

The background is a vibrant, abstract composition of numerous small, glowing spheres in shades of purple, blue, yellow, and white. These spheres are arranged in a way that suggests a molecular structure or a data visualization. The overall effect is a sense of dynamic energy and scientific discovery. A large, dark blue geometric shape, resembling a stylized 'A' or a search icon, is overlaid on the left side of the image. A white line graphic, resembling a stylized 'C' or a search icon, is overlaid on the right side of the image.

CAS SCIFINDER®

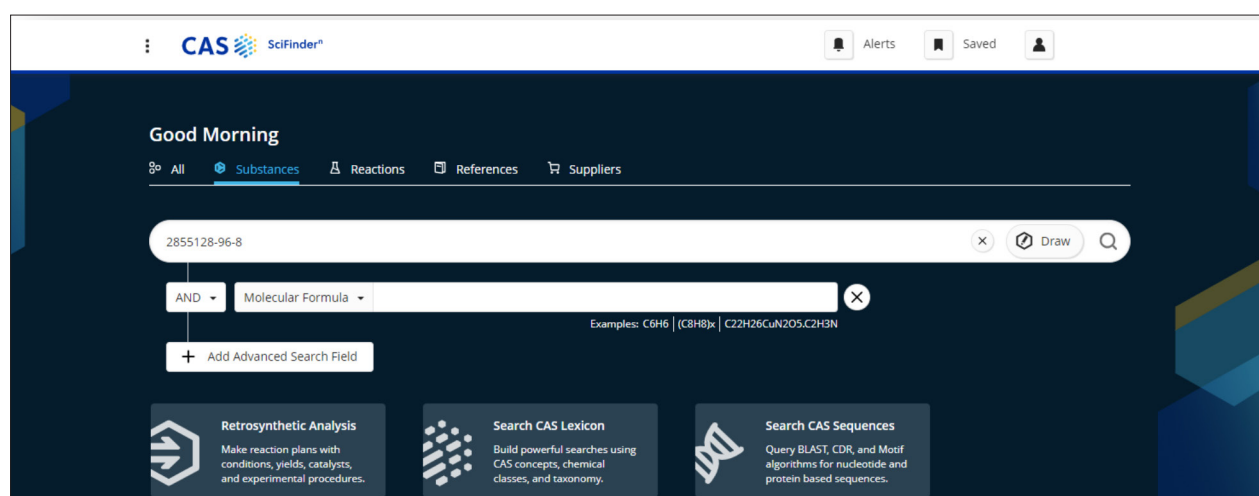
# QUICK START GUIDE FOR PERFORMING A SEARCH

# Get started using CAS SciFinder

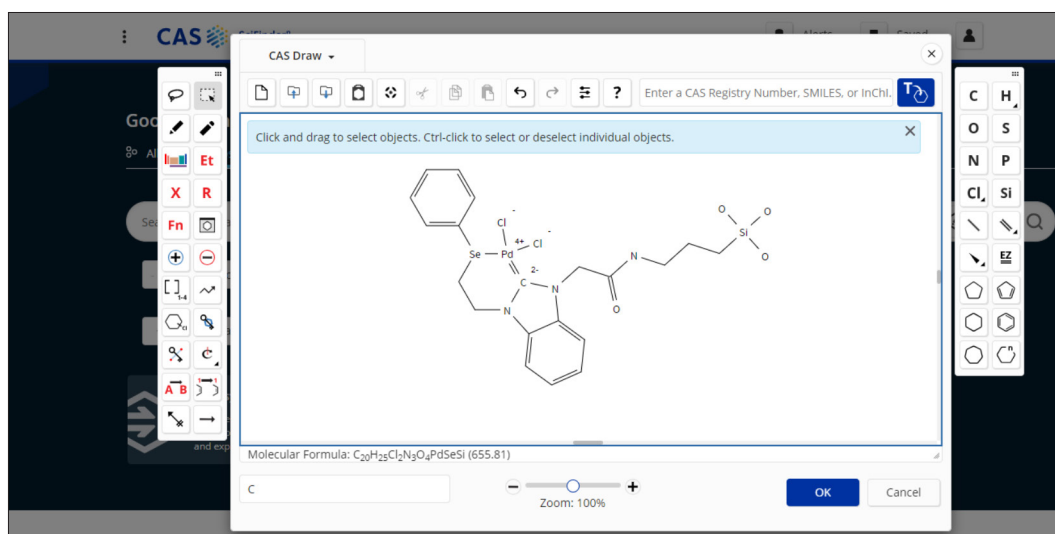
This guide provides you with step-by-step instructions for performing various searches in CAS SciFinder. To begin, visit the login page on cas.org and enter the credentials provided by your organization. Once you are logged in, follow the steps below for your desired search type.

