

Searching the CSD online – WebCSD 101



CCDC

Learning outcomes

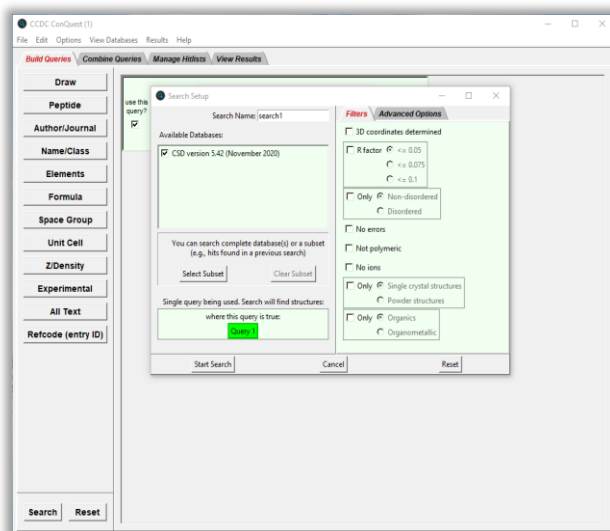
After this session you will know how to search the CSD online.

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.

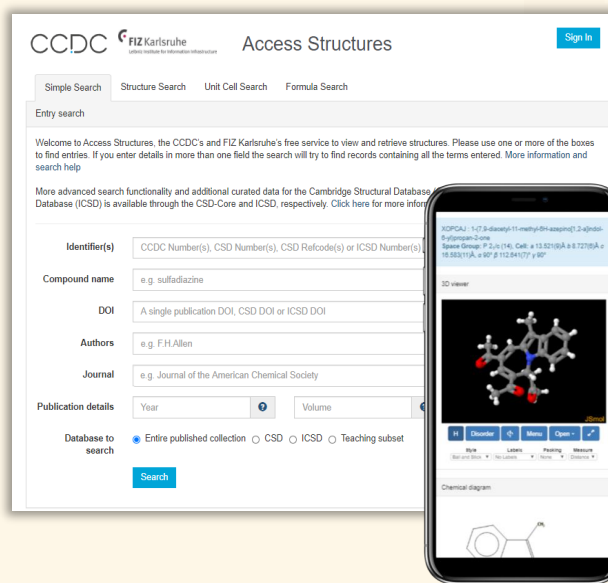
Show One: Structure searching

Desktop



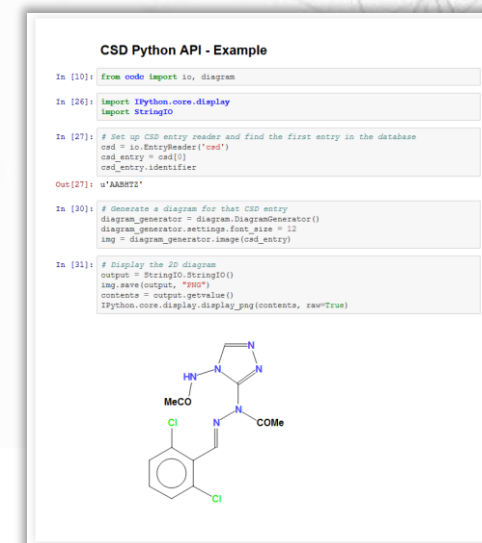
ConQuest

Web Browser



WebCSD /
Access Structures

Programmatic

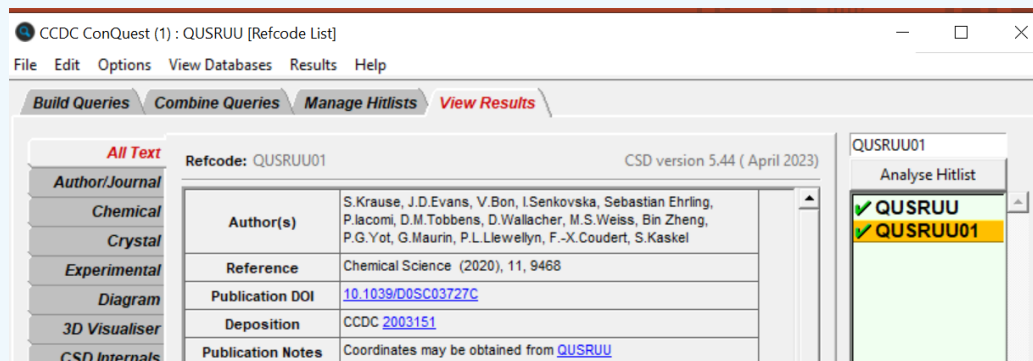


CSD Python API

Desktop vs Web

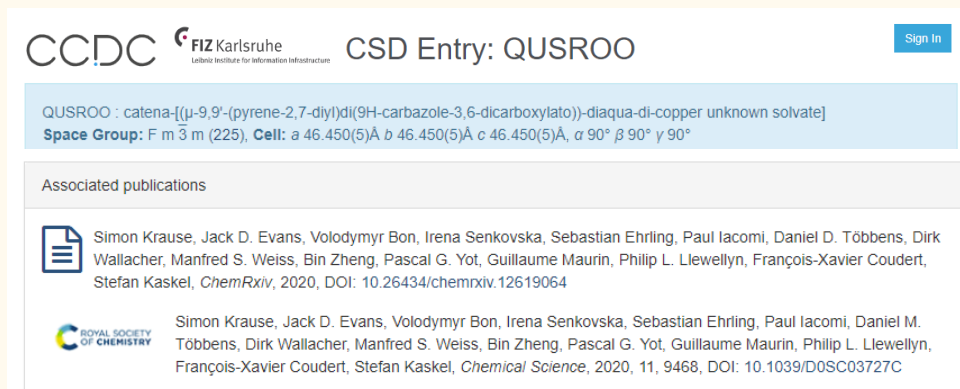
Desktop

- 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)



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.



The screenshot displays the CCDC Access Structures web portal. At the top, there are search tabs: Simple Search, Structure Search, Unit Cell Search, and Formula Search. Below these is an 'Entry search' section with a welcome message and search instructions. A search form is visible with fields for Identifier(s), Compound name, DOI, Authors, Journal, Publication details, and Database to. To the right, a 3D viewer shows a molecular structure, and below it, a chemical diagram is displayed. A 'Download deposited CIF' dialog box is open in the foreground, offering options to download CIF files with or without structure factor data, and including checkCIF reports. In the background, a smartphone displays the same interface, showing a 3D viewer and chemical diagram.

