

# **E2020 – Soft skills II – Information Literacy**

## **4. Databases: Practical**

01.03.2022

Mgr. Ludovic Mayer

[\*ludovic.mayer@recetox.muni.cz\*](mailto:ludovic.mayer@recetox.muni.cz)

# Content

- Lecture divided into 2 parts:
  - 1<sup>st</sup> part: Theoretical – to understand how is the information stored
    - how to access it
  - 2<sup>nd</sup> part: Practical – **you are at the helm and you find the information!**

# Content

– 2<sup>nd</sup> part: Practical – you are at the helm and you find the information!

- Publication databases
  - Properties databases
  - Spectral databases
  - Registration (legal) databases
  - Protein and DNA databases
  - Patent database
- 
- This week
- Next week

# Publication database

- <https://www.scopus.com/search/form.uri?display=basic#basic>
  - <https://www.webofscience.com/wos/woscc/basic-search>
  - <https://scholar.google.com/>
- 
- **Task 0**: Let's look together for a research paper
    - Topic?

# Proficient search

- How to build an advance request?
  - By using logical operator:  
AND, OR, etc.

## Basic Search

Search for records from our product indexes. All successful searches are added to the [Search History](#) table. Remember to follow all applicable [search rules](#) when creating your search queries.

You can select up to three fields on the Search page as your default search fields. You can enter up to 6,000 terms in a search query.

Adding a new field also sets the second field to the AND operator. You can change the AND operator to OR or NOT.

Please note that your settings are applied to all product databases in your subscription package.

**Note:** Administrators may set to display one to three search fields as the default search fields for their entire institution.

## Interface Language

The interface language that you select determines the language of the on-screen instructions and help information. Consequently, search queries must always be in English. The results of your search are always in English.

See [Selecting an Interface Language](#).

## Search Operator Precedence

If you use different operators in your search, the search is processed according to this order of precedence:

1. NEAR/x
2. SAME
3. NOT
4. AND
5. OR

[More Information?](#)

# Proficient search

– <https://www.webofscience.com/wos/woscc/basic-search>

## – Filter a results

- By adding a keyword
- Restrictions by publication type: article, review, etc.
- Time limit: eg the last 10 years

The screenshot displays the Web of Science search interface. At the top, there are navigation links for 'Search', 'Marked List', 'History', and 'Alerts'. The main header reads 'Discover multidisciplinary content from the world's most trusted global citation database.' Below this, there are two tabs: 'DOCUMENTS' (selected) and 'RESEARCHERS'. The search area is set to 'Web of Science Core Collection' and 'Editions: All'. There are three sub-tabs: 'DOCUMENTS', 'CITED REFERENCES', and 'STRUCTURE'. The search criteria are: 'Topic' (dropdown) with 'Epoiconazole' in the input field, and 'And' (dropdown) with 'Topic' (dropdown) and 'toxicity' in the input field. A '+ Add row' button is visible. A dropdown menu is open, showing a list of search fields: 'All Fields', 'Topic' (highlighted), 'Title', 'Author', 'Publication Titles', 'Year Published', 'Affiliation', 'Funding Agency', and 'Publisher'. A tooltip for 'Topic' explains that it searches title, abstract, author keywords, and Keywords Plus, with an example: 'robot\* control\* "input shaping"'. There are 'Clear' and 'Search' buttons at the bottom right of the search area. The footer includes 'Clarivate' logo, '© 2022 Clarivate', 'Data Correction', 'Copyright Notice', and 'Follow Us'.

# Proficient search

– <https://www.webofscience.com/wos/woscc/basic-search>

## – Filter a results

- By adding a keyword
- Restrictions by publication type: article, review, etc.
- Time limit: eg the last 10 years

The screenshot displays the Web of Science search interface. At the top, there are navigation links for 'Search', 'Marked List', 'History', and 'Alerts'. The main heading reads 'Discover multidisciplinary content from the world's most trusted global citation database.' Below this, there are tabs for 'DOCUMENTS' and 'RESEARCHERS'. The search area is set to 'Web of Science Core Collection' and 'Editions: All'. There are three tabs: 'DOCUMENTS', 'CITED REFERENCES', and 'STRUCTURE'. The search criteria are: 'Topic' (dropdown), 'Epoiconazole' (input field), 'And' (operator), 'Topic' (dropdown), and 'toxicity' (input field). A dropdown menu is open under the second 'Topic' dropdown, listing various search fields: 'All Fields', 'Topic', 'Title', 'Author', 'Publication Titles', 'Year Published', 'Affiliation', 'Funding Agency', and 'Publisher'. A tooltip for 'Topic' explains that it searches title, abstract, author keywords, and Keywords Plus, with an example: 'robot\* control\* "input shaping"'. There are 'Clear' and 'Search' buttons at the bottom right of the search area. The footer includes 'Clarivate' logo and copyright information.








# For the rest of the lecture






- IS: open word .doc
- with list of tasks


iS > Files > Study Materials > Study materials posted under the course PŘF:E2020 > Learning Materials > 04. hodina - databáze

## PŘF:E2020 Soft-skills II - Information Literacy

FILES DOCUMENTS OFFICIAL NOTICE BOARD **STUDY MATERIALS** MY WEB FILE DEPOSITORY

    ZIP    

✓	NAME	POSTED BY	UPLOADE...	RIGHTS
↑	<b>04. seminar - databases</b> 04_hodina_-_databaze /2	Šebej, P.	12/3/2021	
<input type="radio"/>	 <u>4._Database_2_Instruction_EN.docx</u>	Mayer, L.	1/3/2022	
<input type="radio"/>	 Database_ressource_list_link.docx	Mayer, L.	1/3/2022	

 Fewer options



# Properties databases

Task 1: Follow the link below, for Chlorpyrifos, what kind of information can we find on that website?

<https://www.reaxys.com/#/structure-editor> :

# Properties databases

<https://www.reaxys.com/#/structure-editor> :

Reaxys<sup>®</sup>

[Quick search](#) [Query builder](#) [Results](#) [Retrosynthesis](#) [History](#)

[Register >](#)

[Sign in](#)



Search substances, reactions and documents

in Reaxys, PubChem, SigmaAldrich and Commercial Substances

Import

Search Reaxys

Find >

Documents, e.g. [publications about quasicrystals](#)

AND



# Properties databases















<https://www.reaxys.com/#/structure-editor> :

Reaxys

[Quick search](#) Query builder Results Retrosynthesis History

Results for "chlorpyrifos"

New  Edit 

	353	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>
	17,217	Documents	Titles, Abstracts, Keywords : "chlorpyrifos" Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>
	3	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>

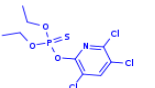
# Properties databases


<https://www.reaxys.com/#/structure-editor> :

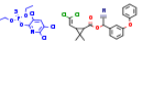

Reaxys® Quick search Query builder **Results** Retrosynthesis History


353 Filters  
Limit to > Exclude >

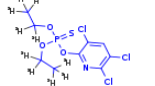

353 Substances out of 10,262 Documents, containing 39 Reactions  
0 selected Limit To Exclude Export Preparations


1  **Chlorpyrifos**  
C9H11NP3Cl3O3 350.59 1545756 2921-88-2  
Identification Physical Data - 80 Bioactivity - 1,871  
Druglikeness Spectra - 65 Other Data - 815

19 

2  **Chlorpyrifos-ethyl + cypermethrin**  
C9H11Cl3NO3PS\*C22H19Cl2NO3 766.894 30654072  Retrieve CAS RN  
Identification  
Druglikeness



3  **chlorpyrifos-D10**  
C9H(2)H10Cl3NO3PS 360.511 34850076  Retrieve CAS RN  
Identification  
Druglikeness  
Physical Data - 1  
Spectra - 1

8 

# Properties databases

<https://www.reaxys.com/#/structure-editor> :

Reaxys® Quick search Query builder Results Retrosynthesis History

27

1

353

Preview

Filters

Limit to > Exclude >

By Structure ▾

Substances Classes ▾

Molecular Weight ▾

Number of Fragments ▾

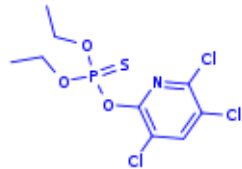
Availability ▾

353 Substances out of 10,262 Documents, containing 39 Reactions

1 selected

Limit To Exclude Export Preparations

1



19

**Chlorpyrifos**

C<sub>9</sub>H<sub>11</sub>NPSCl<sub>3</sub>O<sub>3</sub> 350.59 1545756 2921-88-2

Identification	Physical Data - 80	Bioactivity - 1,871
Druglikeness	Spectra - 65	Other Data - 815

# Properties databases

Task 1: Follow the link below, for Chlorpyrifos, what kind of information can we find on that website?

<https://www.reaxys.com/#/structure-editor> :

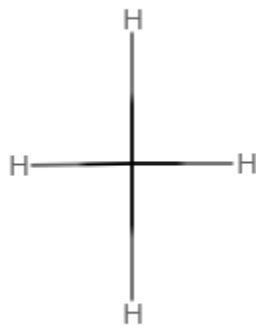
- Physical properties (molecular weight, density, melting point, log  $K_{ow}$  (log P)
- CAS RN
- Concentration in Environment
- Transport through matrices
- Distribution in organisms
- Toxicology data
- Existing reaction

***Main advantage: contains references***

# Properties databases

**Task 2: draw a methane (CH<sub>4</sub>) molecule with apparent bonds, in 2D and in 3D**

<https://www.reaxys.com/#/structure-editor> :



# Properties databases

Reaxys® Quick search Query builder Results Retrosynthesis History

Structure editor selected:  MarvinJS  ChemDrawJS

Search Reaxys

Substance CAS Registry Number, e.g. 102625-70-7

AND

As drawn





# Properties databases

**Task 3:** Follow the link below and look for properties information on **Fonofos (pesticide)** using EpiSuite values

- if experimental value exists: give experimental, if not, give predicted values

<http://www.chemspider.com/>

Give information for:

- Vapor pressure:
- Log  $K_{ow}$ :
- Solubility in water:
- Half life in air:

# Properties databases

Task 3: Follow the link below and look for properties information on **Fonofos (pesticide)** using EpiSuite values

- if experimental value exists: give experimental, if not, give predicted values

<http://www.chemspider.com/>

## Why Episuite ?

Software developed by US-EPA:

- predicting physico chemical properties
- based on experimental data for compound
- and predicted values based on modelling

# Properties databases

**Task 3: Follow the link below and look for properties information on Fonofos (pesticide) using EpiSuite values**

- if experimental value exists: give experimental, if not, give predicted values

<http://www.chemspider.com/>

Give information for:

- Vapor pressure:
- Log  $K_{ow}$ :
- Solubility in water:
- Half life in air:

# Properties databases

Home About us Web APIs Help Sign in

## ChemSpider

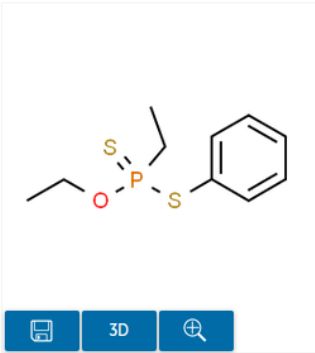
Search and share chemistry

For medical information relating to Covid-19, please consult the [World Health Organisation](#) or local healthcare provision.