## To search for Substances:

1. Select **Substances** on the search options menu above the main search query bar.
2. Using the main search bar, input substance names, CAS Registry Numbers®, and/or document identifiers (such as patent number or DOI).
3. Press "Enter" or click the magnifying glass to submit your query.



4. If you prefer to search for a substance by chemical structure:
  - a. Click the Draw button on the right side of the main search bar.
  - b. Create your desired structure using CAS Draw.
  - c. Click the OK button to close the CAS Draw window and return to the home page.



- d. Your structure now appears in the search bar. If further modifications to the search are needed, text can be combined with structure searches.
- e. Click the magnifying glass to submit your query.

5. When your search is submitted, relevant results are displayed. You can further refine your results with:
  - a. Structure Match – Use the selection tool on the left to define the desired structure match (for structure queries).
  - b. Filter – Select from a variety of filters found on the left-hand menu.
  - c. Sort – Rearrange your results based on relevance, molecular weight, and more using the drop-down found above them.

6. Clicking a CAS Registry Number opens the substance detail view, which provides information such as experimental properties, predicted properties, experimental spectra, predicted spectra, other names, synonyms, and more.

CAS Registry Number: 152342-19-3

Reference (1) Reactions (3) Supplier (1)

CCCCNC(=O)CN1C=C(C2=CC=CC=C2)N3C=CC=CC=C13

$C_{22}H_{23}N_3O$   
4H-Pyrrolo[1,2-a]benzimidazole-4-acetamide, N-butyl-2-phenyl- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	345.44	-
Boiling Point (Predicted)	467.6±45.0 °C	Press: 760 Torr
Density (Predicted)	1.16±0.1 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr

## To search for Reactions:

1. Select **Reactions** on the search options menu above the main search query bar.
2. Using the main search bar, input substance names, CAS Registry Numbers, CAS Reaction Numbers, and/or document identifiers (such as patent number or DOI).
3. Press "Enter" or click the magnifying glass to submit your query.

