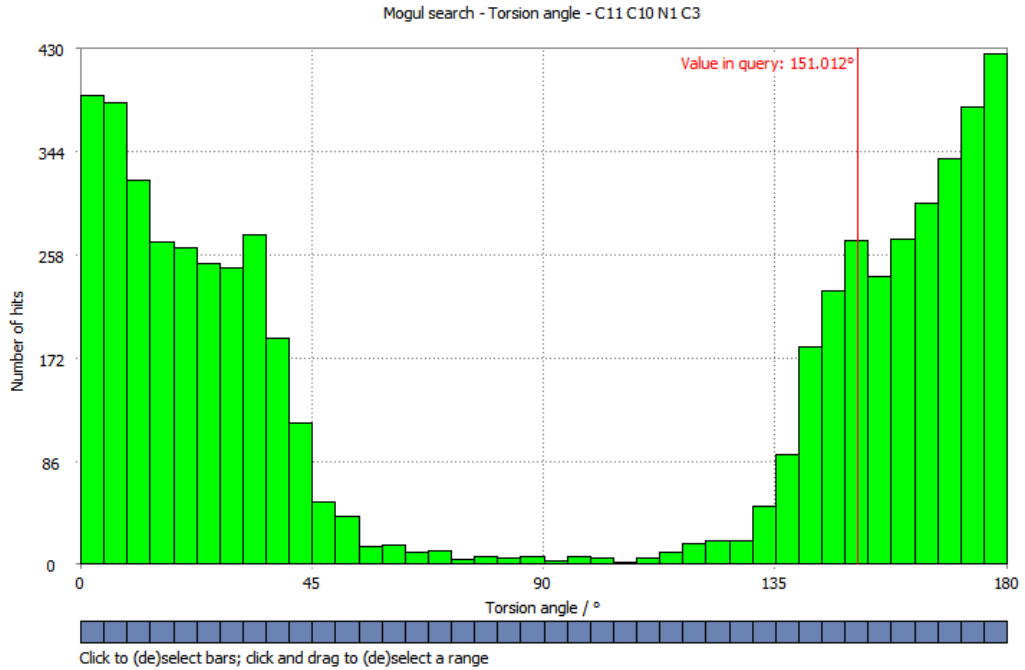
- Compare in more detail the conformations using Mogul Geometry Check.
- Compare fragments of target molecule to similar fragments in CSD to learn about expected values for bonds, angles and torsion angles.

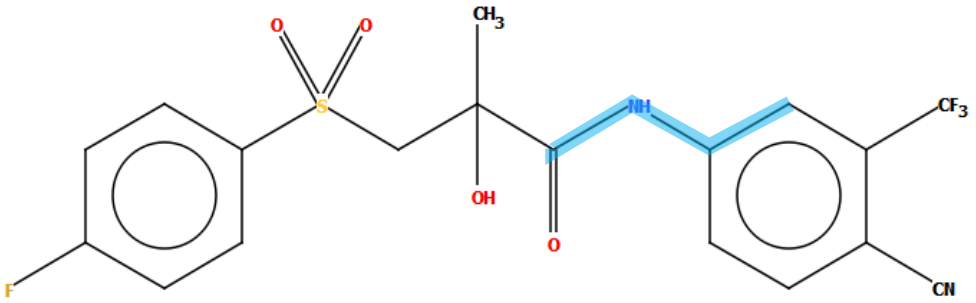
- Focus on torsion angles here.

