# Searching the CSD online – WebCSD 101


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# Learning outcomes

After this session you will know how to search the CSD online.

In particular, you will know:

- What the CSD, Access Structures and WebCSD are.
- How to build a search, navigate hitlists and export results in WebCSD.
- How to construct a 2D structure search of the CSD.
- How WebCSD can be used to find similar structures of interest.
- How to perform advanced 3D structure searches to explore distances, angles, rings, vectors and planes.

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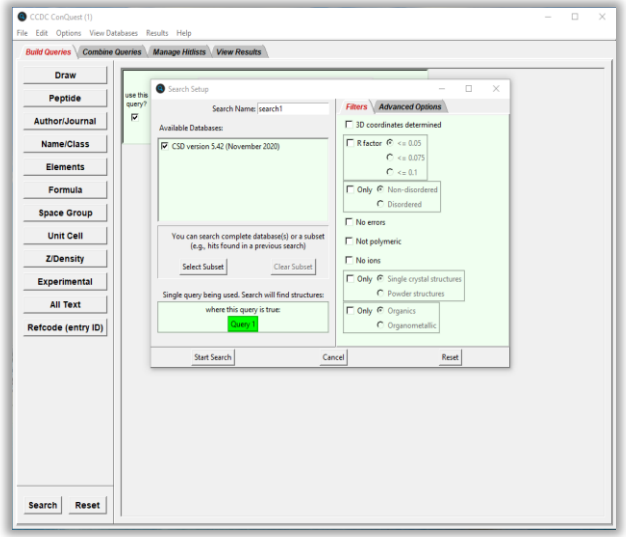
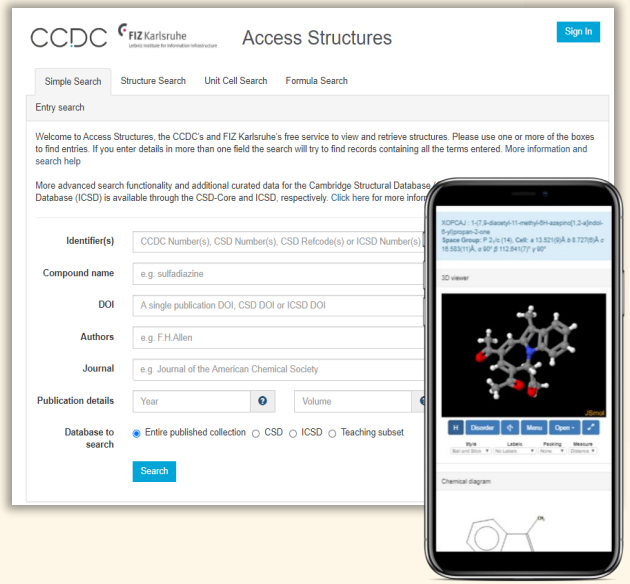
# *Show One:* Structure searching

## Desktop



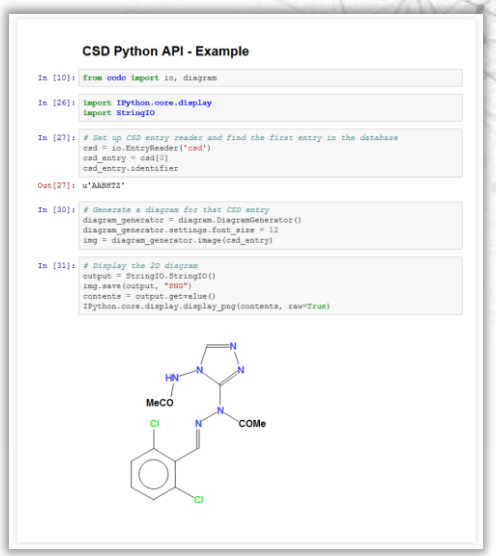

ConQuest

## Web Browser




WebCSD / Access Structures

## Programmatic




CSD Python API

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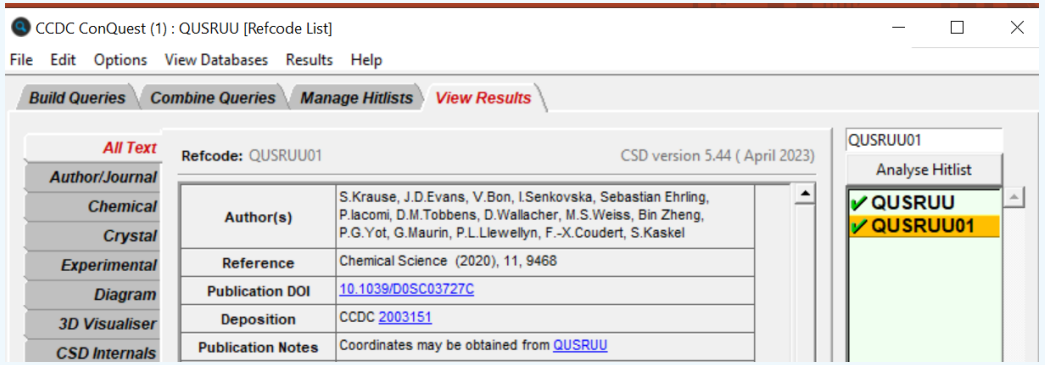
# Desktop vs Web

## Desktop

- **Quarterly** data updates
- One entry per publication/dataset combination
- **Advanced options**
- Searches the **CSD**




## Web Browser

- **Up to the minute** data updates
- One entry per deposited dataset
- **Free and advanced** options
- Access Structures searches **CSD + ICSD** (WebCSD just CSD)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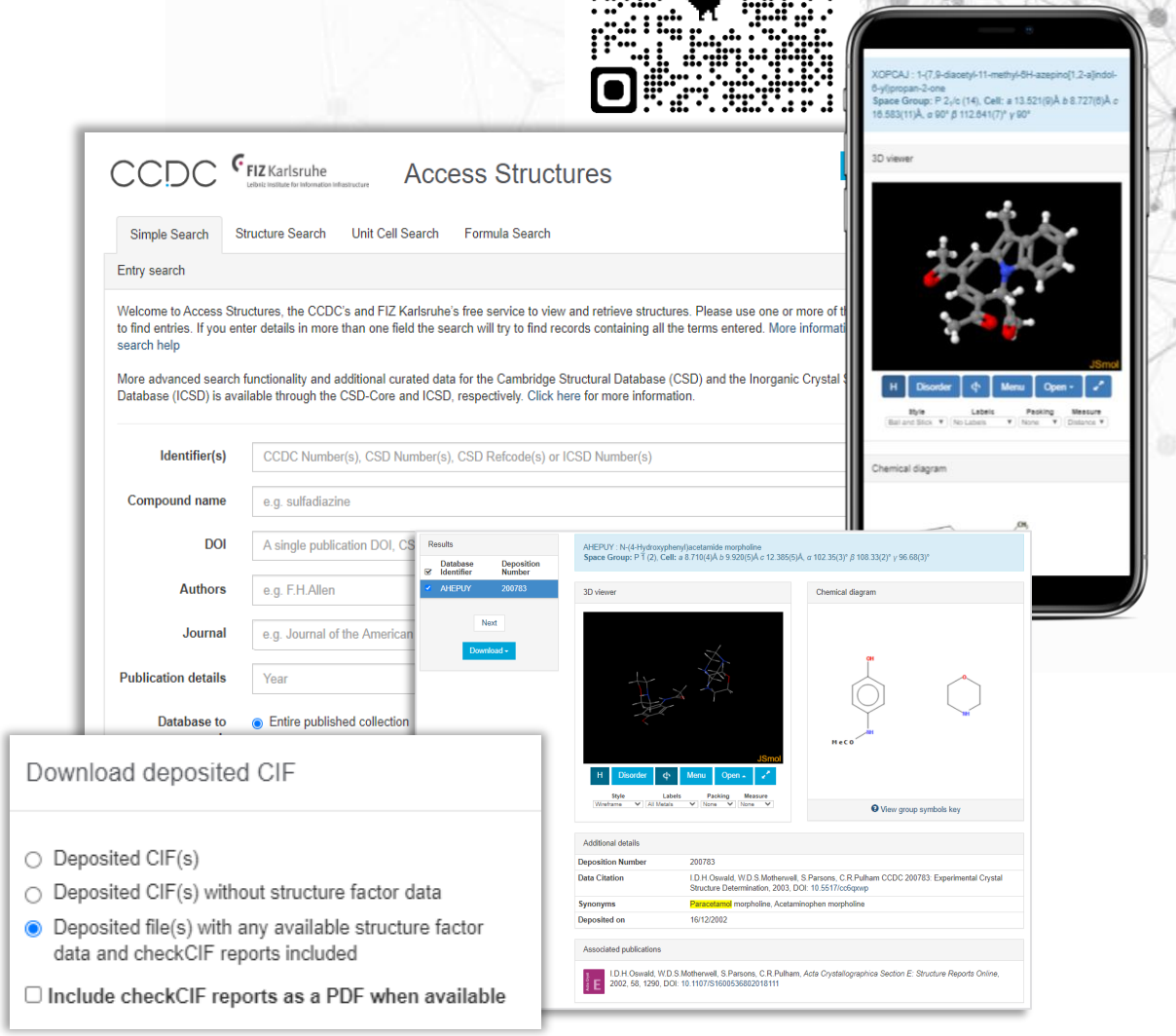
# Access Structures

- Online portal to access the CSD and ICSD.
- Free to view and retrieve individual structures.
- Basic searching and information.
- Accessed through any standard internet browser – no local installation of software required.