Good Afternoon

All Substances **Reactions** References Suppliers

synthesis of 1,5-Diamino-9,10-anthracenedione

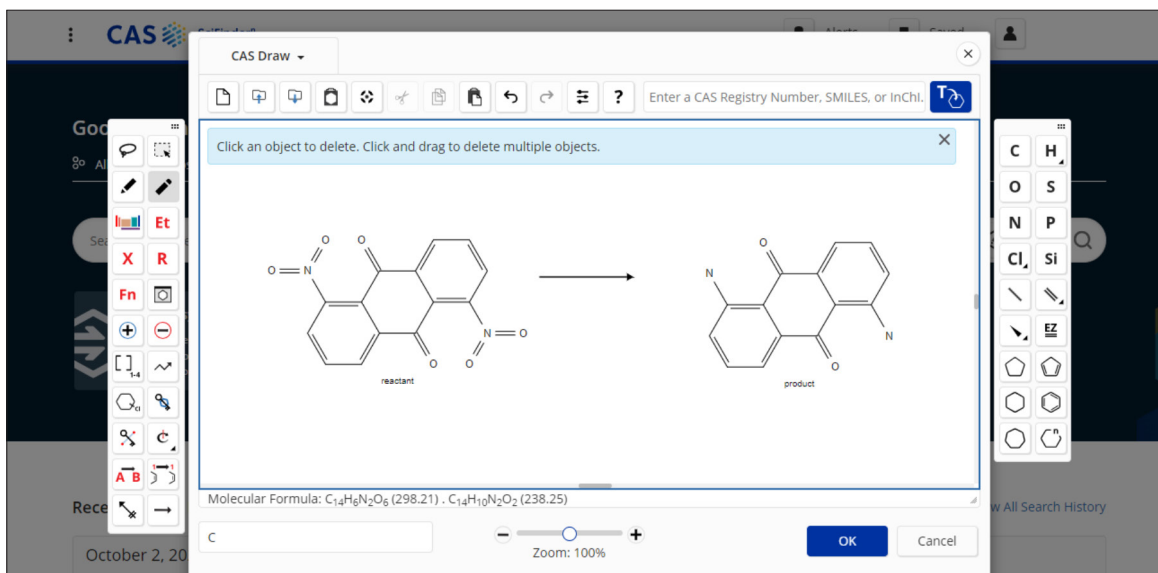
Retrosynthetic Analysis  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search CAS Lexicon  
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Search CAS Sequences  
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.



4. If you prefer to search for reactions using chemical structures:
  - a. Click the Draw button on the right side of the main search bar.
  - b. Create your desired structures to form a reaction using CAS Draw.
  - c. Click the OK button to close the CAS Draw window and return to the home page.



- d. Your reaction now appears in the search bar. If further modifications to the search are needed, text can be combined with reaction searches.
- e. Click the magnifying glass to submit your query.

The screenshot shows the CAS SciFinder home page. At the top, there is a navigation bar with the CAS SciFinder logo and user options like Alerts, Saved, and a profile icon. Below this is a "Good Afternoon" greeting and a navigation menu with "All", "Substances", "Reactions", "References", and "Suppliers". The main search bar contains the text "Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and has an "Edit" button and a magnifying glass icon. Below the search bar are three main sections: "Retrosynthetic Analysis" (Make reaction plans with conditions, yields, catalysts, and experimental procedures.), "Search CAS Lexicon" (Build powerful searches using CAS concepts, chemical classes, and taxonomy.), and "Search CAS Sequences" (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.). A small drawing tool is visible in the bottom right corner of the page.

5. When your search is submitted, relevant results are displayed. You can further refine your results with:
  - a. Structure Match – Use the selection tool on the left to define the desired structure match (for structure queries).
  - b. Filter – Select from a variety of filters found on the left-hand menu.
  - c. Sort – Rearrange your results based on relevance, molecular weight, and more using the drop-down found above them.

**CAS SciFinder** Reactions search for drawn structure

References [icon] [icon] [icon] Save and Alert

Structure Match: **As Drawn (6)**, Substructure (77), Similarity (237K)

Filter Behavior: Filter by, Exclude

Search Within Results: Yield (90-100% (2), No Yield Available (4)), Number of Steps (1 (6))

6 Results | Group: By Scheme | Sort: Relevance | View: Expanded

Scheme 1 (1 Reaction) | Steps: 1 | Yield: 94%

Chemical reaction scheme showing the reduction of a nitroanthraquinone derivative to an aminoanthraquinone derivative.

Suppliers (36) | Suppliers (75)

31-522-CAS-7415743 | Steps: 1 | Yield: 94%

1.1 Reagents: [Sodium borohydride](#)

Synthesis of aminoanthraquinones by sodium borohydride reductions of nitroanthraquinones

By: Morley, John O. Synthesis (1976), (8), 528-30

Full Text [icon]

Collapse Scheme [icon]

6. Clicking a CAS Reaction Number opens the reaction detail view, which provides information such as the reagents, solvents, catalysts, and reaction conditions; source reference bibliography; reaction notes; and reaction transformation.