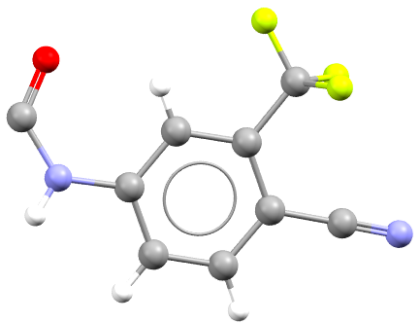


Learn more in the CSDU module

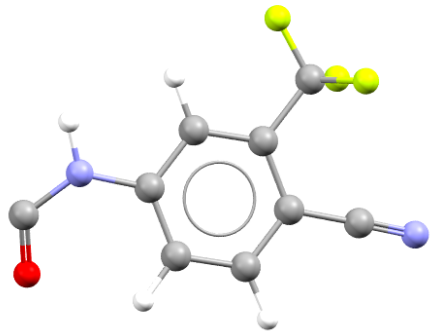
Molecular conformation







JAYCES02

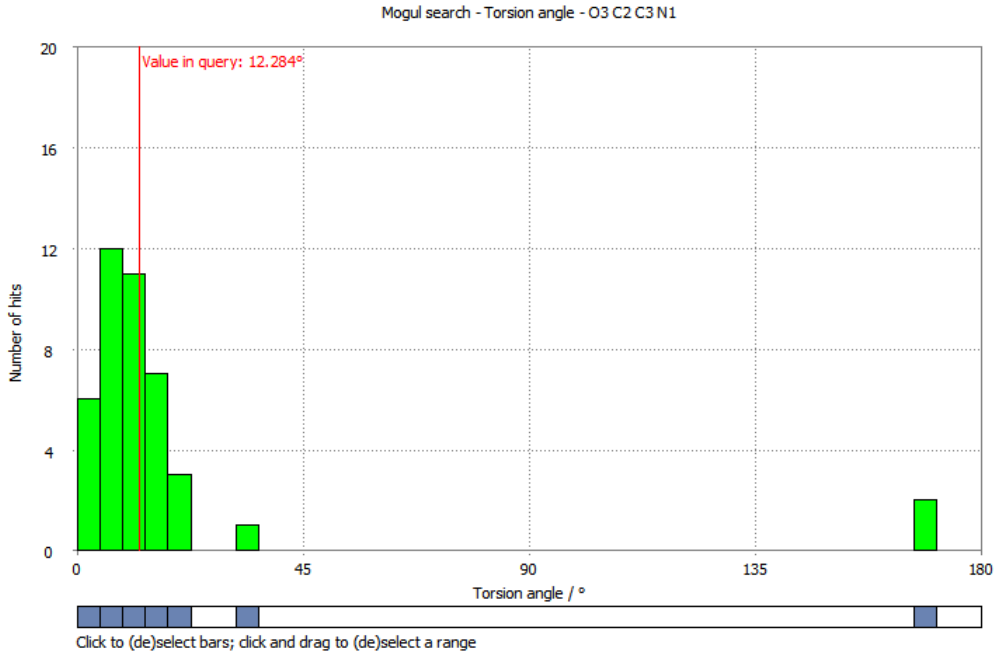


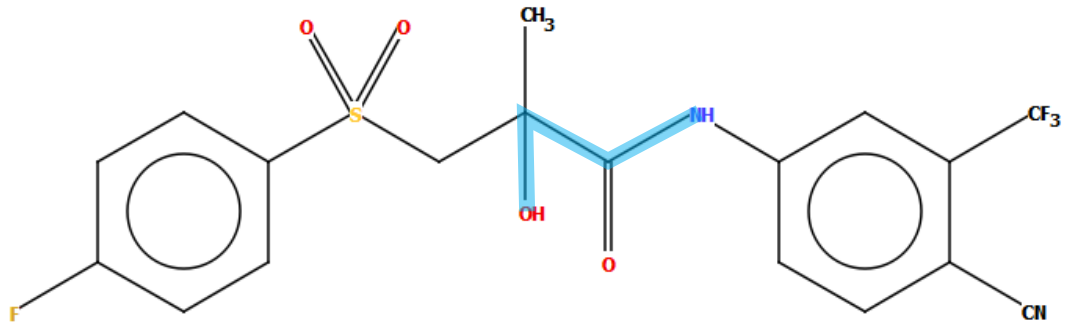
JAYCES03

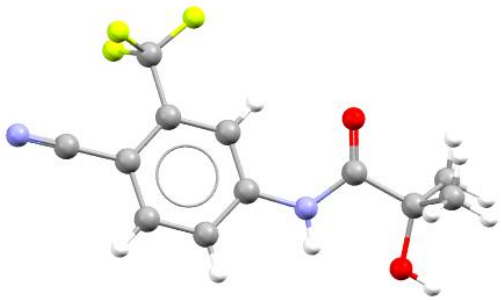
Both modes represented in polymorphs

CCDC

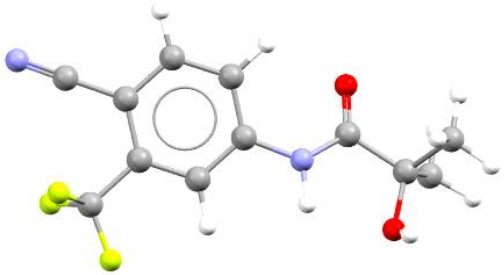
Molecular conformation







JAYCES03

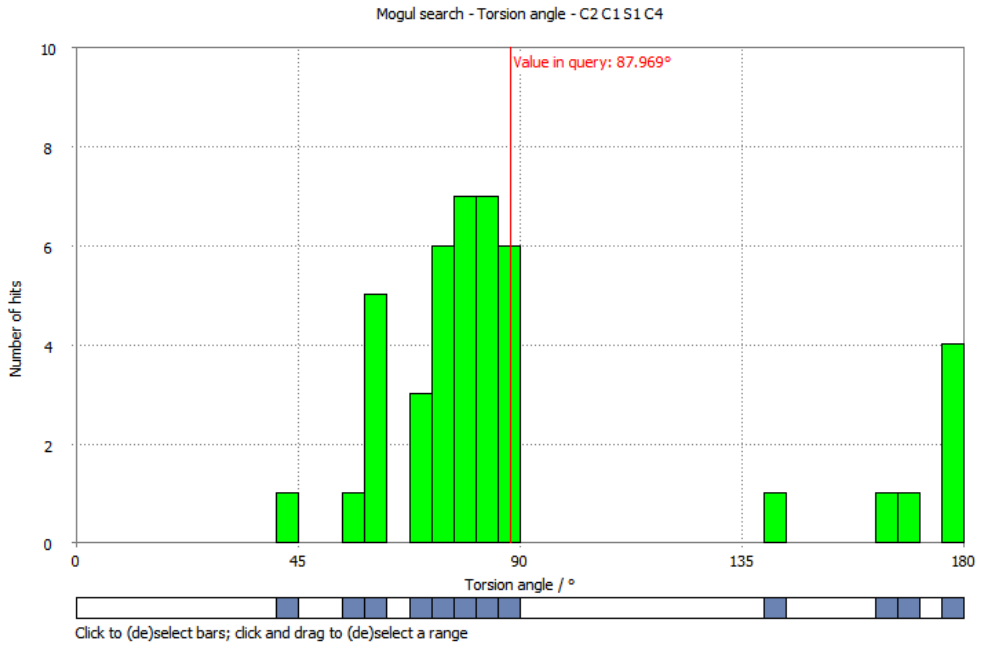


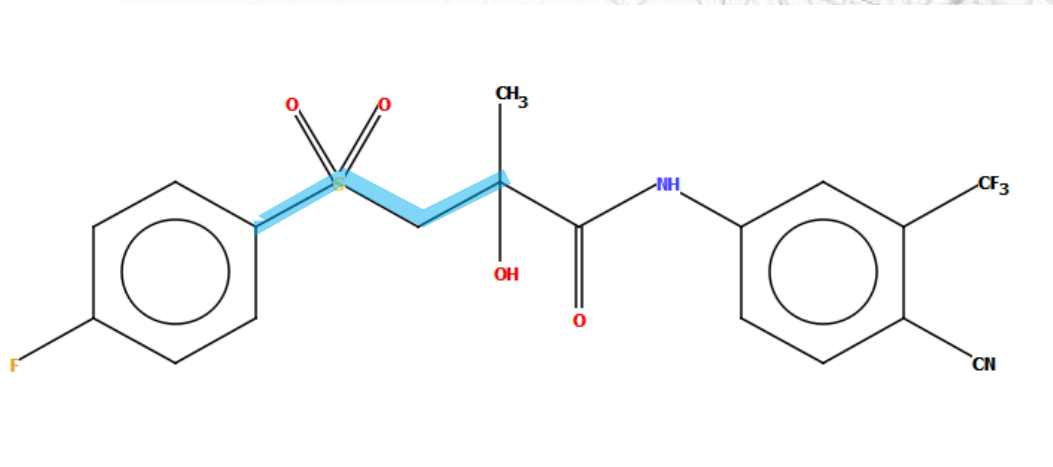
JAYCES02

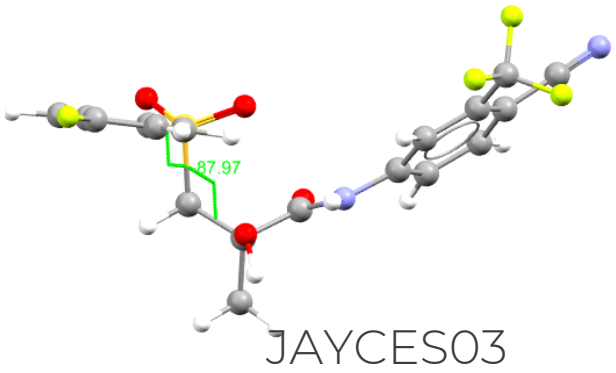
Major mode represented in polymorphs

CCDC

Molecular conformation







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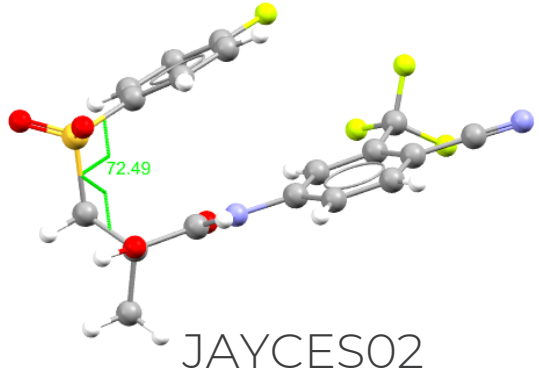


JAYCES02

Not very many hits, but can see usual ± 60°, 180° expected for saturated carbons. Flexibility expected and polymorphs show different conformations

CCDC

Context from CSD

JAYCES03

O4 C3 N1 C10	Not unusual (enough hits)	1093	5.897		0.000	**0.993**
C2 C3 N1 C10	Not unusual (enough hits)	86	-175.997		0.000	**0.988**
C2 C1 S1 O1	Not unusual (enough hits)	86	28.544		0.000	**0.209**
C2 C1 S1 O2	Not unusual (enough hits)	86	156.366		0.000	**0.198**
C2 C1 S1 C4	Not unusual (enough hits)	43	-87.969		0.000	**0.442**
O3 C2 C1 S1	Not unusual (enough hits)	40	56.932		0.000	**0.650**
C3 C2 C1 S1	Not unusual (enough hits)	41	-63.316		0.000	**0.634**
C18 C2 C1 S1	Not unusual (enough hits)	41	179.240		0.000	**0.585**
O3 C2 C3 O4	Not unusual (enough hits)	45	-169.517		0.000	**0.622**
O4 C3 C2 C1	Not unusual (enough hits)	45	-49.981		0.000	**0.600**
O4 C3 C2 C18	Not unusual (enough hits)	42	68.128		0.000	**0.619**
O3 C2 C3 N1	Not unusual (enough hits)	42	12.284		0.000	**0.833**
C1 C2 C3 N1	Not unusual (enough hits)	45	131.820		0.000	**0.622**
C18 C2 C3 N1	Not unusual (enough hits)	42	-110.070		0.000	**0.595**
C5 C4 S1 O1	Not unusual (enough hits)	3428	-27.176		0.000	**0.242**
C5 C4 S1 O2	Not unusual (enough hits)	3428	-156.564		0.000	**0.242**
C5 C4 S1 C1	Not unusual (enough hits)	1611	89.341		0.000	**0.439**
C9 C4 S1 O1	Not unusual (enough hits)	3428	152.182		0.000	**0.239**
C9 C4 S1 O2	Not unusual (enough hits)	3428	22.794		0.000	**0.238**
C9 C4 S1 C1	Not unusual (enough hits)	1611	-91.301		0.000	**0.435**
C11 C10 N1 C3	Not unusual (enough hits)	5718	151.012		0.000	**0.188**
C15 C10 N1 C3	Not unusual (enough hits)	5718	-30.686		0.001	**0.187**
F2 C16 C12 C11	Not unusual (enough hits)	5739	0.215		0.000	**0.144**
F2 C16 C12 C13	Not unusual (enough hits)	2164	-179.117		0.000	**0.173**
F3 C16 C12 C11	Not unusual (enough hits)	5739	-120.517		0.000	**0.278**
F3 C16 C12 C13	Not unusual (enough hits)	2164	60.152		0.000	**0.326**
F4 C16 C12 C11	Not unusual (enough hits)	5739	121.409		0.000	**0.277**
F4 C16 C12 C13	Not unusual (enough hits)	2164	-57.923		0.000	**0.332**

"Not Unusual" classification for torsions in both polymorphs
Conformations different, but not expecting one to be much higher in energy

CCDC

Cocrystals of the antiandrogenic drug bicalutamide: screening, crystal structures, formation thermodynamics and lattice energies†

Artem O. Surov,[a] Katarzyna A. Solanko,[b] Andrew D. Bond,‡[b] Annette Bauer-Brandl[b] and German L. Perlovich*[a]

4822 | *CrystEngComm*, 2016, **18**, 4818–4829

CrystEngComm

Bicalutamide is known to be a flexible molecule, which displays the so-called conformational polymorphism in the solid state.[19] Comprehensive conformational analysis performed by Dhaked *et al.*[39] and Le *et al.*[10] using quantum chemical calculations has indicated that molecular conformations of **Bic** in polymorphs I and II belong to different energy minima separated by a relatively low energy barrier. The form II conformation, however, was found to be a relatively higher-energy state, at least in the gas phase.

Form II

Table 2 Different torsion angles (°), absolute and relative energies of various conformations of bicalutamide at B3LYP/6-31+G(d,p) method

Structures	τ1	τ2	τ3	τ5	τ6	OH13 interaction	NH17 interaction	Absolute energy[a] (a.u.)	Relative energy (kcal/mol)
1	−171	−70	130	−177	−26	H···O9	N17–H···O13	−1902.04437	0.00
1a	−165	−49	71	180	−88	H···O16	–	−1902.03189	7.83
1b	159	177	125	178	53	H···O10	N17–H···O13	−1902.04532	−0.60
1c	165	158	−79	179	−98	H···O16	–	−1902.03014	8.93
1d	−171	89	−58	−177	−130	H···O16	N17–H···O10	−1902.04258	1.12
1e	148	56	−75	−172	−110	H···O16	N17–H···O10	−1902.03944	3.09
2	79	−73	139	0	−34	H···O10	N17–H···O13	−1902.04431	0.04

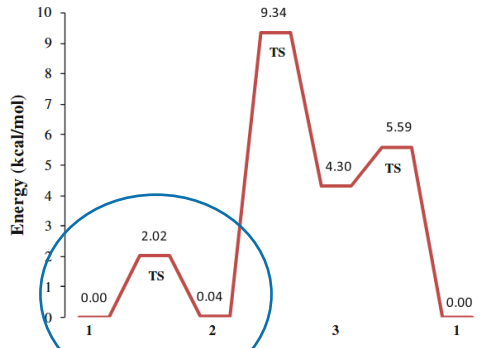
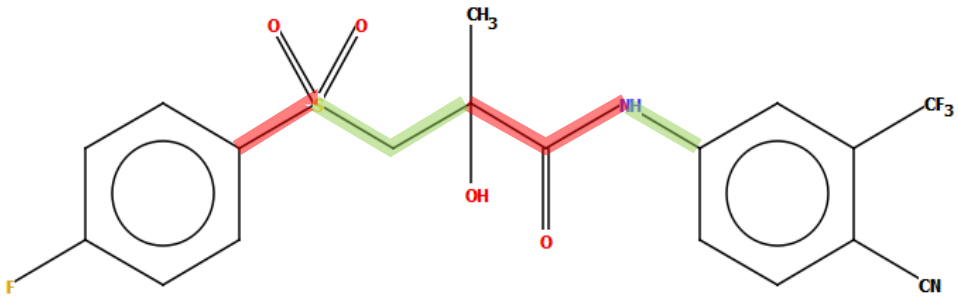


Fig. 4 Energy profile (kcal/mol) for the interconversion of conformations **1**, **2**, and **3** in the gas phase calculated at B3LYP/6-31+G(d,p) level of theory

Molecular conformation

- Identify parts of the molecule which have potential to be flexible.
- Understand how geometry of polymorphs differ.
- Understand if torsion angles are unusual.
- Gain insights into risk of polymorphism.



