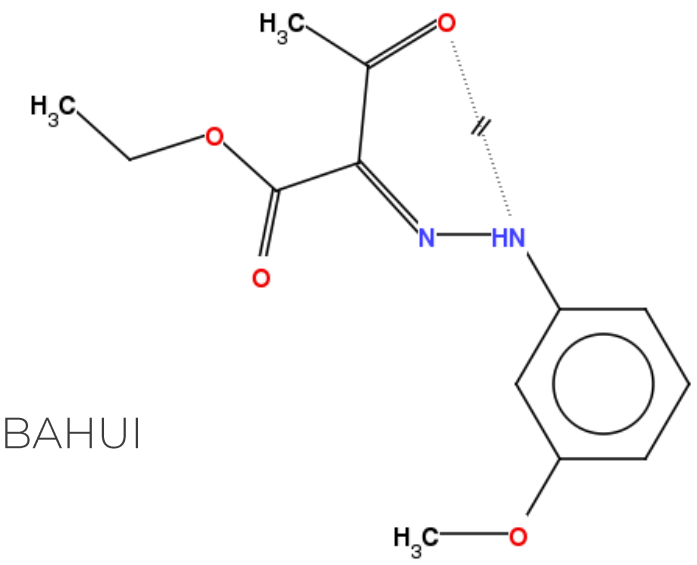
Other API features

Generating 2D diagrams

`ccdc.diagram` module allows you to create 2D diagrams from CSD entries or substructures.



CSD-ABAHUI

Crystal Module

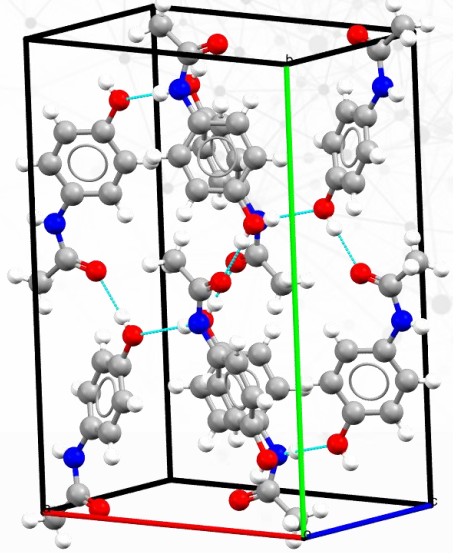
`crystal.contacts()`

The `Crystal` module contains information on close contacts within the structure

`.length`
`.strength`
`.type`
`.intermolecular`

`crystal.hbonds()`

Information on hydrogen bonds within the crystal structure



Combined Searches

The `CombinedSearch` class allows combination of different types of searches.

CCDC

Molecule

`molecule.rings`

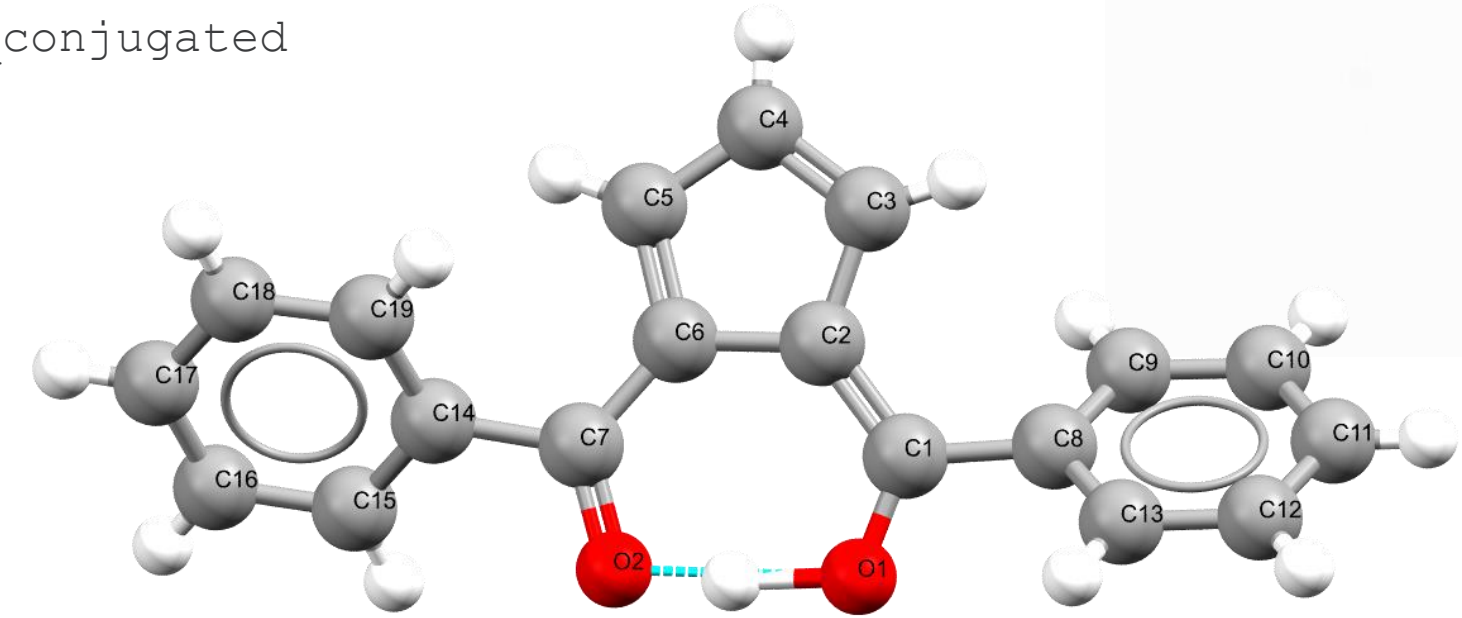
Access to rings of a molecule

```
.is_aromatic
.is_fused
.is_fully_conjugated
```