Simple Structure Advanced History

Found 1 result

Search term: **Fonofos** (Found by approved synonym)



fonofos

Molecular Formula	C <sub>10</sub> H <sub>15</sub> OPS <sub>2</sub>
Average mass	246.329 Da
Monoisotopic mass	246.030197 Da
ChemSpider ID	13087

insecticide

Names Properties Searches Spectra Vendors Articles More

Experimental data Predicted - ACD/Labs **Predicted - EPISuite** Predicted - ChemAxon

Predicted data is generated using the [US Environmental Protection Agency's EPISuite™](#)

# Properties databases

Task 4: Follow the link below and look for information on Fonofos (pesticide) using EpiSuite values

- if experimental value exists: give experimental, if not, give predicted values

<http://www.chemspider.com/>

Give information for:

- Vapor pressure: 3.38 e-4 (25°C) mmHg
- Log  $K_{ow}$ : 3.94
- Solubility in water: 15.70 mg/L
- Half life in air: 1.493 hours

# Also Available on IS

- IS: open word .doc
- with list of tasks

iS > Files > Study Materials > Study materials posted under the course PŘF:E2020 > Learning Materials > 04. hodina - databáze

## PŘF:E2020 Soft-skills II - Information Literacy



✓	NAME	POSTED BY	UPLOADE...	RIGHTS
↑	<b>04. seminar - databases</b> 04_hodina_-_databaze /2	Šebej, P.	12/3/2021	
<input type="radio"/>	<b>W</b> 4_ Database_2_Instruction_EN.docx	Mayer, L.	1/3/2022	
<input type="radio"/>	<b>W</b> <u>Database_ressource_list_link.docx</u>	Mayer, L.	1/3/2022	

Fewer options

E2020: Soft-Skills 2 : Information Literacy

Ressources, a non-exhaustive list of link for database and useful link

**Database of information and articles:**

scifinder.cas.org

reaxys.com/#/search/quick

chemspider.com

isiknowledge.com

pubchem.ncbi.nlm.nih.gov

ncbi.nlm.nih.gov

<http://polysearch.ca/> (biomedical text mining to discover potential associations between various types of biomedical entities)

<https://www.storkapp.me/> (alerts for papers based on keywords)

**Spectra database**

webbook.nist.gov/chemistry

sdb.sdb.aist.go.jp/sdb/cgi-bin/direct\_frame\_top.cgi

echa.europa.eu/home (European Chemical agency)

MassBank (jp, eu, na) – mass spectra

**Database of chemical manufacturers and sellers (just a few examples):**

sigmaaldrich.com

acros.com

tcichemicals.com/en/cz

<https://www.emolecules.com/> (Structure searching)

<https://zinc.docking.org/> (Commercially available compound database)

**Database of biological structures and biomolecules:**

www.uniprot.org

web.expasy.org/protparam

reactome.org

brenda-enzymes.or



# Compounds and Spectra databases

<https://webbook.nist.gov/chemistry/>

- Environmental/human samples
- How to analyse them?
  - **Chromatography: to separate constituents of a sample**
  - **Mass spectrometry: to determine constituent of a sample**

Exist databases of spectra to help identify what is present in samples

The screenshot shows the NIST Chemistry WebBook search page. At the top, there is a navigation bar with the NIST logo and the text 'National Institute of Standards and Technology U.S. Department of Commerce' and 'NIST Chemistry WebBook, SRD 69'. Below the navigation bar, there are links for 'Search', 'NIST Data', and 'About'. The main heading is 'Search for Species Data by Chemical Name'. Below this, there is a prompt: 'Please follow the steps below to conduct your search (Help):'. The steps are: 1. Enter a chemical species name or pattern: (e.g., methane, \*2-hexene) with a text input field containing 'chlorpyrifos'. 2. Select the desired units for thermodynamic data: with radio buttons for 'SI' (selected) and 'calorie-based'. 3. Select the desired type(s) of data: with two columns of checkboxes. The 'Thermodynamic Data' column includes: Gas phase, Condensed phase, Phase change, Reaction, Ion energetics, and Ion cluster. The 'Other Data' column includes: IR spectrum, THz IR spectrum, Mass spectrum, UV/Vis spectrum, Gas Chromatography, Vibrational & electronic energy levels, Constants of diatomic molecules, and Henry's Law. 4. Press here to search: with a 'Search' button.



# Compounds and Spectra databases

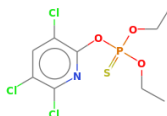
<https://webbook.nist.gov/chemistry/>

**NIST** National Institute of Standards and Technology  
U.S. Department of Commerce **NIST Chemistry WebBook, SRD 69**

Search ▾ NIST Data ▾ About ▾

## Chlorpyrifos

- **Formula:** C<sub>9</sub>H<sub>11</sub>Cl<sub>3</sub>NO<sub>3</sub>PS
- **Molecular weight:** 350.586
- **IUPAC Standard InChI:** InChI=1S/C9H11Cl3NO3PS/c1-3-14-17(18,15-4-2)16-9-7(11)5-6(10)8(12)13-9/h5H,3-4H2,1-2H3  InChI v1.06
- **IUPAC Standard InChIKey:** SBPBAQFVLVIOKP-UHFFFAOYSA-N 
- **CAS Registry Number:** 2921-88-2
- **Chemical structure:**

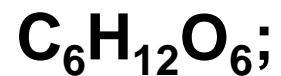


This structure is also available as a [2d Mol file](#) or as a [computed 3d SD file](#).  
The 3d structure may be viewed using [Java](#) or [Javascript](#).

- **Other names:** Dursban; Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl) ester; Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridyl) ester; Chlorpyrifos; Chlorpyrifos; Chlorpyrifos; Chlorpyrifos; Dowco 179; Dursban 4E; ENT 27,311; Killmaster; Lorsban; O,O-Diethyl O-(3,5,6-Trichloro-2-pyridyl) phosphorothioate; Brodan; Chlorpyrifos-ethyl; Chlorpyrifos-ethyl; Detmol U.A.; O,O-Diethyl O-(3,5,6-trichloro-2-pyridyl)monothiophosphate; Dursban F; ENT 27311; OMS-0971; 2-Pyridinol, 3,5,6-trichloro-, O-ester with O,O-diethyl phosphorothioate; Pyrinex; Stipend; Dursban 10CR; suSCon; Chlorpyrifos; Dursban 2E; Empire 20; Equity; Lentrex; Lock-On; OMS 971; Pageant; Piridane; Silrifos; Spannir; Suscon blue; Suscon green; Trichlorpyrifos; Zidil; Bonidel; Coroban; Danusban; Durmet; Dursban R; Ethyl chlorpyrifos; Geodinfos; O,O-Diethyl O-(3,5,6-trichloro-2-pyridinyl)phosphorothioate; Radar; Tafaban; Terial; XRM 429; XRM 5160; m-Chlorpyrifos; O,O-Diethyl O-(3,5,6-trichloropyridin-2-yl) thiophosphate
- **Permanent link** for this species. Use this link for bookmarking this species for future reference.
- **Information on this page:**
  - [Notes](#)
- **Other data available:**
  - [Phase change data](#)
  - [IR Spectrum](#)
  - [Mass spectrum \(electron ionization\)](#)
  - [Gas Chromatography](#)
- **Options:**
  - [Switch to calorie-based units](#)

# Compounds and Spectra databases


**Task 4: Look for Spectra for D-glucose, using only the number of atoms:**



**Copy/paste the spectra below and indicate the associated InChI of the molecule**

[https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

# Compounds and Spectra databases

Spectral Database for Organic Compounds SDBS [Japanese](#) [Introduction](#) [Disclaimer](#) [HELP](#) [Contact](#) [What's New](#) [RIO-DB](#) [FAQ](#) [LINK](#) 

## SDBS Compounds and Spectral Search

**Compound Name:**

**Molecular Formula:**   
C, H, then the other elements are alphabetical order, "%,"\* for the wild card

**Molecular Weight:**  to   
Numbers between left and right columns  
Up to the first place of a decimal point

**CAS Registry No.:**   
"%,"\* for the wild card.

**SDBS No.:**   
"%,"\* for the wild card.

**Atoms:**

C(Carbon)	<input type="text"/>	to	<input type="text"/>
H(Hydrogen)	<input type="text"/>	to	<input type="text"/>
N(Nitrogen)	<input type="text"/>	to	<input type="text"/>
O(Oxygen)	<input type="text"/>	to	<input type="text"/>
F(Fluorine)	<input type="text"/>	to	<input type="text"/>
Cl(Chlorine)	<input type="text"/>	to	<input type="text"/>
Br(Bromine)	<input type="text"/>	to	<input type="text"/>
I(Iodine)	<input type="text"/>	to	<input type="text"/>
S(Sulfur)	<input type="text"/>	to	<input type="text"/>
P(Phosphorus)	<input type="text"/>	to	<input type="text"/>
Si(Silicon)	<input type="text"/>	to	<input type="text"/>

Numbers between left and right columns.

**Spectrum:**  
Check the spectra of your interest.  
 MS  IR  
 <sup>13</sup>C NMR  Raman  
 <sup>1</sup>H NMR  ESR

**IR Peaks(cm<sup>-1</sup>):**  Allowance  ± 10  
"," or space is the separator for multiple peaks.  
Use "-", to set a range: eg. 550-750,1650-3000-  
Transmittance <  %

**<sup>13</sup>C NMR Shift(ppm):**  Allowance  ± 2.0  
"," is the separator for multiple shifts, eg. 129.3,18.4,...

**No shift regions:**   
Range defined by two numbers separated by a space, eg. 110 78,...

**<sup>1</sup>H NMR Shift(ppm):**  Allowance  ± 0.2  
**No shift regions:**

**MS Peaks and intensities:**   
Mass and its intensity are a set of data separated by a space, eg. 110 22,...

Hit:  Sort by:   Result Display type:  with Structures

# Compounds and Spectra databases

**SDBS Search Results:** 1 - 20 out of 21 hits    Sort by:        

SDBS No	Molecular Formula	Molecular Weight	MS	CNMR	HNMR	IR	Raman	ESR	Compound Name
<a href="#">1137</a>	C6H12O6	180.2	<u>Y</u>	<u>Y</u>	N	<u>Y</u>	N	N	D-mannopyranose
<a href="#">1139</a>	C6H12O6	180.2	<u>Y</u>	<u>Y</u>	N	<u>Y</u>	N	N	D-fructose
<a href="#">1183</a>	C6H12O6	180.2	N	<u>Y</u>	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	D-galactopyranose
<a href="#">2023</a>	C6H12O6	180.2	N	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	N	D-glucopyranose
<a href="#">2046</a>	C6H12O6	180.2	N	<u>Y</u>	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	myo-inositol
<a href="#">2990</a>	C6H12O6	180.2	<u>Y</u>	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	N	L-(-)-sorbose
<a href="#">4571</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	1,3-dihydroxyacetone dimer
<a href="#">5544</a>	C6H12O6	180.2	<u>Y</u>	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	N	D-(+)-talose
<a href="#">10271</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	DL-glyceraldehyde dimer
<a href="#">11513</a>	C6H12O6	180.2	N	N	N	<u>Y</u>	N	N	D-mannose
<a href="#">11521</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	D-glucose
<a href="#">15696</a>	C6H12O6	180.2	<u>Y</u>	<u>Y</u>	<u>Y</u>	<u>Y</u>	N	N	D-tagatose
<a href="#">16041</a>	C6H12O6	180.2	N	<u>Y</u>	<u>Y</u>	N	N	N	beta-D-fructopyranose
<a href="#">16339</a>	C6H12O6	180.2	N	<u>Y</u>	N	N	N	N	alpha-L-mannopyranose
<a href="#">22009</a>	C6H12O6	180.2	<u>Y</u>	N	<u>Y</u>	<u>Y</u>	N	N	L-(-)-mannose
<a href="#">32639</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	alpha-L-sorbopyranose
<a href="#">32672</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	beta-D-glucopyranose
<a href="#">50268</a>	C6H12O6	180.2	<u>Y</u>	N	N	<u>Y</u>	N	N	D-allose
<a href="#">35361</a>	C6H12CuN2O6	271.7	N	N	N	<u>Y</u>	N	N	trans-bis(DL-serinato)copper(II)
<a href="#">35377</a>	C6H12CuN2O6	271.7	N	N	N	<u>Y</u>	N	N	trans-bis(L-serinato)copper(II)