www.ccdc.cam.ac.uk/structures

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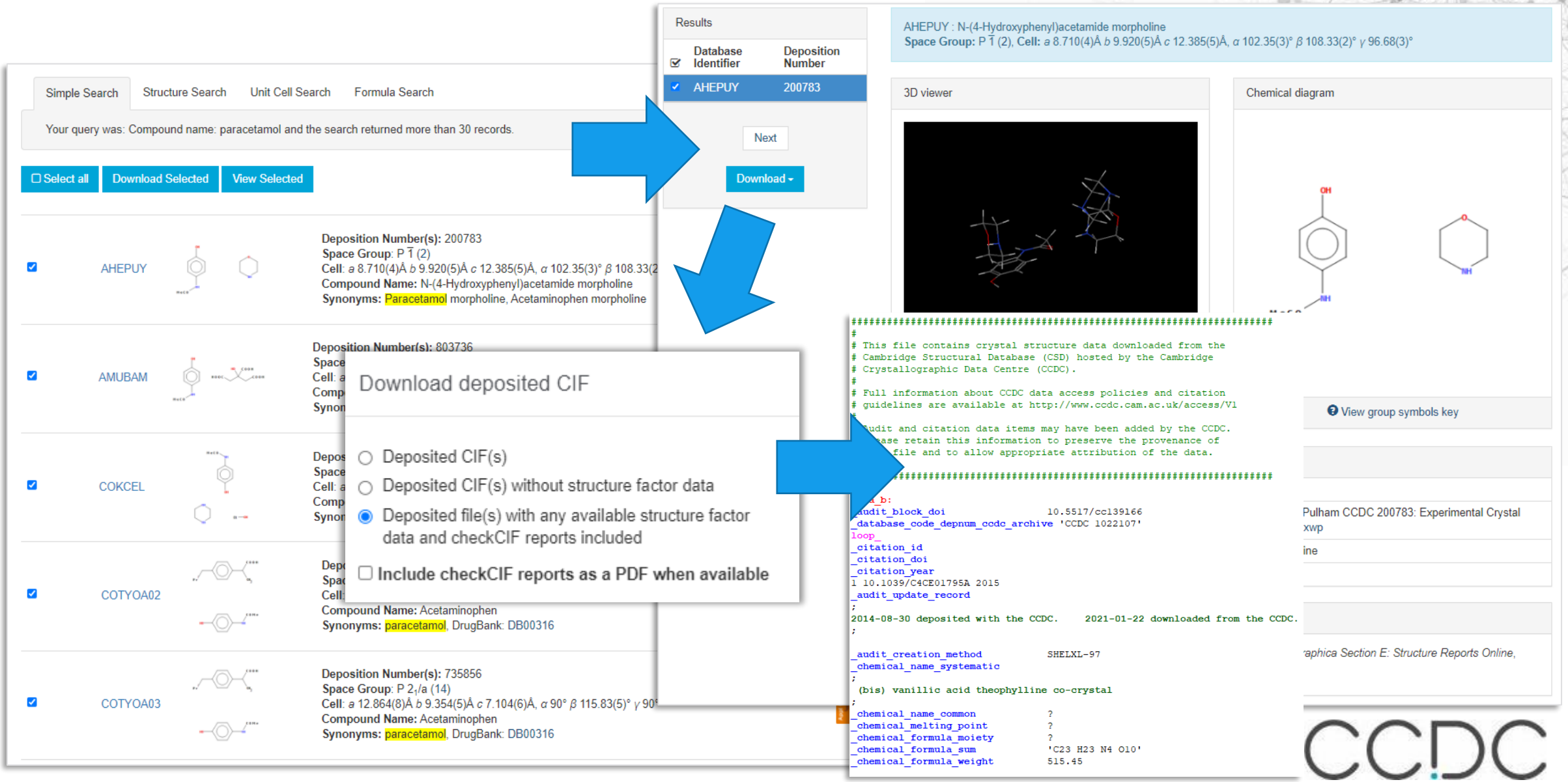
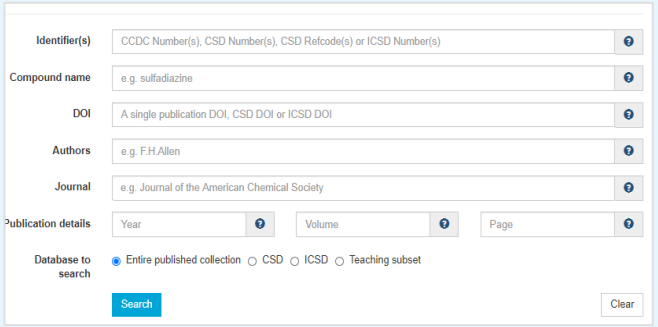
# Search, view and download structures



# Web: Structure searching

## Access structures

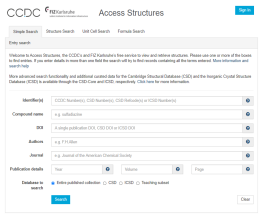
- Free to view and download individual structures.
- Basic searching.
- Basic curated data.
- Access to CSD and ICSD.




## Web Browser

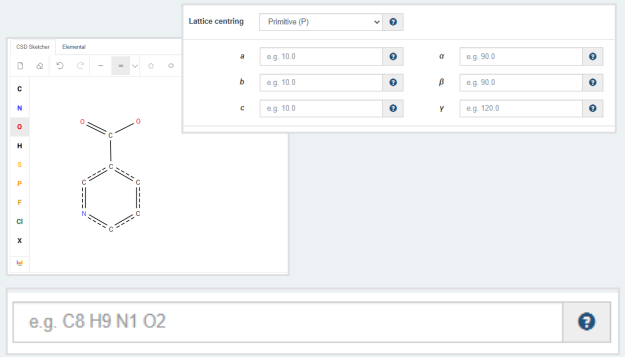
Access Structures + WebCSD

- Web search and access.
- Easy and intuitive.
- Cross-platform and no installation needed
- Up to the minute data



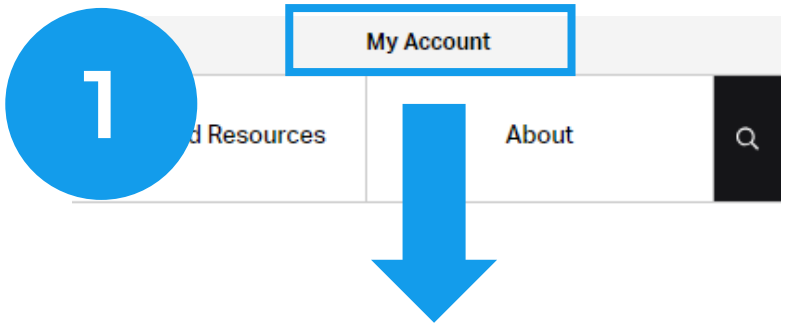

## WebCSD

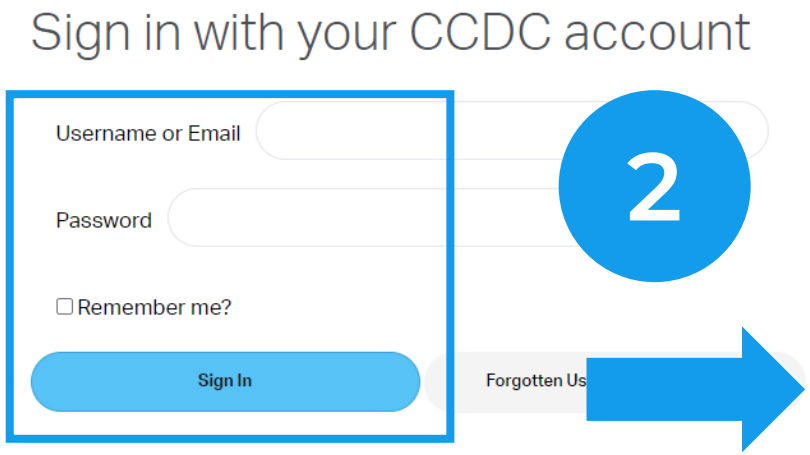
- Licensed software.
- Advanced searching of the CSD.
- Unlimited use.
- Full curated data.

