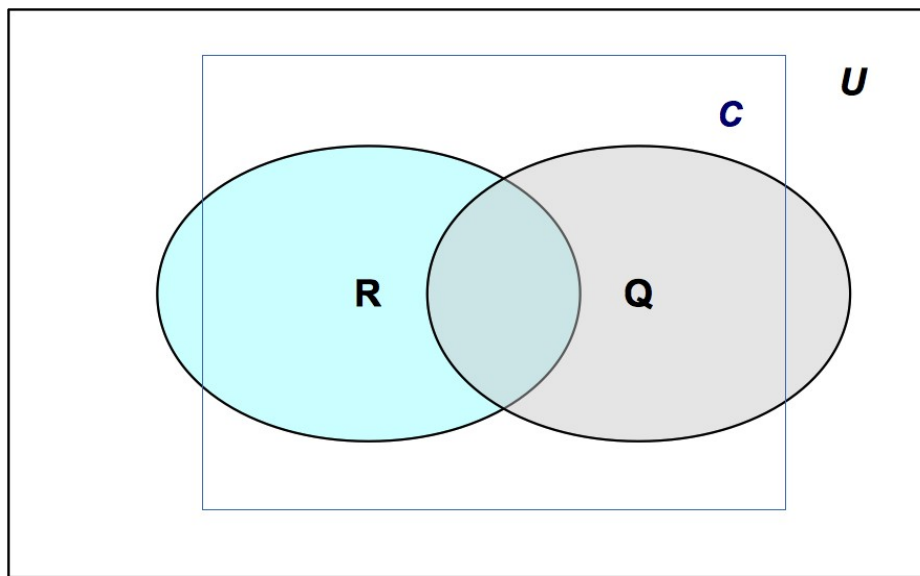




Source: <https://www.publicdomainpictures.net/de/view-image.php?image=100369&picture=tool-box>

Coverage: the forgotten factor



=> the tool you use will determine C

Selected types of search tools

Type	Content
Multidisciplinary databases (WoS, Scopus; EPFL's BEAST)	Articles and some conference proceedings for current events in research
Specialized databases (SciFinder, Pubmed, MathSciNet, etc)	Mainly article references
Scientific search engines (Google Scholar, ...)	Web pages of articles and proceedings
Chemical databases (SciFinder, Reaxys, Chemspider, Pubmed, Cambridge Structure Databases)	Chemical compounds , sometimes reactions , sometimes linked with literature references
Citation tools (most of the above)	Cited scientific and technical articles and proceedings

The right tool for the right job

- **Book DB** or **Multidisciplinary DB (filtering by type: Review)** to have a good overview of an existing subject
- **Multidisciplinary DB** to find current publications (i.e. less than 1 year old) regardless of subject
- **Full text DB** to find information located in the full text such as material, methods, or factual info)
- **Citation tools** to identify the most «prestigious» articles
- **Specialized DB** to find subject-specific information, sometimes from “exotic” sources

Google Scholar

- Research in the Web for scientific publications (peer-reviewed or not)
- More focused and relevant than Google
- Selection of sources' process unknown
- Rankings of results' process unknown
- Citations' origin not transparent

Web of science

Created in 1964, owned by Clarivate Analytics.

~86 mio bibliographic records in the Core Collection (+1 mio)

> 21'000 journals (2023-10-09)

Full indexation of cited references (~1.9 billion citations)

Available at most universities

The screenshot displays the Web of Science search interface. At the top, the Clarivate logo is on the left, and language and product options are on the right. The main search area features a search bar with the text "Web of Science™" and "Search". Below the search bar, there are tabs for "DOCUMENTS" and "RESEARCHERS". The "DOCUMENTS" tab is active, showing a search filter for "Web of Science Core Collection" and "Editions: All". There are also tabs for "DOCUMENTS" and "CITED REFERENCES". A search input field contains the text "Example: liver disease india singh". Below the search field are buttons for "+ Add row", "+ Add date range", and "Advanced Search". A "Clear" button and a "Search" button are also present. At the bottom of the search area, there is a promotional banner for a personalized homepage dashboard with a "Sign in to access" button. The footer contains the Clarivate logo, the tagline "Accelerating innovation", the year "© 2022 Clarivate", and links for "Data Correction", "Copyright Notice", "Manage cookie preferences", and "Follow Us".

Scopus




Created in 2004, owned by Elsevier.