1 2

# Compounds and Spectra databases

## SDBS Information

SDBS No.: 11521

**Compound Name:**  
D-glucose

**Molecular Formula:** C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>

**Molecular Weight:** 180.2

**CAS Registry No.:**  
50-99-7

**Spectral Code:**

[Mass :](#)

[IR : nujol mull](#)

[Chemical Information:](#)

[Return to Search:](#)

[Return to Result:](#)

**URL for this Compound:**

<https://sdb.sdb.aist.go.jp/sdb/cg1-bin/landingpage?sdbno=11521>

**External Information:**

external link displays in a separate page

- [Japan Chemical Information Link Center](#) (in Japanese)
  - [JST Nikkaji Web](#) (in Japanese)

## SDBS-Mass

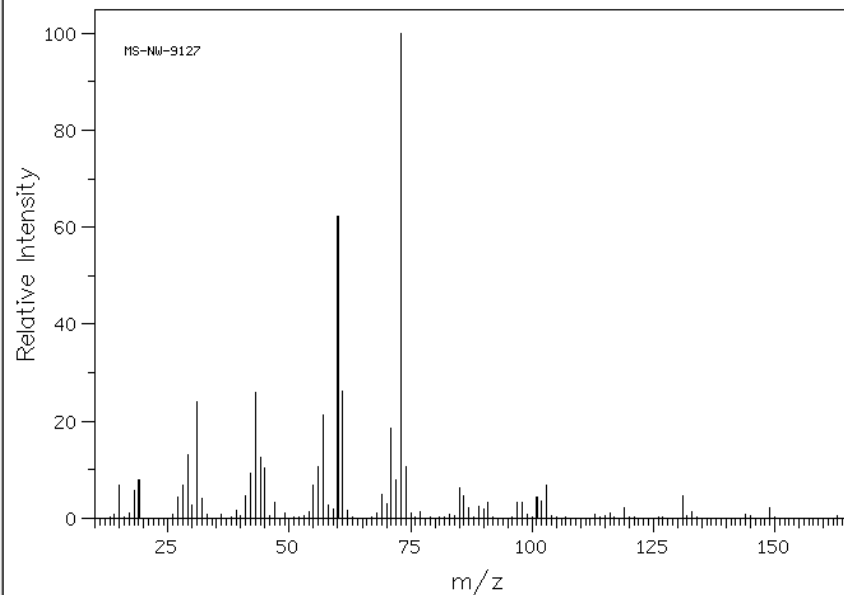
MS-NW-9127

SDBS NO. 11521

D-glucose

(Mass of molecular ion: 180)

C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>



Source Temperature: 200 °C  
Sample Temperature: 140 °C  
Direct, 75 eV

peak data

MS-NW-9127 SDBS NO. 11521

DOI:

**Sample InChI:**

InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h1,3-6,8-12H,2H2/t3-,4+,5+,6+/m0/s1

**Sample InChIKey:**

GZCGUPFRVQAUEE-SLPGGIOYSA-N

# Small molecule mass spectral databases

- Typically mass spectra compound are shared as text files with limited ease of use
- Spectral matching is a key component of a compound identification

NAME: Phosmet  
RETENTIONTIME: 25.331  
PRECURSORMZ: 316.992126464844  
PRECURSORTYPE: [M]<sup>+</sup>  
IONMODE: Positive  
COLLISIONENERGY: 70  
FORMULA: C10H7NO4  
SMILES: COP(=S)(OC)SCN1C(=O)C2=CC=CC=C2C1=O  
INCHIKEY: WQINSVOOIJ DOLJ-UHFFFAOYSA-N  
Num Peaks:15

76.03039	938223
77.03818	1629764
78.91741	417336
78.99396	406285
79.05384	448837
93.00958	2273096
104.02512	1400371
105.03298	1295700
124.94133	446127
124.98142	449841
130.02811	1679535
133.02771	3772589
160.03839	32462268
161.0417	3305389
192.01024	413541

# Small molecule mass spectral databases

- <https://massbank.eu/> : hosts spectra for around 15 000 compounds
  - Pros: diverse instrumentation and ionization modes
  - Cons: intensity of spectra are very different from what we can encounter in biological or environmental samples
- <https://metlin.scipps.edu/> : hosts spectra for 1 million compounds
  - Pro: easy search, good indexing
  - Con: proprietary spectra, not available for download, only for LC-MS/MS



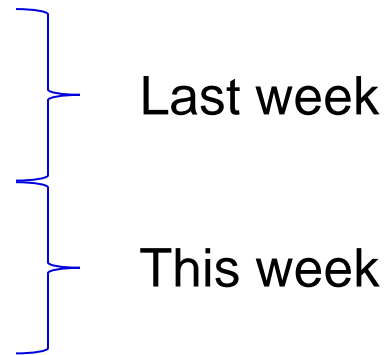
# Small molecule mass spectral databases

- <https://gnps.ucsd.edu/>: hosts spectra for around 255 000 compounds
  - Pros: easy to compare spectra with many tools & links to molecular networking
  - Cons: contain natural products,  
uses MGF text format which loses information such as chromatographic retention
- <https://hmdb.ca/>: hosts spectra for 100 000 compounds
  - Pro: integrated with many other databases and user-friendly tools
  - Con: merged in silico and experimental spectra  
only cover humans

# Content

– 2<sup>nd</sup> part: Practical – you are at the helm and you find the information!

- Publication databases
- Properties databases
- Spectral databases
- Biological databases
- Registration databases
- Patent database

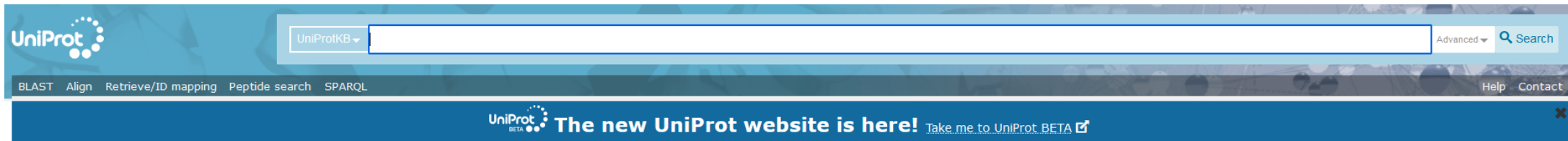


# Biological databases

- Protein and DNA databases
- They work similarly to chemical DB
- Focus on biomolecules and biologically important objects

# Protein databases

– Sequence, structure, function, domains, localization, interactions, related proteins...



The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

The image shows the main content area of the UniProt website. It is divided into several sections. On the left, there are two boxes for UniProtKB: 'Swiss-Prot (566,996)' which is 'Manually annotated and reviewed' and contains records with information from literature and curator-evaluated computational analysis; and 'TrEMBL (230,328,648)' which is 'Automatically annotated and not reviewed' and contains records that await full manual annotation. In the center, there are three boxes: 'UniRef' (The UniProt Reference Clusters), 'UniParc' (a comprehensive and non-redundant database), and 'Proteomes' (the set of proteins thought to be expressed by an organism). Below these is a 'Supporting data' section with icons for Literature citations, Cross-ref. databases, Taxonomy, Diseases, Subcellular locations, and Keywords. On the right, there is a 'News' section with a 'View SARS-CoV-2 Proteins and Receptors' link and several news items including 'Forthcoming changes', 'UniProt release 2022\_01', 'UniProt release 2021\_04', and 'UniProt release 2021\_03'. There are also social media icons for Blog, Twitter, Facebook, and RSS.

<https://www.uniprot.org/>

# Protein databases

## UniProtKB - P04554 (PRM2\_HUMAN)

### Display

Help video

BLAST

Align

Format

Add to basket

History

Entry

Publications

Feature viewer

Feature table

Protein **Protamine-2**

Gene **PRM2**

Organism *Homo sapiens (Human)*

Status Reviewed - Annotation score: ●●●●●● - Experimental evidence at protein level<sup>1</sup>

### Function<sup>1</sup>

Protamines substitute for histones in the chromatin of sperm during the haploid phase of spermatogenesis. They compact sperm DNA into a highly condensed, stable and inactive complex.

By similarity

#### GO - Molecular function<sup>1</sup>

- cadmium ion binding Source: CAFA
- DNA binding Source: ProtInc
- zinc ion binding Source: CAFA

[Complete GO annotation on QuickGO ...](#)

#### GO - Biological process<sup>1</sup>

- chromosome condensation Source: UniProtKB-KW
- DNA packaging Source: ProtInc
- nucleus organization Source: GO\_Central
- spermatid development Source: GO\_Central
- spermatogenesis Source: UniProtKB

[Complete GO annotation on QuickGO ...](#)

#### Keywords<sup>1</sup>

Molecular function	Developmental protein, DNA-binding
--------------------	------------------------------------

- None
- Function
  - Names & Taxonomy
  - Subcellular location
  - Pathology & Biotech
  - PTM / Processing
  - Expression
  - Interaction
  - Structure
  - Family & Domains
  - Sequences (2)
  - Similar proteins
  - Cross-references
  - Entry information
  - Miscellaneous

▲ Top

# Protein databases

## Sequences (2)<sup>i</sup>

Sequence status<sup>i</sup>: Complete.

Sequence processing<sup>i</sup>: The displayed sequence is further processed into a mature form.