`molecule.contacts()`

Close contacts identified within the molecule

```
.atoms
.intermolecular
.length
.strength
```



`molecule.hbonds()`

Hydrogen bonds within the molecule

```
.atoms
.angle
.length
.da_distance
```

CSD-POCTOS

Barbara Enk, Benno Bildstein, Klaus Wurst, *Zeitschrift fur Kristallographie - New Crystal Structures*, 2009, 224, 544

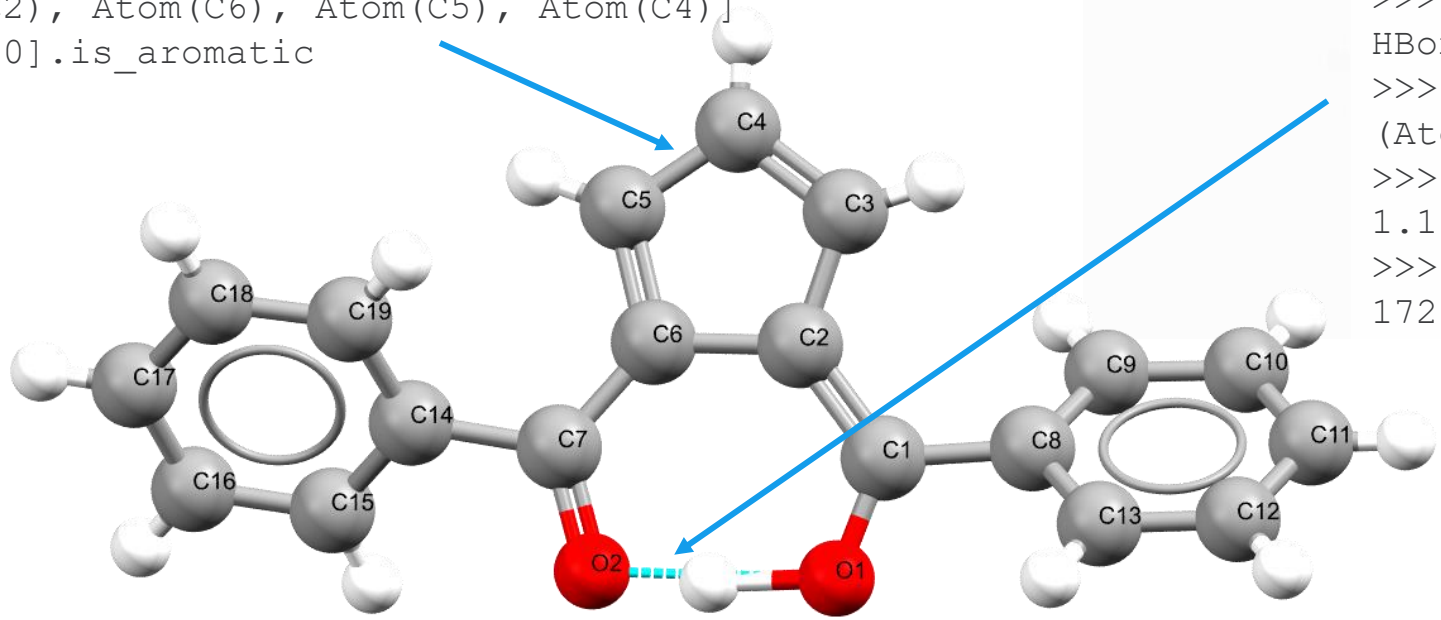
CCDC

Molecule

```
p = csd.entry('POCTOS')
poctos = p.molecule
```

molecule.rings

```
>>> poctos.rings[0]
Atom(C3)-Atom(C2)-Atom(C6)-Atom(C5)-Atom(C4)
>>> poctos.rings[0].atoms
[Atom(C3), Atom(C2), Atom(C6), Atom(C5), Atom(C4)]
>>> poctos.rings[0].is_aromatic
False
```



molecule.hbonds()

```
>>> poctos.hbonds()[0]
HBond(Atom(O2)-Atom(H1)-Atom(O1))
>>> poctos.hbonds()[0].atoms
(Atom(O2), Atom(H1), Atom(O1))
>>> poctos.hbonds()[0].length
1.1758648276493127
>>> poctos.hbonds()[0].angle
172.08777970837588
```