Polymorphs have different conformations but no unusual torsion angles. Don't expect one conformation to be significantly different in energy to the other.

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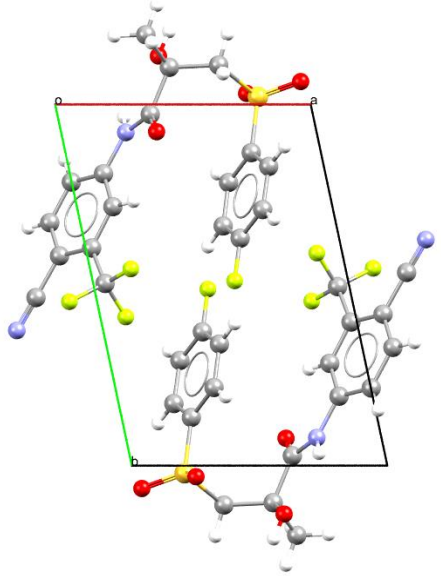
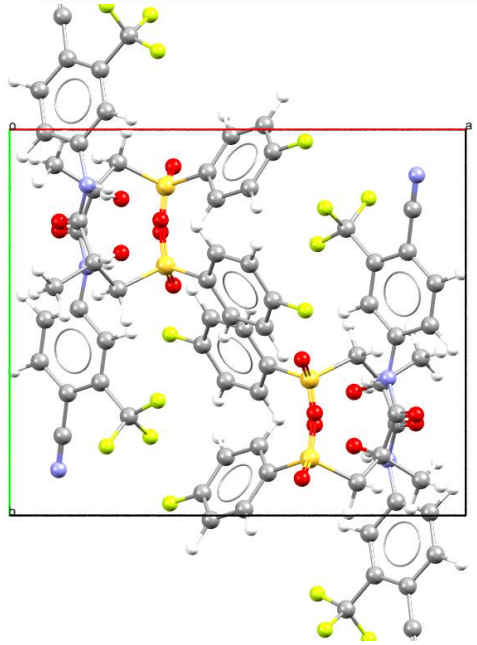
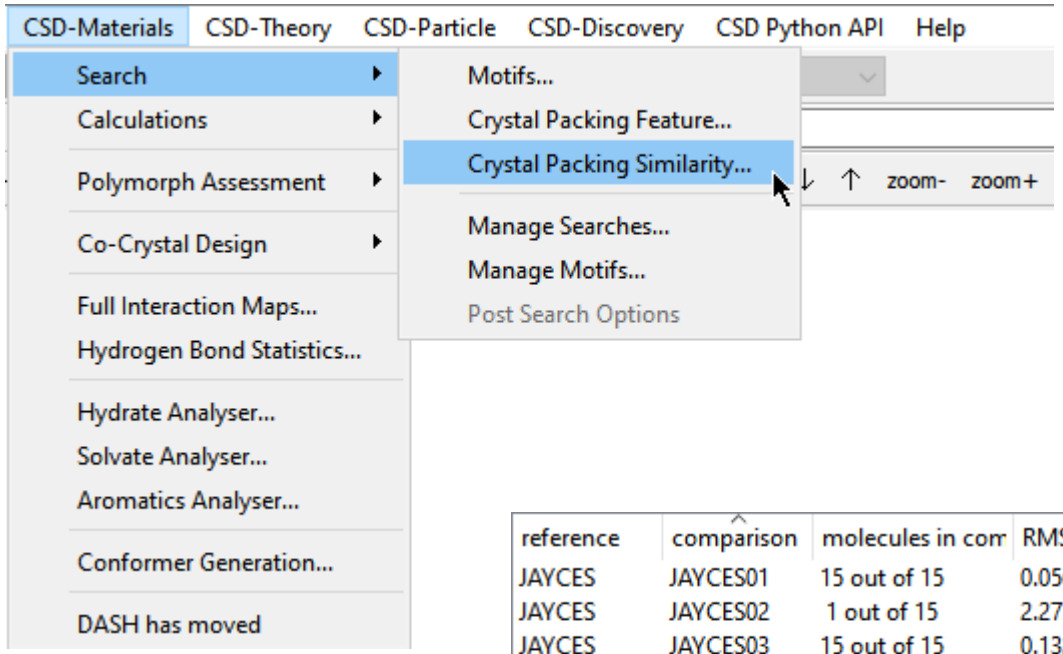
Intermolecular interactions and packing

- Look at the packing environment of the molecules using a range of tools.
- Use CSD for context (unusual hydrogen bond parameters for example) as well as enabling comparison of structures.

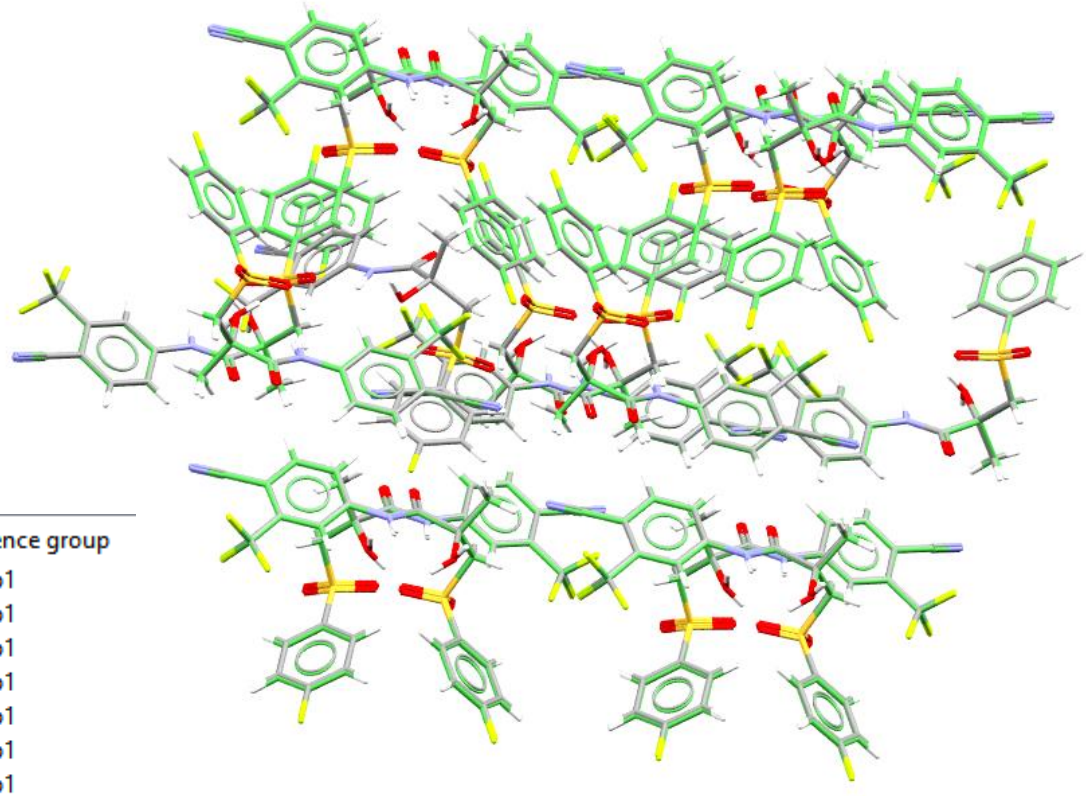




Packing

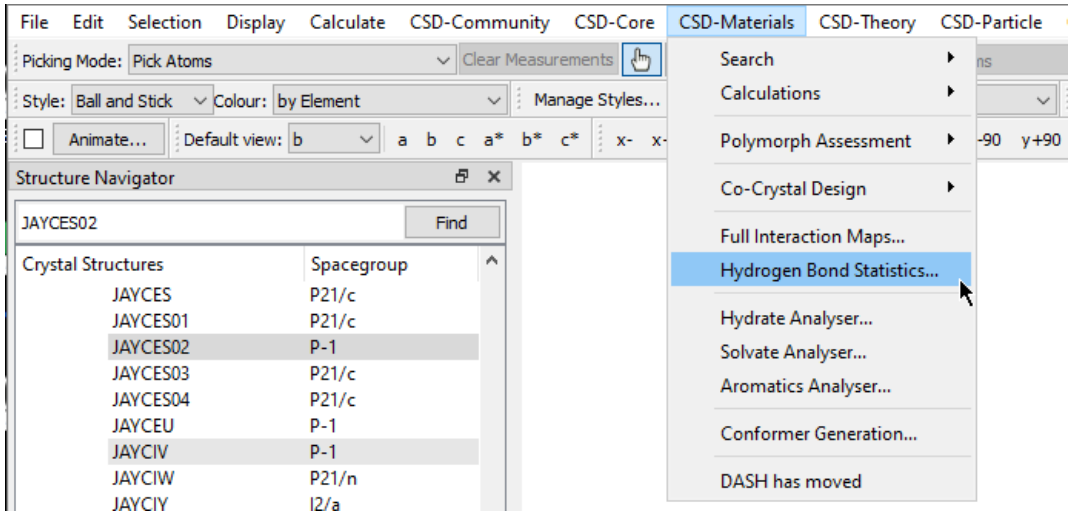


reference	comparison	molecules in com	RMS	reference group
JAYCES	JAYCES01	15 out of 15	0.056	group1
JAYCES	JAYCES02	1 out of 15	2.275	group1
JAYCES	JAYCES03	15 out of 15	0.132	group1
JAYCES	JAYCES04	15 out of 15	0.011	group1
JAYCES01	JAYCES02	1 out of 15	2.277	group1
JAYCES01	JAYCES03	15 out of 15	0.16	group1
JAYCES01	JAYCES04	15 out of 15	0.058	group1
JAYCES02	JAYCES03	1 out of 15	2.269	group2
JAYCES02	JAYCES04	1 out of 15	2.275	group2
JAYCES03	JAYCES04	15 out of 15	0.125	group1



CCDC

Intermolecular Interactions: Hydrogen bonds



- Using standardised functional group definitions searches for hydrogen bonds in CSD to compare to those found in the target structure.
- Returns assessment of length and angle of Hbond with respect to CSD-derived distributions.