CCDC FIZ Karlsruhe
Access Structures

Simple Search Structure Search Unit Cell Search Formula Search

Entry search

Welcome to Access Structures, the CCDC's and FIZ Karlsruhe's free service to view and retrieve structures. Please use one or more of the search options to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. More information on search help

More advanced search functionality and additional curated data for the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD) is available through the CSD-Core and ICSD, respectively. Click here for more information.

Identifier(s) CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s)

Compound name e.g. sulfadiazine

DOI A single publication DOI, CSD DOI or ICSD DOI

Authors e.g. F.H.Allen

Journal e.g. Journal of the American Chemical Society

Publication details Year

Database to ☒ Entire published collection

Download deposited CIF

- ☐ Deposited CIF(s)
- ☐ Deposited CIF(s) without structure factor data
- ☒ Deposited file(s) with any available structure factor data and checkCIF reports included
- ☐ Include checkCIF reports as a PDF when available

Results

Database Identifier	Deposition Number
<input checked="" type="checkbox"/> AHEPLY	200783

Next Download

AHEPLY: N-(4-Hydroxyphenyl)acetamide morpholine
Space Group: P 2₁ (2), Cell: a 8.710(4)Å b 9.920(5)Å c 12.306(5)Å α 102.36(3)° β 108.33(2)° γ 96.68(3)°

3D viewer

Chemical diagram

Additional details

Deposition Number	200783
Data Citation	I.D.H. Oswald, W.D.S. Motherwell, S. Parsons, C.R. Pulham CCDC 200783: Experimental Crystal Structure Determination, 2003, DOI: 10.5517/ccdcgroup
Synonyms	Paracetamol morpholine, Acetaminophen morpholine
Deposited on	16/12/2002

Associated publications

Journal	Volume	Page	DOI
I.D.H. Oswald, W.D.S. Motherwell, S. Parsons, C.R. Pulham, Acta Crystallographica Section E: Structure Reports Online	2002, 58, 1290	DOI: 10.1107/S1600536802016111	

www.ccdc.cam.ac.uk/structures

CCDC

Search, view and download structures

Simple Search

Structure Search

Unit Cell Search

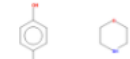


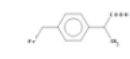
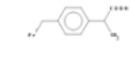
Formula Search

Your query was: Compound name: paracetamol and the search returned more than 30 records.

Select all

Download Selected

View Selected

<input checked="" type="checkbox"/>	AHEPUY		Deposition Number(s): 200783 Space Group: P $\bar{1}$ (2) Cell: <i>a</i> 8.710(4)Å <i>b</i> 9.920(5)Å <i>c</i> 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)° Compound Name: N-(4-Hydroxyphenyl)acetamide morpholine Synonyms: Paracetamol , morpholine, Acetaminophen morpholine
<input checked="" type="checkbox"/>	AMUBAM		Deposition Number(s): 803736 Space Group: P $\bar{1}$ (2) Cell: <i>a</i> 8.710(4)Å <i>b</i> 9.920(5)Å <i>c</i> 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)° Compound Name: N-(4-Hydroxyphenyl)acetamide morpholine Synonyms: Paracetamol , morpholine, Acetaminophen morpholine
<input checked="" type="checkbox"/>	COKCEL		Deposition Number(s): 803736 Space Group: P $\bar{1}$ (2) Cell: <i>a</i> 8.710(4)Å <i>b</i> 9.920(5)Å <i>c</i> 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)° Compound Name: N-(4-Hydroxyphenyl)acetamide morpholine Synonyms: Paracetamol , morpholine, Acetaminophen morpholine
<input checked="" type="checkbox"/>	COTYOA02		Deposition Number(s): 735856 Space Group: P $\bar{1}$ (2) Cell: <i>a</i> 8.710(4)Å <i>b</i> 9.920(5)Å <i>c</i> 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)° Compound Name: Acetaminophen Synonyms: paracetamol , DrugBank: DB00316
<input checked="" type="checkbox"/>	COTYOA03		Deposition Number(s): 735856 Space Group: P $\bar{1}$ (2) Cell: <i>a</i> 8.710(4)Å <i>b</i> 9.920(5)Å <i>c</i> 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)° Compound Name: Acetaminophen Synonyms: paracetamol , DrugBank: DB00316

Results

<input checked="" type="checkbox"/> Database Identifier	Deposition Number
<input checked="" type="checkbox"/> AHEPUY	200783

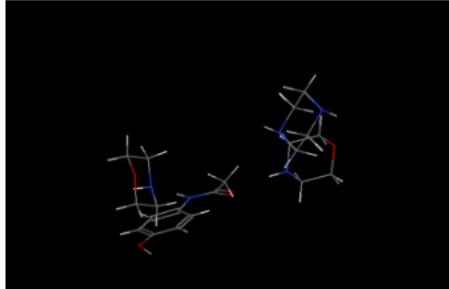
Next

Download

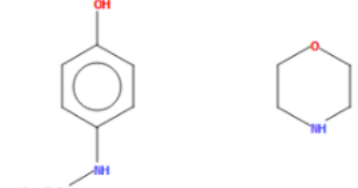
AHEPUY : N-(4-Hydroxyphenyl)acetamide morpholine

Space Group: P $\bar{1}$ (2), Cell: *a* 8.710(4)Å *b* 9.920(5)Å *c* 12.385(5)Å, α 102.35(3)° β 108.33(2)° γ 96.68(3)°

3D viewer



Chemical diagram



View group symbols key

Pulham CCDC 200783: Experimental Crystal xwp

ine

raphica Section E: Structure Reports Online,

CCDC

Download deposited CIF

☐ Deposited CIF(s)

☐ Deposited CIF(s) without structure factor data

☒ Deposited file(s) with any available structure factor data and checkCIF reports included

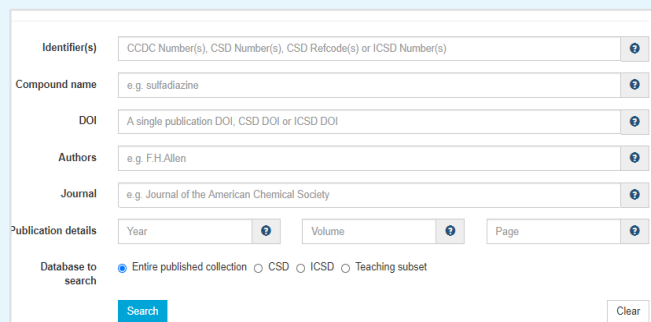
☐ Include checkCIF reports as a PDF when available

```
#####
#
# This file contains crystal structure data downloaded from the
# Cambridge Structural Database (CSD) hosted by the Cambridge
# Crystallographic Data Centre (CCDC).
#
# Full information about CCDC data access policies and citation
# guidelines are available at http://www.ccdc.cam.ac.uk/access/V1
#
# Audit and citation data items may have been added by the CCDC.
# Please retain this information to preserve the provenance of
# the file and to allow appropriate attribution of the data.
#####
_audit_block_id 10.5517/cc139166
_audit_block_doi 10.5517/cc139166
_audit_block_depnum_ccdc_archive 'CCDC 1022107'
loop_
_citation_id
_citation_doi
_citation_year
1 10.1039/C4CE01795A 2015
_audit_update_record
;
2014-08-30 deposited with the CCDC. 2021-01-22 downloaded from the CCDC.
;
_audit_creation_method SHELXL-97
_chemical_name_systematic
;
(bis) vanillic acid theophylline co-crystal
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety ?
_chemical_formula_sum 'C23 H23 N4 O10'
_chemical_formula_weight 515.45
```