CSD-POCTOS

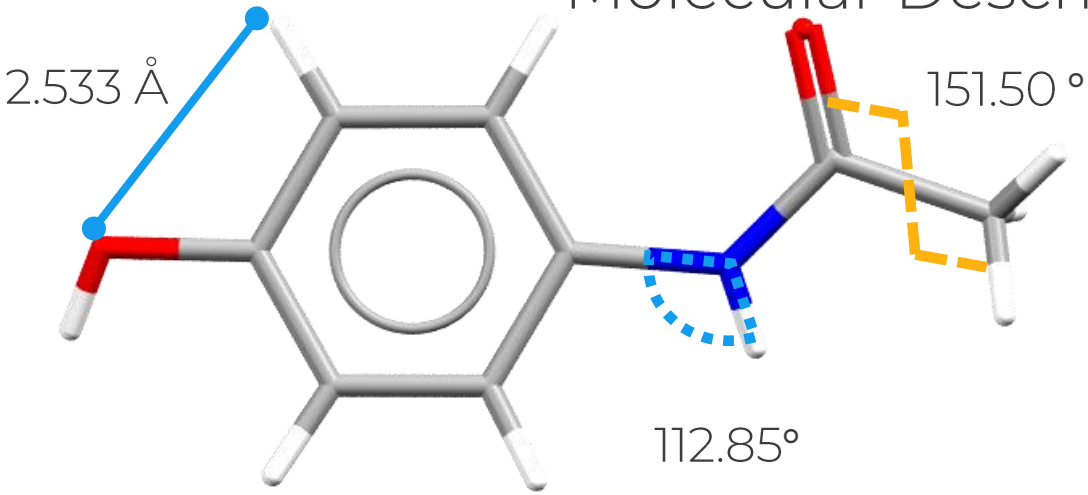
Barbara Enk, Benno Bildstein, Klaus Wurst, *Zeitschrift fur Kristallographie - New Crystal Structures*, 2009, 224, 544

CCDC

Descriptors

The `ccdc.descriptors` module contains a number of classes for calculating descriptors.

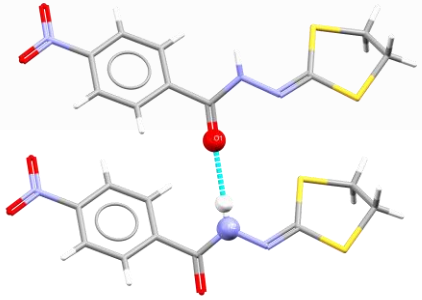
Molecular Descriptors



Statistical Descriptors

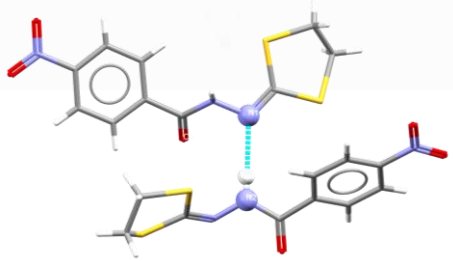
- Ranking statistics

Hydrogen Bond Propensities



DEDMUX

Form I

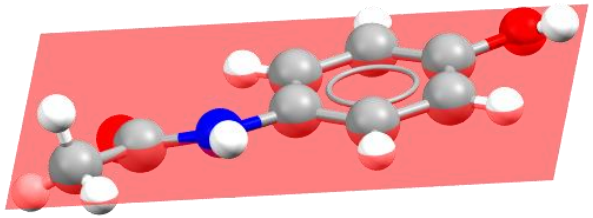


DEDMUX02

Form II

Geometric Descriptors

- Planes, Vectors, Spheres



Documentation: https://downloads.ccdc.cam.ac.uk/documentation/API/modules/descriptors_api.html

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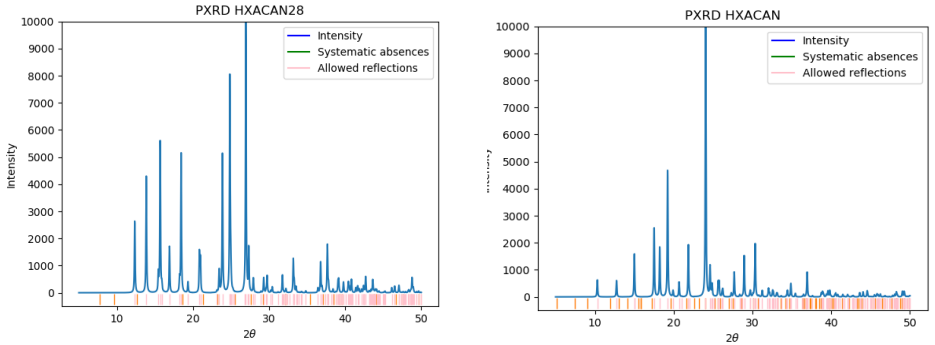
Descriptors