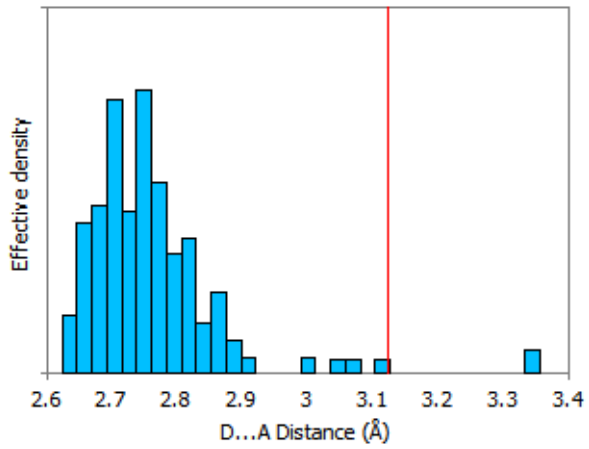
CCDC

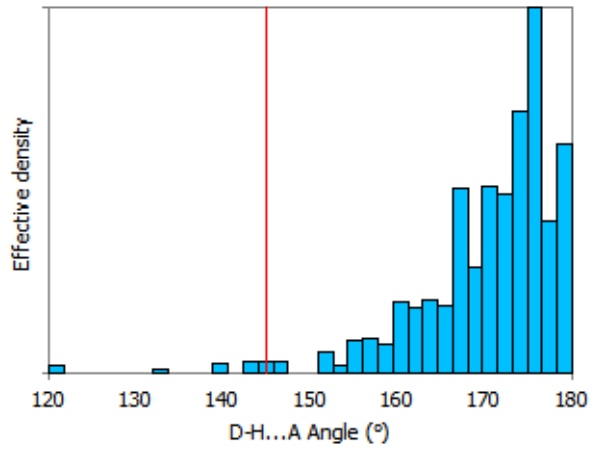
Hydrogen bonds

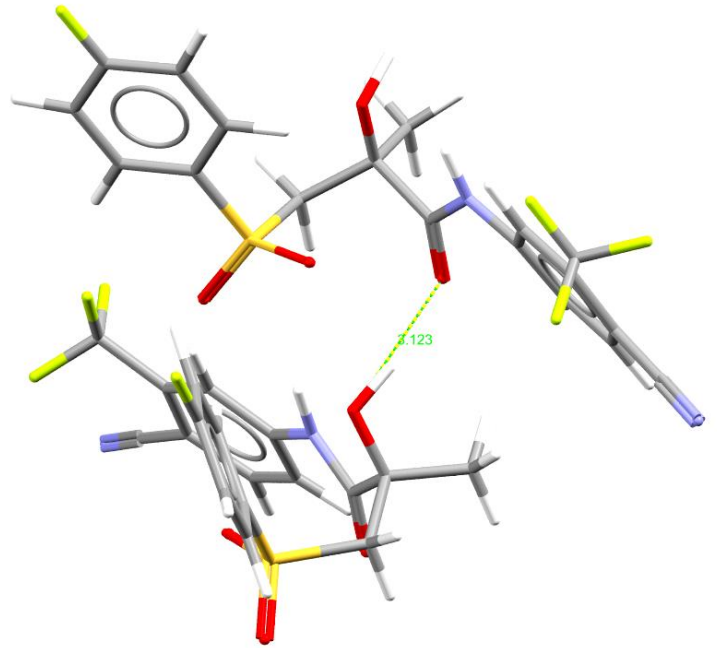
Hydrogen Bond Statistics ... JAYCES03

	Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
1	N1 (ar_al_trans_amide)	O2 (ar_al_sulfone)	**3.51**	Unusual	(2.94, 3.50)	8	3.22	0.25	2.91	3.51	152.93	Not Unusual	122.61	8	149.32	16.38	120.08	167.94
2	O3 (acyclic_al_oh)	O4 (ar_al_trans_amide)	**3.12**	Unusual	(2.65, 2.90)	103	2.76	0.10	2.63	3.34	**144.89**	Unusual	145.38	103	168.70	11.45	120.67	179.23

Results and analysis | View structures







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Hydrogen bonds

Hydrogen Bond Statistics ... JAYCES02

	Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
1	N1 (ar_al_trans_amide)	O2 (ar_al_sulfone)	3.15	Not Unusual	(2.94, 3.50)	8	3.22	0.25	2.91	3.51	148.17	Not Unusual	122.61	8	149.32	16.38	120.08	167.94
2	O3 (acyclic_al_oh)	N2 (ar_nitrile)	2.99	Not Unusual	(2.81, 3.08)	56	2.93	0.10	2.78	3.31	171.44	Not Unusual	143.84	56	167.95	12.75	125.90	179.54

- Hydrogen Bond Statistics allows you to assess hydrogen bond parameters in context of similar interactions from the CSD. Unusual geometries may suggest less stabilising interactions.

Hydrogen bonding is different between polymorphs, but both polymorphs show trans-amide to sulfone interaction

Not very many hits in CSD

H-bonding in JAYCES03 is classified as unusual: long non-linear interactions

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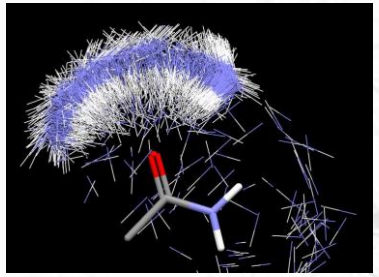
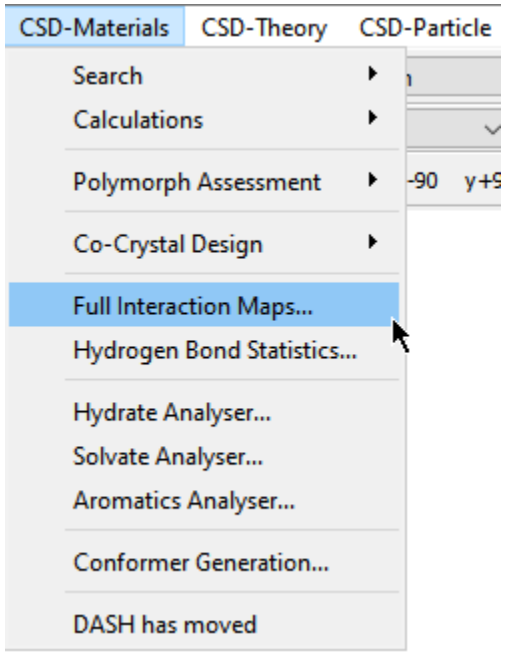
Full Interaction Maps