> 90 mio bibliographic records

44'737 serials (journals, book series...) (2023-10-09)

Cited references 1970-2023 (est. ~1.8 billion citations)


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+ Add search field [Add date range](#) [Advanced document search](#) ▶ [Search Q](#)

[Search History](#) [Saved Searches](#) New


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Scifinder & Chemical Abstracts

CAS SciFinder

Return to Home

Good Morning, Alain

The effect of antibiotic residues on dairy products

Featured Search

- Prior Art Discovery**
Discover prior art in patents and non-patent literature using AI-enhanced search technologies.
- Patent Markush**
Search Patent Markush by structure and view associated references.
- Advanced Search**
Select data fields and search operators to create a focused query.
- Retrosynthetic Analysis**
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

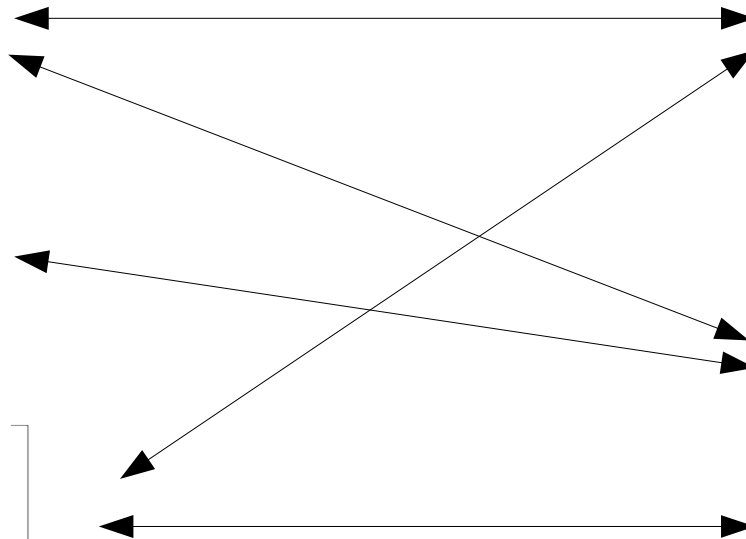
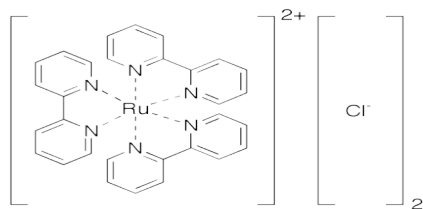
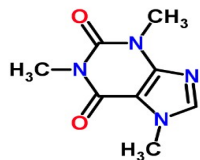
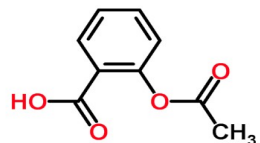
History **New**⁴ NEW

CAPLus: > 59 mio bibliographic records. Allegedly the most exhaustive DB for chemistry.

Registry: > 275 mio substances

CASReact: > 150 mio reactions

Scifinder's distinctive feature



Scifinder's query processing (before 2019)

- 1) Natural language processing engine => concept extraction
- 2) Presence or absence of some concepts + where (title, abstract, keywords)
= relevance ranking
- 3) Filters
- (4) Boolean combination of result sets by the user)

Scifinder concept extraction (before 2019):

applications of platinum chelates in medicine



Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "applications of platinum chela..."

REFERENCES ⓘ

Select All Deselect All

0 of 9 Research Topic Candidates Selected

- 3 references were found containing all of the concepts "applications", "platinum chelates" and "medicine".
- 29 references were found containing the two concepts "applications" and "platinum chelates" closely associated with one another.
- 197 references were found where the two concepts "applications" and "platinum chelates" were present anywhere in the reference.
- 64815 references were found containing the two concepts "applications" and "medicine" closely associated with one another.
- 150553 references were found where the two concepts "applications" and "medicine" were present anywhere in the reference.
- 10 references were found containing the two concepts "platinum chelates" and "medicine".
- 6176681 references were found containing the concept "applications".
- 2082 references were found containing the concept "platinum chelates".
- 1182050 references were found containing the concept "medicine".

Get References

Comparison:

applications platinum chelates medicine



Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "applications platinum chelates..."

REFERENCES ⓘ

Select All Deselect All

0 of 2 Research Topic Candidates Selected

- No References were found containing both of the concepts "applications platinum" and "chelates medicine".
- 12159 references were found containing the concept "applications platinum".
- 705 references were found containing the concept "chelates medicine".

Get References

Very different behavior in 2025 : 162 refs (disable interpretation : 1'083'217 with preps, 505'109 without)

2023 : with prepositions 521'414 refs, without => 112'705

2022 : 474'539 vs 9'712'109 in 2022!)

Tutorials for the 2023-2024 version :

<https://www.cas.org/training/module/reference-searching>

Extended Boolean searching in SciFinder 2023-2024: the way it used to be...

lead AND perovskite AND solar AND cells

<https://scifinder-n.cas.org/search/reference/635b9ceef2fe9e7a888488bb/1>

=> all 4 words must be present

lead perovskite solar cells

<https://scifinder-n.cas.org/search/reference/6165538d3e8b173419fa7735/1>

=> at least 1 is present, many more results

Feedback on Scifinder-n results

Display of results

- **By relevance**
- **By date** to find the most recent references
- **By times cited** to find the most popular/important articles

Too many results -> increase precision

- Add terms or use more specific ones
- Use the AND and NOT operators in Advanced Search
- **Use filters**
- Advanced search : search in specific fields (i.e. Title vs Abstract/Keywords, or special identifiers,...)