This entry describes **2** isoforms<sup>i</sup> produced by **alternative splicing**. [Align](#) [Add to basket](#)

**Isoform 1** (identifier: **P04554-1**) [UniParc] [FASTA](#) [Add to basket](#)

*This isoform has been chosen as the canonical<sup>i</sup> sequence. All positional information in this entry refers to downloadable versions of the entry.*

[« Hide](#)

```

10      20      30      40      50
MVR YR VRSLS ERSHEVYRQQ LHGQE QGHG QEEQGLSPEH VEVYERTHGQ
60      70      80      90     100
SHYRRRHCSR RRLHRIHRRQ HRSCRRRKRR SCRHRRRHRR GCRTRKRTCR
    
```

RH

**Isoform 2** (identifier: **P04554-2**) [UniParc] [FASTA](#) [Add to basket](#)

*The sequence of this isoform differs from the canonical sequence as follows:*

91-102: GCRTRKRTCRRH → ESLG DPLNQNFLSQAAEPGREHAEGTKLPGPLTPSWKLRKSRPKHQVRP

[Show »](#)

				Positively charged			Negatively charged	12.1 or 6.0: pKa of side chain Sulfur or Selenium	
Arginine Arg <b>R</b>	Histidine His <b>H</b>	Lysine Lys <b>K</b>	Aspartic Acid Asp <b>D</b>		Glutamic Acid Glu <b>E</b>				
				Polar uncharged					Special cases
Serine Ser <b>S</b>	Threonine Thr <b>T</b>	Asparagine Asn <b>N</b>	Glutamine Gln <b>Q</b>		Glycine Gly <b>G</b>	Proline Pro <b>P</b>	Cysteine Cys <b>C</b>	Selenocysteine Sec <b>U</b>	
					Hydrophobic				Hydrophobic
Alanine Ala <b>A</b>	Valine Val <b>V</b>	Isoleucine Ile <b>I</b>	Leucine Leu <b>L</b>	Methionine Met <b>M</b>		Phenylalanine Phe <b>F</b>	Tyrosine Tyr <b>Y</b>	Tryptophan Trp <b>W</b>	

Thomas Ryckmans 2021

BLAST  [GO](#)

# Protein databases

- Sequence, structure, function, domains, localization, interactions, related proteins...
- [UniProt KB](#) - aggregation of other databases, Specialized
- Physico-chemical parameters from the sequence - [ProtParam](#)
- Biological pathways - [Reactome](#)
- Enzymes - [Brenda](#)
- Proteomics - [ProteomicsDB](#)
- Posttranslational modifications - [iPTMnet](#)
- Domains - [Pfam](#)
- And many others

UniProt

BLAST Align Retrieve/ID mapping Peptide

UniProtKB - P00512

Display

Entry

Publications

Feature viewer

Feature table

None

<input checked="" type="checkbox"/>	Function
<input checked="" type="checkbox"/>	Names & Taxonomy
<input checked="" type="checkbox"/>	Subcellular location
<input checked="" type="checkbox"/>	Pathology & Biotech
<input checked="" type="checkbox"/>	PTM / Processing
<input checked="" type="checkbox"/>	Expression
<input checked="" type="checkbox"/>	Interaction
<input checked="" type="checkbox"/>	Structure
<input checked="" type="checkbox"/>	Family & Domains
<input checked="" type="checkbox"/>	Sequences (4+)
<input checked="" type="checkbox"/>	Similar proteins
<input checked="" type="checkbox"/>	Cross-references
<input checked="" type="checkbox"/>	Entry information
<input checked="" type="checkbox"/>	Miscellaneous

▲ Top

# DNA sequence database

- BLAST = Basic Local Alignment Search Tool
- Search and comparison of sequences
- → GenBank
- Finding protein from DNA sequence
- Also for exists proteins (BLAST protein)

The screenshot shows the NCBI BLAST Standard Nucleotide BLAST interface. At the top, there are logos for NIH (U.S. National Library of Medicine) and NCBI (National Center for Biotechnology Information). The main heading is "BLAST >> blastn suite". Below this, the page is titled "Standard Nucleotide BLAST".

The interface is divided into several sections:

- Enter Query Sequence:** A text area containing a DNA sequence: "1 atgaaaaga atacattaag tgcgatatta atgactttat ttttattat accttgraat 61 aattcagga aagtgggga tctgcactc actaatctc ctgacgagtc tgcgaaagg 121 cctaatttta cagaaataag caaaaaatt acagattcta atgcatttgt acttgctgt". There are "Clear" and "Query subrange" options.
- Or, upload file:** A button labeled "Procházet..." and a text input field "Soubor nevybrán."
- Job Title:** A text input field with the placeholder "Enter a descriptive title for your BLAST search".
- Choose Search Set:** A section with radio buttons for "Standard databases (nr etc.)", "rRNA/ITS databases", "Genomic + transcript databases", and "Betacoronavirus". A dropdown menu shows "Nucleotide collection (nr/nt)". There are checkboxes for "Exclude" (Models (XM/XP), Uncultured/environmental sample sequences) and "Limit to" (Sequences from type material). An "Entrez Query" field is also present.
- Program Selection:** Radio buttons for "Highly similar sequences (megablast)", "More dissimilar sequences (discontiguous megablast)", and "Somewhat similar sequences (blastn)". A "Choose a BLAST algorithm" dropdown is also shown.

At the bottom, there is a "BLAST" button and a checkbox for "Show results in a new window". A link for "Algorithm parameters" is at the very bottom.



# BLAST

- BLAST = Basic Local Alignment Search Tool
- Widely used sequence similarity search tool
  - Finds high scoring local alignments between two sequences (Protein or DNA)

# BLAST

I have a DNA or protein sequence

- What is it related to? What does it do? (Homology, conserved domains)
- Is it already in the database (identification)?
  - Find matching sequence in the database or organism of origin
- Where is it located? How is it organized in a genome?

# BLAST

<https://blast.ncbi.nlm.nih.gov/Blast.cgi>

## Basic Local Alignment Search Tool

**BLAST** finds regions of similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance. [Learn more](#)

NEWS

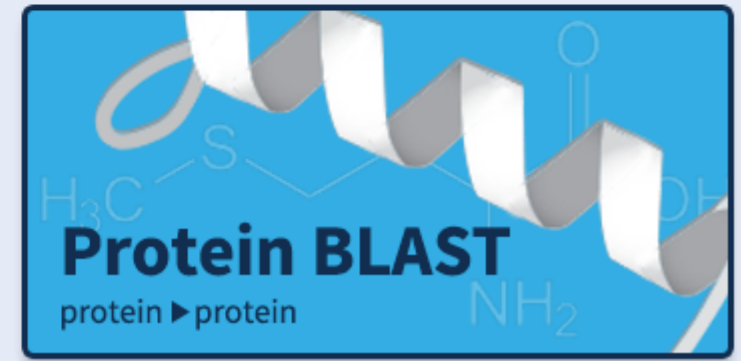
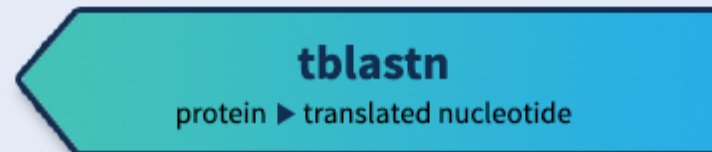
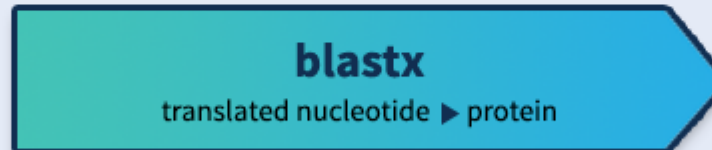
### ElasticBLAST is here!

ElasticBLAST is a new cloud based tool to run your BLAST searches faster and make you more effective.

Mon, 07 Feb 2022 12:00:00 EST

[More BLAST news...](#)

## Web BLAST



# BLAST



## **Task 5: Identification search:**

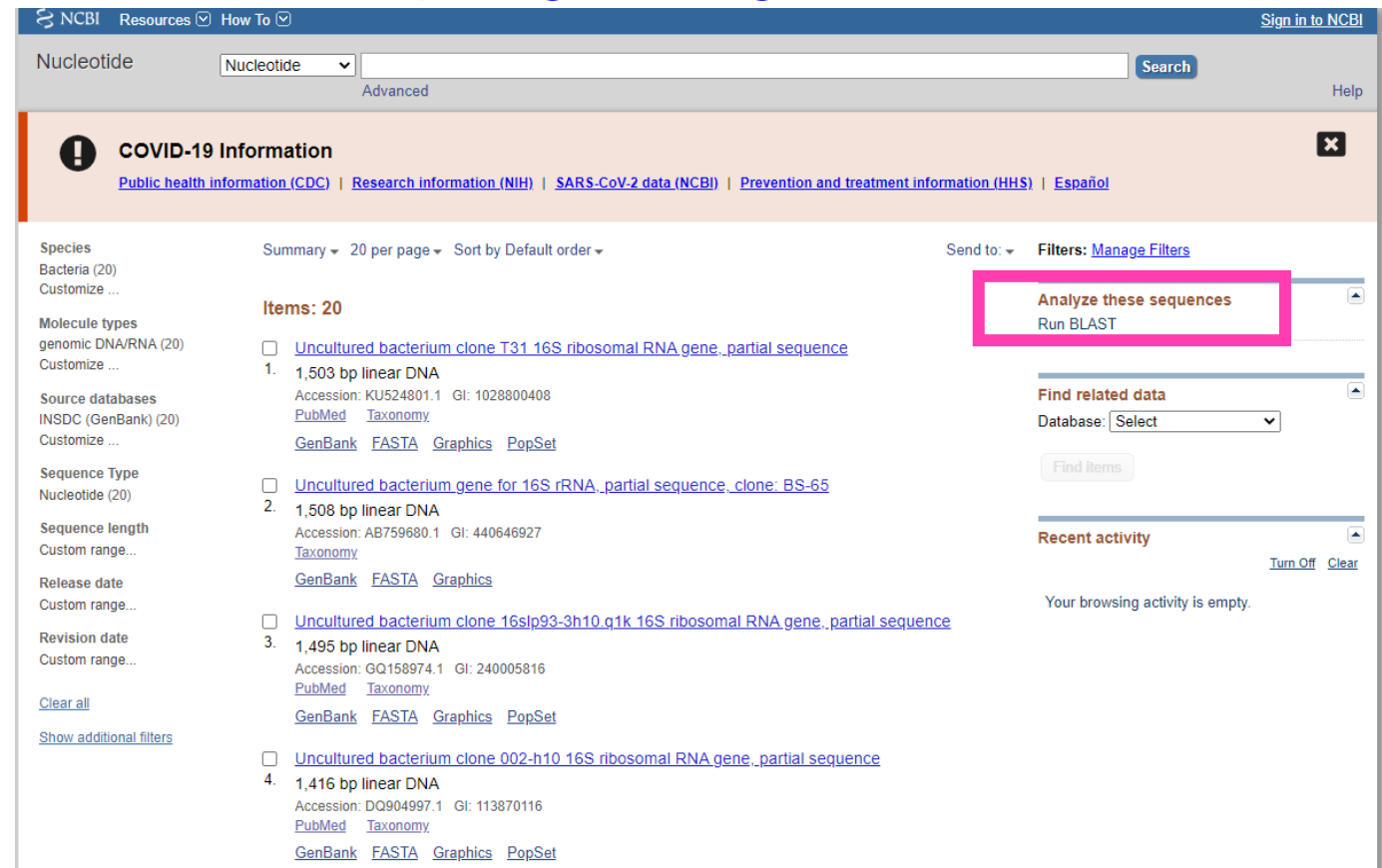
- Look within the 16S rRNA type strains database
- Visualize distance trees of results
- Manipulate tree viewer display
- Use MOLE-BLAST tool
  
- <https://blast.ncbi.nlm.nih.gov/Blast.cgi>

# BLAST

20 uncultured bacterias; Link to retrieve data: <https://go.usa.gov/xUEX4>

Available on IS:  
Word document:

NAME	POSTED BY
04. seminar - databases 04_hodina_-_database /2	Šebej, P.
<input type="radio"/>  4. Database 2. Instruction EN.docx	★ Mayer, L.
<input type="radio"/>  Database_resource_list_link.docx	Mayer, L.