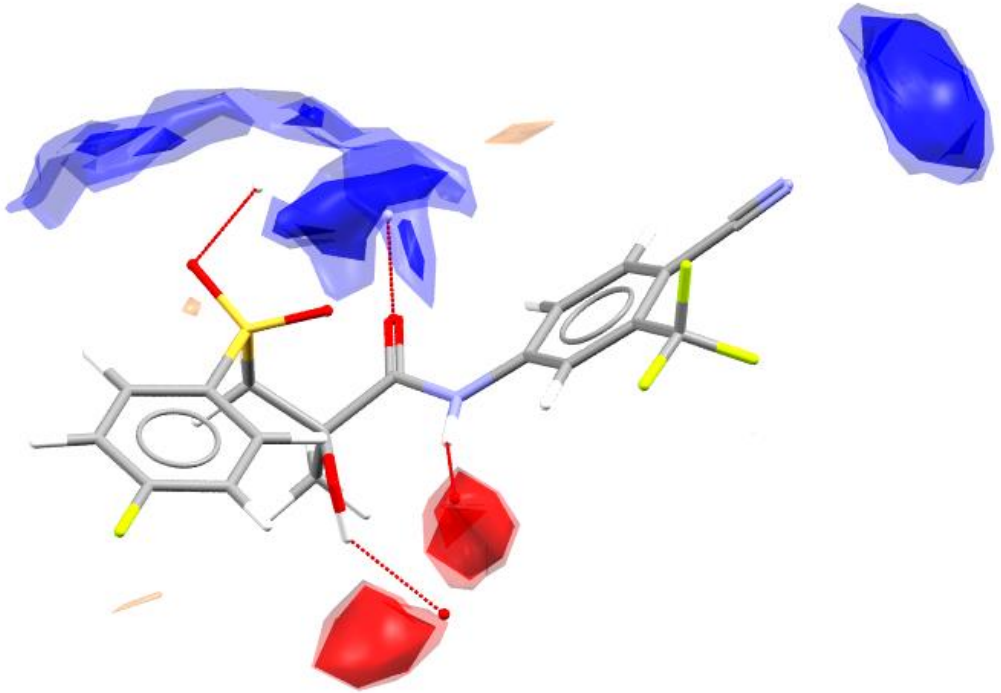




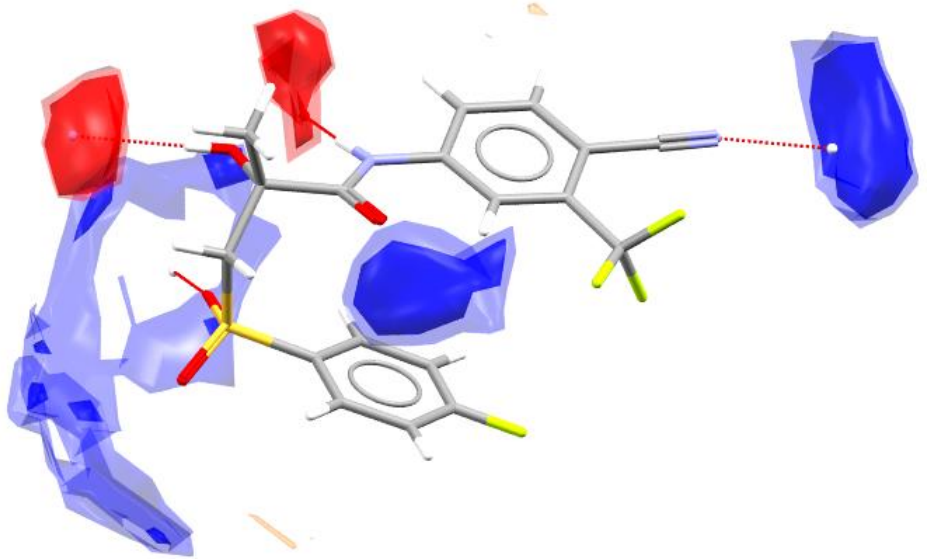
- Shows density maps for where functional groups are expected to be found for target molecule.
- Uses central groups (to model target molecule) and “probe” groups to map where interactions are expected.
- Very visual tool – allows you to see what an ideal packing environment should provide.

Learn more in the CSDU module

- Poor geometry of hydrogen bonds seen in FIMs too. Ideal packing environment not matched in either polymorph.

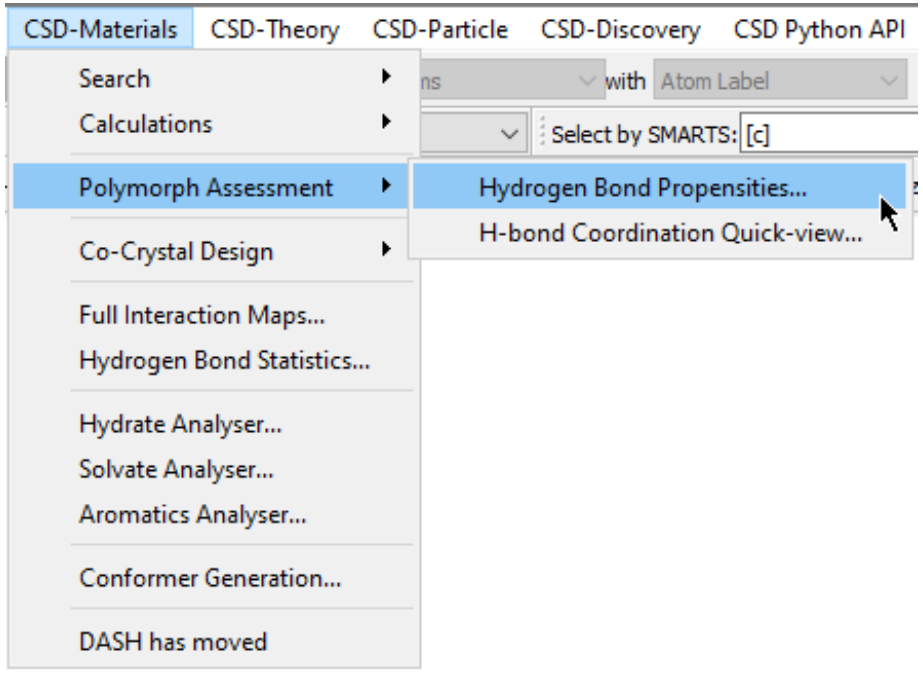


JAYCES03



JAYCES02

Hydrogen Bond Propensities



- Assesses donor-acceptor pairings and use of functional groups by modelling behaviour of functional groups in relevant structures from the CSD.
- For more details see: https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-materials-workshops/
  - "Exploring Hydrogen Bond Propensities" and "Investigating solid form stability: understanding Hydrogen Bond Propensities"

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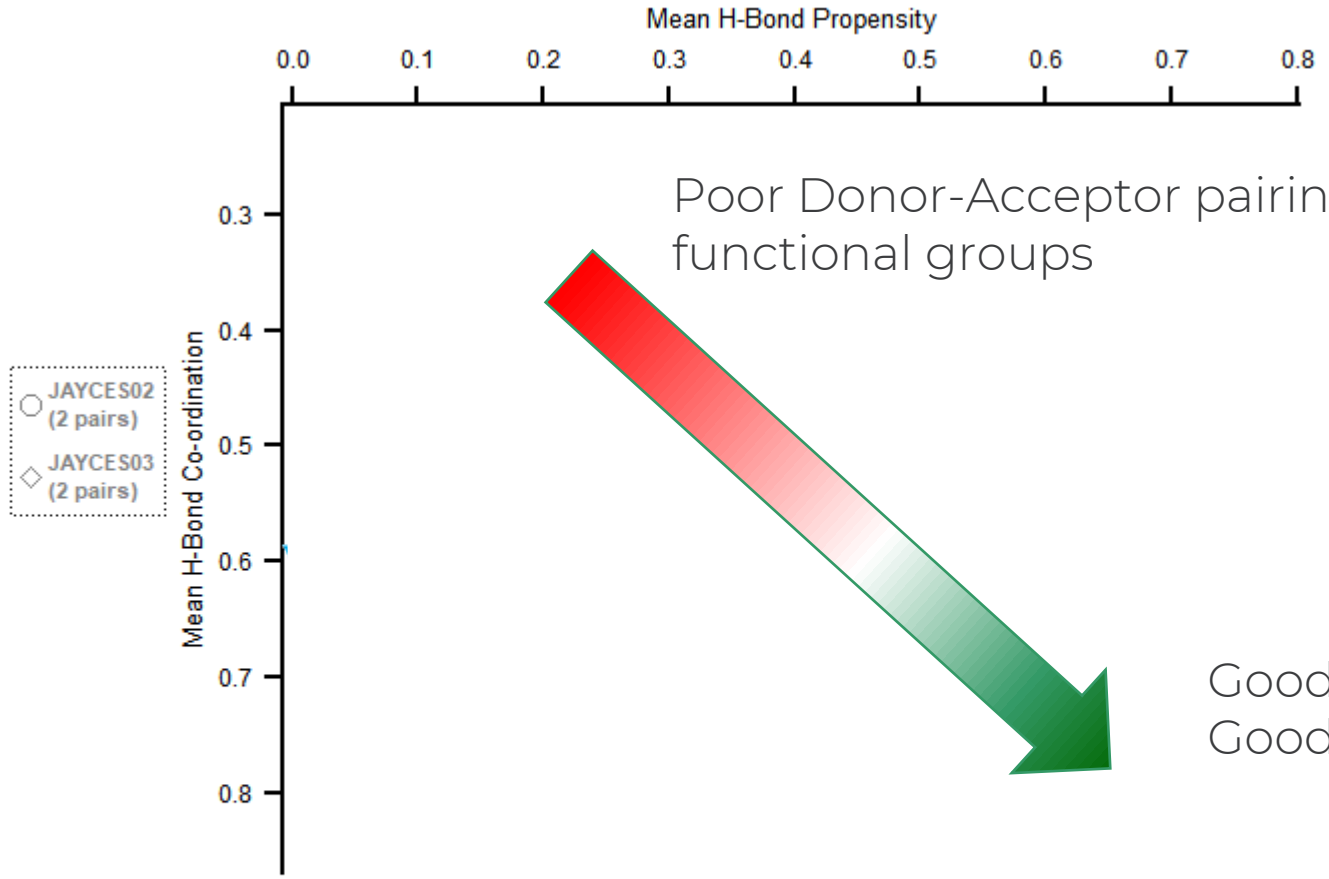
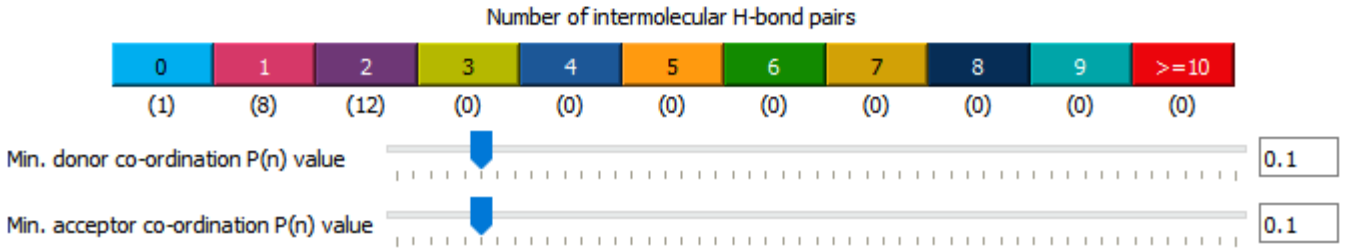
Hydrogen bond networks