Web: Structure searching

Access structures

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



Identifier(s) CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s) ?

Compound name e.g. sulfadiazine ?

DOI A single publication DOI, CSD DOI or ICSD DOI ?

Authors e.g. F.H.Allen ?

Journal e.g. Journal of the American Chemical Society ?

Publication details Year ? Volume ? Page ?

Database to search ☒ Entire published collection ☐ CSD ☐ ICSD ☐ Teaching subset

Search Clear

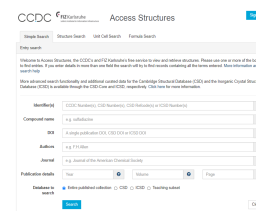
Web Browser

Access Structures



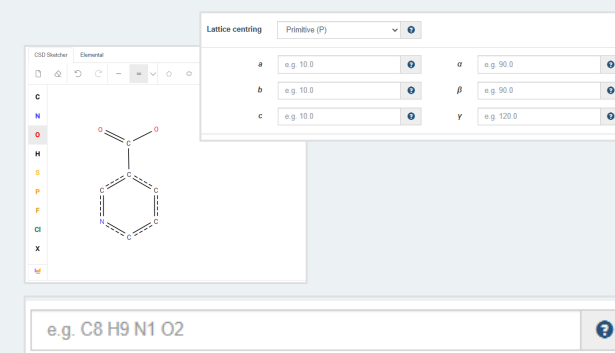
WebCSD

- 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.



Lattice centring Primitive (P) ?

a e.g. 10.0 ? α e.g. 90.0 ?

b e.g. 10.0 ? β e.g. 90.0 ?

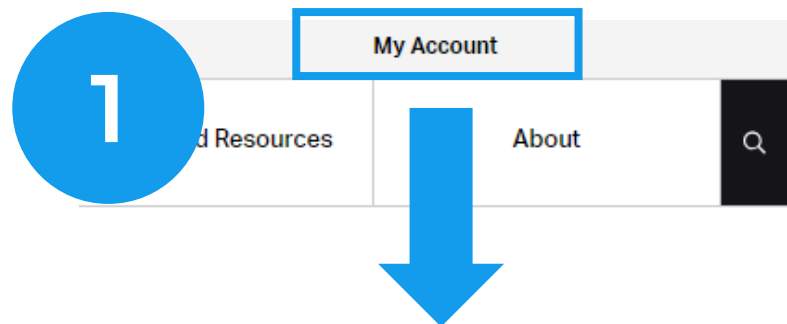
c e.g. 10.0 ? γ e.g. 120.0 ?

Chemical structure diagram

e.g. C8 H9 N1 O2 ?

Logging into WebCSD

Option I.

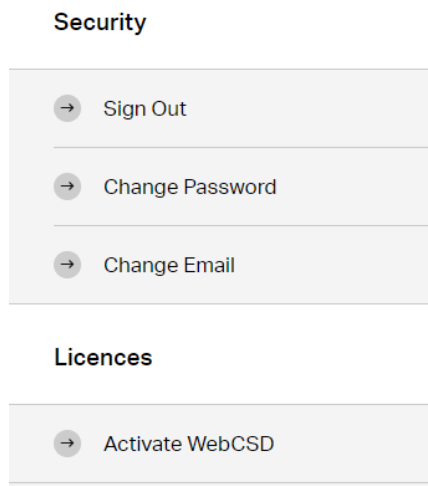
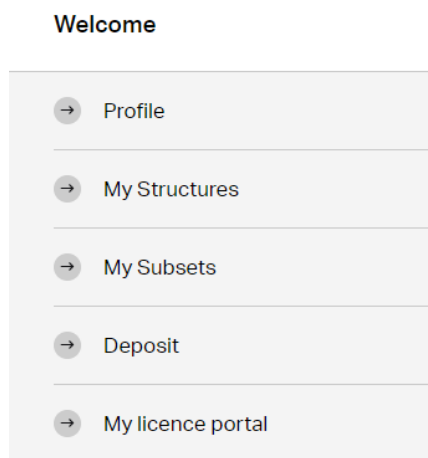


Sign in with your CCDC account

A login form with the following elements:

- Input field for 'Username or Email'
- Input field for 'Password'
- Checkbox for 'Remember me?'
- Blue 'Sign In' button
- Link for 'Forgotten Us' (partially visible)

A large blue circle with the number '2' is positioned to the right of the form, and a blue arrow points from the 'Sign In' button towards the 'Licences' section of the dashboard.



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.

Activate WebCSD Licence

A screenshot of the 'Activate WebCSD Licence' form. It contains the following elements:

- Input field for 'Licence Customer Number *'
- Input field for 'Licence Activation Key *'
- Captcha field
- Blue 'Activate' button

A large blue circle with the number '4' is positioned to the right of the form, and a blue arrow points from the 'Activate WebCSD' link in the dashboard to this form.