The screenshot shows the NCBI BLAST search results page. At the top, there is a search bar with 'Nucleotide' selected and a 'Search' button. Below the search bar, there is a 'COVID-19 Information' banner with links to CDC, NIH, SARS-CoV-2 data, and HHS. The main content area displays a list of 20 items, with the first four items visible. Each item is a link to a sequence, followed by its length and accession number. The first item is 'Uncultured bacterium clone T31 16S ribosomal RNA gene, partial sequence' (1,503 bp linear DNA, Accession: KU524801.1). The second item is 'Uncultured bacterium gene for 16S rRNA, partial sequence, clone BS-65' (1,508 bp linear DNA, Accession: AB759680.1). The third item is 'Uncultured bacterium clone 16slp93-3h10.q1k 16S ribosomal RNA gene, partial sequence' (1,495 bp linear DNA, Accession: GQ158974.1). The fourth item is 'Uncultured bacterium clone 002-h10 16S ribosomal RNA gene, partial sequence' (1,416 bp linear DNA, Accession: DQ904997.1). On the right side of the page, there is a 'Send to' section with a 'Filters: Manage Filters' link. Below this, there is a 'Find related data' section with a 'Database: Select' dropdown and a 'Find items' button. At the bottom right, there is a 'Recent activity' section with 'Turn Off' and 'Clear' links.

# BLAST

BLAST<sup>®</sup> » blastn suite

Standard Nucleotide BLAST

blastn

blastp

blastx

tblastn

tblastx

BLASTN programs search nucleotide databases using a nucleotide query. [more...](#)

## Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) [?](#) [Clear](#)

KU524801.1  
AB759680.1  
GQ158974.1  
DQ904997.1

Query subrange [?](#)

From

To

Or, upload file

No file chosen [?](#)

Job Title

Enter a descriptive title for your BLAST search [?](#)

Align two or more sequences [?](#)

## Choose Search Set

Database

Standard databases (nr etc.):  rRNA/ITS databases  Genomic + transcript databases  Betacoronavirus

Nucleotide collection (nr/nt)  [?](#)

Organism

Optional

Enter organism name or id—completions will be suggested  exclude

Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown [?](#)

Exclude

Optional

Models (XM/XP)  Uncultured/environmental sample sequences

Limit to

Optional

Sequences from type material

Entrez Query

Optional

[YouTube](#) [Create custom database](#)

Enter an Entrez query to limit search [?](#)

# BLAST

BLAST® » blastn suite

Standard Nucleotide BLAST

blastn

blastp

blastx

tblastn

tblastx

BLASTn programs search nucleotide databases using a nucleotide query. [more...](#)

## Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) [?](#) [Clear](#)

KU524801.1  
AB759680.1  
GQ158974.1  
DQ904997.1

Query subrange [?](#)

From

To

Or, upload file

No file chosen [?](#)

Job Title

Enter a descriptive title for your BLAST search [?](#)

Align two or more sequences [?](#)

## Choose Search Set

Database

Standard databases (nr etc.):  rRNA/ITS databases  Genomic + transcript databases  Betacoronavirus

◆ 16S ribosomal RNA sequences (Bacteria and Archaea) [?](#) [Targeted Loci Project Information](#)

Organism

Optional

exclude

Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown [?](#)

Exclude

Optional

Models (XM/XP)  Uncultured/environmental sample sequences

Limit to

Optional

Sequences from type material

Entrez Query

Optional

[YouTube](#) [Create custom database](#)

Enter an Entrez query to limit search [?](#)

# BLAST

Job Title: gb|KU524801.1|

---

Request ID	1YBMVEFY016
Status	Searching
Submitted at	Wed Mar 2 03:45:15 2022
Current time	Wed Mar 02 03:45:20 2022
Time since submission	00:00:05

This page will be automatically updated in 2 seconds

Link to get results:

<https://blast.ncbi.nlm.nih.gov/Blast.cgi?CMD=Get&RID=NH1S873K015>



# BLAST

BLAST® » blastn suite » results for RID-NH1S873K015

[Home](#) [Recent Results](#) [Saved Strategies](#) [Help](#)

[← Edit Search](#)

[Save Search](#)

[Search Summary](#) ▾

[? How to read this report?](#)

[▶ BLAST Help Videos](#)

[↶ Back to Traditional Results Page](#)

Job Title	KU524801:Uncultured bacterium clone T31 16S...
RID	<a href="#">NH1S873K015</a> <small>Search expires on 10-27 09:02 am</small> <a href="#">Download All</a> ▾
Results for	1:gb KU524801.1 Uncultured bacterium clone T31 16S ribosomal RN. ▾
Program	BLASTN <a href="#">?</a> <a href="#">Citation</a> ▾
Database	rRNA_typestrains/prokaryotic_16S_ribosomal_RNA <a href="#">See details</a> ▾
Query ID	<a href="#">KU524801.1</a>
Description	Uncultured bacterium clone T31 16S ribosomal RNA gene ...
Molecule type	nucleic acid
Query Length	1503
Other reports	<a href="#">Distance tree of results</a> <a href="#">MSA viewer</a> <a href="#">?</a>

## Filter Results

**Organism** only top 20 will appear  exclude

Type common name, binomial, taxid or group name

[+ Add organism](#)

---

**Percent Identity**  to

**E value**  to

**Query Coverage**  to

[Filter](#) [Reset](#)

**Descriptions**

[Graphic Summary](#)

[Alignments](#)

[Taxonomy](#)

Sequences producing significant alignments

Download ▾

**New** Select columns ▾

Show  ▾

[?](#)

select all 100 sequences selected

[GenBank](#)

[Graphics](#)

[Distance tree of results](#)

**New** [MSA Viewer](#)

# BLAST

## — Identification

Descriptions		Graphic Summary	Alignments	Taxonomy					
Sequences producing significant alignments									
Download <span>New</span> Select columns <span>Show</span> 100 <span>?</span>									
<input checked="" type="checkbox"/> select all 100 sequences selected									
<a href="#">GenBank</a> <a href="#">Graphics</a> <a href="#">Distance tree of results</a> <span>New</span> <a href="#">MSA Viewer</a>									
	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	<a href="#">Shigella dysenteriae strain ATCC 13313 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella dysenter...</a>	2713	2713	99%	0.0	99.00%	1487	<a href="#">NR_026332.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia fergusonii ATCC 35469 16S ribosomal RNA, complete sequence</a>	<a href="#">Escherichia fergu...</a>	2693	2693	100%	0.0	99.00%	1542	<a href="#">NR_074902.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia marmotae strain HT073016 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia mar...</a>	2676	2676	100%	0.0	99.00%	1504	<a href="#">NR_136472.1</a>
<input checked="" type="checkbox"/>	<a href="#">Shigella flexneri strain ATCC 29903 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella flexneri</a>	2660	2660	99%	0.0	99.00%	1488	<a href="#">NR_026331.1</a>
<input checked="" type="checkbox"/>	<a href="#">Shigella sonnei strain CECT 4887 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella sonnei</a>	2652	2652	99%	0.0	99.00%	1530	<a href="#">NR_104826.1</a>
<input checked="" type="checkbox"/>	<a href="#">Shigella boydii strain P288 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella boydii</a>	2651	2651	98%	0.0	99.00%	1515	<a href="#">NR_104901.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia fergusonii ATCC 35469 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia fergu...</a>	2623	2623	98%	0.0	99.00%	1473	<a href="#">NR_027549.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia albertii strain Albert 19982 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia albertii</a>	2623	2623	98%	0.0	99.00%	1494	<a href="#">NR_025569.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia fergusonii strain NBRC 102419 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia fergu...</a>	2615	2615	97%	0.0	99.00%	1467	<a href="#">NR_114079.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia coli strain NBRC 102203 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia coli</a>	2615	2615	97%	0.0	99.00%	1467	<a href="#">NR_114042.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter amalonaticus strain CECT 863 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter amal...</a>	2579	2579	99%	0.0	98.00%	1504	<a href="#">NR_104823.1</a>
<input checked="" type="checkbox"/>	<a href="#">Salmonella enterica subsp. enterica serovar Typhi 16S ribosomal RNA, partial sequence</a>		2577	2577	100%	0.0	98.00%	1534	<a href="#">NR_074799.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter koseri strain LMG 5519 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter koseri</a>	2560	2560	98%	0.0	98.00%	1494	<a href="#">NR_118105.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter farmeri strain CDC 2991-81 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter farmeri</a>	2558	2558	99%	0.0	98.00%	1511	<a href="#">NR_024861.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter amalonaticus strain LMG 7873 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter amal...</a>	2553	2553	98%	0.0	98.00%	1494	<a href="#">NR_118106.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia coli strain U 5/41 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia coli</a>	2553	2553	96%	0.0	98.00%	1450	<a href="#">NR_024570.1</a>
<input checked="" type="checkbox"/>	<a href="#">Salmonella enterica subsp. arizonae strain ATCC 13314 16S ribosomal RNA, partial sequence</a>	<a href="#">Salmonella enteri...</a>	2551	2551	99%	0.0	98.00%	1491	<a href="#">NR_041696.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter koseri strain CDC-8132-86 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter koseri</a>	2534	2534	97%	0.0	98.00%	1469	<a href="#">NR_104890.1</a>
<input checked="" type="checkbox"/>	<a href="#">Salmonella bongori strain DSM 13772 16S ribosomal RNA, partial sequence</a>	<a href="#">Salmonella bongori</a>	2523	2523	96%	0.0	98.00%	1443	<a href="#">NR_116124.1</a>
<input checked="" type="checkbox"/>	<a href="#">Citrobacter koseri strain CIP 82.87 16S ribosomal RNA, partial sequence</a>	<a href="#">Citrobacter koseri</a>	2512	2512	97%	0.0	98.00%	1459	<a href="#">NR_118588.1</a>

# BLAST

BLAST® » blastn suite » results for RID-NH1S873K015 Home Recent Results Saved Strategies Help

[← Edit Search](#)
[Save Search](#)
[Search Summary ▾](#)

[? How to read this report?](#)
[BLAST Help Videos](#)
[↶ Back to Traditional Results Page](#)

Job Title	KU524801:Uncultured bacterium clone T31 16S...
RID	NH1S873K015 <small>Search expires on 10-27 09:02 am</small> <a href="#">Download All ▾</a>
Results for	1:gb KU524801.1 Uncultured bacterium clone T31 16S ribosomal RN. ▾
Program	BLASTN <a href="#">?</a> <a href="#">Citation ▾</a>
Database	rRNA_typestrains/prokaryotic_16S_ribosomal_RNA <a href="#">See details ▾</a>
Query ID	<a href="#">KU524801.1</a>
Description	Uncultured bacterium clone T31 16S ribosomal RNA gene ...
Molecule type	nucleic acid
Query Length	1503
Other reports	<a href="#">Distance tree of results</a> <a href="#">MSA viewer</a> <a href="#">?</a>

**Filter Results**

**Organism** only top 20 will appear  exclude

[+ Add organism](#)