Poor Donor-Acceptor pairings, Poor use of functional groups

Good Donor-Acceptor pairings, Good use of functional groups



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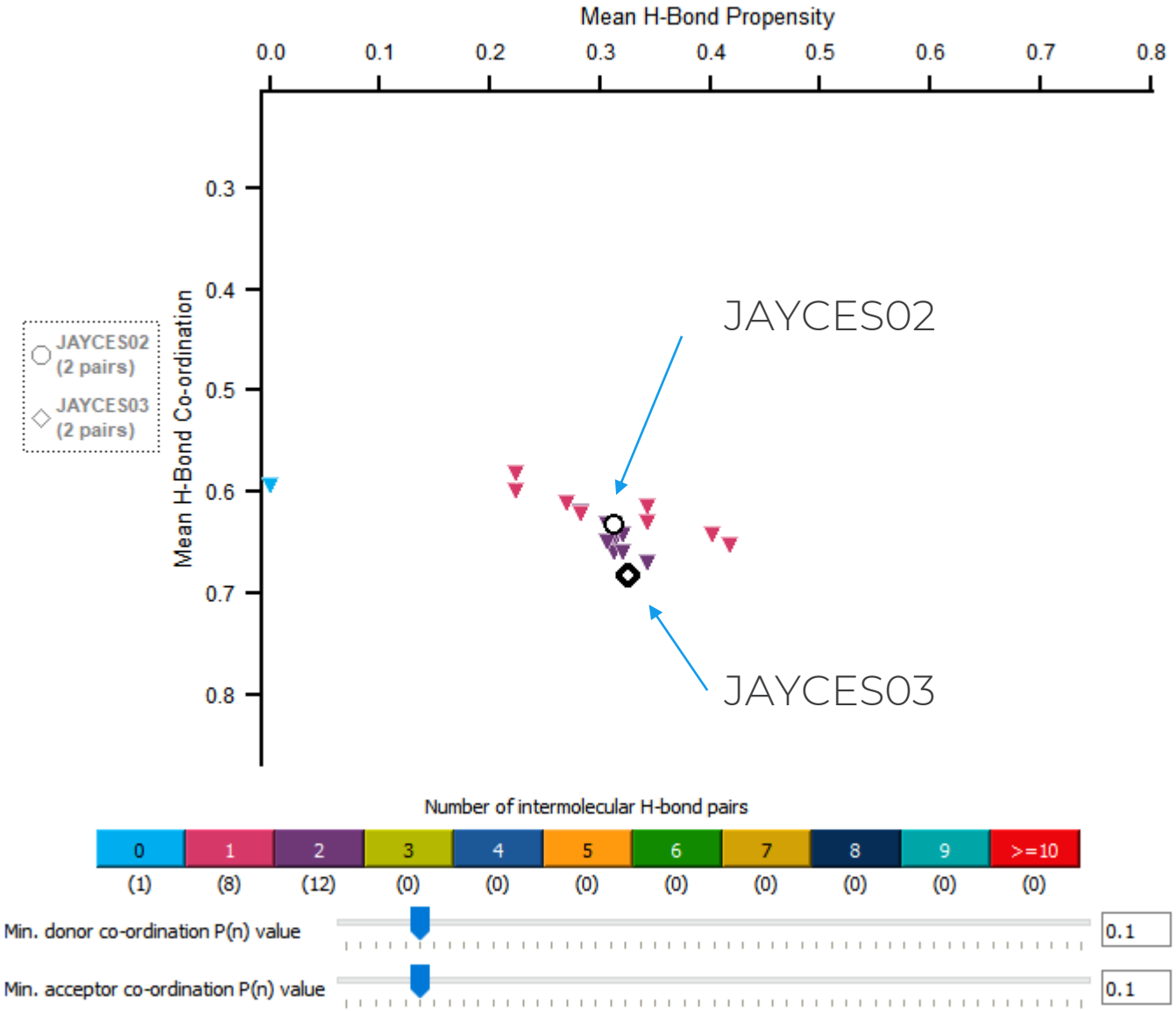
Hydrogen bond networks



Modelling from H-bond interactions in CSD suggests that JAYCES03 has a more likely H-bond network but propensities of interactions low

Donor	Acceptor	Polymorph
Acyclic_OH	O of trans_amide	JAYCES03
Acyclic_OH	N of ar_nitrile	JAYCES02
N of trans_amide	O of sulfone	JAYCES02/03

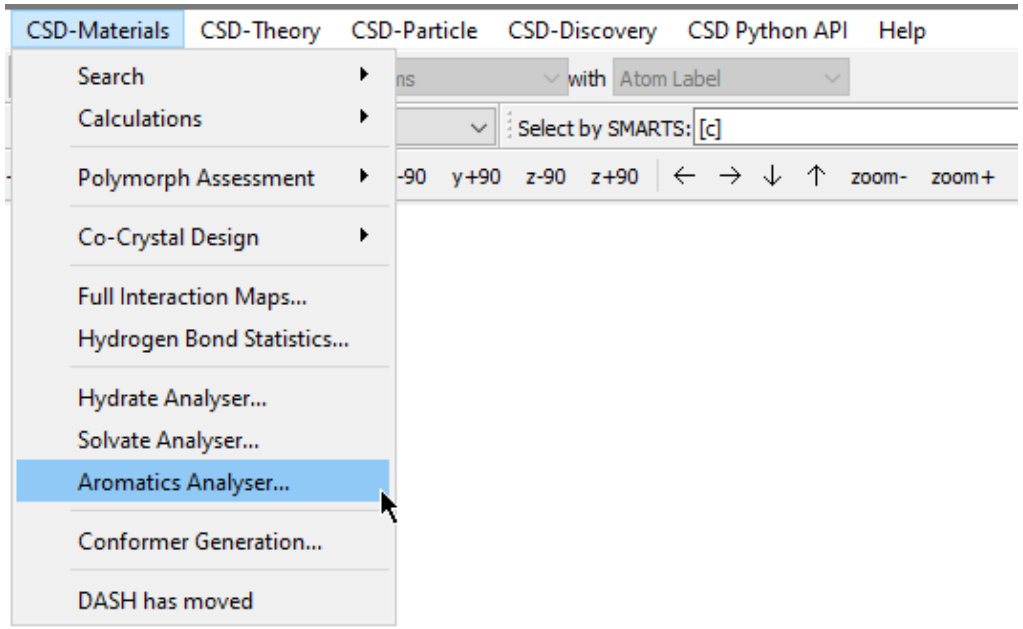
Hydrogen Bonding

- Use the CSD for context to understand if hydrogen bonds have unusual geometries and hence might be less stabilising.
- Understand the use of different donors and acceptors in the polymorphs in terms of predictions based on CSD data. Allows "ranking" of structures.
- Compare how packing environment matches "ideal" environment from Full Interaction Maps.

JAYCES02 has better geometry of interactions but poorer donor-acceptor pairings. Amide to sulfone interaction is "unusual" and Hydrogen bond propensities for both polymorphs are low.

CCDC

Aromatic Interactions



- Dataset of 25,000 benzene-ring pairs generated.
- Energies of interaction calculated.
- Neural network learned relationship between geometric parameters and energy.
- Assessment of strength of interaction between C_6 rings.

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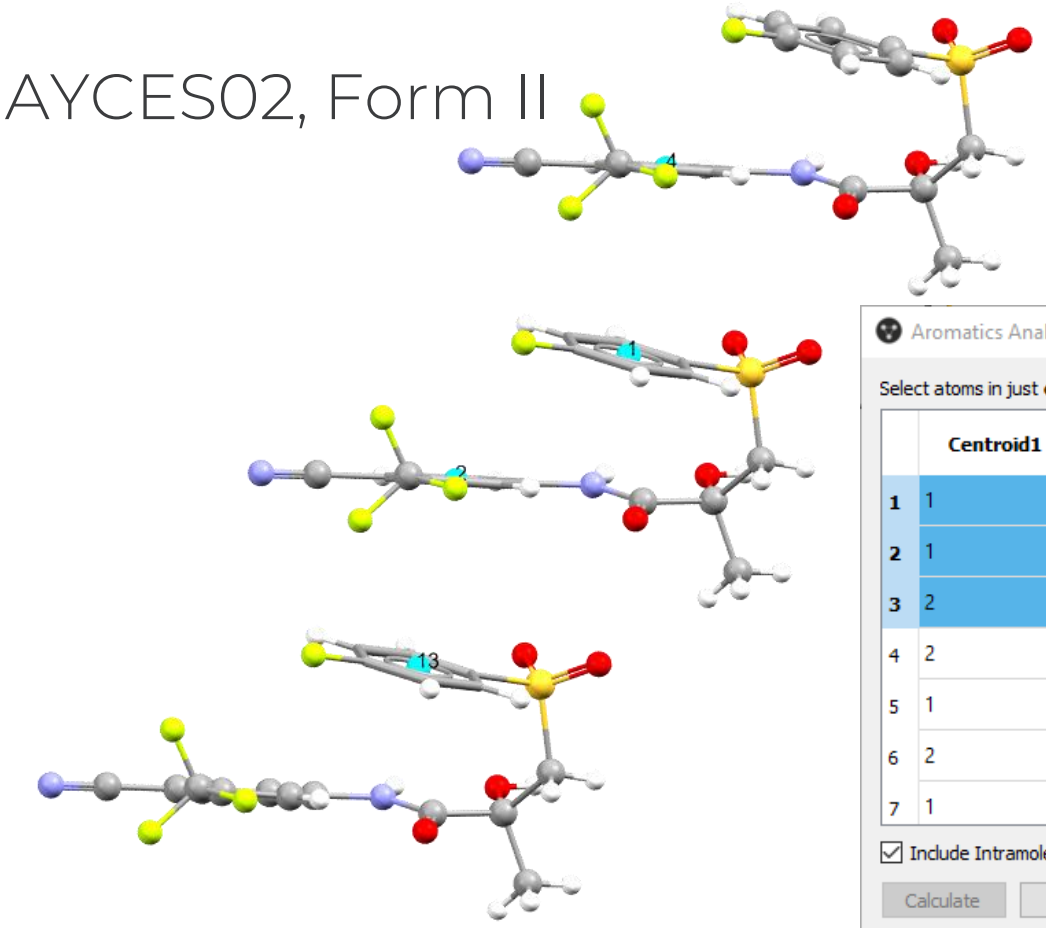
Aromatic Interactions