Powder Pattern

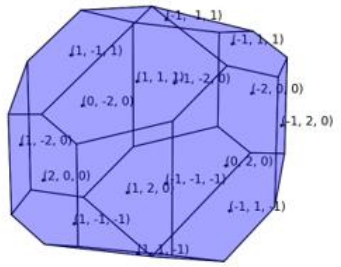


H Bond Coordination

	Atom (D/A)	= 0	= 1	= 2	= 3
1	N1 of acyclic_amide (d)	0.034	0.944	0.021	0.000
2	O1 of ar_oh (d)	0.028	0.930	0.043	0.000
3	O1 of ar_oh (a)	0.650	0.334	0.016	0.000
4	O2 of acyclic_amide (a)	0.027	0.765	0.200	0.009

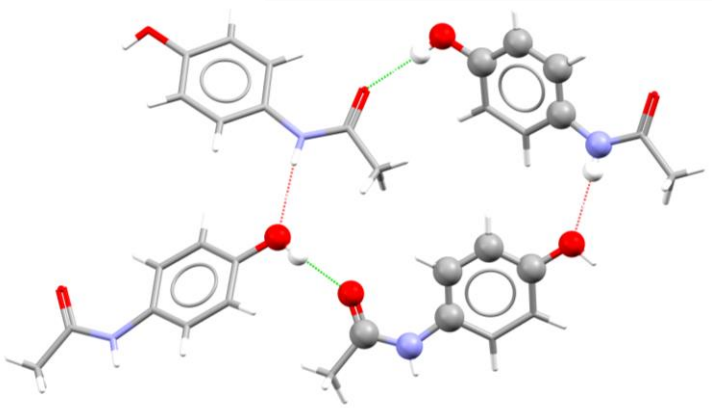
Calculates hydrogen bond coordination predictions.

Morphology



Calculates the BFDH morphology

Graph Set Search



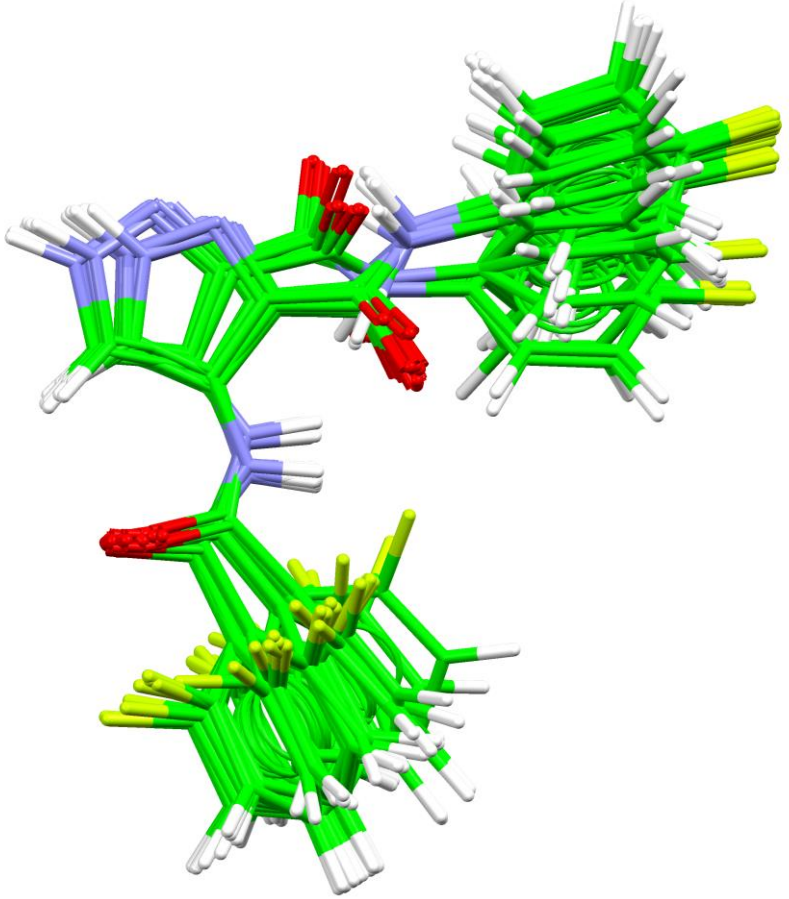
Calculates hydrogen bonding networks

Documentation: https://downloads.ccdc.cam.ac.uk/documentation/API/modules/descriptors_api.html

CCDC

Conformer Generation

- The `ccdc.conformer` module can be used to generate conformers
- The three main classes within the module:
  - `ConformerGenerator`
  - `MoleculeMinimser`
  - `GeometryAnalyser`
- Data from the CSD is used to optimise conformers.