Too few results -> increase recall

- Add or use broader terms
- Use the OR operator in Advanced Search
- Run a different search and combine the result sets
- (Use a different tool?)
- (The subject is very very recent and few things are published yet?)

Automated searching: alerts (formerly known as Keep Me Posted)

Satisfied with your search? From now on, let the computer work for you

The screenshot displays the CAS SciFinder search results page. At the top, there is a search bar with the text "CAS SciFinder" and "Edit Search Enter a query...". Below the search bar, there is a navigation bar with "Return to Advanced Search" and "References Advanced search for 3 fields".

The main content area shows search results for "7,242,214 Results". The first result is titled "Novel electrochemical approach to discriminate the coordination of two polymers using polymer-modified carbon paste electrodes" by Loughmari, S.; Oubaouz, M.; Oukbab, M.; Haddouchy, H.; Visseaux, M.; El Bouadili, A.; El Quatli, S.-E.; Chtaini, A. The abstract text is visible, starting with "To discriminate the structures of two polymers, 1,4-transpolymyrce (TPM) and 1,4- cis polymyrce (CPM), at mol. level, NMR (NMR) was herein used as the main method. However, to enhance the reliability of findings, this method involves a longer ordering time, which results in higher costs. A simple electrochem. technique, based on the use of cyclic voltammetry (CV), square wave voltammetry (SWV) and electrochem. impedance spectroscopy (EIS), was incorporated into the approach of this study. CV provided information on the polymers' electronic properties, while EIS enabled to assess electroche..."

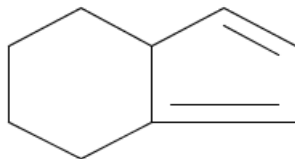
On the right side of the interface, there is a "Save and Alert" button circled in green. Below it, there is a "Copy Search to Clipboard" button. The "Analyze Results" section shows a bar chart titled "Top Document Types" with categories: Journal (purple), Patent (green), Review (orange), Conf... (teal), Pre (red), and Re (blue).

On the left side, there is a "Filter Results" section with a "New" button and a "Document type" filter set to "Journal (5M)".

- Scientific information as a network
- Elementary information retrieval
- The world of scientific information
- **(really basic) Elements of cheminformatics**

Theoretical bases

Chemical searching: what's in a name?



CAS Registry Number: 96288-37-8

Molecular formula: C₉ H₁₂

CAS name: 4*H*-Indene, 3a,5,6,7-tetrahydro-

IUPAC name: 4,5,6,7-Tetrahydro-1*H*-indene

SMILES: C1CCC2=CC=CC2C1

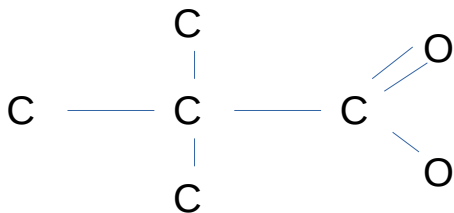
InChi: 1S/C9H12/c1-2-5-9-7-3-6-8(9)4-1/h3,6H,1-2,4-5,7H2

Substructure searching: the hard part

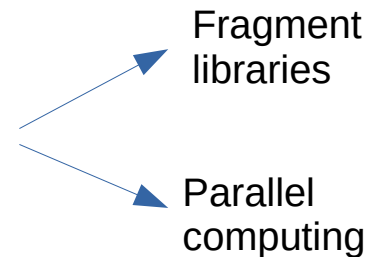
Indexing molecules and fragments is much more difficult than words

This — is — a — sentence

- Linear sequence
- Large vocabulary (you use 20'000-35'000 words routinely in your native language)
- For searching purposes, the user will not mind if the order is different



- Branches (and cycles) possible
- Small vocabulary (118 elements, basic organic chemistry deals with just 5)
- Huge number of possible structures (10^{60} for molecules up to 300-500 Da)
- Connectivity **ESSENTIAL**



Artificial Intelligence : are words useful again ?

- Active research in the application of language processing methods to chemical problems ; for example reaction prediction using transformers (as in «Generative Pre-trained Transformer»...)