- JAYCES02, Form II



Aromatics Analyser... JAYCES02

Select atoms in just **one** molecule

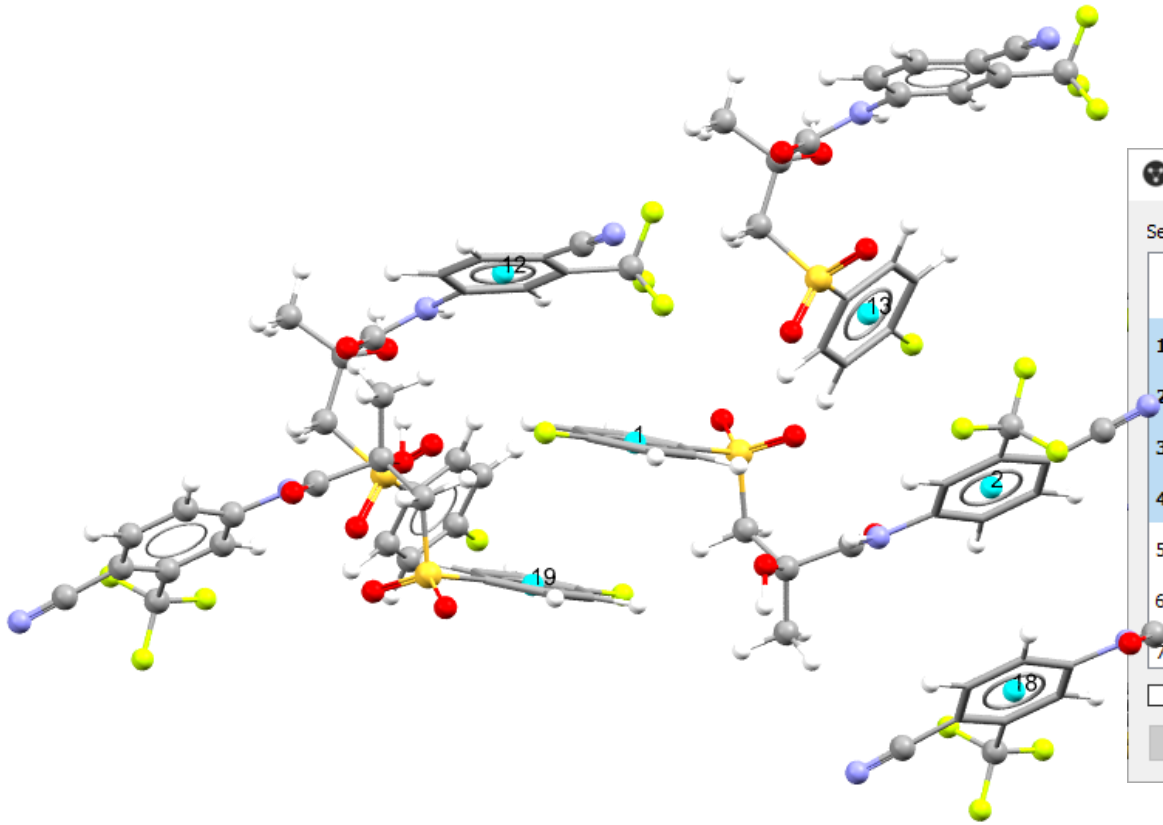
	Centroid1	Centroid2	Distance	Relative Orientation	Inter-molecular	Score	Assessment
1	1	2	5.03	13.3	No	7.7	Strong
2	1	4	3.89	13.3	Yes	7.7	Strong
3	2	13	3.89	13.3	Yes	7.7	Strong
4	2	24	5.19	0	Yes	5.8	Moderate
5	1	17	7.24	0	Yes	2.3	Weak
6	2	28	7.28	0	Yes	2.3	Weak
7	1	15	7.46	0	Yes	1.8	Weak

☑ Include Intramolecular pairs ☐ Exclude symmetry equivalent interactions

Calculate | Export | Atom info | Close

CCDC

- JAYCES03, Form I. Both aromatic rings show 2 strong interactions



Aromatics Analyser... JAYCES03

Select atoms in just **one** molecule

	Centroid1	Centroid2	Distance	Relative Orientation	Inter-molecular	Score	Assessment
1	1	19	4.33	0	Yes	8.6	Strong
2	2	18	4.7	0	Yes	7.8	Strong
3	1	12	5.1	25.64	Yes	7	Strong
4	2	13	5.1	25.64	Yes	7	Strong
5	1	21	6.78	0	Yes	3.6	Moderate
6	1	25	6.53	64.77	Yes	3.3	Moderate
7	1	27	6.53	64.77	Yes	3.3	Moderate

Include Intramolecular pairs Exclude symmetry equivalent interactions

Calculate Export m info Close

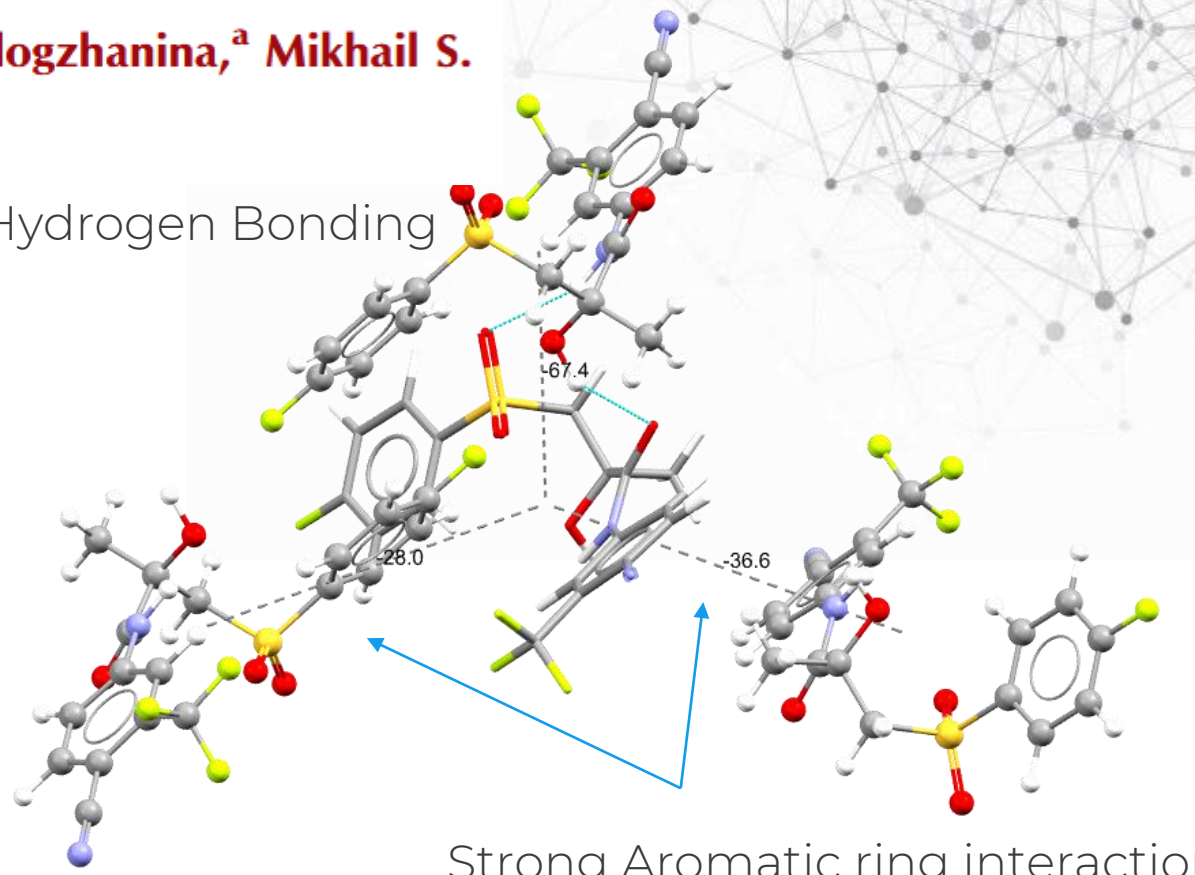
Charge density view on bicalutamide molecular interactions in the monoclinic polymorph and androgen receptor binding pocket

IUCrJ (2020). **7**, 71–82

Alexander A. Korlyukov,[a]‡ Maura Malinska,[b]‡ Anna V. Vologzhanina,[a] Mikhail S. Goizman,[c] Damian Trzybinski[b] and Krzysztof Wozniak[b]*

Table 3
Energies (kJ mol^{-1}) of intermolecular interactions in the **Bic** crystal structure calculated by the UNI force field and the dimer interaction energies calculated using *Crystal Explorer* based on the PIXEL method [CE-B3LYP/6-31 G(d,p)].

		UNI empirical force field	CE-B3LYP/6-31G(d,p)				
Symmetry operation	Dimer	E_{tot}	E_{el}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
$x, 1/2 - y, z - 1/2$	Dimer 1	−65.2	−42.9	−16.4	−54.0	52.7	−71.6
$-x, 1 - y, 1 - z$	Dimer 2	−37.0	−16.2	−4.5	−36.6	23.2	−37.9
$1 - x, 1/2 + y, 3/2 - z$	Dimer 3	−29.6	−17.8	−4.3	−13.1	6.8	−29.2
$1 - x, -y, 1 - z$	Dimer 4	−24.1	−8.8	−4.5	−34.6	24.3	−27.7
$x, 3/2 - y, z - 1/2$	Dimer 5	−17.4	−12.1	−4.5	−19.9	14.4	−24.5
$x, -1 + y, z$	Dimer 6	−16.8	−14.3	−4.6	−15.3	15.1	−22.6



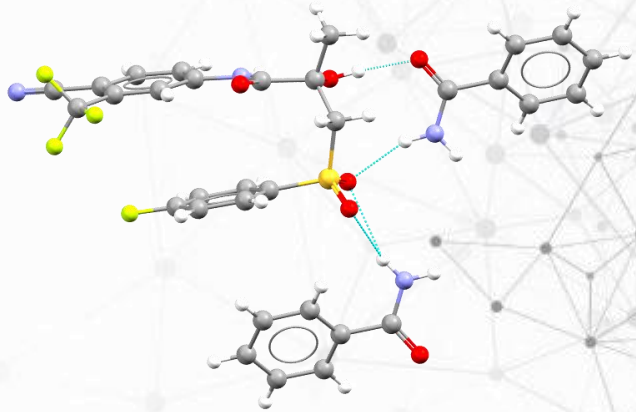
CCDC

What did we learn?