WebCSD

Simple Search

Structure Search

Unit Cell Search

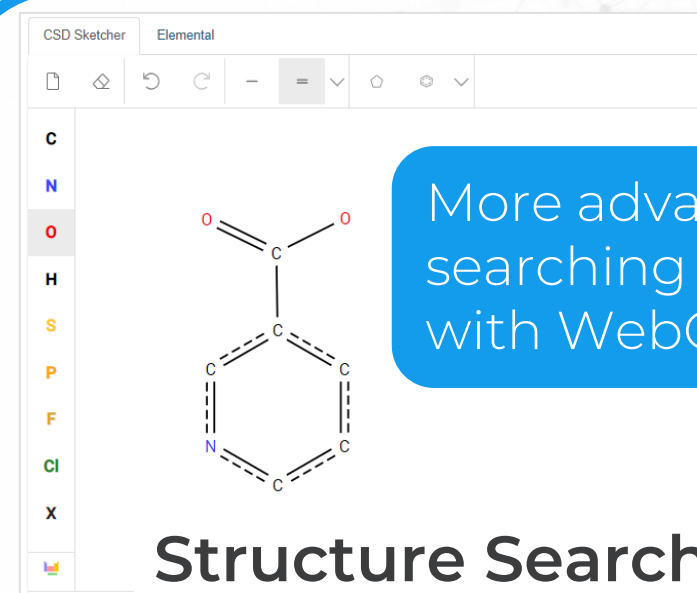
Formula Search

Access Structures and WebCSD

Search interface for Simple Search:

- Identifier(s): CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s)
- Compound name: e.g. sulfadiazine
- DOI: A single publication DOI, CSD DOI or ICSD DOI
- Authors: e.g. F.H.Allen
- Journal: e.g. Journal of the American Chemical Society
- Publication details: Year, Volume, Page
- Database to search: ☒ Entire published collection ☐ CSD ☐ ICSD ☐ Teaching subset
- + Add New Search Field
- Search

Simple Search



Unit Cell Search

Search interface for Unit Cell Search:

Lattice centring: Primitive (P)

a	e.g. 10.0	α	e.g. 90.0
b	e.g. 10.0	β	e.g. 90.0
c	e.g. 10.0	γ	e.g. 120.0

Formula Search

e.g. C8 H9 N1 O2


CCDC

Searching specific information fields

CCDC

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

WebCSD

 Licensed to: CCDC Main Site

Simple Search Structure Search Unit Cell Search Formula Search

Simple text and numeric searching

Welcome to WebCSD. This service now includes the ability to search for inorganic structures through the CCDC's and FIZ Karlsruhe's joint Access Service using the Simple Search tab. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. [More information and search help](#)

Identifier(s)	CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s) ?	
Compound name	e.g. sulfadiazine ?	
DOI	A single publication DOI, CSD DOI or ICSD DOI ?	
Authors	e.g. F.H.Allen ?	
Journal	e.g. Journal of the American Chem ?	
Publication details	Year ?	Page ?
Database to search	<input checked="" type="radio"/> Entire published collection <input type="radio"/> CS	
	<div>+ Add New Search Field</div>	
	<div>+ Add New Search Field</div>	
	<div>Bioactivity</div>	
	<div>Crystal colour</div>	
	<div>Disorder</div>	
	<div>Habit</div>	
	<div>Phase transitions</div>	
	<div>Polymorph</div>	
	<div>Recrystallisation solvent</div>	
	<div>Search</div>	<div>Clear</div>

CCDC

Formula Searching

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

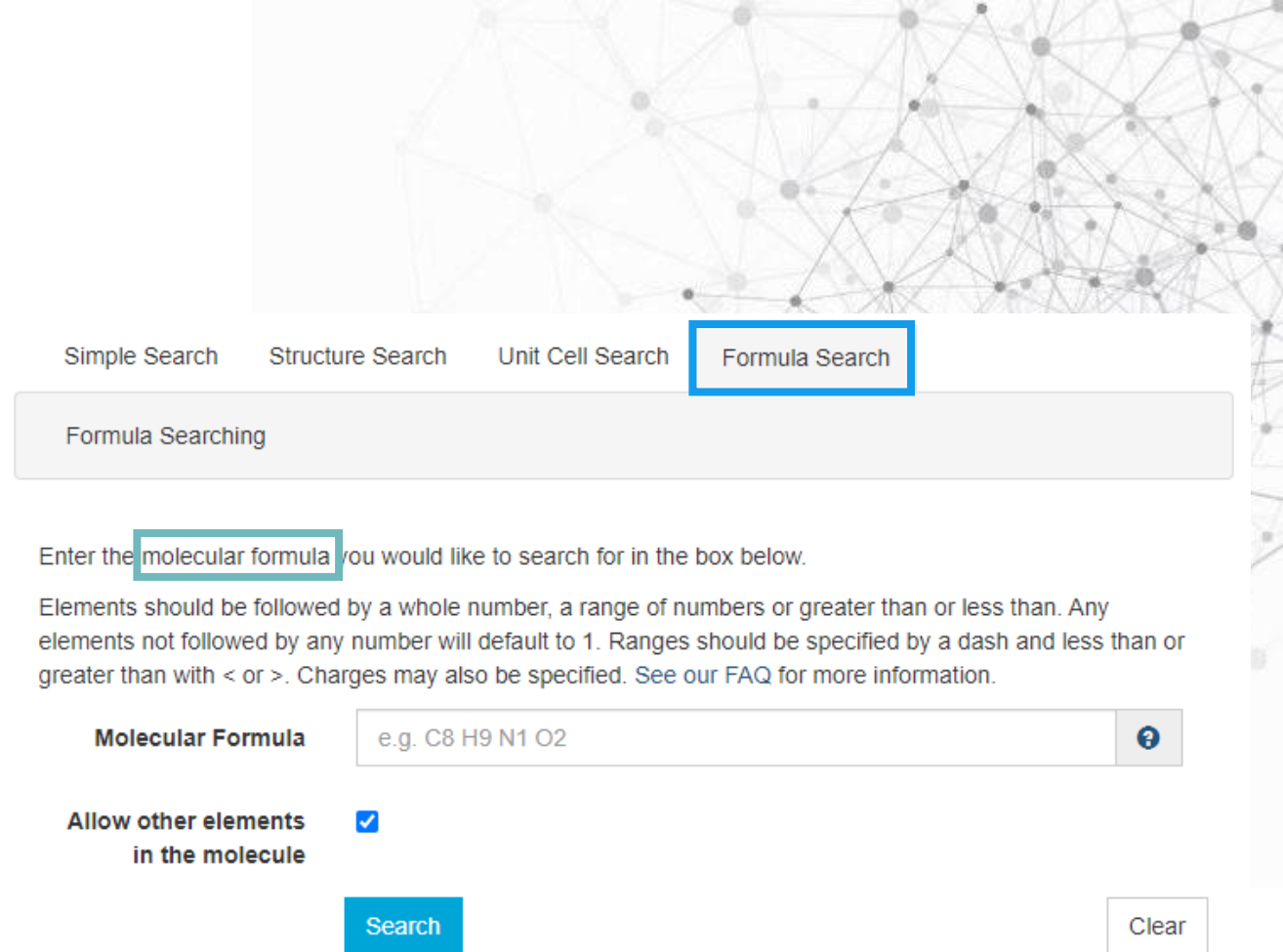
- e.g. **Cd C5 O2**
- Assumes number of atoms is 1 if no number given

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)



The screenshot shows the CCDC Formula Searching interface. At the top, there are four tabs: 'Simple Search', 'Structure Search', 'Unit Cell Search', and 'Formula Search' (which is highlighted with a blue border). Below the tabs is a header bar labeled 'Formula Searching'. The main content area contains instructions: 'Enter the **molecular formula** you would like to search for in the box below.' followed by a detailed explanation of the search syntax: 'Elements should be followed by a whole number, a range of numbers or greater than or less than. Any elements not followed by any number will default to 1. Ranges should be specified by a dash and less than or greater than with < or >. Charges may also be specified. See our FAQ for more information.' Below this is a search form with a label 'Molecular Formula' and a text input field containing 'e.g. C8 H9 N1 O2'. To the right of the input field is a help icon. Below the input field is a checkbox labeled 'Allow other elements in the molecule' which is checked. At the bottom of the form are two buttons: 'Search' and 'Clear'.