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RETURN TO ISSUE < PREV RESEARCH ARTICLE NEXT >

Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction

Philippe Schwaller*, Teodoro Laino, Théophile Gaudin, Peter Bolgar, Christopher A. Hunter, Costas Bekas, and Alpha A. Lee*

Cite this: *ACS Cent. Sci.* 2019, 5, 9, 1572–1583
 Publication Date: August 30, 2019
<https://doi.org/10.1021/acscentsci.9b00576>
 Copyright © 2019 American Chemical Society

Article Views: 25297 Altmetric: 151 Citations: 105

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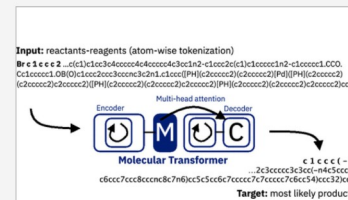
Read Online PDF (1 MB)

SUBJECTS: Reagents, Chemical reactions, v

ACS Central Science

Abstract

Organic synthesis is one of the key stumbling blocks in medicinal chemistry. A necessary yet unsolved step in planning synthesis is solving the forward problem: Given reactants and reagents, predict the products. Similar to other work, we treat reaction prediction as a machine translation problem between simplified molecular-input line-entry system (SMILES) strings (a text-based representation) of reactants, reagents, and the products. We show that a multihed attention Molecular Transformer model outperforms all algorithms in the literature, achieving a top-1 accuracy above 90% on a common benchmark data set. Molecular Transformer makes predictions by inferring the correlations between the



Too many hits?

- Use more detailed fragments
- Add explicit hydrogens or lock atoms to prevent unwanted substitutions
- Lock rings
- Use filters (substance role, Refine, etc.)

CAS Draw

Draw or change atoms or bonds.

Molecular Formula: C₂H₆ (30.07)

Zoom: 100%

Cancel OK

Coordination compounds

Use precision analysis to explicitly request the exact substructure you have drawn (otherwise the system will be allowed to rearrange bonds in the vicinity of the metal)

The screenshot displays the CAS SciFinder interface. On the left, the 'Structure Match' filter is expanded, showing 'As Drawn (1)', 'Substructure (593)', and 'Similarity (2,510)'. Below this, the 'Structure Precision' section is highlighted with a green box, containing 'Conventional Results (463)' and 'Tautomers and Zwitterions (130)'. The main search results area shows a list of substances. The first result is '483309-89-3', which is a complex iron coordination compound. Its chemical structure is shown as a central iron atom coordinated to four nitrogen atoms in a tetraazacyclohexane ring and two additional ligands. The second result is '180676-18-0', which is a dichloro complex of the same ligand system. The interface includes a search bar at the top, navigation buttons, and a feedback icon at the bottom right.

Materials

Structure search doesn't really work for materials in Scfinder. A crystal structure database (Cambridge or ICSD) would work better but doesn't contain much information beyond the X-ray structure.

- Use formula search with “molecular” fragment:
CH₃NH₃PbI₃ perovskite → Advanced search «Molecular formula» CH₅N.H.I₃Pb (CASRN 69507-98-8) (and a few deuterated variants)
- Non-stoichiometric or doped substances: combine the results of several searches; for example if you wanted to mix chloride and iodide in various proportions
 - CH₅N . H . I₃Pb as substance then retrieve associated references
 - CH₅N . H . Cl₃Pb as substance (→ CASRN 69276-12-6) then references
 - “69507-98-8D with chloride” as a keyword search
 - “69276-12-6D with iodide” as a keyword searchYou can then apply filters to the combine reference set.

Searching for reactions

Same as structure searching... plus an arrow.

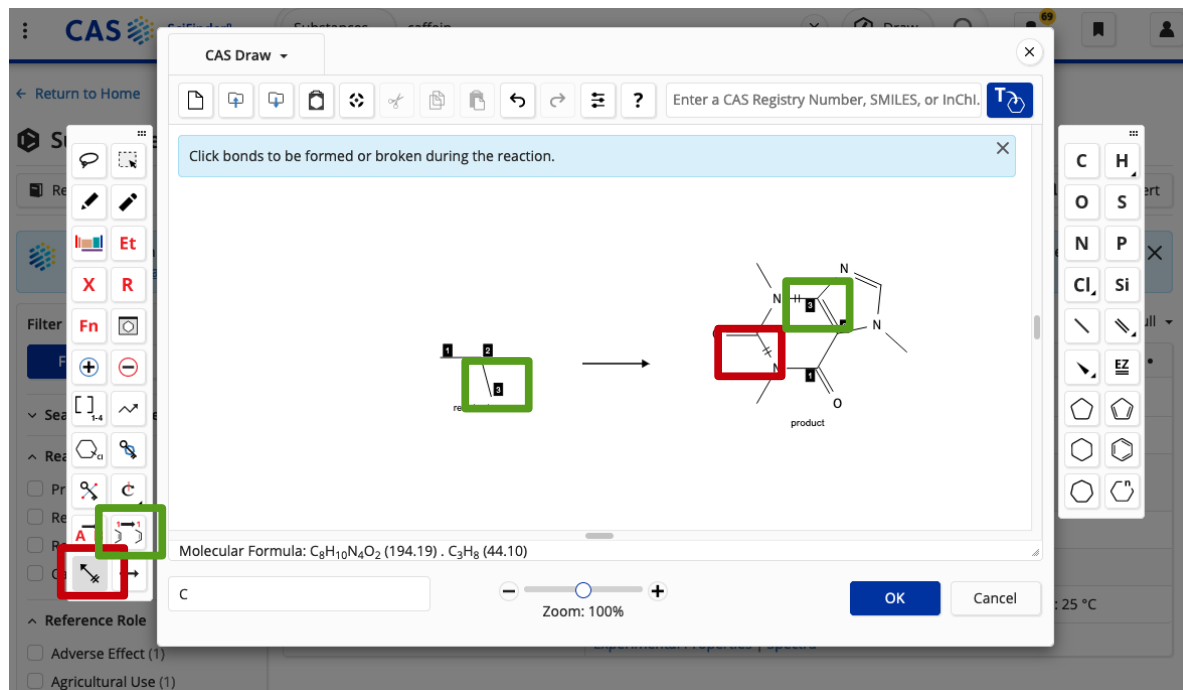
The screenshot shows the CAS Draw application window. At the top, there is a search bar with the text "Enter a CAS Registry Number, SMILES, or InChI." Below this is a toolbar with various icons. The main drawing area contains a reaction scheme: a reactant (a simple line structure) followed by an arrow pointing to a product (a complex heterocyclic structure). Below the drawing area, the molecular formula is displayed: "Molecular Formula: C₈H₁₀N₄O₂ (194.19) · C₃H₈ (44.10)". At the bottom of the window, there is a zoom slider set to 100% and buttons for "OK" and "Cancel".