**CAS SciFinder** Reactions Enter a query...

Return to Results | Prev (Scheme 2, Reaction 1 of 1) Next

**CAS Reaction Number: 31-522-CAS-15114748**

Get Similar Reactions [icon] [icon] [icon] Save

Chemical reaction scheme showing the reduction of a nitroanthraquinone derivative to an aminoanthraquinone derivative.

Suppliers (42) | Suppliers (36) | Suppliers (75) | Suppliers (13)

Reaction Overview: Steps: 1 | Yield: -

PATENT: Method for dye preparation using waste slag formed from production of 1-aminoanthraquinone. By: Wang, Qingjun; et al

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Disodium sulfide</a>	-	<a href="#">Water</a>	rt → 95 °C; 1 h, 95 °C

Alternative Steps (0)

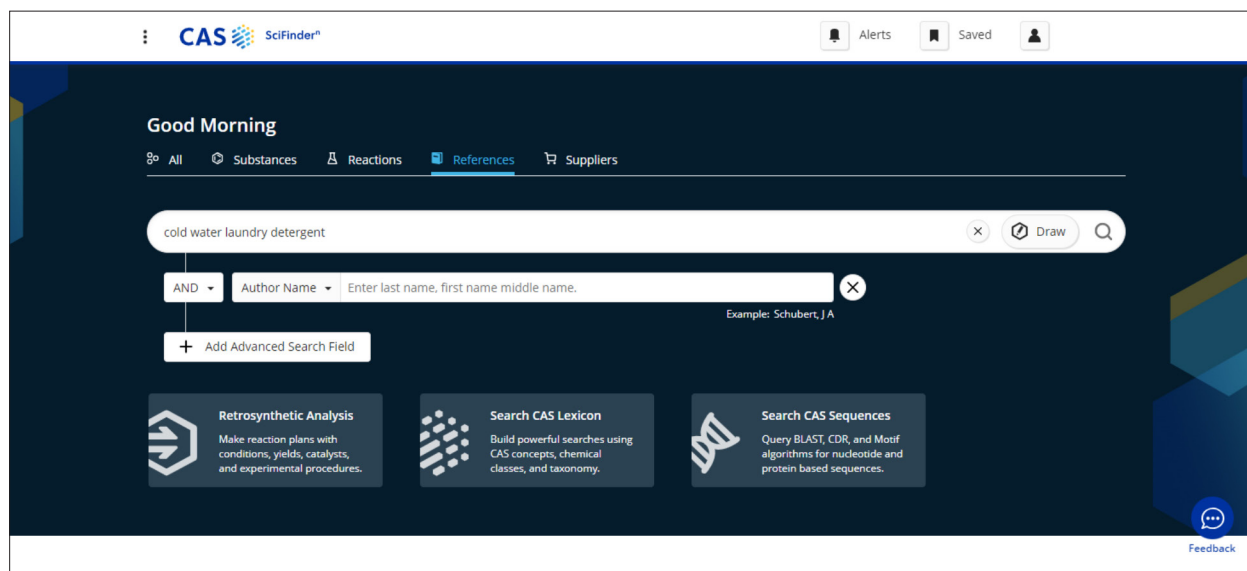
Transformations: 1. Reduction of Nitro Compounds to Amines