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)

Unit Cell Search

Simple Search

Structure Search

Unit Cell Search

Formula Search

Unit Cell Searching

Mandatory fields

Lattice centring

Primitive (P)

a

e.g. 10.0

Cell length *a* (Å)

α

e.g. 90.0

b

e.g. 10.0

β

e.g. 90.0

Cell angle *β* (°)

c

e.g. 10.0

γ

e.g. 120.0

Advanced

Tolerance options

Tolerances

Length tolerance

1.5

Angle tolerance

2.0

Search

% cell length tolerance of longest cell dimension

Angle tolerance (°)

Clear

CCDC

Structure Search

Tip: Hover over the buttons to see more information

Simple Search **Structure Search** Unit Cell Search Formula Search

Chemical structure searching

Bond types

More templates

Autogenerate H-atoms and connections and change settings

Upload Mol file

☐ AUTO GENERATE

Editing features

Ring templates

Zoom in and out

Pan or reset view

Quick access to elements

Any element

Periodic table

Add 3D parameters

Select an element then left click in space to add an atom

Left click and drag from an atom to attach an atom

Right click on an atom or bond to edit or add extra properties to it

Suggestions and tips can be displayed as you draw.

See advanced options (SMARTS)

Version: 1.9.40 - [Enabled Features](#)

Match condition: ☐ Substructure ☒ Similarity

Select search type

☒ Toggle Hints

Advanced

CCDC

Results

Results listed
by REFCODE

Simple Search Structure Search Unit Cell Search Formula Search

Search Complete - 1000 Results Found

Progress bar

100%

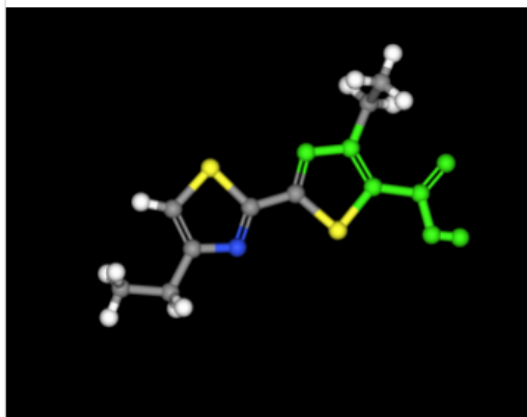
Modify Search New Search

Database Identifier	Deposition Number
<input checked="" type="checkbox"/> ARILUL	2022486
<input checked="" type="checkbox"/> ARIMAS	2022487
<input checked="" type="checkbox"/> ASIREZ	220759
<input checked="" type="checkbox"/> ASUSIS	1014639
<input checked="" type="checkbox"/> AVEMUK	839256
<input checked="" type="checkbox"/> AVEMUK01	1443393
<input checked="" type="checkbox"/> AWABEG	805484
<input checked="" type="checkbox"/> AYAVAY	756717
<input checked="" type="checkbox"/> AYEBIP	242352
<input checked="" type="checkbox"/> AYIKEZ	710956
<input checked="" type="checkbox"/> AYIKEZ01	842925
<input checked="" type="checkbox"/> AYIKEZ02	906630
<input checked="" type="checkbox"/> AYINOM	845206
<input checked="" type="checkbox"/> AYIYAJ	845248
<input checked="" type="checkbox"/> AYOYUK	1509954
<input checked="" type="checkbox"/> AZOKAE	2074661
<input checked="" type="checkbox"/> AZOKUW	850471
<input checked="" type="checkbox"/> BADNOM	1413573
<input checked="" type="checkbox"/> BAFKEA	774582
<input checked="" type="checkbox"/> BAWHIR	210815
<input checked="" type="checkbox"/> BETKUH	237120
<input checked="" type="checkbox"/> BEWVIM	2099287
<input checked="" type="checkbox"/> 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°

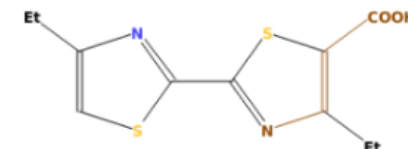
3D viewer

Ball and Stick No Labels



No Packing H Disorder

Chemical diagram



View group symbols key

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

Chemical details

3D viewer and 2D
chemical diagram

The substructure
searched is
highlighted.

More bibliographic,
chemical, crystal and
experimental details

CCDC DOI

Link to
publication

CCDC


Results

Download
results

<input checked="" type="checkbox"/>	AYIJAJ	845248
<input checked="" type="checkbox"/>	AYOYUK	1509954
<input checked="" type="checkbox"/>	AZOKAE	2074661
<input checked="" type="checkbox"/>	AZOKUW	850471
<input checked="" type="checkbox"/>	BADNOM	1413573
<input checked="" type="checkbox"/>	BAFKEA	774582
<input checked="" type="checkbox"/>	BAWHIR	210815
<input checked="" type="checkbox"/>	BETKUH	237120
<input checked="" type="checkbox"/>	BEWVIM	2099287
<input checked="" type="checkbox"/>	BEWVOS	2099289
<input checked="" type="checkbox"/>	BEWWEJ	2099288
<input checked="" type="checkbox"/>	BICYER	1110283
<input checked="" type="checkbox"/>	BIHHIM	1855210
<input checked="" type="checkbox"/>	BIJZAZ	2256588
<input checked="" type="checkbox"/>	BIJZED	2256589
<input checked="" type="checkbox"/>	BIKDAE	1817775
<input checked="" type="checkbox"/>	BIMYED	932966

31 - 60 of 1000 items

Download

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, <i>Journal of the American Chemical Society</i> , 2004, 126, 4318, DOI: 10.1021/ja0397916
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 α 90° β 113.443(4)° γ 90°
Cell volume	2454.64
Reduced cell	a 5.188Å b 11.625Å c 21.160Å 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	
PubChem	86035535