---

**Percent Identity**  to 
**E value**  to 
**Query Coverage**  to

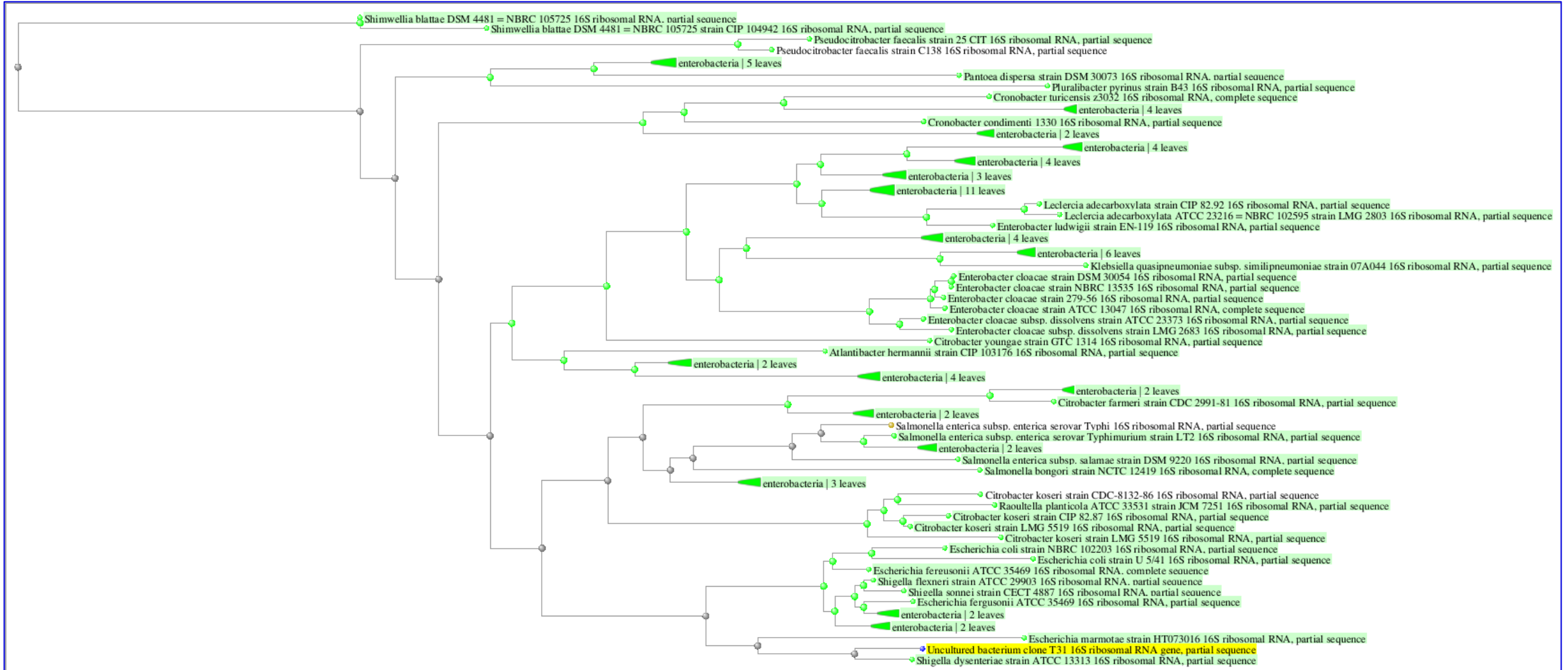
[Descriptions](#)
[Graphic Summary](#)
[Alignments](#)
[Taxonomy](#)

**Sequences producing significant alignments** Download ▾ **New** Select columns ▾ Show  [?](#)

select all 100 sequences selected 
[GenBank](#)
[Graphics](#)
[Distance tree of results](#)
**New** [MSA Viewer](#)

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	<a href="#">Shigella dysenteriae strain ATCC 13313 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella dysenter...</a>	2713	2713	99%	0.0	99.00%	1487	<a href="#">NR_026332.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia fergusonii ATCC 35469 16S ribosomal RNA, complete sequence</a>	<a href="#">Escherichia ferg...</a>	2693	2693	100%	0.0	99.00%	1542	<a href="#">NR_074902.1</a>
<input checked="" type="checkbox"/>	<a href="#">Escherichia marmotae strain HT073016 16S ribosomal RNA, partial sequence</a>	<a href="#">Escherichia mar...</a>	2676	2676	100%	0.0	99.00%	1504	<a href="#">NR_136472.1</a>
<input checked="" type="checkbox"/>	<a href="#">Shigella flexneri strain ATCC 29903 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella flexneri</a>	2660	2660	99%	0.0	99.00%	1488	<a href="#">NR_026331.1</a>
<input checked="" type="checkbox"/>	<a href="#">Shigella sonnei strain CECT 4887 16S ribosomal RNA, partial sequence</a>	<a href="#">Shigella sonnei</a>	2652	2652	99%	0.0	99.00%	1530	<a href="#">NR_104826.1</a>

# BLAST




# MOLE-BLAST

- Extension tool: cluster things together
- <https://blast.ncbi.nlm.nih.gov/moleblast/moleblast.cgi>
- Does BLAST search, but also full multiple sequence alignment
- Will give a tree that cluster the 20 sequences
  - With 16s sequences
  - also with each other
- ***For time constraining reason: Copy/paste the first 3 sequences (see word document)***

KU524801.1  
AB759680.1  
GQ158974.1  
DQ904997.1  
EU488411.1  
KX431275.1  
EU556993.1  
FM873915.1  
FM874039.1  
HM124388.1  
FJ624883.1  
FJ625334.1  
EU236261.1  
EF508875.1  
DQ814438.1  
HM779760.1  
HM780090.1  
EF604165.1  
EF604435.1  
EF604230.1


# MOLE-BLAST

**MOLE-BLAST** This is a BLAST test site 

**Neighbor Search Tool**

MOLE-BLAST is an experimental tool that helps taxonomists find closest database neighbors of submitted query sequences. It computes a multiple sequence alignment (MSA) between the query sequences along with sequences from different genes or loci, MOLE-BLAST can cluster them and compute an MSA and a phylogenetic tree for each locus separately. This tool may eventually be incorporated into our supported suite.

**Nucleotide**

MOLE-BLAST searches for closest neighbors... 

**Enter Query Sequences**

Enter nucleotide accessions, gis, or FASTA sequences (up to 300 input sequences with up to 5000 bases each)  [Clear](#)

DQ814438.1  
HM779760.1  
HM780090.1  
EF604165.1  
EF604435.1  
EF604230.1


Or, upload FASTA file

No file chosen

Job Title

**Choose Search Set**


Database

16S ribosomal RNA sequences (Bacteria and Archaea) 

# MOLE-BLAST

MOLE-BLAST

Neighbor Search Tool

 Please, do not close the browser before the processing is completed

Mole-BLAST Request ID	1YDFTD4F413
Status	Calculating
Submitted at	Wed Mar 02 04:16:35 2022
Current time	Wed Mar 02 04:16:41 2022
Time since submission	6 seconds

This page will be automatically updated in 10 seconds

- Then we wait!
- *(Let it run in the background while we continue, it will take a few minutes...)*
- [https://www.youtube.com/watch?v=JKD5laNtwSc&ab\\_channel=TheNationalLibraryofMedicine](https://www.youtube.com/watch?v=JKD5laNtwSc&ab_channel=TheNationalLibraryofMedicine) (source for the exercise)

# Registration databases

- Look for the status of a compound (authorized for use vs banned)
- ECHA: European Chemical Agency
  - Shows substances registered for use in EU
  - Toxicity criteria and labelling
  - Somehow of a mess to find registration status
  - **Chemicals under REACH Legislation**
    - REACH = Registration, Evaluation, Authorization, Chemicals**
    - Applies to all chemicals sold on the European market (more than 1 tonne per year)
    - Insure safety of chemicals used for humans and environment
- <https://echa.europa.eu/home>



# Registration databases



The screenshot displays the ECHA website interface. At the top, it identifies itself as 'An agency of the European Union' and provides a 'Sign In' link and language selection for 'English (en)'. The ECHA logo and 'EUROPEAN CHEMICALS AGENCY' are prominently featured. Navigation links for 'About Us', 'Contact', and 'Jobs' are present, along with a search bar for the website. A main menu includes 'LEGISLATION', 'CONSULTATIONS', 'INFORMATION ON CHEMICALS', and 'SUPPORT'. The main content area features a 'Search our data' section with a checkbox for accepting legal notices, a search input field with an example (e.g., Formaldehyde, or 200-001-8 or 50-00-0, or 605-001-00-5), and buttons for 'Search for chemicals' and 'Search SCIP database'. An 'ADVANCED SEARCH' link is also available. To the right, there is a 'COVID-19 information' section with a warning icon and a link to read more about IT application maintenance. Below this is a 'Follow us' section with social media icons for Facebook, LinkedIn, Twitter, and YouTube, and buttons for 'Read ECHA Weekly news' and 'Subscribe to our news'. At the bottom right, there is a banner for 'EU CHEMICALS LEGISLATION FINDER' with the tagline 'Know how EU laws affect your business'. On the left side of the main content area, there is a news article titled 'Do you have information on uses of eight substances proposed for authorisation?' dated 02/02/2022, with a 'REACH' tag. The article text states: 'ECHA invites comments on its proposal to include eight substances of very high concern in the REACH Authorisation List. Comments can be given by 2 May 2022.' The article is accompanied by an image of laboratory glassware.

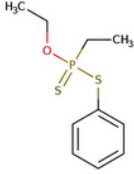
# Registration databases

IC Substance Infocard [See a problem or have feedback?](#) RSS

## Fonofos

Regulatory process names 23 Translated names 43 CAS names 1 IUPAC names 1 Other identifiers 6 OBL

<b>Substance identity</b> <span>?</span>	<b>Hazard classification &amp; labelling</b> <span>?</span>
<b>EC / List no.:</b> 213-408-0 <b>CAS no.:</b> 944-22-9 <b>Mol. formula:</b> C10H15OPS2	  <p><i>Danger!</i> According to the <b>harmonised classification and labelling</b> (CLP00) approved by the European Union, this substance is fatal if swallowed, is fatal in contact with skin, is very toxic to aquatic life and is very toxic to aquatic life with long lasting effects.</p>



about INFOCARD - Last updated: 21/12/2021

### Key datasets

?

Brief Profile REACH registered substance factsheets **C&L Inventory** Biocidal active substance factsheets PACT tool Regulatory Obligations

### Regulatory context

?

Here you can find all of the regulations and regulatory lists in which this substance appears, according to the data available to ECHA. This substance has been found in the following regulatory activities (directly, or inheriting the regulatory context of a parent substance):

# Registration databases

– **Task 5: Find EU authorization status of the following compound, using following links**

– <https://go.drugbank.com/> (Drug database)

– [https://ec.europa.eu/food/plants/pesticides/eu-pesticides-database\\_en](https://ec.europa.eu/food/plants/pesticides/eu-pesticides-database_en) (EU pesticide database)

– <https://www.echemportal.org/echemportal/> (EU chemical portal)

– <https://risctox.istas.net/en/> (Toxic substance database)

– <https://echa.europa.eu/home> (ECHA website)

**For these compounds:**

**Dicloxacillin – Epoxiconazole – Decachlorobiphenyl**

# Registration databases

DRUGBANK Online

Browse COVID-19 Search Interaction Checker Downloads Solutions About

Drugs

Discover published papers by academic researchers that use DrugBank data. [Read Blog!](#)

## Dicloxacinin

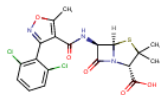
Watch 0 Star 0

**Summary** Dicloxacinin is a penicillin used to treat penicillinase-producing bacterial infections that are susceptible to the drug.