On the left side of the CAS Draw window, there is a vertical toolbar with various icons. A green box highlights the arrow icon, which is used to add a reaction arrow to the drawing.

On the right side of the CAS Draw window, there is a vertical toolbar with various icons for drawing chemical structures, including atoms (C, H, O, S, N, P, Cl, Si), bonds, and rings (pentagon, hexagon, octagon).

Too many hits?

- **Map atoms:** explicitly associate some atoms in the reactant(s) with corresponding atoms in the product(s)
- **Mark bonds:** tag reactant bonds that will be broken or product bonds that will be formed



Reaxys



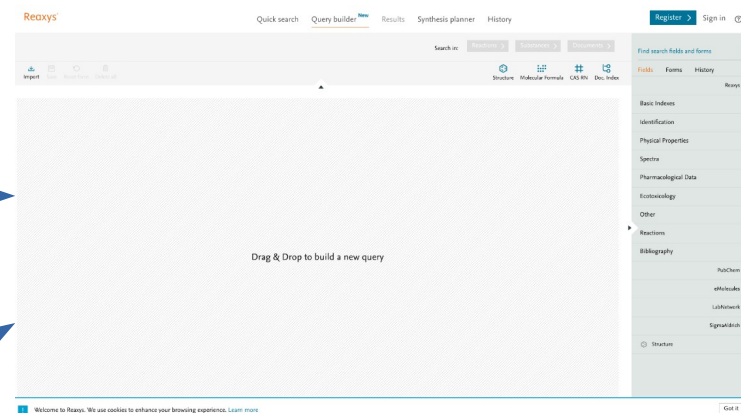
Beilstein: organic chemistry
(175 journals starting 1771),
8'000'000 compounds.



+ Gmelin: inorganic
chemistry (62 journals
starting 1772), 2'200'000
compounds

+ newer content
(Patent Chemistry database, PubChem...)