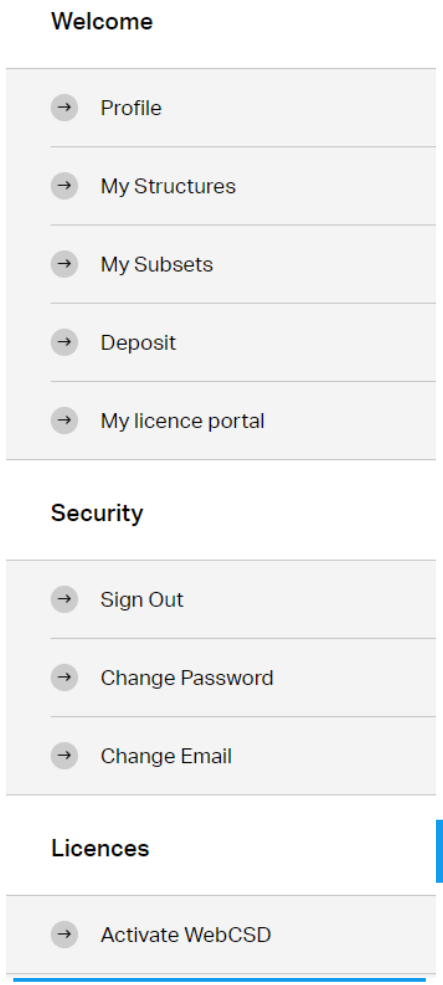


# Logging into WebCSD

## Option I.



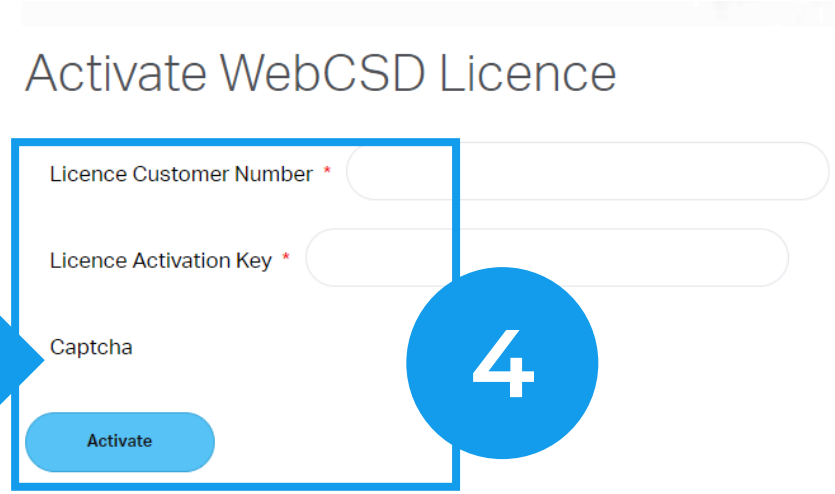




## Two ways to log into WebCSD:

I. **Create an account** on the CCDC website and **activate WebCSD** using your customer number and activation key.

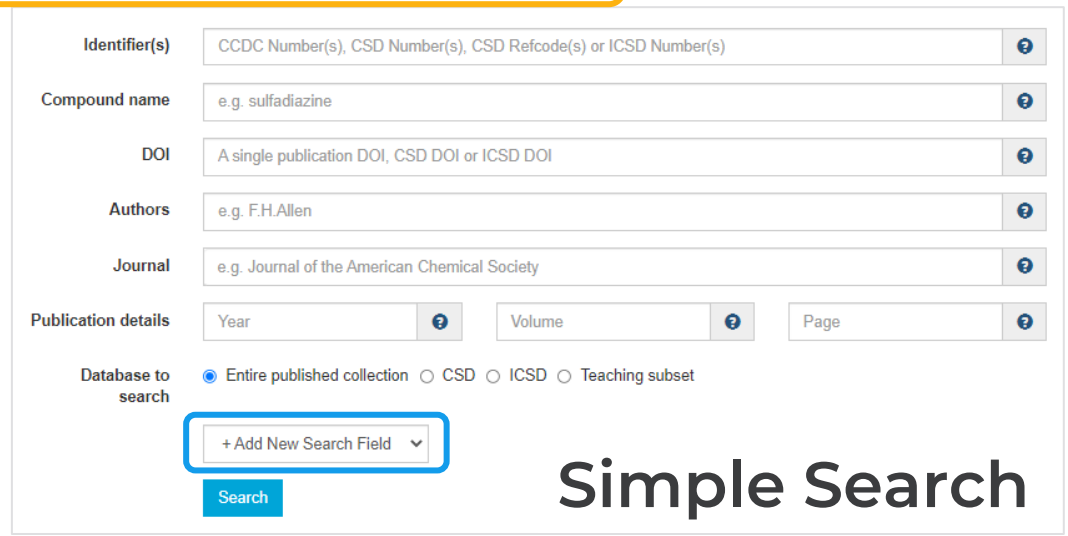
II. **Email** admin@ccdc.cam.ac.uk to **add your IP address(es)** to your customer account.



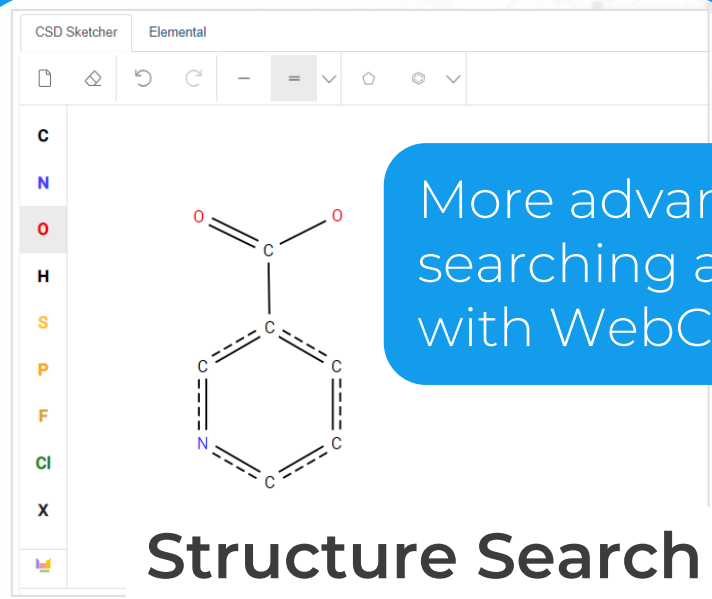
# WebCSD

Simple Search | Structure Search | Unit Cell Search | Formula Search

## Access Structures and WebCSD



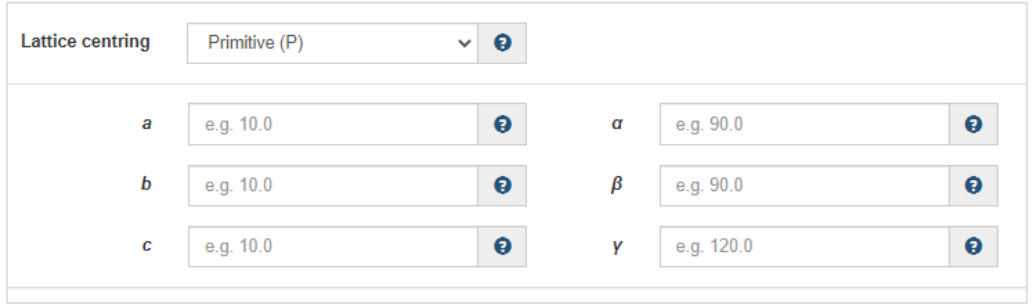

### Simple Search




More advanced searching available with WebCSD

### Structure Search

### Unit Cell Search




### Formula Search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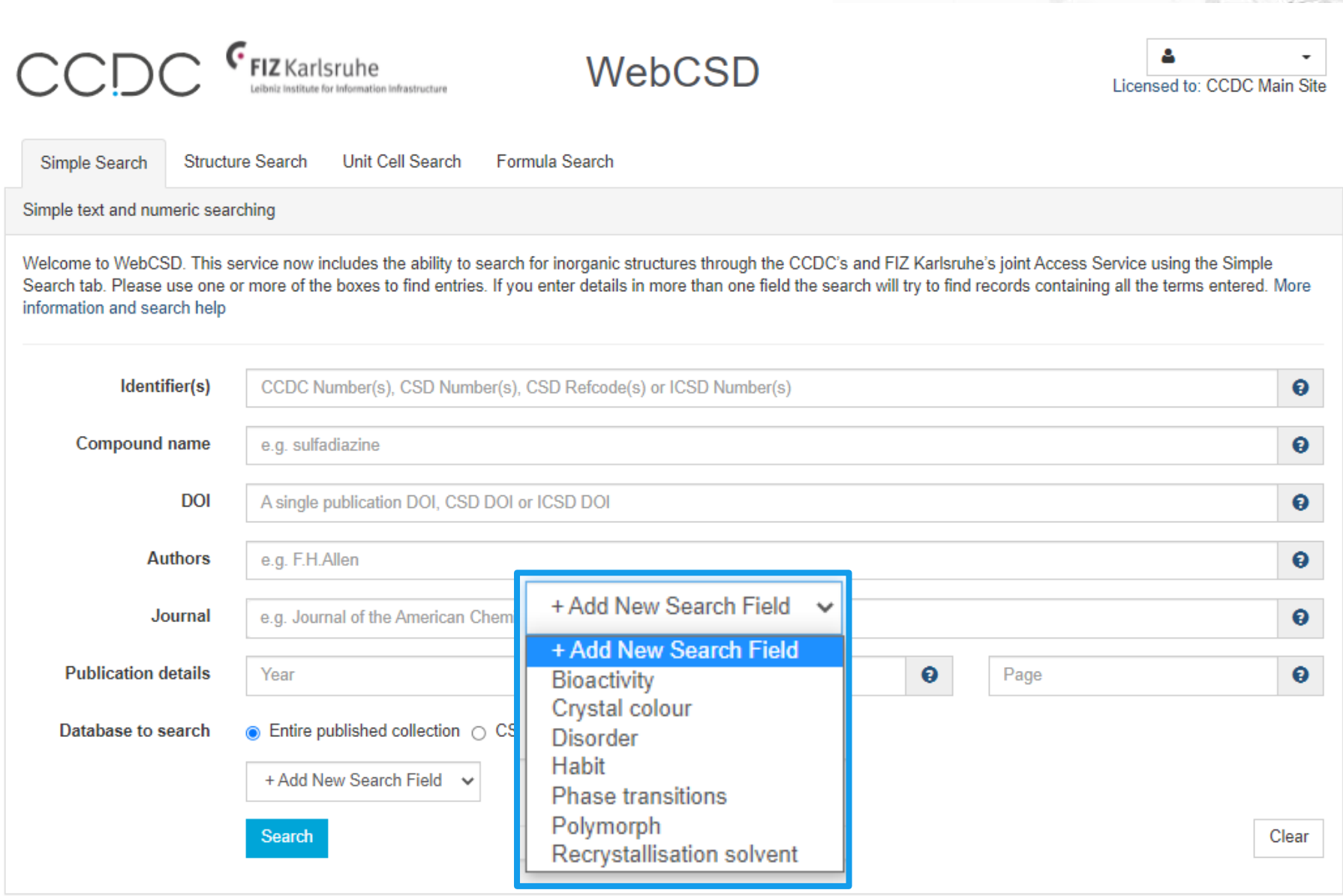
# Searching specific information fields