- Molecule has potential to be conformationally flexible – and different conformations realised in polymorphs.
- Conformations different but no suggestion that one is significantly higher in energy.
- Hydrogen bond interactions differ and geometry looks better in JAYCES02 but donor-acceptor pairings look better in JAYCES03. Neither structure has very good interactions.
- Aromatic interactions look very good in JAYCES03.
- Happy with hydroxy proton position? Multicomponent forms?

CCDC

Experimentally



- JAYCES03 is more stable polymorph.
- 4 cocrystals and 1 solvate of bicalutamide in CSD – and in all multicomponent forms, no bicalutamide-bicalutamide hydrogen bonding is retained.

- Get to know your polymorphs better!
  Comparison of polymorphs and the addition of context from the CSD can help understand the difference between the solid forms and may highlight areas to explore experimentally

CCDC

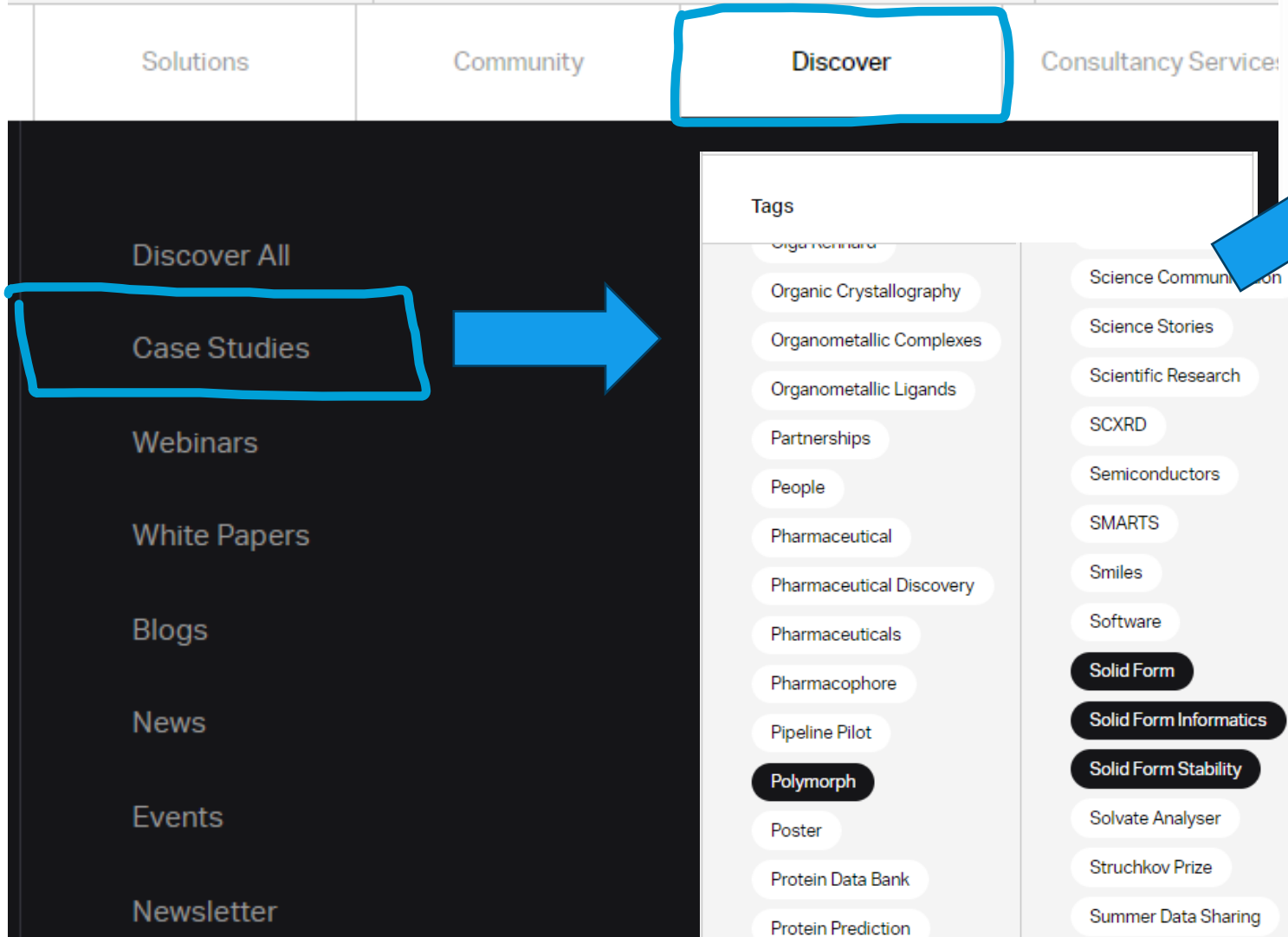
What have we learnt today?

- Understood the value of analysing polymorphic structures to assess their stability.
- Re-familiarised with the basics of Mercury, Mogul and Isostar.
- Explored what tools are available in the CSD-Materials suite and learnt how they can be used to compare solid forms, including:
    - Mogul Geometry Check, Hydrogen Bond Statistics, Hydrogen Bond Propensities, Aromatics Analyser, Overlay tools and Full Interaction Maps (FIMs).
- Learnt how these tools have been used in industry and what a workflow for assessing solid forms might look like.
- Gained confidence in the software used today so you can apply the techniques on your own systems/structures.

CCDC

Want to explore more?

Case studies



Unlocking Solid Form Innovation in CSD-Materials

Blog Hydrogen Bond Mercury Solid Form Stability

Investigating Solid Form Stability: Understanding Hydrogen Bond Propensity in Mercury

Blog CSD Landscape Generator. CSD-Theory Polymorph Solid Form Informatics

How to Generate a Solid Form Landscape without a Crystal Structure with C

Blog CSD-Materials Solid Form Informatics

How to Analyse Hydroge

Blog CSD-Materials Drug Development Matwall Pharmace

Matwall: materials knowl development to comme

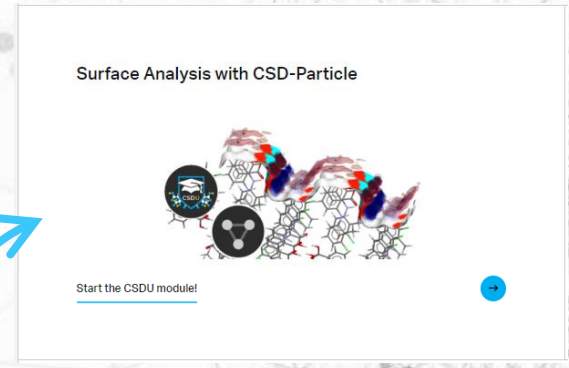
Want to explore more?

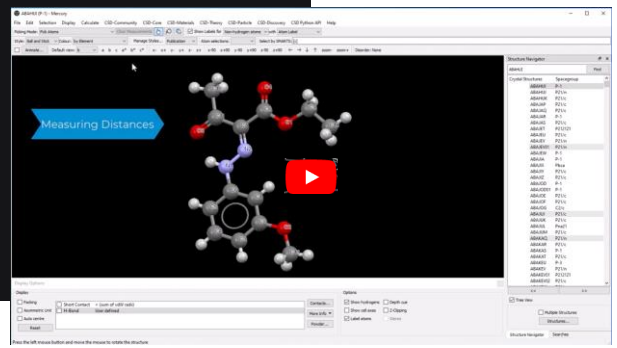
On-demand training resources

Solutions | Community | Discover | Consultancy

- Access/Deposit Structures
- CCDC for the Community
- Education and Outreach
- Events
- Free Products
- Training and Learning

- Free Online Courses
- Self-Guided Workshops
- Training and Support Videos





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Free online training courses

With completion certificates!

CSDU

On-demand modules to learn how to use the CSD software at your own pace.

UWatch • UTry • UTest

Mercury

Python API

WebCSD

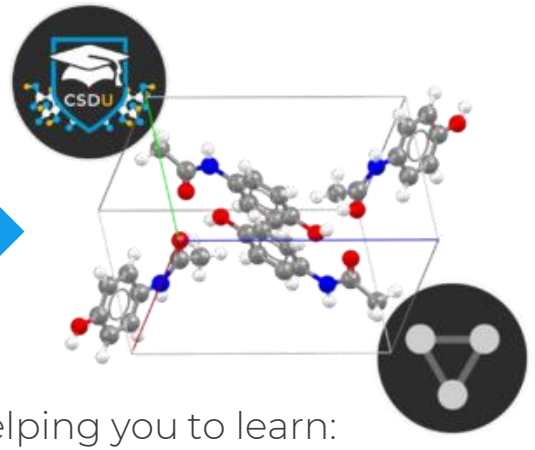
GOLD Docking

Mogul

FIMs

Particle

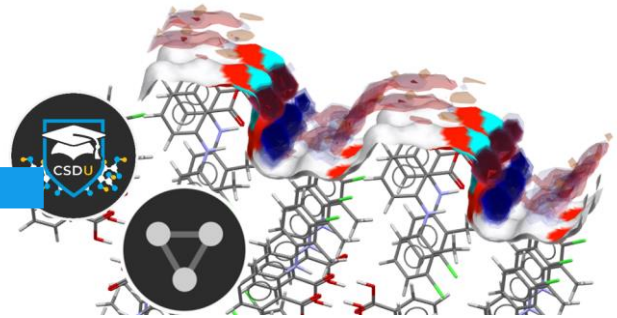
Visualization 101



Helping you to learn:

- The basics of Mercury software.
- How to explore and pack structures.
- How to create high resolution images.

Surface analysis



Helping you to learn:

- The basics of CSD-Particle.
- How to perform a surface analysis.
- How to visualise likely interactions with the surface using Full Interaction Maps (also a CSDU course!).

https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/

Upcoming Events

CCDC Webinar: The Role of Quality Data in Advancing AI and ML in Life Sciences

Date: 30 May 2024

Read More →

Find all webinars, training and events and links to registration from this webpage!

https://www.ccdc.cam.ac.uk/community/events/

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