More bibliographic,
chemical, crystal and
experimental details

CCDC DOI

Link to
publication

Other links
– if available

CCDC

Selecting search type

The screenshot shows the 'Chemical structure searching' interface. At the top, there are four tabs: 'Simple Search', 'Structure Search' (selected), 'Unit Cell Search', and 'Formula Search'. Below the tabs is a search bar labeled 'Chemical structure searching'. A blue box highlights the 'AUTO GENERATE' button and the 'Auto Generate Settings' dialog. The dialog has three options: 'Exact' (selected), 'Generate Connections', and 'Generate Hydrogens'. Below the dialog, a chemical structure of a substituted benzene ring is shown, with an arrow pointing to its expanded representation where atoms are labeled with indices (e.g., CH₃^(X4), CH₂^(X4), NH₁^(X3)). At the bottom, a blue box highlights the 'Match condition' section, which has two options: 'Substructure' and 'Similarity' (selected). The version '1.9.40 - Enabled Features' is displayed at the bottom left.

Simple Search Structure Search Unit Cell Search Formula Search

Chemical structure searching

AUTO GENERATE

Auto Generate Settings

- ☒ Exact
- ☐ Generate Connections
- ☐ Generate Hydrogens

Find out more about the Tanimoto coefficient in the glossary of the hand-out

Match condition: ☐ Substructure ☒ Similarity

Version: 1.9.40 - [Enabled Features](#)

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.

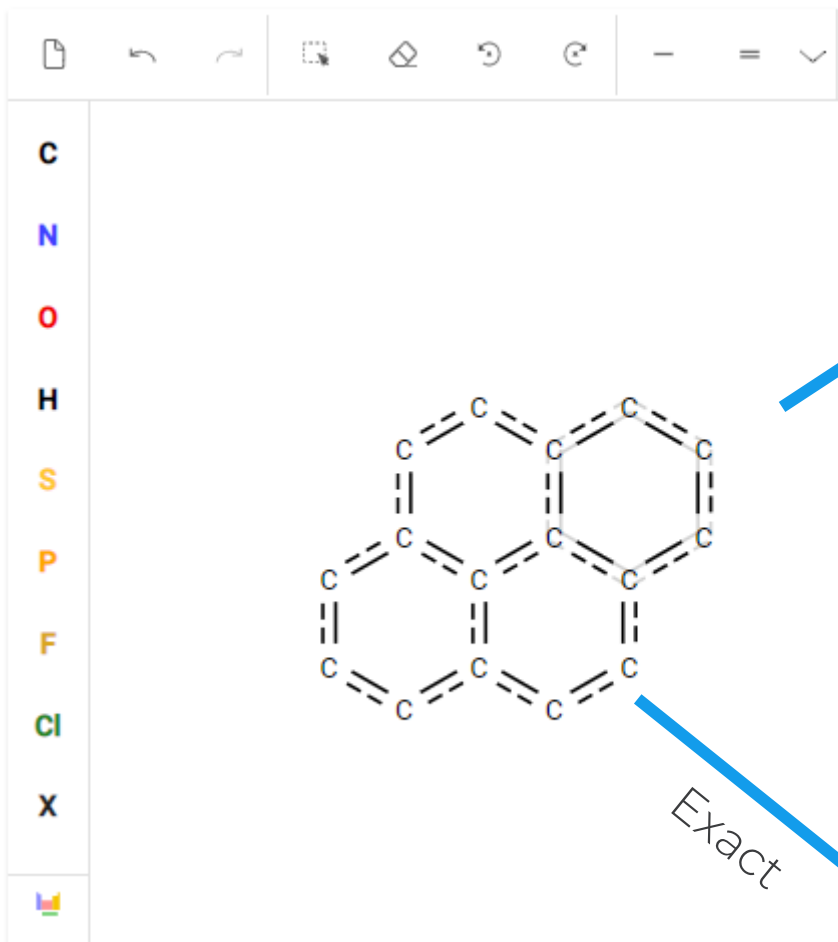
Similarity

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



Simple Search Structure Search Unit Cell Search Formula Search

Search Complete **1000 Results Found**

100%

Modify Search New Search

Results

Database Identifier	Deposition Number
ABALIZ	244177
ABIBEW	2072185
ABIBIA	2072186
ABIBOG	2072187
ABICAT	2072188
ABICEX	2072189
ABIKOP	2080990
ABINIM	2091443
ABUHEN	1434681
ABUJIT	1448617
ABUJIU	2076486
ABUREW	830174
ABURIA	830175

ABALIZ : 2,5,8,10,15,17-hexakis(t-butyl)-(bc,ef,hi,uv)tetrabenzovalene hexane solvate
Space Group: P c a b (61), Cell: a 17.2333(8)Å b 24.8954(8)Å c 29.6704(9)Å, α 90° β 90° γ 90°

3D viewer

Ball and Stick No Labels

Chemical diagram

View group symbols key

Simple Search Structure Search Unit Cell Search Formula Search

Search Complete **385 Results Found**

100%

Modify Search New Search

Results

Database Identifier	Deposition Number
ABUJIU	2076486
ABUTEY	823544
AGORAS	1847617
AGORAS01	1847613
AGOREW	1847618
AGOREW01	1847616
AGOREW02	1847615
AKACUM	1451536
AKACUM01	1451537
AKECEA	1449783
AKIVEX	998244
ASULOS	1893487
ATAMAM	2062107
ATAMEQ	2062108

ASULOS : (2-[[3-(pyridin-2-yl)-1H-pyrazol-1-yl]methyl]-3-[[3-(pyridin-2-yl)-1H-pyrazol-1-yl]methyl]quinoxaline)-silver perchlorate hemikis(pyrene)
Space Group: P 2₁/c (14), Cell: a 10.771(2)Å b 19.080(4)Å c 15.000(3)Å, α 90° β 93.45(3)° γ 90°