# Formula Searching

Type **desired formula** into the box with the number of the atoms in the structure after each element

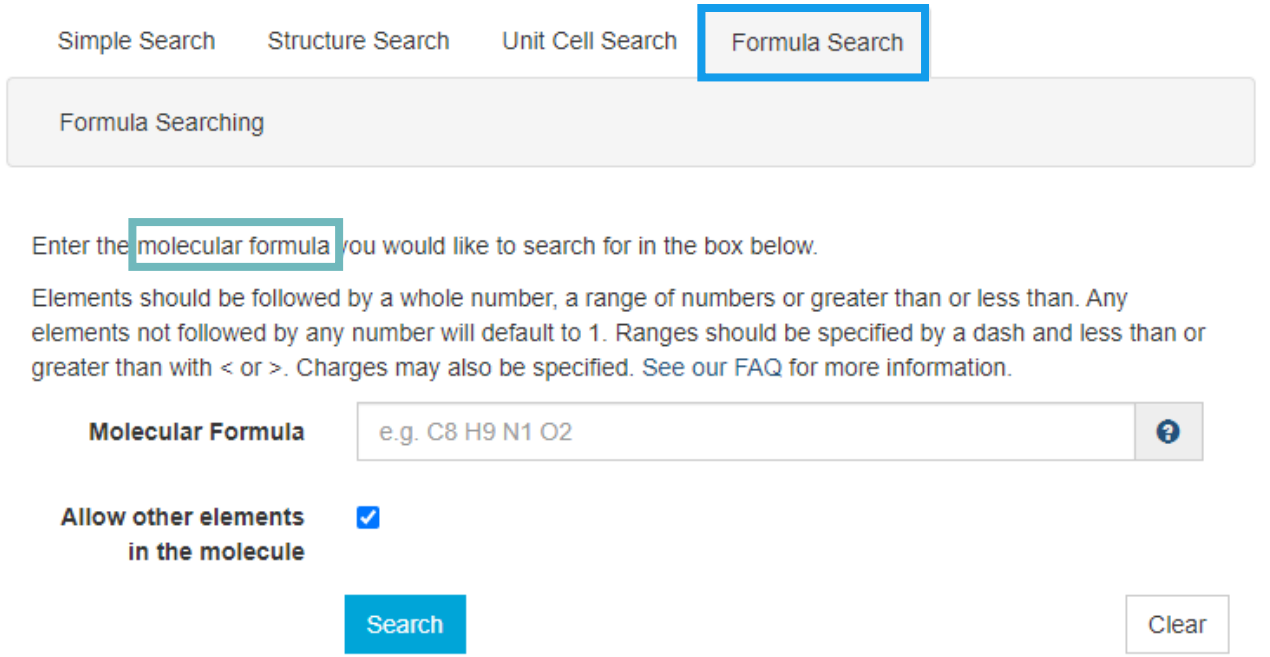
- e.g. **Cd C5 O2**
- Assumes number of atoms is 1 if no number given

Are there **elements you don't want** in your structure?

- Put a 0 after the element in the formula
- e.g. **Cd C5 O2 Cl0** (excludes structures with Cl)

Want **atoms within a range**?

- include the range after element separated by a **-**
- e.g. **Cd C1-3 O2 Cl0** (This will find structures with 1-3 carbons in them)




Want **more or less than a certain number of atoms** of an element?

- Use > or < after the element
- e.g. **Fe N3-4 O>6** (finds structures with more than 6 O)

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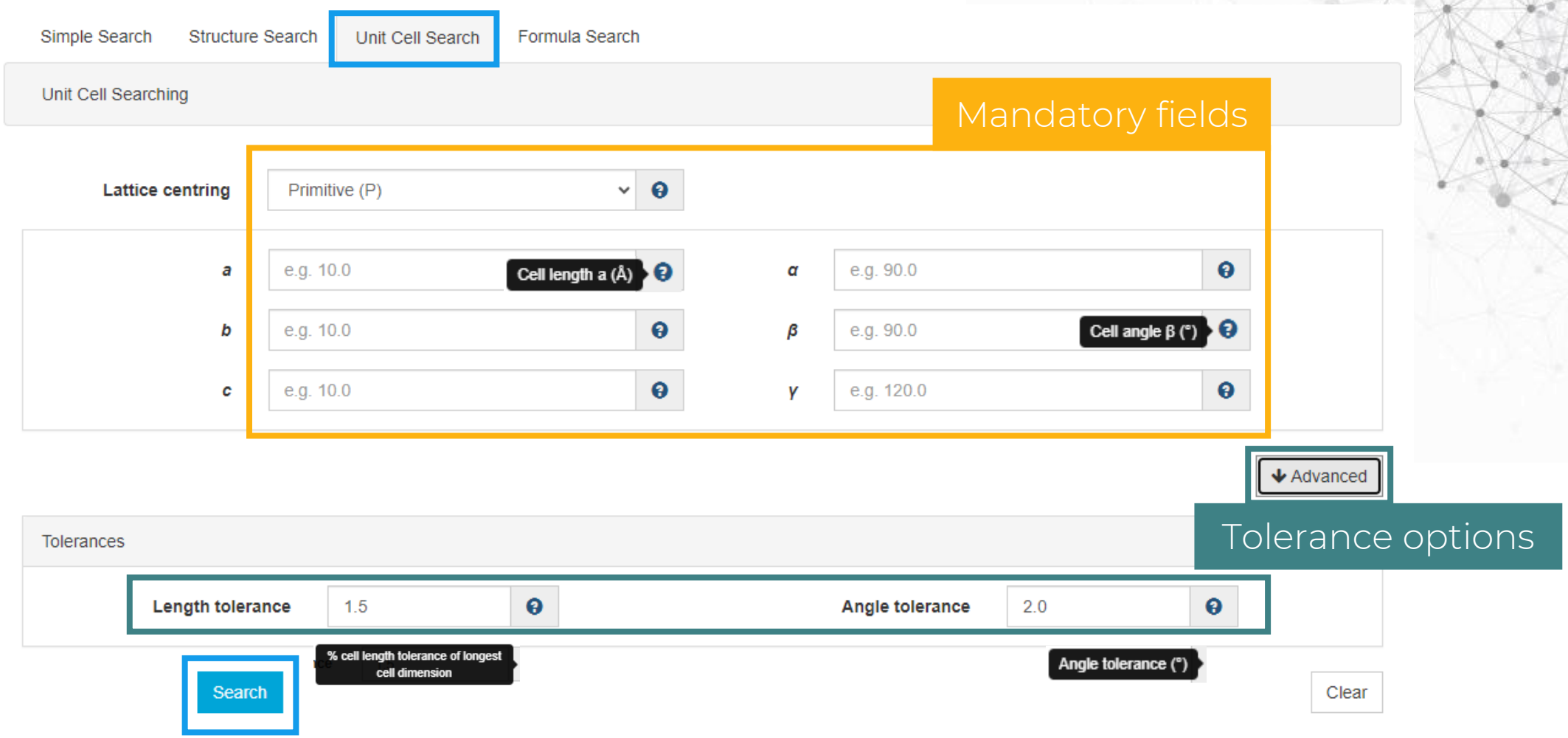
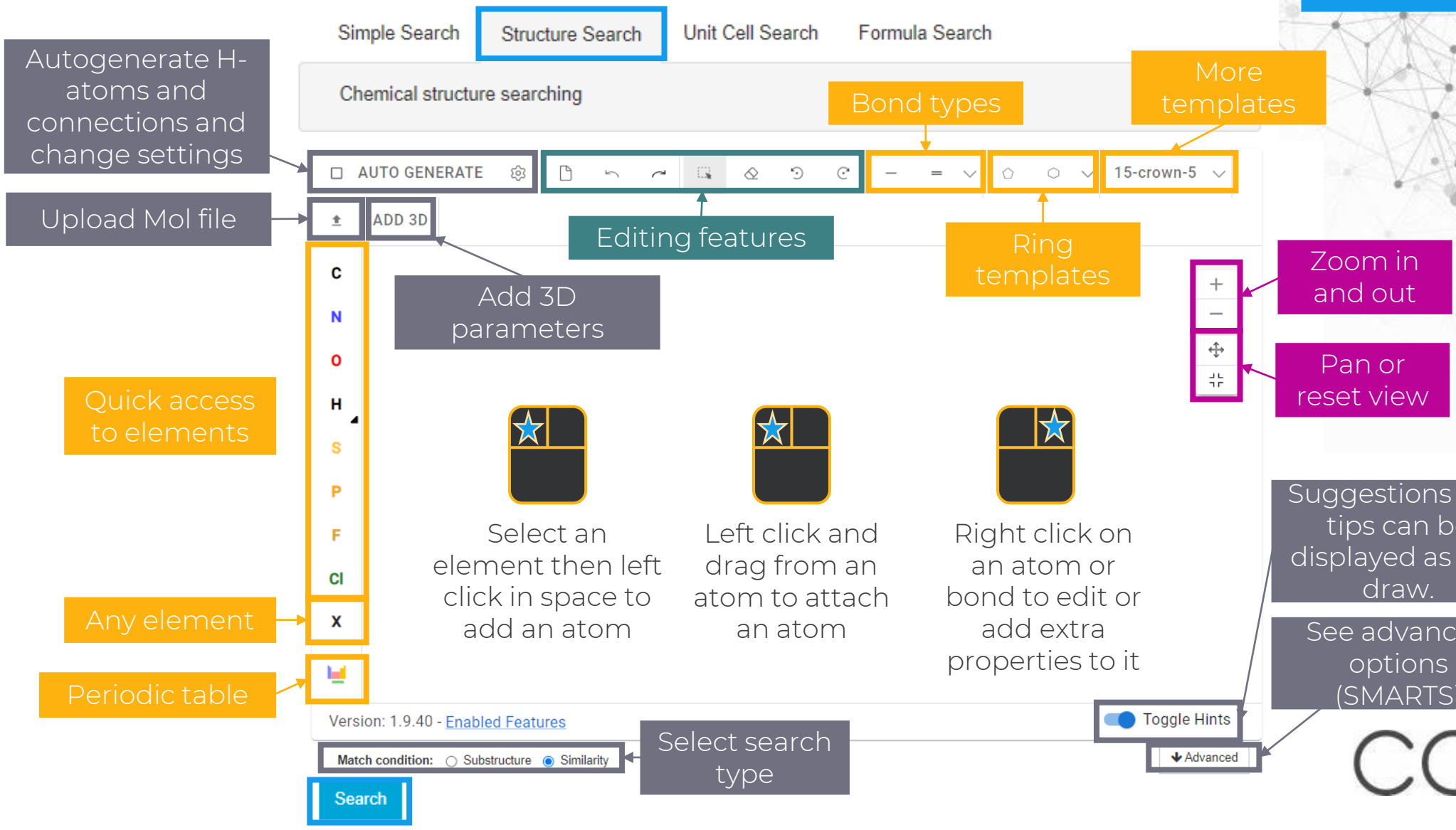
# Unit Cell Search