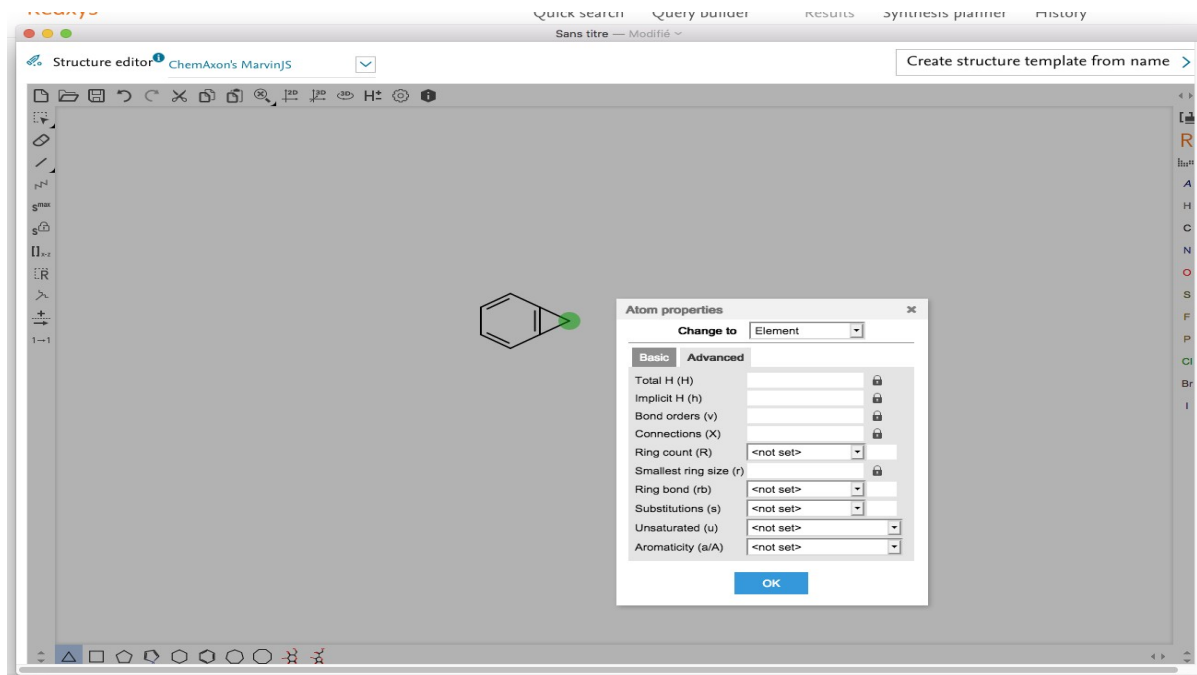
= <https://www.reaxys.com>



Structure searching with Reaxys

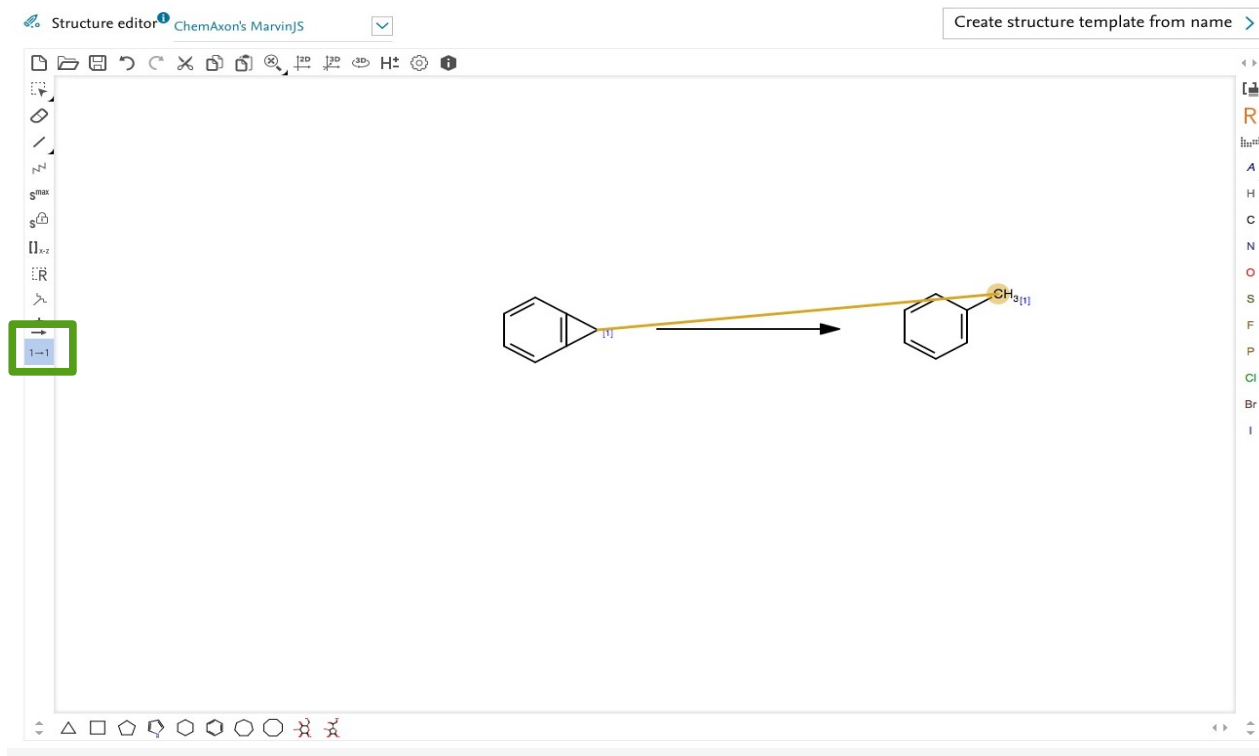
Features similar to Scifinder (usually : right-click instead of a tool button):

Lock atom equivalent
(right-click,
«Atom properties»):



Reaction searching with Reaxys

Map atoms



Searching for properties

Reaxys allows sophisticated searches, for example:

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation options: Quick search, Query builder (highlighted), Results, Synthesis planner, and History. On the right, there are buttons for Register and Sign in. Below the navigation, there are tabs for Reactions, Substances, and Documents. A search bar is present with the text "Search in:". Below the search bar, there are icons for Structure, Molecular Formula, CAS RN, and Doc. Index. On the left, there are icons for Import, Save, Reset form, and Delete all. The main area is divided into several sections:

- Structure:** A large box containing the chemical formula U^{5+} .
- Magnetic Susceptibility:** A section with a "Find any" button and a dropdown menu set to "Show fields". The selected fields are "(Magnetic Susceptibility, 10-6cm³mol⁻¹, Temperature, °C)".
- NMR Spectroscopy:** A section with a "Find any" button and a dropdown menu set to "Hide fields". The selected fields are:
 - Description (NMR Spectroscopy)
 - 1h
 - Coupling Nuclei
 - Solvents (NMR Spectroscopy)

On the right side, there is a sidebar titled "Find search fields and forms" with a search icon. It lists various search fields and forms, including:

- Solubility Product
- Solution Behaviour
- Sound Properties
- Space Group
- Static Dielectric Constant
- Surface Tension
- Thermal Expansion
- Transition Point(s) of Crystalline Modification(s)
- Transition Point(s) of Liquid Modification(s)
- Transport Data
- Transport Phenomena
- Triple Point
- Vapour Pressure
- Spectra
 - NMR Spectroscopy
 - IR Spectroscopy
 - Mass Spectrometry


Contains at least U^{5+} ion + Magnetic susceptibility study + 1H -NMR spectrum

Searching for publications in Reaxys

The screenshot displays the Reaxys search interface. At the top, there are three tabs for search types: 'Reactions', 'Substances', and 'Documents'. The 'Documents' tab is selected and highlighted with a green circle. Below the tabs, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. To the right, there are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. The search bar contains the query 'iridium AND catalysis' with a dropdown menu set to 'contains'. On the right side, there is a sidebar titled 'Find search fields and forms' with a search icon. The sidebar lists various search fields under 'Fields', 'Forms', and 'History'. The 'Fields' section includes: Document Basic Index, Identification, Physical Properties, Spectra, Pharmacological Data, Ecotoxicology, Other, Reactions, Bibliography, Document Type, Authors, Patent Assignee, Journal Title, Publication Year, Common Patent Number, Journal Publication Status, Indexing Status, and Citation Number. A 'Feedback' button is located at the bottom right of the sidebar.


Used to be weak, now it has become better. Compare with Scopus ?

Analyzing publications in Reaxys

Reaxys® Quick search Query builder **Results** Retrosynthesis History Register > Sign in 

222 Documents with 466 Substances, 117 Reactions, 0 Targets

0 selected Limit To Exclude Export

Sort by Publication Year ↓ Bioactivity Visualization 

Filters

222 Search

Limit to > Exclude >

Publication Year

Document Type

- article 142
- review 59
- conference paper 14
- chapter 3
- short survey 2
- note 1
- conference review 1

Authors/Inventors

- dorn, harry c 15
- zhao, yuliang 13
- sun, baoyun 13
- shinohara, hisanori 12
- xing, gengmei 10
- wilson, lon j 9
- dunsch, lothar 9

Filter by value View more

Current Patent Office

Patent Office

Journal Title

Substance Classes

Reaction Classes

1 Structurally Defined Water-Soluble Metallofullerene Derivatives towards Biomedical Applications [Cited 4 times](#)
 Li, Yanbang; Biswas, Rohit; Kopcha, William P.; Dubroca, Thierry; Abella, Laura; Sun, Yue; Crichton, Ryan A.; (...) Hill, Stephen; Zhang, Jianyuan
 [Angewandte Chemie - International Edition, 2023, vol. 62, # 3, art. no. E202211704][Angew. Chem., 2022, vol. 135, # 3]
 Abstract Index Terms Substances 26 Reactions 28 Full Text

Index Terms hit: {...Contrast Agents, Endohedral Fullerenes, Rare Earth Compounds...}

2 Recent advances and futuristic potentials of nano-tailored doxorubicin for prostate cancer therapy [Cited 4 times](#)
 Sawpari, Rana; Samanta, Sovan; Banerjee, Jhimli; Das, Swarnali; Dash, Shib Shankar; Ahmed, Rubai; Giri, Biplob; Dash, Sandeep Kumar [Journal of Drug Delivery Science and Technology, 2023, vol. 81, art. no. 104212]
 Abstract Index Terms Substances 35 Full Text

Index Terms hit: {...docetaxel, gadolinium texaphyrin, prednisone...}


3 Innovative nanomaterials for cancer diagnosis, imaging, and therapy: Drug delivery applications [Cited 7 times](#)
 Pourmadadi, Mehrab; Mahdi Eshaghi, Mohammad; Ostovar, Shima; Mohammadi, Zahra; Sharma, Rakesh K.; Paiva-Santos, Ana Cláudia; Rahmani, Erfan; Rahdar, Abbas; Pandey, Sadanand [Journal of Drug Delivery Science and Technology, 2023, vol. 82, art. no. 104357]
 Abstract Index Terms Full Text