"Knowledge-Based Conformer Generation Using the Cambridge Structural Database", J. C. Cole, O. Korb, P. McCabe. M. G. Read and R. Taylor, J. Chem. Inf. Model., 58, 615-629, 2018, DOI: 10.1021/acs.jcim.7b00697.

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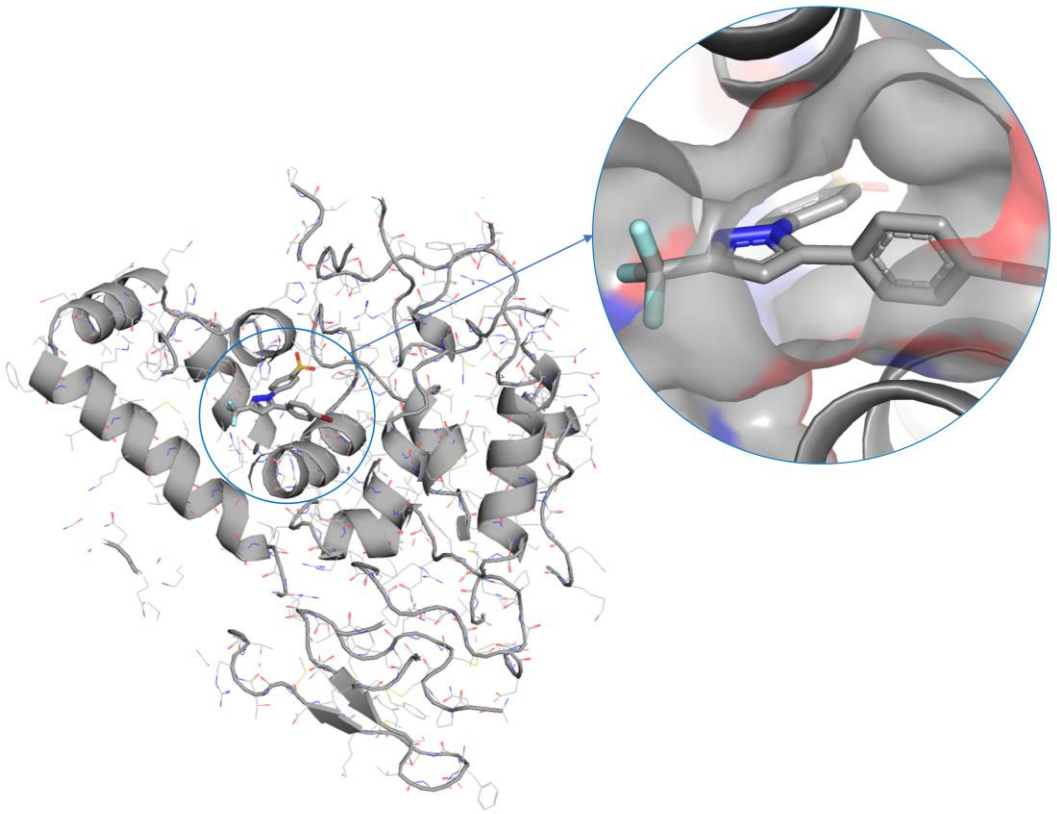
Docking



- `ccdc.docking` module provides an API to protein-ligand docking.
- Docking module contains classes to:
  - set up a docking run
    - define the binding site in different ways
    - set constraints to the docking
  - inspect the results of a docking run
  - rescore ligand(s) with alternative scoring functions

"Molecular recognition of receptor sites using a genetic algorithm with a description of desolvation", G. Jones, P. Willett and R. C. Glen, J. Mol. Biol., 245, 43-53, 1995, DOI: 10.1016/S0022-2836(95)80037-9.