# Structure Search




Tip: Hover over the buttons to see more information

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# Results

Simple Search | Structure Search | Unit Cell Search | Formula Search

Search Complete - **1000** Results Found

Progress bar

100%

Modify Search | New Search

Results listed by REFCODE

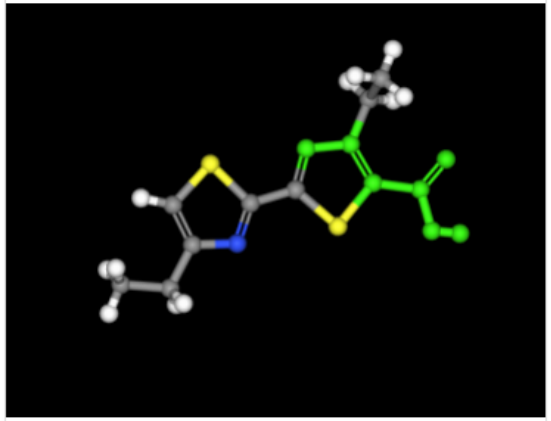
Results

| Database Identifier | Deposition Number |
|---|---|
| ARILUL | 2022486 |
| ARIMAS | 2022487 |
| ASIREZ | 220759 |
| ASUSIS | 1014639 |
| AVEMUK | 839256 |
| AVEMUK01 | 1443393 |
| AWABEG | 805484 |
| AYAVAY | 756717 |
| AYEBIP | 242352 |
| AYIKEZ | 710956 |
| AYIKEZ01 | 842925 |
| AYIKEZ02 | 906630 |
| AYINOM | 845206 |
| AYIYAJ | 845248 |
| AYOYUK | 1509954 |
| AZOKAE | 2074661 |
| AZOKUW | 850471 |
| BADNOM | 1413573 |
| BAFKEA | 774582 |
| BAWHIR | 210815 |
| BETKUH | 237120 |
| BEWVIM | 2099287 |
| BEWVOS | 2099289 |

BETKUH : 5-Carboxy-4,4'-diethyl-2,2'-bithiazole
**Space Group:** C 2/c (15), **Cell:** *a* 22.664(6)Å *b* 5.1881(14)Å *c* 22.754(6)Å, *α* 90° *β* 113.443(4)° *γ* 90°

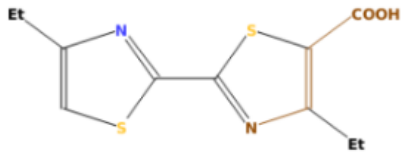
3D viewer

Ball and Stick | No Labels



No Packing | H | Disorder

Chemical diagram




View group symbols key

3D viewer and 2D chemical diagram

The substructure searched is highlighted.

Additional details

| | |
|---|---|
| **Deposition Number** | 237120 |
| **Data Citation** | M.D.Curtis, Jie Cao, J.W.Kampf CCDC 237120: Experimental Crystal Structure Determination, 2004, DOI: 10.5517/cc7yr1y |
| **Deposited on** | 13/09/2004 |

Associated publications

M.D.Curtis, Jie Cao, J.W.Kampf, *Journal of the American Chemical Society*, 2004, 126, 4318, DOI: 10.1021/ja0397916

Link to publication

Chemical details

More bibliographic, chemical, crystal and experimental details

CCDC DOI

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# Results

| | | |
|---|---|---|
| ☑ | AYIYAJ | 845248 |
| ☑ | AYOYUK | 1509954 |
| ☑ | AZOKAE | 2074661 |
| ☑ | AZOKUW | 850471 |
| ☑ | BADNOM | 1413573 |
| ☑ | BAFKEA | 774582 |
| ☑ | BAWHIR | 210815 |
| ☑ | BETKUH | 237120 |
| ☑ | BEWVIM | 2099287 |
| ☑ | BEWVOS | 2099289 |
| ☑ | BEWWEJ | 2099288 |
| ☑ | BICYER | 1110283 |
| ☑ | BIHHIM | 1855210 |
| ☑ | BIJZAZ | 2256588 |
| ☑ | BIJZED | 2256589 |
| ☑ | BIKDAE | 1817775 |
| ☑ | BIMYED | 932966 |

31 - 60 of 1000 items

Download

Download results

## Additional details

| | |
|---|---|
| **Deposition Number** | 237120 |
| **Data Citation** | M.D.Curtis, Jie Cao, J.W.Kampf CCDC 237120: Experimental Crystal Structure Determination, 2004, DOI: 10.5517/cc7yr1y |
| **Deposited on** | 13/09/2004 |

More bibliographic, chemical, crystal and experimental details

CCDC DOI

## Associated publications

M.D.Curtis, Jie Cao, J.W.Kampf, *Journal of the American Chemical Society*, 2004, 126, 4318, DOI: 10.1021/ja0397916

Link to publication

## Chemical details

| | |
|---|---|
| **Formula** | $C_{11}$ $H_{12}$ $N_2$ $O_2$ $S_2$ |

## Crystal details

| | |
|---|---|
| **Space group** | C 2/c (15) |
| **Unit cell** | ***a*** 22.664(6)Å ***b*** 5.1881(14)Å ***c*** 22.754(6)Å<br>***α*** 90° ***β*** 113.443(4)° ***γ*** 90° |
| **Cell volume** | 2454.64 |
| **Reduced cell** | ***a*** 5.188Å ***b*** 11.625Å ***c*** 21.160Å<br>***α*** 82.393° ***β*** 82.958° ***γ*** 77.106° |
| **Z, Z'** | 8, 1 |
| **Habit** | irregular |
| **Recrystallisation solvent** | acetonitrile |
| **Colour** | orange |

## Experimental details

| | |
|---|---|
| **R-factor (%)** | 2.94 |
| **Temperature (K)** | 158 |
| **Density (CCDC)** | 1.452 |
| **Radiation probe** | x-ray |
| **Experiment type** | single crystal |