Index Terms hit: {...solid lipid nanoparticle, fullerene derivative, nanomaterial...}

4 Nanoscale Porosity of High Surface Area Gadolinium Oxide Nanofoam Obtained With Combustion Synthesis [Cited 1 times](#)
 de Boer, Roos M.; Chen, Xiaodan; Cvejn, Daniel; Peterek Dědková, Kateřina; van Huis, Marijn A.; Mendes, Rafael G. [Advanced Materials Interfaces, 2023, vol. 10, # 13, art. no. 2300060]
 Abstract Index Terms Substances 1 Full Text

Index Terms hit: {...electron tomography, gadolinium oxide, in situ TEM...}

5 Stabilization of γ -/ α -Fe nanocrystalline phases inside carbon nanotube buckypapers and functionalization with Gd [Cited 1 times](#)
 Guo, Xilong; Wang, Shanling; Gu, Aiqun; He, Yi; Zheng, Shuping; Guo, Jian; Boi, Filippo S. [Diamond and Related Materials, 2023, vol. 136, art. no. 110042]

Feedback 

AI... because yes, of course

The screenshot shows the Reaxys website interface. At the top left is the Reaxys logo. The navigation menu includes 'Quick search', 'Query builder', 'Results', and 'Retrosynthesis'. The 'Quick search' menu is open, and 'Reaxys AI Search Beta' is highlighted with a red circle. In the top right corner, there are icons for a refresh button, a notification bell, a help icon with a '19' badge, and a user profile icon labeled 'AB' with a red circle around it.

Discover a more intuitive way to search — with Reaxys AI Search Beta.

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances

Import [↓](#)

Search Reaxys

Target Name, e.g. Polo-like kinase 1

Find >

AND

[Draw](#)

Content Overview | Latest update: 23. September 2025 >

350M	71M	122M	47M	50M
Substances	Reactions	Documents	Patents	Bioactivities

Pubchem

- for molecules & bioassays
- data is free to re-use without constraints

PubChem Statistics (Documentation) TOP

Search Documents

- About
- News
- Citation Guidelines
- Publications
- Tutorials
- Data Organization
- Data Sources
- Search and Tools
- Submissions
- Downloads
- Programmatic Access
- Widgets
- RDF
- Glossary
- Data Specification
- Statistics**
- Archive

Collection	Live Count	Description	Last Updated
Periodic Table of Elements	118	Interactive periodic table with up-to-date element property data collected from authoritative sources	September 12, 2025
Compounds	122,271,373	Unique chemical structures extracted from contributed PubChem Substance records	September 26, 2025
Substances	338,294,418	Information about chemical entities provided by PubChem contributors	September 28, 2025
BioAssays	1,768,874	Biological experiments provided by PubChem contributors	September 28, 2025
Pathways	250,942	Interactions between chemicals, genes, and proteins	September 26, 2025
Proteins	258,037	Proteins in PubChem including those found in BioAssays, Pathways, and Patents	September 26, 2025
Genes	166,217	Genes in PubChem including those found in BioAssays, Pathways, and Patents	September 26, 2025
Taxonomies	329,269	Organisms in PubChem including those found in BioAssays, Pathways, and Patents	September 26, 2025
Patents	73,126,479	Patents with links in PubChem	September 26, 2025
Literature	43,872,279	Scientific publications with links in PubChem	September 8, 2025
Cell Lines	2,009	Information about cell lines	September 26, 2025
BioActivities	297,992,506	Biological activity data points reported in PubChem BioAssays	September 29, 2025

Speaker

<https://pubchemdocs.ncbi.nlm.nih.gov/statistics> accessed on 2025-10-01

Properties: more sources

Other sources can be better if you know exactly the molecule of interest :

- CRC Handbook of Chemistry and Physics
- NIST Chemistry Webbook <http://webbook.nist.gov/chemistry/>
- Springer Materials <http://www.springermaterials.com>

Another database for substance searches according to properties:

- EchemPortal <http://www.echemportal.org>

X-Ray Structures:

Inorganic Crystal Structure Database (ICSD)

<https://icsd.fiz-karlsruhe.de/>

Content info : <https://icsd.products.fiz-karlsruhe.de/>

- ~320'000 structures (+12K/yr)
- Inorganic crystal structures
- EPFL license

X-Ray Structures:

Cambridge Structural Database (CSD)

<https://www.ccdc.cam.ac.uk/structures>

Content info : <https://www.ccdc.cam.ac.uk/solutions/CSD-System/Components/CSD/>

- 1.3 mio structures
- Small organic or organometallic molecules
- Free basic access, advanced searching for licensed institutions (ETHZ also for EPFL)

X-Ray Structures: Crystallography Open Database

<http://www.crystallography.net/cod/>

- ~0.5 mio structures
- Small organic or organometallic molecules
- Free access, public-domain data