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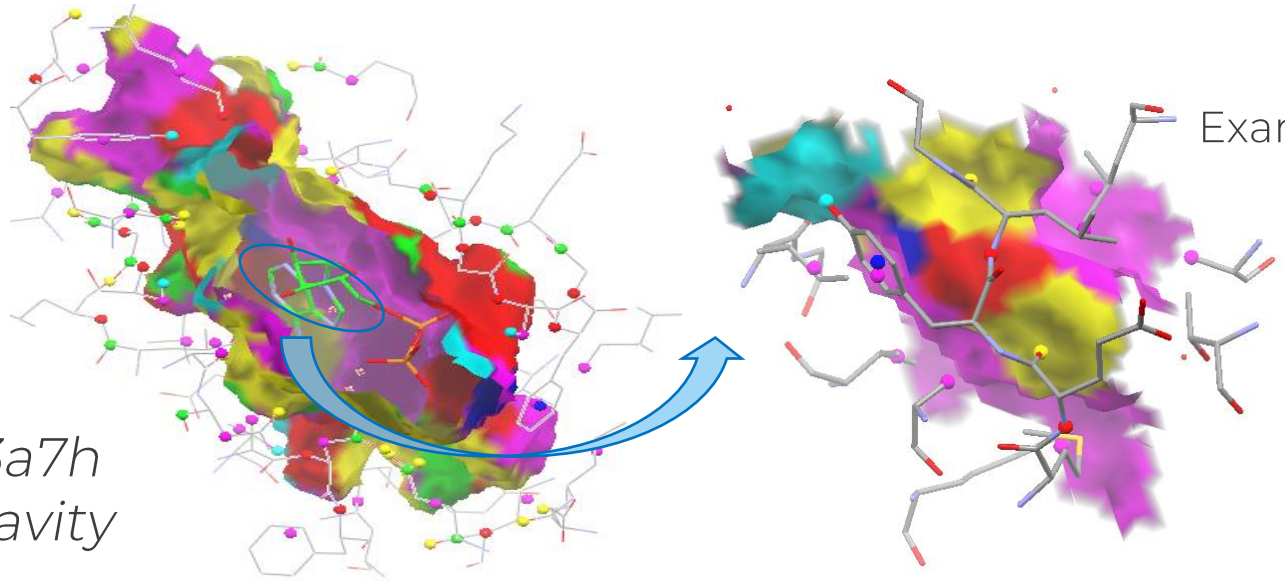
Cavities

- `ccdc.cavity` module provides API for cavity searching and comparison.
  - Uses database of protein cavities (LIGSITE)
  - API contains three different (non sequence-based) cavity comparison methods

Visualisation of cavity identifiers output by search script in **PYMOL**



3a7h cavity

3a7h subcavity

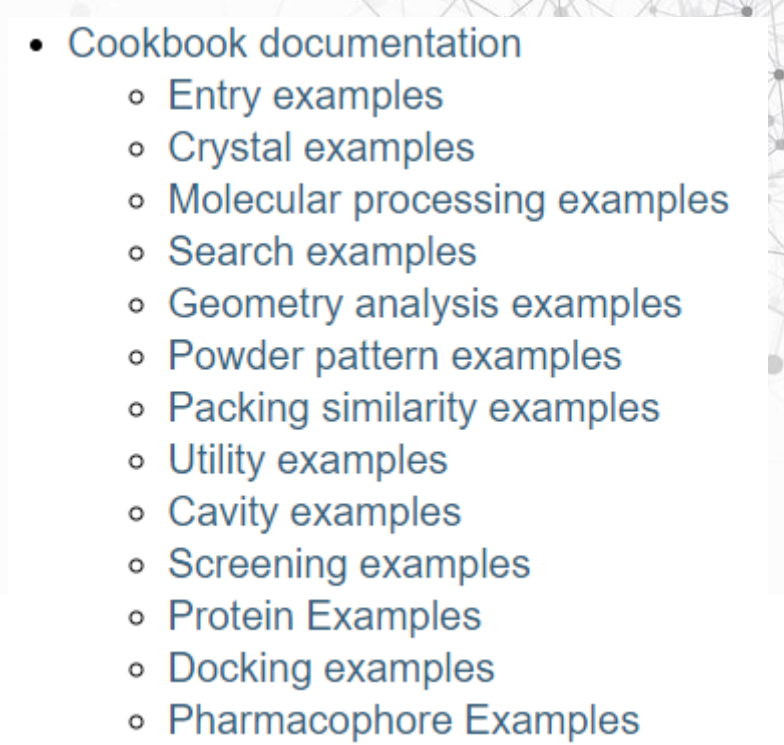
Example script: *`cavity_subcavity_compare_filter.py`*

- Acceptor
- Aliphatic
- Donor
- Aromatic
- Donor-Acceptor
- Pi

CCDC

CSD Python API Cookbook

- API cookbook is available from CSD Python API documentation page.
- There are lots of great example scripts using the different CSD modules that you could use for inspiration.