## Links

Other links – if available

| | |
|---|---|
| **PubChem** | 86035535 |

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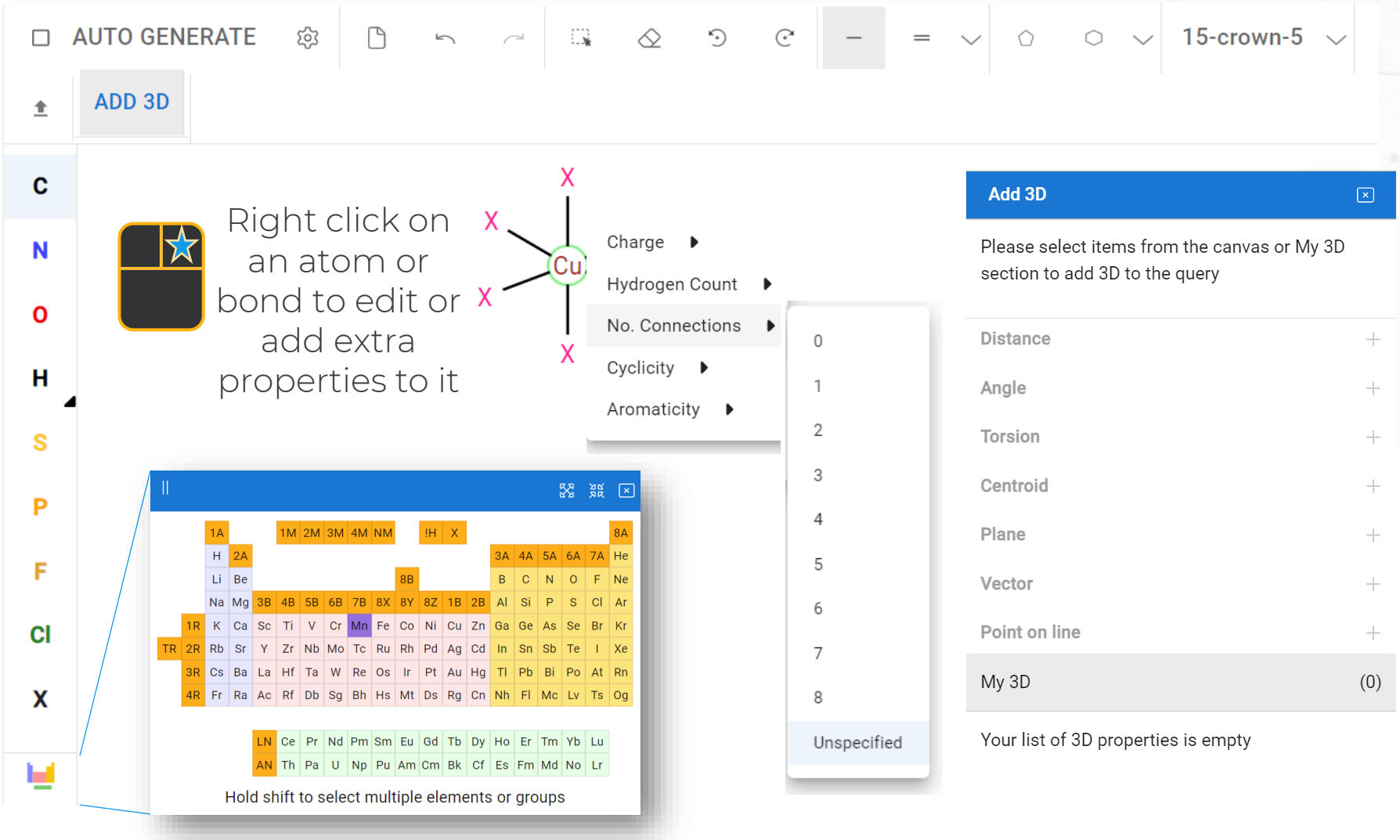
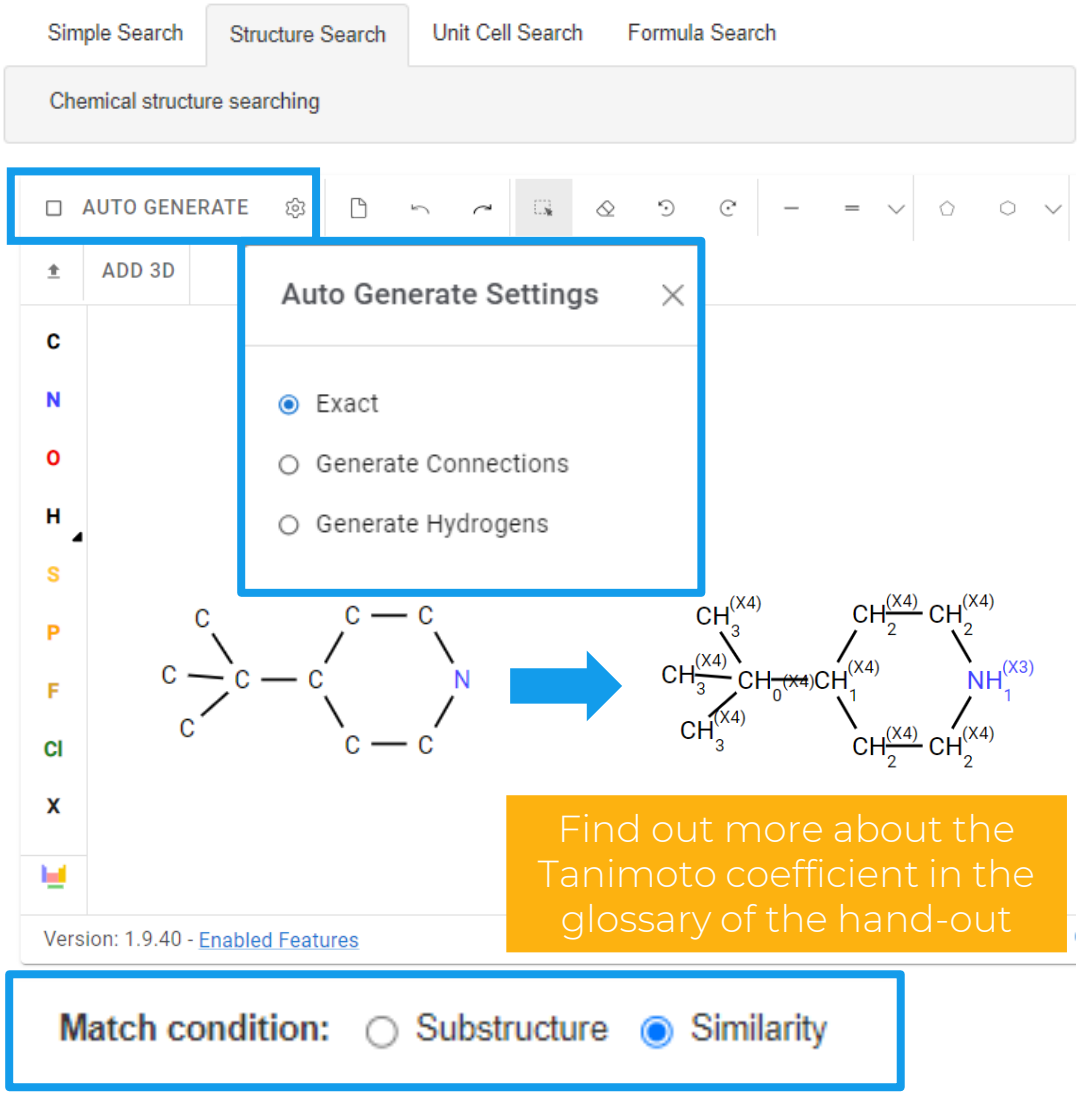
# Advanced structure searching



# Selecting search type




## Substructure

Returns hits where the draw query is a part of any molecule (similar to ConQuest).

## Exact

To return structures that contain the exact molecule as it is drawn, tick Auto Generate and from the Auto Generate Settings select Exact. Select Substructure in Match condition.

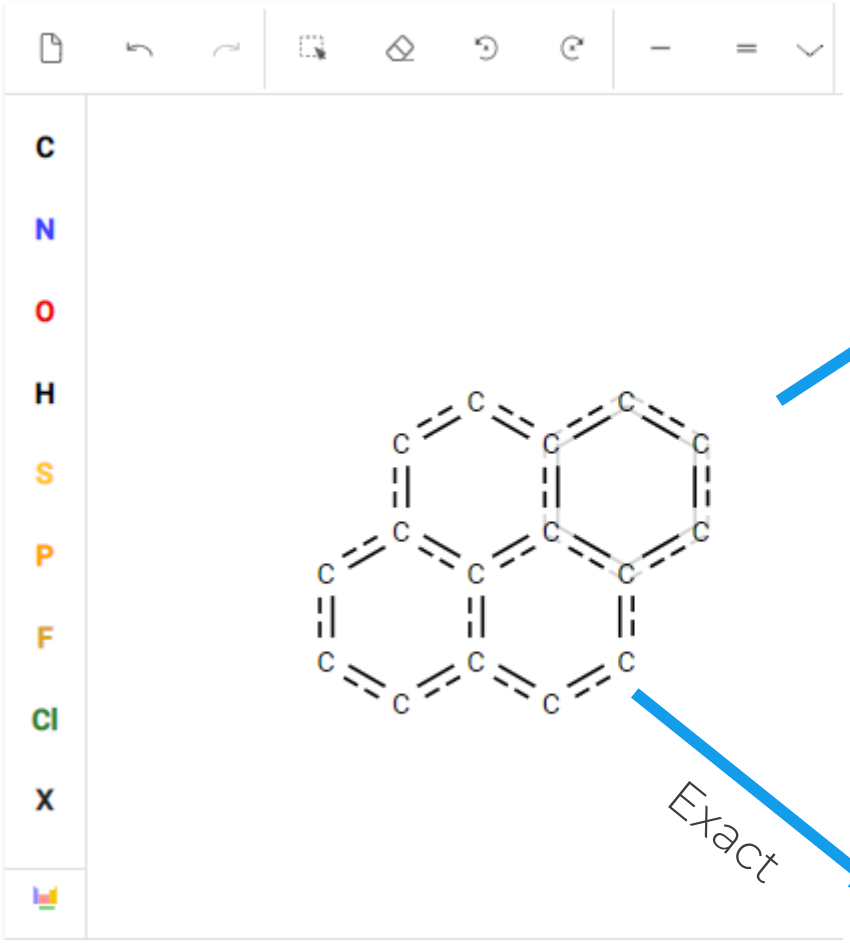
## Similarity

Calculates a molecular fingerprints for the drawn molecule and compares that to pre-calculated fingerprints for structures in the CSD using the Tanimoto coefficient .

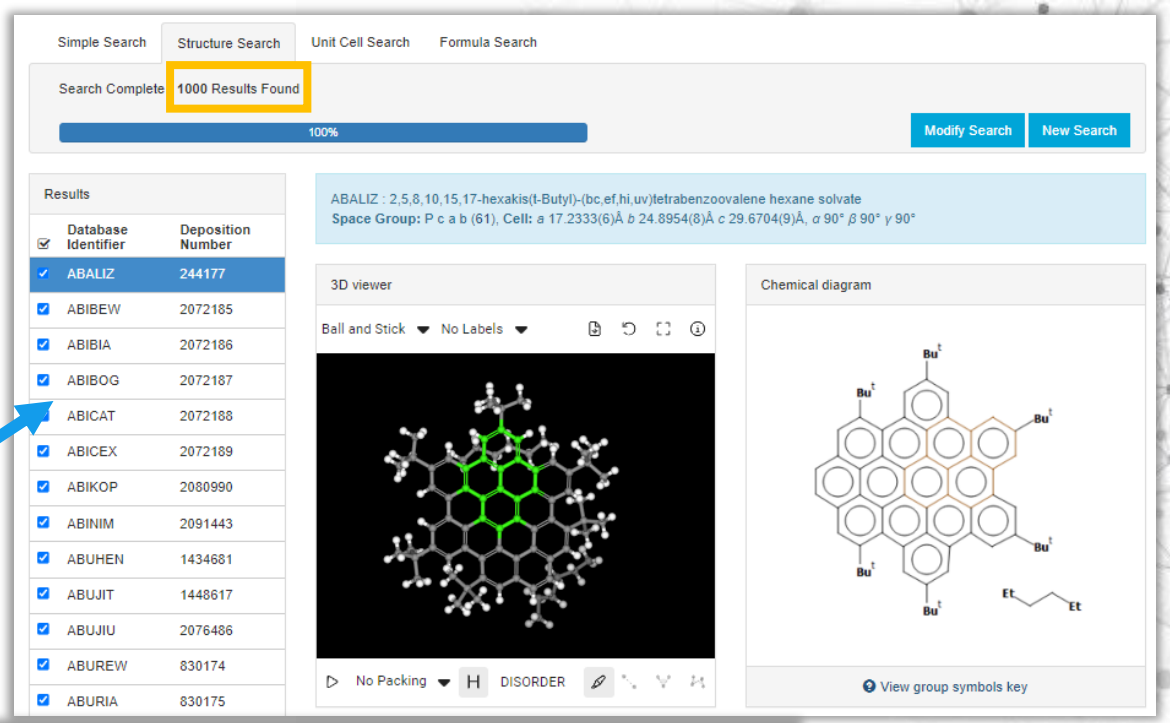
Required: Full molecule drawn, but connectivity and missing H will automatically be assigned during the search.