3D viewer

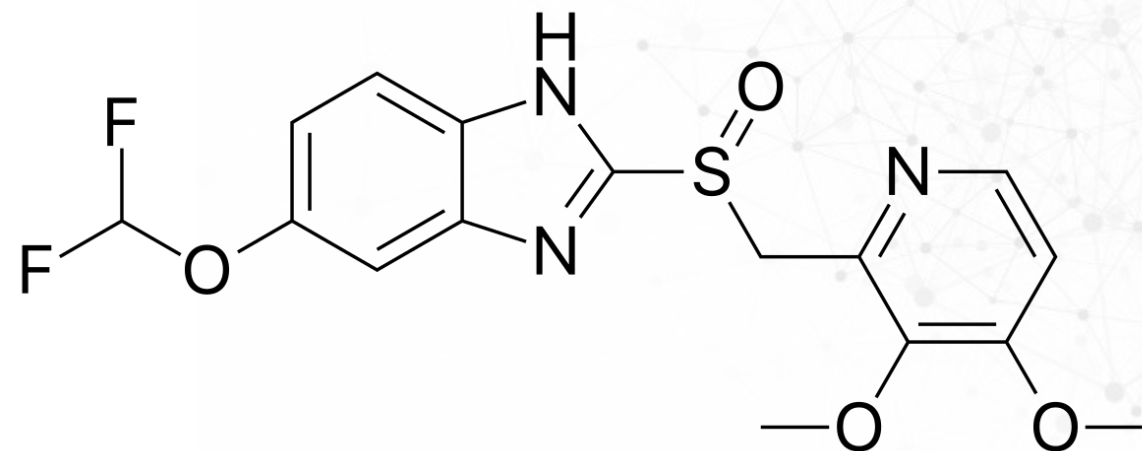
Ball and Stick No Labels

Chemical diagram

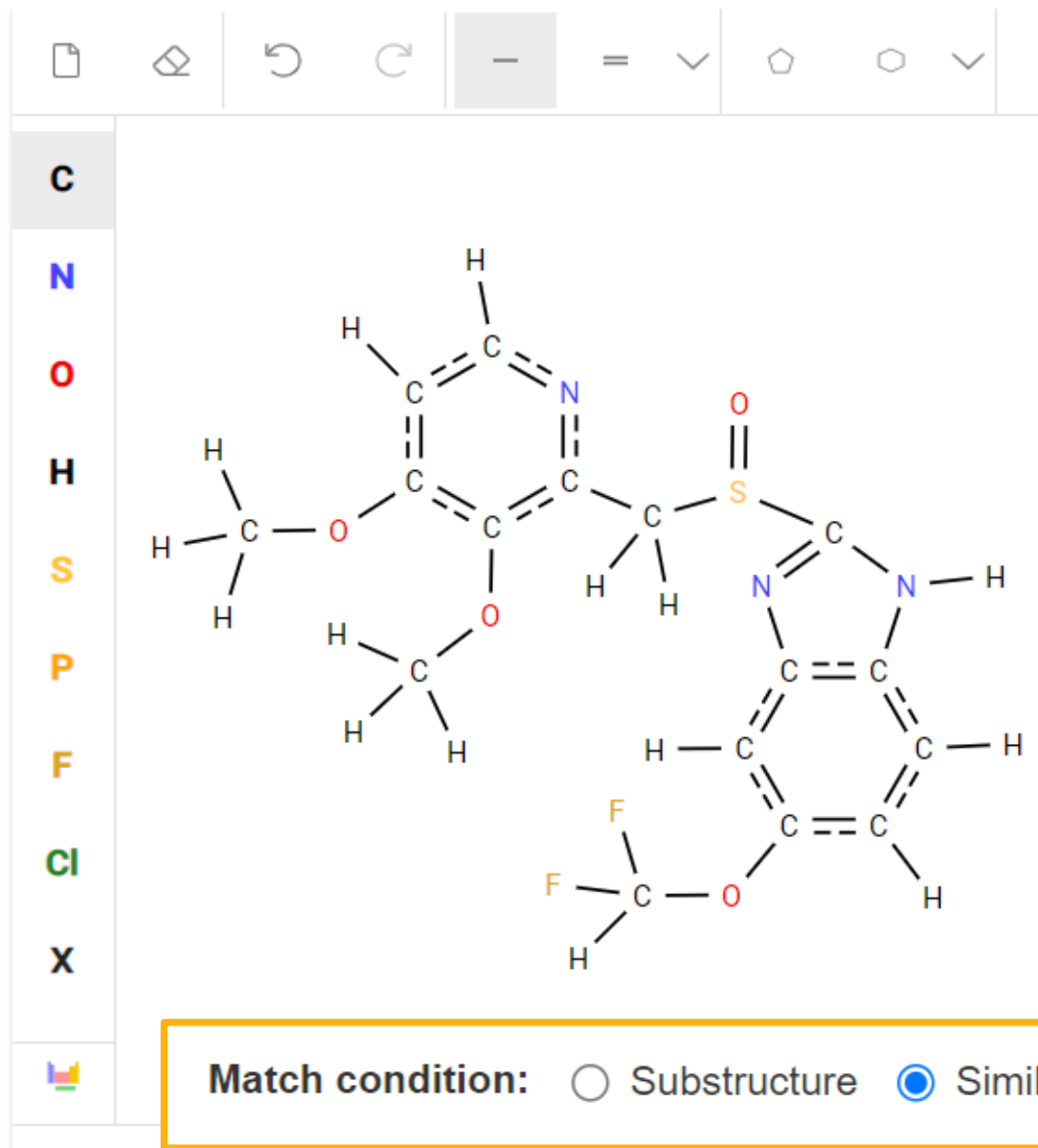
View group symbols key

385 hits
Only structures with
pyrene on its own

☒ Similarity



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



The image shows a chemical structure editor interface. On the left is a vertical toolbar with buttons for Carbon (C), Nitrogen (N), Oxygen (O), Hydrogen (H), Sulfur (S), Phosphorus (P), Fluorine (F), Chlorine (Cl), and Xenon (X). Below these is a small icon of a multi-colored bar. The main area displays a chemical structure of a complex molecule with multiple fused and linked rings, including benzene, pyridine, and a sulfonamide group. At the bottom, a box contains the text "Match condition:" followed by two radio buttons: "Substructure" (unselected) and "Similarity" (selected).