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

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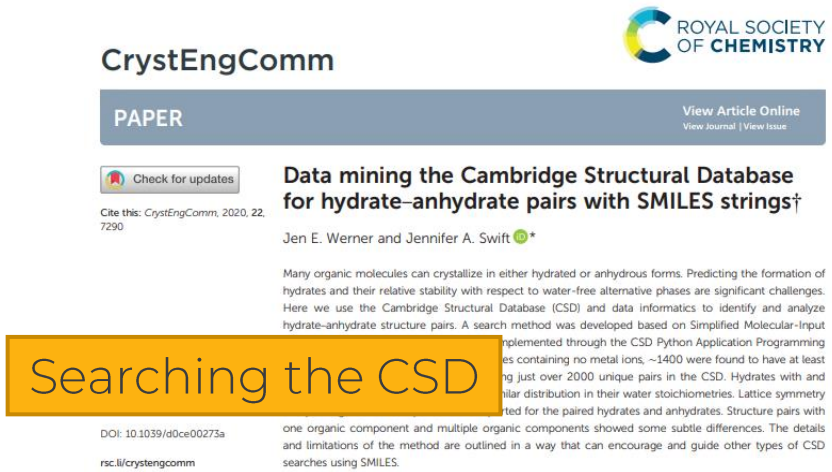
Publications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Cite this: *CrystEngComm*, 2020, 22, 7290

Data mining the Cambridge Structural Database for hydrate–anhydrate pairs with SMILES strings†

Jen E. Werner and Jennifer A. Swift *

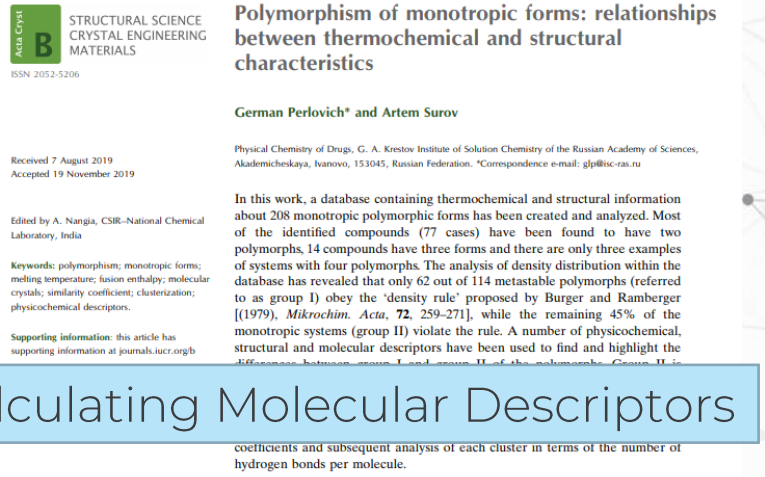
Many organic molecules can crystallize in either hydrated or anhydrous forms. Predicting the formation of hydrates and their relative stability with respect to water-free alternative phases are significant challenges. Here we use the Cambridge Structural Database (CSD) and data informatics to identify and analyze hydrate-anhydrate structure pairs. A search method was developed based on Simplified Molecular-Input ...mplemented through the CSD Python Application Programming ...es containing no metal ions, ~1400 were found to have at least ...ng just over 2000 unique pairs in the CSD. Hydrates with and ...ilar distribution in their water stoichiometries. Lattice symmetry ...rted for the paired hydrates and anhydrates. Structure pairs with one organic component and multiple organic components showed some subtle differences. The details and limitations of the method are outlined in a way that can encourage and guide other types of CSD searches using SMILES.

DOI: 10.1039/d0ce00273a

rsc.li/crystengcomm

Searching the CSD

DOI: https://doi.org/10.1039/D0CE00273A


Acta Cryst B

STRUCTURAL SCIENCE CRYSTAL ENGINEERING MATERIALS

ISSN 2052-5206

Polymorphism of monotropic forms: relationships between thermochemical and structural characteristics

German Perlovich* and Artem Surov

Physical Chemistry of Drugs, G. A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Akademicheskaya, Ivanovo, 153045, Russian Federation. *Correspondence e-mail: glp@isc-ras.ru

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Keywords: polymorphism; monotropic forms; melting temperature; fusion enthalpy; molecular crystals; similarity coefficient; clusterization; physicochemical descriptors.

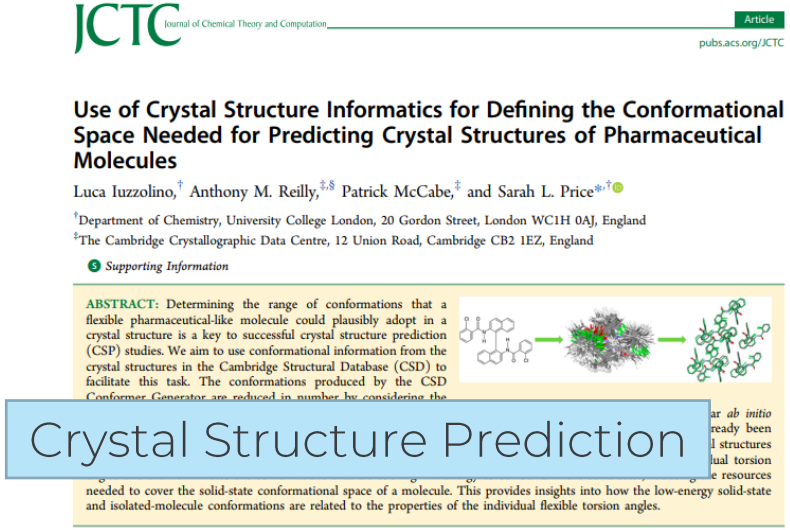
Supporting information: this article has supporting information at journals.iucr.org/b