**Generic Name** Dicloxacinin **DrugBank Accession Number** DB00485






**Background** One of the penicillins which is resistant to penicillinase.

**Type** Small Molecule **Groups** Approved, Investigational, Vet approved

**Structure**  
  
3D Download Similar Structures

**Weight** Average: 470.326  
Monoisotopic: 469.026596773

**Chemical Formula** C<sub>19</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>5</sub>S

**Synonyms** [Show All Synonyms](#)  
Dicloxacinina  Dicloxacinin  Dicloxacillina  Dicloxacilline  Dicloxacillinum 

**External IDs** [View As Table](#)  
Bayer 5488 BRL 1702 BRL-1702 P 1011 R 13423 R-13423

PHARMACOLOGY

# Registration databases



English

Search

European Commission > Food, farming, fisheries > Food Safety > Plants > Pesticides > EU Pesticides database

Search Active substances, safeners and synergists

## Search options

### Type

Nothing selected

### Status

Nothing selected

### Legislation

Nothing selected

### Authorised in

## Active substances, safeners and synergists (1 matching records)

[Export Active substances](#)

epoxiconazole

CURRENT APPROVAL PERIOD 01/05/2009 - 30/04/2020

NOT APPROVED

**Epoxiconazole**

# Registration databases

An agency of the European Union Sign In English (en)

**ECHA**  
EUROPEAN CHEMICALS AGENCY

About Us Contact Jobs

LEGISLATION CONSULTATIONS INFORMATION ON CHEMICALS SUPPORT




ECHA > Substance Information

## IC Substance Infocard See a problem or have feedback?

RSS

### Decachloro-1,1'-biphenyl

Regulatory process names 6 IUPAC names 2 Other identifiers 3 | Groups:

<b>Substance identity</b> EC / List no.: 218-115-1 CAS no.: 2051-24-3 Mol. formula: C12Cl10 	<b>Hazard classification &amp; labelling</b>  <i>Warning!</i> According to the classification provided by companies to ECHA in <b>CLP notifications</b> this substance is very toxic to aquatic life, is very toxic to aquatic life with long lasting effects and may cause damage to organs through prolonged or repeated exposure.	<b>Properties of concern</b>  Persistent Organic Pollutant
---	---	--

## POP - Persistent Organic Pollutants Regulations

- List of substances subject to POPs Regulation

Substances whose production and use are banned or severely restricted under the POPs Regulation and/or which are subject to release reduction provisions under the POPs Regulation.



# Registration databases

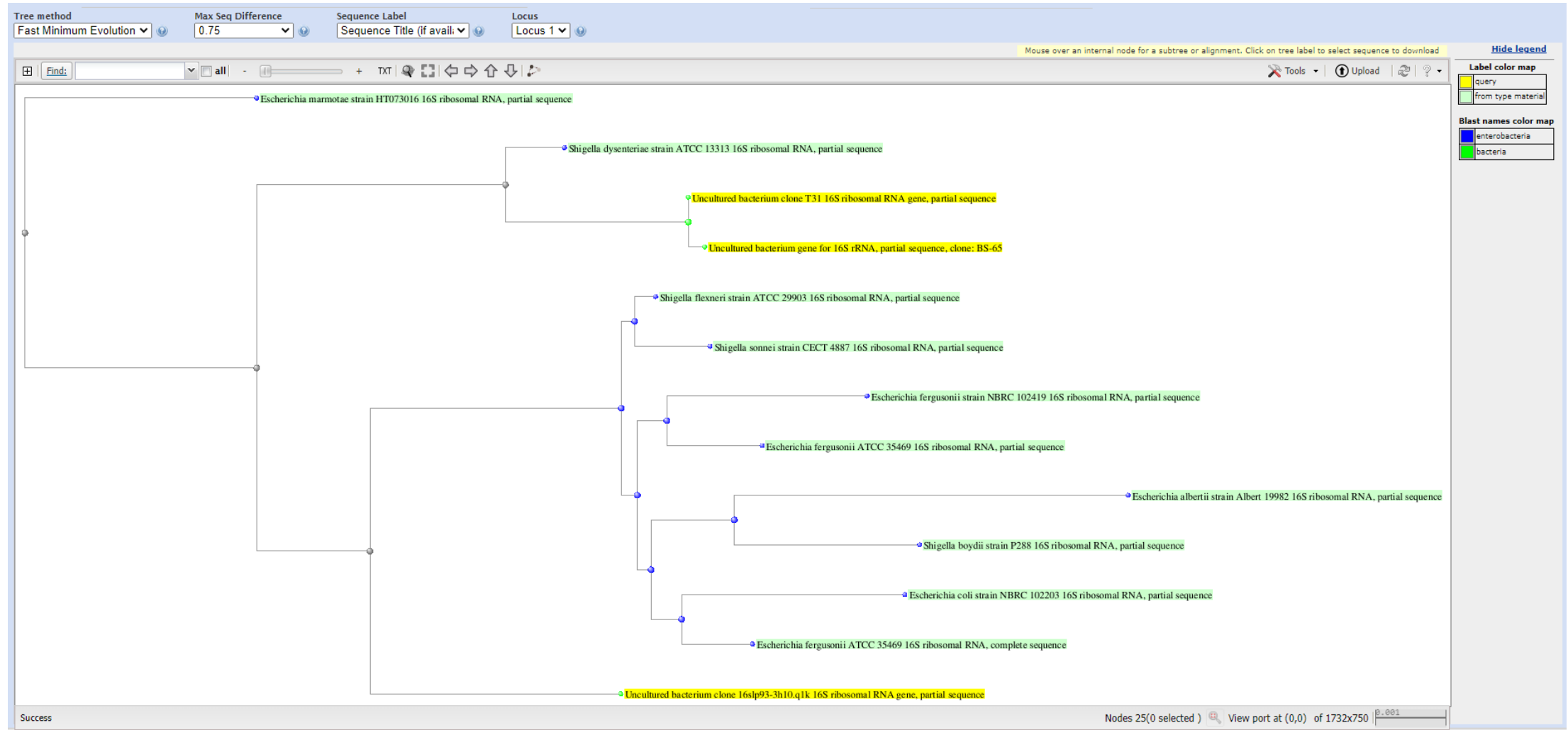
- Very clear DB for some type of compounds:
  - Pesticides
  - Drugs
- But not for other types of compounds
  
- Alternatives: googling it, news articles can be useful or EU legislation text
- But information can be very complicated to find
- Public information / private company → *Full disclosure legislation doesn't exist*

# Registration databases

- Other sources of chemical information (incl. Databases)
  - Manufacturers and dealers: Merck, TCI, Acros,...
  - Large projects: NIH library (US -National Institute of Health, etc.)



# MOLE-BLAST





# Magazine database

- Publishers (industry-specific or broad-based)
- Larger consortia or aggregators
- Other organizations: e.g., NIH

# Magazine database

– <https://pubs.acs.org/> (American Chemical society)

The screenshot shows the ACS Publications website homepage. At the top, there is a navigation bar with 'ACS Publications', 'C&EN', and 'CAS' on the left, and 'Access provided by MASARYK UNIV BRNO | Log in' on the right. Below this is the ACS Publications logo and a search bar. The main content area is divided into sections: 'FOR ORGANIZATIONS', 'FOR AUTHORS', 'EVENTS & CONFERENCES', and 'OPEN SCIENCE'. The central focus is a large blue banner with the text 'Most Trusted. Most Cited. Most Read.' and a 'Get Access' button. To the right of this banner is a 'NEW & NOTEWORTHY' section with three items: 'ACS Wins Bronze Brandon Hall Group HCM Excellence Award', 'Learning to Create Effective Patents: A New ACS Guide Chapter', and 'ChemRxiv Surpasses 10,000 Preprints Posted'. Below the banner is a 'Browse Content' section with seven colored tiles representing different scientific fields: 'All Subjects', 'Analytical', 'Applied', 'Biological', 'Materials Science & Engineering', 'Organic-Inorganic', and 'Physical'. At the bottom of the page, there are four white buttons: 'Publish with ACS', 'New Products & Services', 'ACS Open Science', and 'Explore ACS Solutions'.

# Magazine database



## NARROW RESULTS

### CONTENT TYPE

Book Chapter	28
Reference/Standard	2
C&EN Article	32
Journal Article	204

### ARTICLE SUBJECT

Article	134
News	26
Review	8
Concentrates	4
Features	4

MORE (15)

### PUBLICATION DATE

RESULTS: 1 - 20 of 301

Follow results:

REFINE SEARCH

PER PAGE: 20 50 100

SORT: RELEVANCE

1 2 3 4 5 6 7

Article

## Synthesis of Multi-core-shell Magnetic Molecularly Imprinted Microspheres for Rapid Recognition of Dicofol in Tea

Hongyuan Yan\*, Xiaoling Cheng, and Ning Sun

*Journal of Agricultural and Food Chemistry* 2013, 61, 11, 2896-2901 (Article) Subscribed

Publication Date (Web): February 23, 2013

DOI: 10.1021/jf400847b

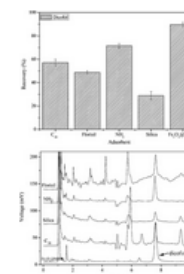
Abstract

Full text

PDF



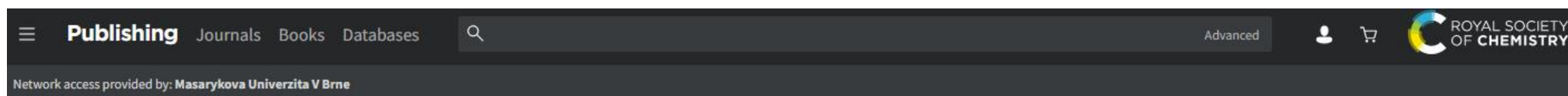
ABSTRACT



JOURNAL OF  
**AGRICULTURAL AND  
FOOD CHEMISTRY**

# Magasine database

– <https://pubs.rsc.org/> (Royal Society of Chemistry)



The Royal Society of Chemistry's

## Journals, Books and Databases

### Our journals

[View all journals](#)



Search our journals

### About our publications

The Royal Society of Chemistry publishes 48 peer-reviewed journals, around 2,000 book titles and a collection of online databases and literature updating services.

Our international publishing portfolio covers the core chemical sciences including related fields such as biology, biophysics, energy and environment, engineering, materials, medicine and physics. As a not-for-profit publisher, we reinvest surplus funds back into the global scientific community, supporting our mission to advance excellence in the chemical sciences.

# Other magazine publishers

- Elsevier
- Wiley & Sons.
- Nature publishing group
- AAAS
- Hindawi
- Universities, AV, Research organizations
- Many other...



# https://www.sciencedirect.com/



ScienceDirect

Journals & Books



Register

Sign in

Search for peer-reviewed journal articles and book chapters (including [open access](#) content)



Advanced search

Elsevier journals offer the latest peer-reviewed research papers on climate change, biodiversity, renewable energy and other topics addressing our planet's climate emergency. Join us in working towards a sustainable future with our editorially independent report on creating a Net Zero future.

Get the Net Zero report

Explore scientific, technical, and medical research on ScienceDirect

Physical Sciences and Engineering

Life Sciences

Health Sciences

Social Sciences and Humanities



# CAS: Chemical Abstracts Services

- Published by ACS as an abstract review journal
  - It included more than 8,000 magazines and conferences, as well as technical reports, dissertations, etc.
  - 1907-2010• Today, its role has been taken over by online databases...
- Abstract databases
  - They no longer make much sense
  - Replaced by general ones
- More wider databases•
  - PubChem - one of the CAS substitutes
  - And one of the databases operated by NIH NLM: [ncbi.nlm.nih.gov](http://ncbi.nlm.nih.gov)

# PUBCHEM



National Library of Medicine  
National Center for Biotechnology Information



[About](#)

[Blog](#)

[Submit](#)

[Contact](#)

## Explore Chemistry

Quickly find chemical information from authoritative sources



Try [covid-19](#) [aspirin](#) [EGFR](#) [C9H8O4](#) [57-27-2](#) [C1=CC=C\(C=C1\)C=O](#) [InChI=1S/C3H6O/c1-3\(2\)4/h1-2H3](#)

Use Entrez


Compounds

Substances

BioAssays

# PUBCHEM

SEARCH FOR

× 

Treating this as a text search.