Results			
<input checked="" type="checkbox"/>	Database Identifier	Deposition Number	Similarity Score More Info
<input checked="" type="checkbox"/>	BOMQOK	1113696	0.998
<input checked="" type="checkbox"/>	EYEJUP	1511140	0.775
<input checked="" type="checkbox"/>	WETBIJ	1563921	0.763
<input checked="" type="checkbox"/>	CENBIJ	1556811	0.745
<input checked="" type="checkbox"/>	FOPYOZ	692400	0.745
<input checked="" type="checkbox"/>	UDAVIF	633383	0.745
<input checked="" type="checkbox"/>	UDAVIF01	633384	0.745
<input checked="" type="checkbox"/>	UDAVIF02	633385	0.745
<input checked="" type="checkbox"/>	UDAVIF03	633386	0.745
<input checked="" type="checkbox"/>	VAYXOI	1280849	0.745
<input checked="" type="checkbox"/>	VAYXOI01	1280850	0.745
<input checked="" type="checkbox"/>	VAYXOI02	159050	0.745
<input checked="" type="checkbox"/>	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

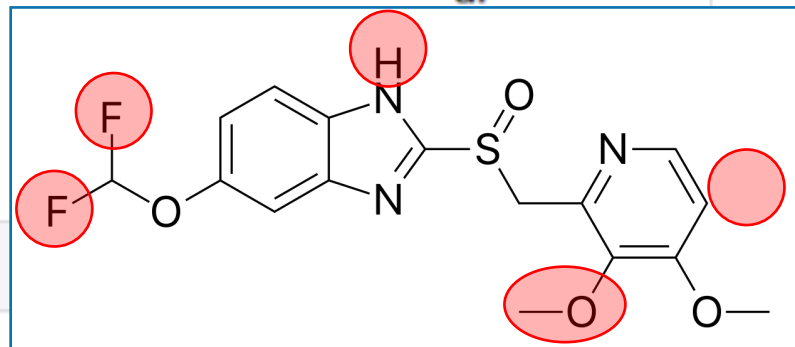
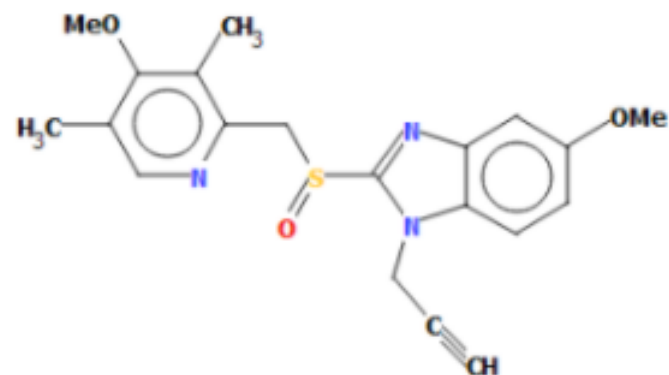
Ball and Stick ▾ No Labels ▾    



 No Packing ▾ **H**

DISORDER 

Chemical diagram



CCDC

Results			
<input checked="" type="checkbox"/>	Database Identifier	Deposition Number	Similarity Score More Info
<input checked="" type="checkbox"/>	BOMQOK	1113696	0.998
<input checked="" type="checkbox"/>	EYEJUP	1511140	0.775
<input checked="" type="checkbox"/>	WETBIJ	1563921	0.763
<input checked="" type="checkbox"/>	CENBIJ	1556811	0.745
<input checked="" type="checkbox"/>	FOPYOZ	692400	0.745
<input checked="" type="checkbox"/>	UDAVIF	633383	0.745
<input checked="" type="checkbox"/>	UDAVIF01	633384	0.745
<input checked="" type="checkbox"/>	UDAVIF02	633385	0.745
<input checked="" type="checkbox"/>	UDAVIF03	633386	0.745
<input checked="" type="checkbox"/>	VAYXOI	1280849	0.745
<input checked="" type="checkbox"/>	VAYXOI01	1280850	0.745
<input checked="" type="checkbox"/>	VAYXOI02	159050	0.745
<input checked="" type="checkbox"/>	VAYXOI03	633382	0.745

⏮

⏪

⏩

⏭





1 - 13 of 13 items

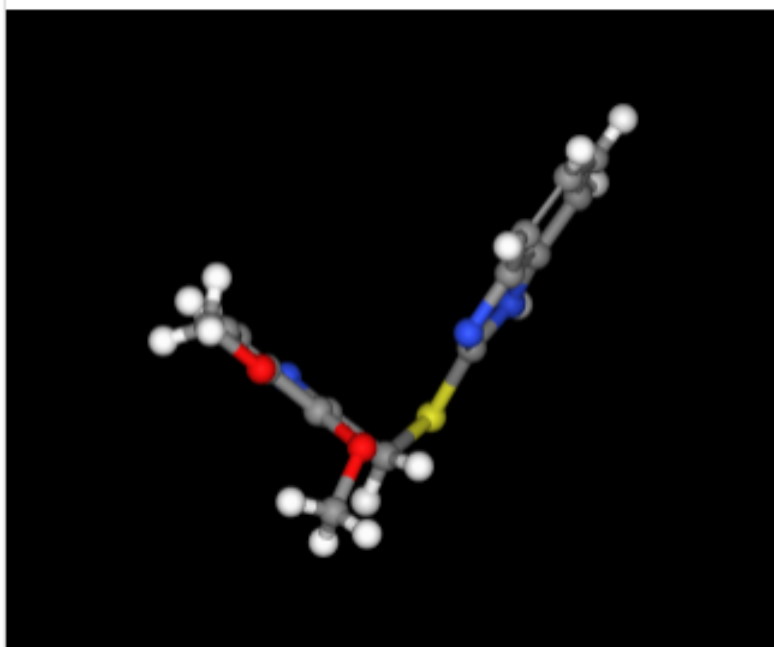
Download ▾

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

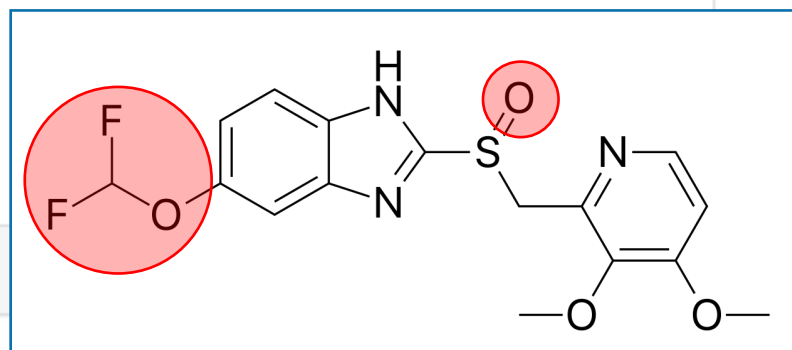
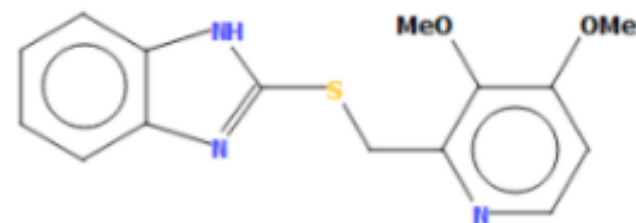
Ball and Stick ▾ No Labels ▾    



▶ No Packing ▾ H

DISORDER

Chemical diagram



CCDC