Returns: Similar structures and a similarity score (where 1 is an identical molecule).

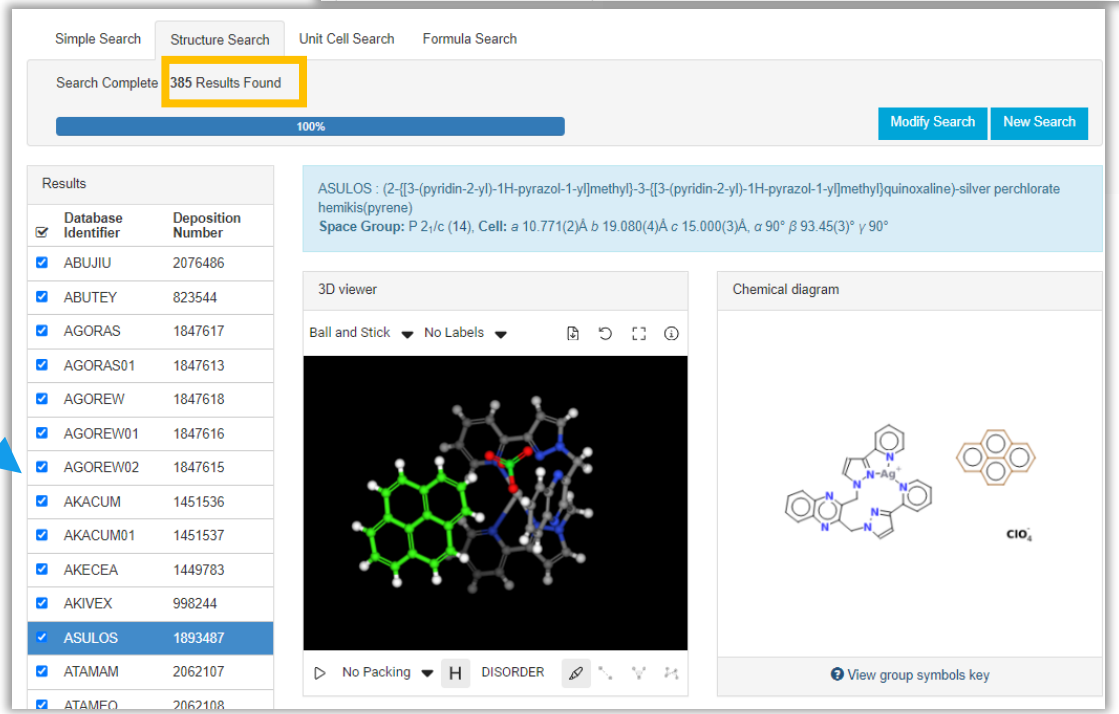
>1,000 hits
Includes structures where pyrene structure is part of a larger molecule




Substructure




Exact




385 hits
Only structures with pyrene on its own

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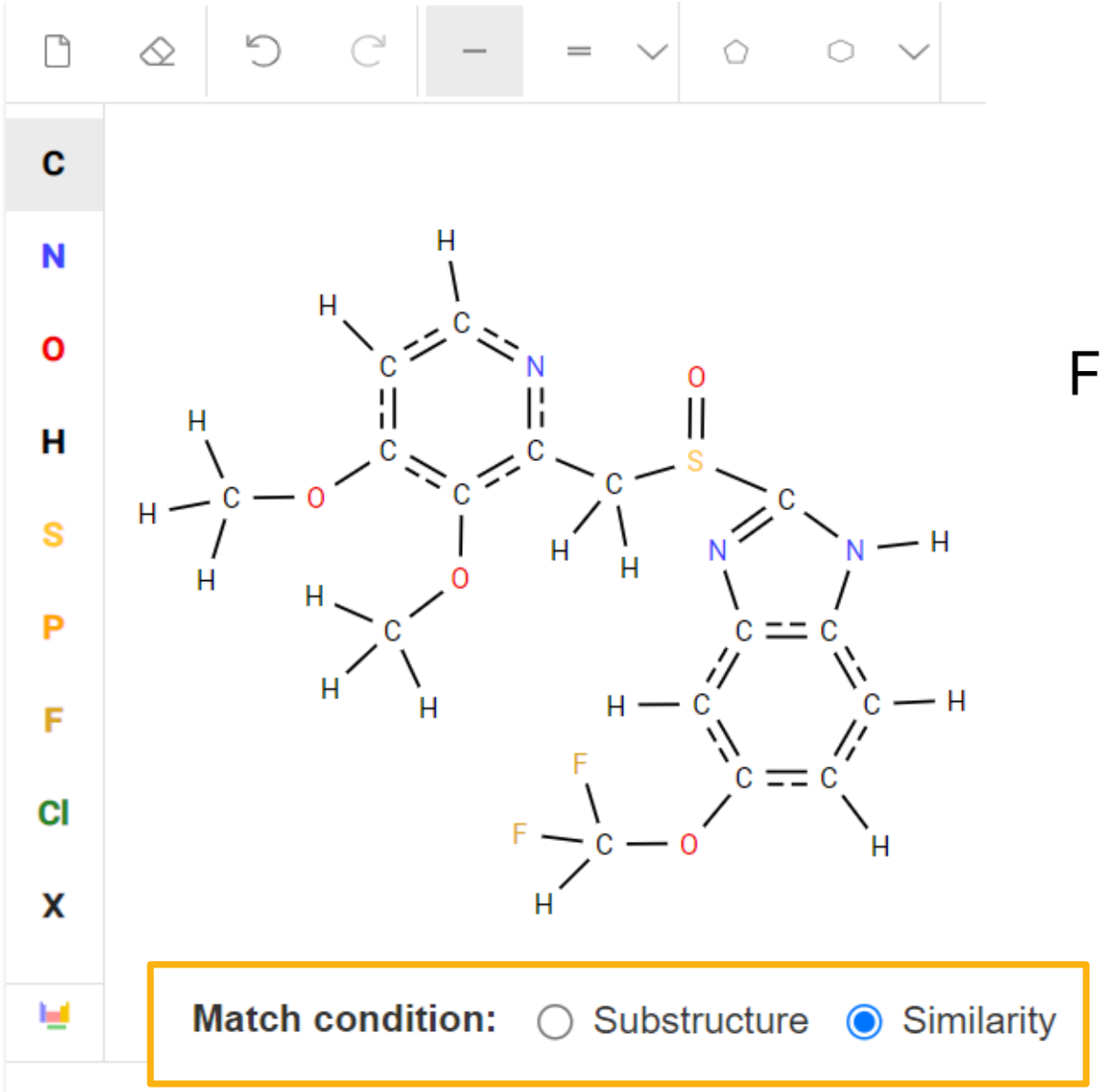
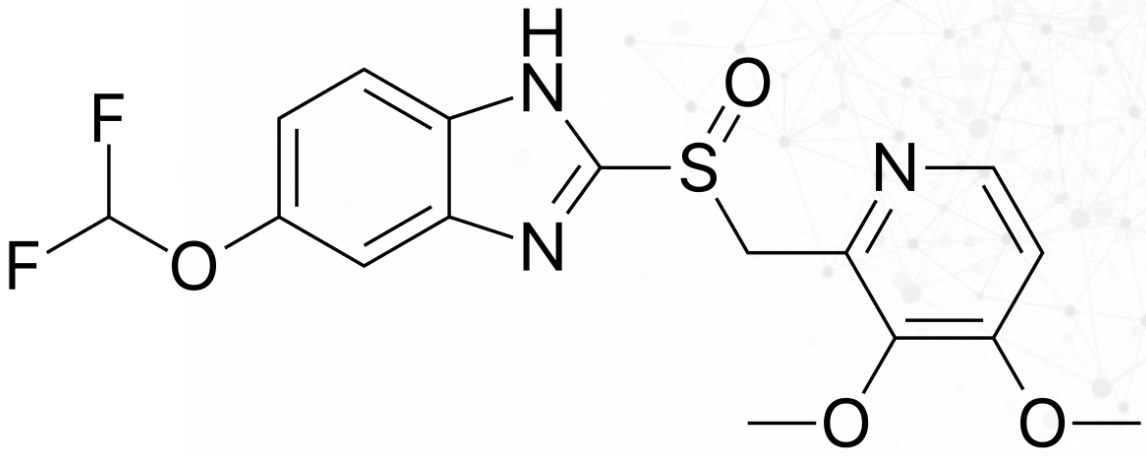