Reaction Notes: Industrial

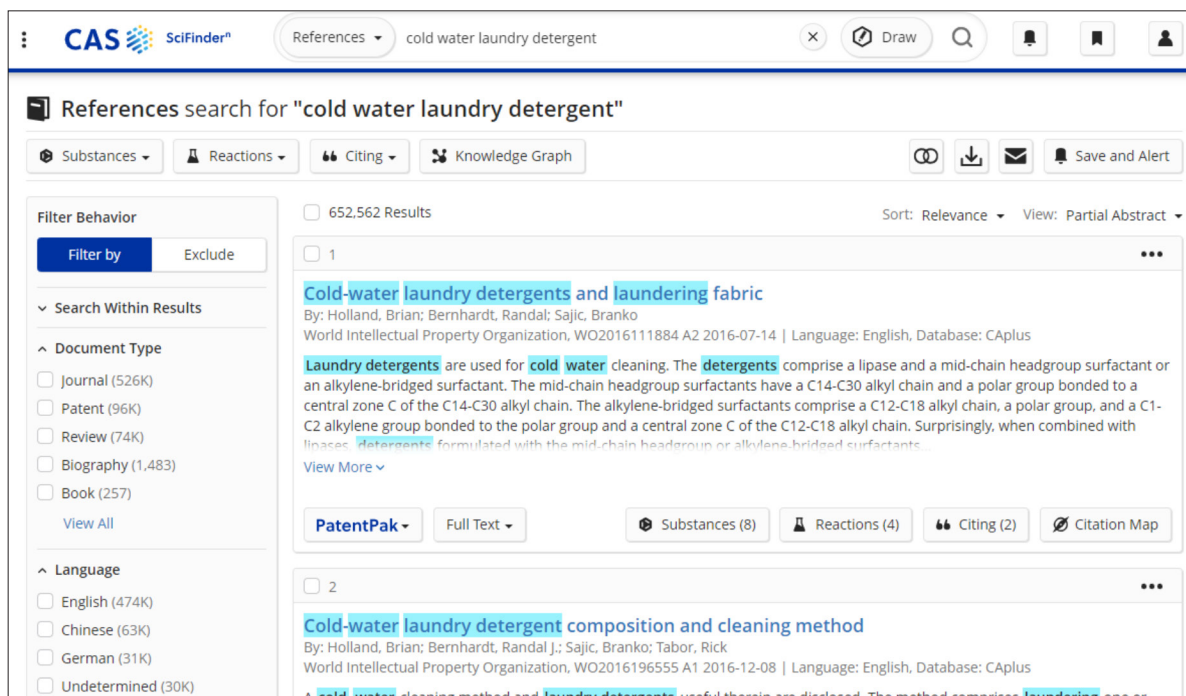


## To search for References:

1. Select **References** on the search options menu above the main search query bar.
2. Using the main search bar, input research topics, keywords, concepts, substance names, CAS Registry Numbers, and/or document identifiers (such as Accession Number, PubMed ID, DOI, or patent number).
3. Press "Enter" or click the magnifying glass to submit your query.



4. When your search is submitted, relevant results are displayed. You can further refine your results with:
  - a. Filter – Select from a variety of filters, such as Document Type or Author, found on the left-hand menu. Multiple filters can be selected to manage and refine results.
  - b. Sort – Rearrange your results based on relevance, publication date, and more using the Sort drop-down found above them.



5. Clicking a reference title opens the reference detail view, which provides bibliographic information, full-text options, patent information, similar references, indexed concepts, indexed substances, indexed formulations, indexed analytical protocols, and cited documents.

The screenshot shows the CAS SciFinder interface. The browser address bar displays 'References - cold water laundry detergent'. The article title is 'Probing Interfacial Behavior and Antifouling Activity of Adsorbed Copolymers at Solid/Liquid Interfaces'. The authors listed are Gao, Jinpeng; Khan, Rubel Md; Wu, Yuchen; Hawker, Dustin D.; Gutowski, Keith E.; Konradi, Rupert; Mayr, Lukas; Hankett, Jeanne M.; Kellermeyer, Matthias; Chen, Zhan. The journal is Langmuir, Volume 39, Issue 13, Pages 4557-4570. The DOI is 10.1021/acs.langmuir.2c03056. The article abstract discusses the antifouling properties of copolymers containing PEG units on PET surfaces, mentioning techniques like SFG and QCM-D. An illustration at the bottom shows a schematic of a copolymer chain on a surface with labels for IR, Vis, and SFG.

For additional training, visit the Training page on [cas.org](https://cas.org) or view the Help and Support section accessible from within CAS SciFinder.

For questions, reach out to the CAS Customer Center at [help@cas.org](mailto:help@cas.org).

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