In this work, a database containing thermochemical and structural information about 208 monotropic polymorphic forms has been created and analyzed. Most of the identified compounds (77 cases) have been found to have two polymorphs, 14 compounds have three forms and there are only three examples of systems with four polymorphs. The analysis of density distribution within the database has revealed that only 62 out of 114 metastable polymorphs (referred to as group I) obey the 'density rule' proposed by Burger and Ramberger [(1979), *Mikrochim. Acta*, **72**, 259–271], while the remaining 45% of the monotropic systems (group II) violate the rule. A number of physicochemical, structural and molecular descriptors have been used to find and highlight the ...

...coefficients and subsequent analysis of each cluster in terms of the number of hydrogen bonds per molecule.

Calculating Molecular Descriptors

DOI: https://doi.org/10.1107/S2052520619015671


JCTC Journal of Chemical Theory and Computation

Article

pubs.acs.org/JCTC

Use of Crystal Structure Informatics for Defining the Conformational Space Needed for Predicting Crystal Structures of Pharmaceutical Molecules

Luca Iuzzolino,† Anthony M. Reilly,‡,§ Patrick McCabe,‡ and Sarah L. Price*,†

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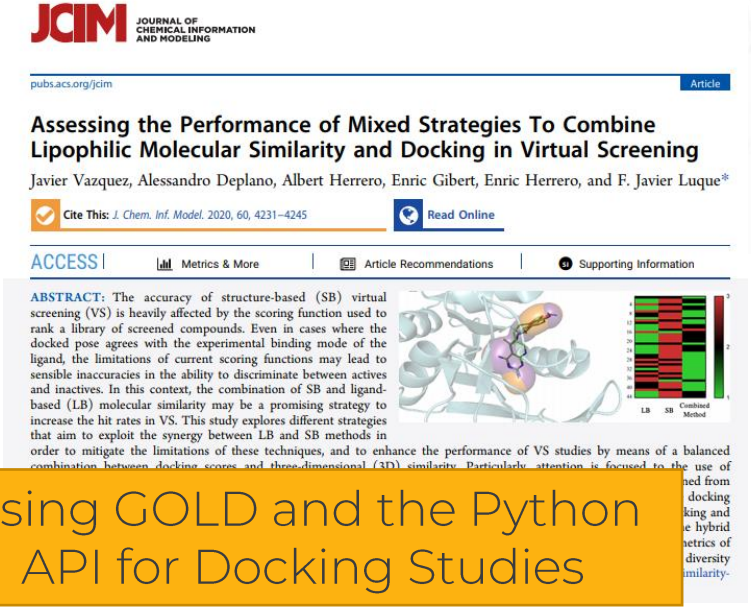
Supporting Information

ABSTRACT: Determining the range of conformations that a flexible pharmaceutical-like molecule could plausibly adopt in a crystal structure is a key to successful crystal structure prediction (CSP) studies. We aim to use conformational information from the crystal structures in the Cambridge Structural Database (CSD) to facilitate this task. The conformations produced by the CSD Conformer Generator are reduced in number by considering the ...ar *ab initio* ...ready been ...l structures ...ual torsion ...e resources needed to cover the solid-state conformational space of a molecule. This provides insights into how the low-energy solid-state and isolated-molecule conformations are related to the properties of the individual flexible torsion angles.

Crystal Structure Prediction

DOI:https://doi.org/10.1021/acs.jctc.7b00623


JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

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Article

Assessing the Performance of Mixed Strategies To Combine Lipophilic Molecular Similarity and Docking in Virtual Screening

Javier Vazquez, Alessandro Deplano, Albert Herrero, Enric Gibert, Enric Herrero, and F. Javier Luque*

Cite This: *J. Chem. Inf. Model.* 2020, 60, 4231−4245

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ABSTRACT: The accuracy of structure-based (SB) virtual screening (VS) is heavily affected by the scoring function used to rank a library of screened compounds. Even in cases where the docked pose agrees with the experimental binding mode of the ligand, the limitations of current scoring functions may lead to sensible inaccuracies in the ability to discriminate between actives and inactives. In this context, the combination of SB and ligand-based (LB) molecular similarity may be a promising strategy to increase the hit rates in VS. This study explores different strategies that aim to exploit the synergy between LB and SB methods in order to mitigate the limitations of these techniques, and to enhance the performance of VS studies by means of a balanced ...ned from ...docking ...king and ...e hybrid ...metrics of ...diversity ...milarity-

Using GOLD and the Python API for Docking Studies

DOI: https://doi.org/10.1021/acs.jcim.9b01191

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