Similarity



**Example: Pantoprazole**, a medication to treat stomach ulcers.
Not currently in the CSD

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Results

| | Database Identifier | Deposition Number | Similarity Score More Info |
|---|---|---|---|
| ☑ | BOMQOK | 1113696 | 0.998 |
| ☑ | EYEJUP | 1511140 | 0.775 |
| ☑ | WETBIJ | 1563921 | 0.763 |
| ☑ | CENBIJ | 1556811 | 0.745 |
| ☑ | FOPYOZ | 692400 | 0.745 |
| ☑ | UDAVIF | 633383 | 0.745 |
| ☑ | UDAVIF01 | 633384 | 0.745 |
| ☑ | UDAVIF02 | 633385 | 0.745 |
| ☑ | UDAVIF03 | 633386 | 0.745 |
| ☑ | VAYXOI | 1280849 | 0.745 |
| ☑ | VAYXOI01 | 1280850 | 0.745 |
| ☑ | VAYXOI02 | 159050 | 0.745 |
| ☑ | VAYXOI03 | 633382 | 0.745 |

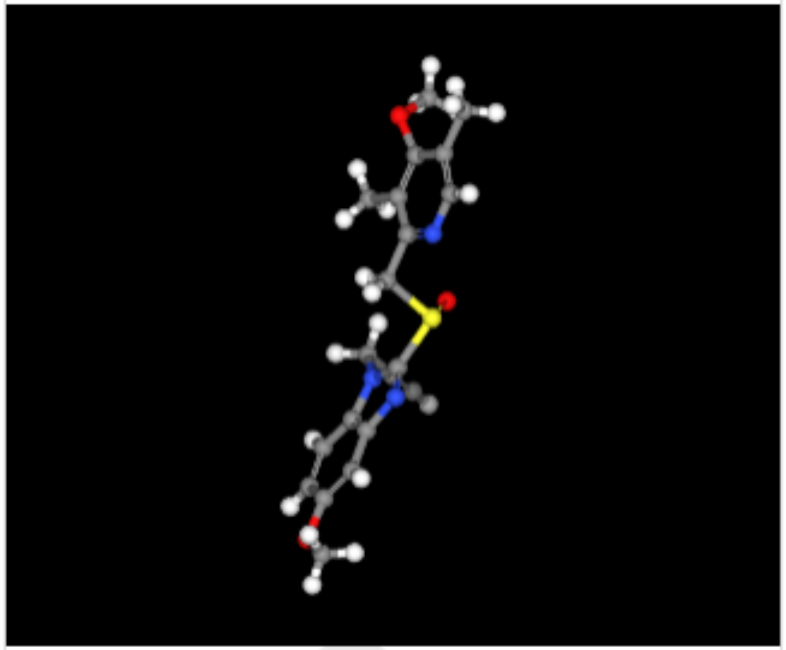
1 - 13 of 13 items

Download

EYEJUP : 5-methoxy-2-(((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)sulfinyl)-1-(prop-2-yn-1-yl)-1H-benzimidazole
**Space Group:** P $2_1/c$ (14), **Cell:** *a* 4.5974(3)Å *b* 30.675(2)Å *c* 13.8090(9)Å, *α* 90° *β* 91.961(1)° *γ* 90°

3D viewer

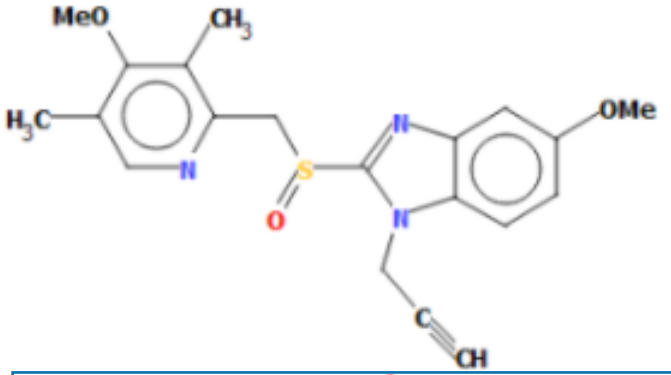
Ball and Stick | No Labels

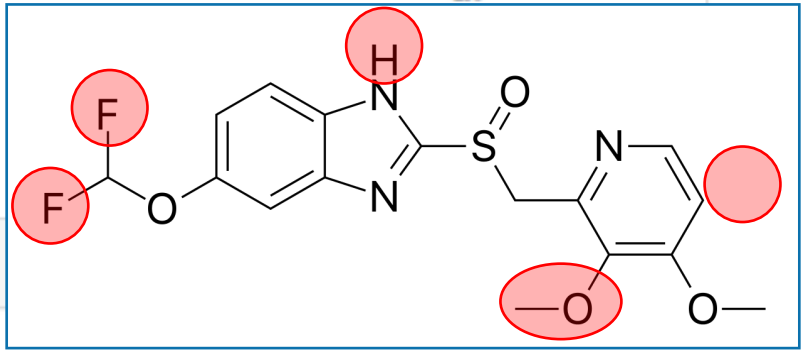


No Packing | H

DISORDER

Chemical diagram




CCDC

Results

| | Database Identifier | Deposition Number | Similarity Score More Info |
|---|---|---|---|
| ☑ | BOMQOK | 1113696 | 0.998 |
| ☑ | EYEJUP | 1511140 | 0.775 |
| ☑ | WETBIJ | 1563921 | 0.763 |
| ☑ | CENBIJ | 1556811 | 0.745 |
| ☑ | FOPYOZ | 692400 | 0.745 |
| ☑ | UDAVIF | 633383 | 0.745 |
| ☑ | UDAVIF01 | 633384 | 0.745 |
| ☑ | UDAVIF02 | 633385 | 0.745 |
| ☑ | UDAVIF03 | 633386 | 0.745 |
| ☑ | VAYXOI | 1280849 | 0.745 |
| ☑ | VAYXOI01 | 1280850 | 0.745 |
| ☑ | VAYXOI02 | 159050 | 0.745 |
| ☑ | VAYXOI03 | 633382 | 0.745 |

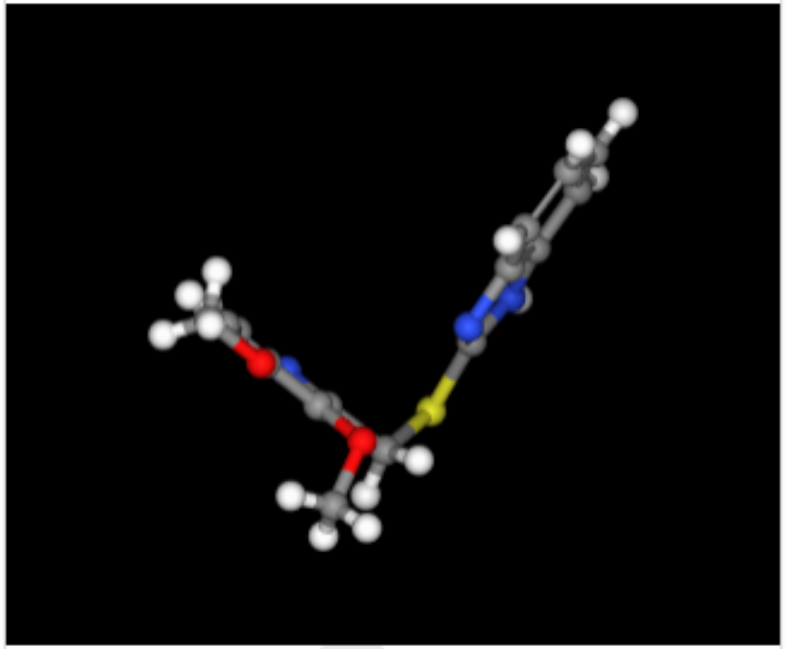
1 - 13 of 13 items

Download

WETBIJ : 2-{[(3,4-dimethoxypyridin-2-yl)methyl]sulfanyl}-1H-benzimidazole
**Space Group:** P $2_1$ $2_1$ $2_1$ (19), **Cell:** *a* 9.1828(16)Å *b* 11.625(2)Å *c* 13.463(2)Å, *α* 90° *β* 90° *γ* 90°

3D viewer

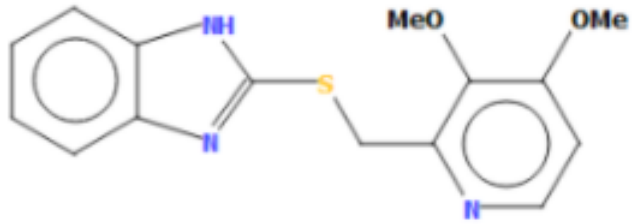
Ball and Stick | No Labels

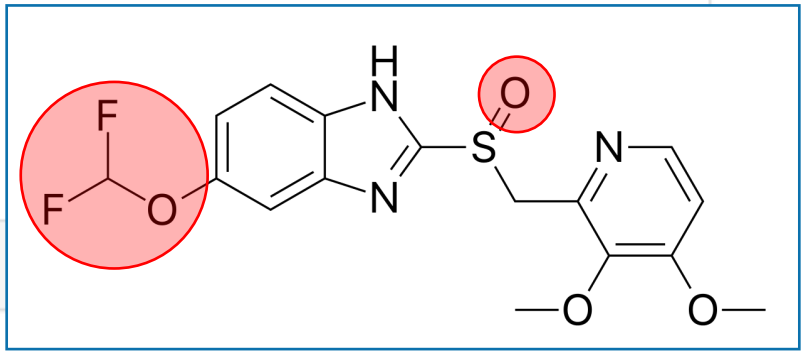


No Packing | H

DISORDER

Chemical diagram




CCDC