## COMPOUND BEST MATCH



Epoxiconazole; 135319-73-2; CHEBI:83758; 1-[[3-(2-chlorophenyl)-2-(4-fluorophenyl)oxiran-2-yl]methyl]-1H-1,2,4-triazole; 133855-98-8; (2RS,3SR)-1-[3-(2-Chlorophenyl)-2,3-epoxy-2-(4-fluorophenyl)propyl]-1H-1,2,4-triazole; BAS 480F; 106325-08-0; ...

Compound CID: 3317081

MF: C<sub>17</sub>H<sub>13</sub>ClFN<sub>3</sub>O MW: 329.8g/mol

IUPAC Name: 1-[[3-(2-chlorophenyl)-2-(4-fluorophenyl)oxiran-2-yl]methyl]-1,2,4-triazole

Isomeric SMILES: C1=CC=C(C(=C1)C2C(O2)(CN3C=NC=N3)C4=CC=C(C=C4)F)Cl

InChIKey: ZMYFCLJBGAQRS-UHFFFAOYSA-N

InChI: InChI=1S/C17H13ClFN3O/c18-15-4-2-1-3-14(15)16-17(23-16,9-22-11-20-10-21-22)12-5-7-13(19)8-6-12/h1-8,10-11,16H,9H2

Create Date: 2005-09-07

[Summary](#) [Similar Structures Search](#) [Related Records](#)



**Compounds** (6)   **Substances** (78)   **Literature** (253)   **Patents** (258)



Searching PubMed abstracts and metadata. [Read More...](#)

253 results

 Filters

SORT BY  Relevance 

 Download 

 Search in PubMed 

### Enantioselective determination of triazole fungicide epoxiconazole bioaccumulation in tubifex based on HPLC-MS/MS

PMID: 24364671 Publication Type: Article

Publication Date: 2014-01-15

Journal: Journal of agricultural and food chemistry



Author(s): Chunxiao Liu, Bo Wang, Peng Xu, Tiantian Liu, Shanshan Di, Jinling Diao



Abstract: In this study, the enantioselective bioaccumulation of epoxiconazole enantiomers in tubifex (*Oligochaeta*, Tubificida) was investigated in two uptake pathways. A sensitive and rapid chiral method was developed for the determination of epoxiconazole enantiomers in tubifex and soil based on high-performance liquid chromatography coupled with triple-quadrupole mass spectrometry (HPLC-MS/MS). In the spiked-water or spiked-soil treatments, enantioselective bioaccumulation of epoxiconazole in tubifex was observed. For spiked-water treatment, (-)-epoxiconazole accumulated in tubifex to a greater extent than (+)-epoxiconazole, leading to enrichments with a composition (-) > (+). However, for spiked-soil treatment, the enantioselectivity in tubifex was reversed with a preferential accumulation of (+)-epoxiconazole. Calculated accumulation factors (AFs) indicated that epoxiconazole in spiked-water treatment had higher bioaccumulation potential than that in spiked-soil treatment. The results from the spiked-soil treatment also revealed that the dissipation of epoxiconazole in soil was enantioselective, and tubifex has positive effects on epoxiconazole diffusion from soil to overlying water.

Linked Compounds Count: [7](#)

#### ACTIONS ON RESULTS WITH ID TYPE:



- PubMed Abstracts
- Compounds
- Substances

 Save for Later 

 Linked Data Sets 

COMPOUND SUMMARY

## Epoxiconazole

<b>PubChem CID</b>	3317081
<b>Structure</b>	 <p>2D 3D</p> <p><a href="#">Find Similar Structures</a></p>
<b>Chemical Safety</b>	 <p>Health Hazard Environmental Hazard</p> <p><a href="#">Laboratory Chemical Safety Summary (LCSS) Datasheet</a></p>
<b>Molecular Formula</b>	$C_{17}H_{13}ClFN_3O$
<b>Synonyms</b>	<p>Epoxiconazole 135319-73-2 1-[[[3-(2-chlorophenyl)-2-(4-fluorophenyl)oxiran-2-yl]methyl]-1,2,4-triazole CHEBI:83758 1-[[[3-(2-chlorophenyl)-2-(4-fluorophenyl)oxiran-2-yl]methyl]-1H-1,2,4-triazole</p> <p><a href="#">More...</a></p>
<b>Molecular Weight</b>	329.8
<b>Dates</b>	<p>Modify Create</p> <p>2023-02-18 2005-09-07</p>
<p>1-[[[3-(2-chlorophenyl)-2-(4-fluorophenyl)oxiran-2-yl]methyl]-1H-1,2,4-triazole is an epoxide that is <i>oxirane</i> substituted by a 2-chlorophenyl, 4-fluorophenyl and a 1H-1,2,4-triazol-1-ylmethyl groups. It is an epoxide, a member of monochlorobenzenes, a member of monofluorobenzenes and a member of triazoles.</p> <p><a href="#">ChEBI</a></p>	

[Cite](#) [Download](#)

**CONTENTS**

- Title and Summary
- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Spectral Information
- 5 Related Records
- 6 Chemical Vendors
- 7 Drug and Medication Information
- 8 Agrochemical Information
- 9 Pharmacology and Biochemistry
- 10 Use and Manufacturing
- 11 Safety and Hazards
- 12 Toxicity
- 13 Literature
- 14 Patents
- 15 Biological Test Results
- 16 Classification
- 17 Information Sources

# Patent Database

- Only partial overlap with articles and monographs
- Different style of text and content
  - European: ESPACENET
  - US: USPTO
  - Japanese
  - Czech
  - and others, eg:
    - [patents.google.com](https://patents.google.com)
    - Patentscope (WIPO)
    - [freepatentsonline.com](https://freepatentsonline.com)

# Patent Database

– <https://worldwide.espacenet.com/>



**Espacenet**  
Patent search

Enter your search terms



My Espacenet

Help

Classification search

Results

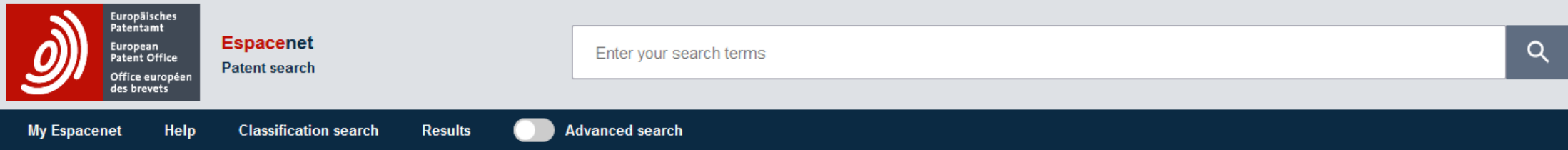


Advanced search

**Espacenet: free access to over 130 million patent documents**

# Patent Database

– <https://worldwide.espacenet.com/>



**Espacenet: free access to over 130 million patent documents**

- Let's look for something
  - Suggestions?

# Patent Database

The screenshot shows the Espacenet Patent search interface. At the top, there is a search bar containing 'epoxiconazole'. Below the search bar, there are navigation tabs: 'My Espacenet', 'Help', 'Classification search', and 'Results'. To the right of these tabs are three toggle switches for 'Advanced search', 'Filters', and 'Popup tips'. Below the navigation, the breadcrumb 'Home > Results' is visible. The main heading indicates '7 832 results found'. Below this, there are dropdown menus for 'List view' (set to 'Text only'), 'List content' (set to 'All'), and 'Sort by' (set to 'Relevance'). A selection summary shows '(0 patents selected) Select the first 20 results'. Three patent results are listed, each with a checkbox, a title, a patent number, a date, and an applicant name. The first result is 'TERNARY FUNGICIDE AGENT COMBINATIONS' by Bayer CropScience AG. The second is 'Preparation method of epoxiconazole intermediate and preparation method of epoxiconazole' by Jiangsu Sevencontinent Green Chemical Co Ltd. The third is 'SYNERGISTIC FUNGICIDAL COMBINATION' by Irvita Plant Prot N V.

Europäisches Patentamt  
European Patent Office  
Office européen des brevets

Espacenet  
Patent search

epoxiconazole

My Espacenet Help Classification search Results Advanced search Filters Popup tips

Home > Results

7 832 results found

List view Text only List content All Sort by Relevance

(0 patents selected) Select the first 20 results

1. **TERNARY FUNGICIDE AGENT COMBINATIONS**  
WO2008061656A2 (A3) • 2008-05-29 • BAYER CROPSCIENCE AG [DE]  
**Earliest priority: 2006-11-24 • Earliest publication: 2008-05-29**  
The novel active agent combinations of spiroxamine, epoxiconazole and tebuconazole or prothioconazole have very good fungicidal properties.

2. **Preparation method of epoxiconazole intermediate and preparation method of epoxiconazole**  
CN106279067A (B) • 2017-01-04 • JIANGSU SEVENCONTINENT GREEN CHEMICAL CO LTD  
**Earliest priority: 2016-08-16 • Earliest publication: 2017-01-04**  
...The invention relates to a preparation method of an epoxiconazole intermediate and a preparation method of epoxiconazole. The preparation method of the epoxiconazole intermediate comprises the following steps: taking O-chlorobenzyl chloride as a raw material and carrying out a... the epoxiconazole intermediate and the preparation method of epoxiconazole, provided by the invention, adopt a Corey epoxidation

3. **SYNERGISTIC FUNGICIDAL COMBINATION**  
WO2011117868A1 • 2011-09-29 • IRVITA PLANT PROT N V [NL]  
**Earliest priority: 2010-03-22 • Earliest publication: 2011-09-29**  
Compositions and methods employing combinations of synergistically effective amounts of folpet and epoxiconazole are provided.



# Conclusions

- Lots of information is available online
- Just need to know where to look for it ...
- ... and how to formulate your query
  
- Accessibility may sometimes be an issue...

# Exam: Assignment 2

- For April 5<sup>th</sup> – as a word document or pdf – submitted on IS
- Instructions: From the following list of journals, select the one that has the same serial number as the last digit of your UČO number:

Last number of your UČO	Journal
1	Environmental Science and Technology
2	Chemosphere
3	ACS Earth and Space Chemistry
4	Science
5	TrAC Trends in Analytical Chemistry
6	Environmental Science & Policy
7	Limnologica
8	Energy & Environmental Science
9	Atmospheric Science Letters
0	Risk Analysis

# Exam: Assignment 2

- **For April 5<sup>th</sup> – as a word document or pdf – submitted on IS**
- Instructions: From the following list of journals, select the one that has the same serial number as the last digit of your UČO number:
  
- Then find out for the journal you have been given:
  - a) the name of the publishing house
  - b) the name of the chairman of the editorial board
  - c) is there a member of the editorial board who has an affiliation with a Czech institution?
  - d) what types of articles does this journal accept for publication (e.g. reports, full papers, letters, reviews, opinions, etc.
  
- Write a small report (10 lines maximum)

# Questions?

– Contact me anytime via email: [ludovic.mayer@recetox.muni.cz](mailto:ludovic.mayer@recetox.muni.cz)