SCIFINDER 功能介绍及使用技巧

黄培益

2022年3月11日

SCIFINDER.CAS.ORG

CAS SciFinder^n is now available!

CAS SciFinder^n helps you do everything you use classic SciFinder for today, plus it provides new tools for retrosynthesis planning, biosequence searching, result set visualizations, and more. Learn about the differences.

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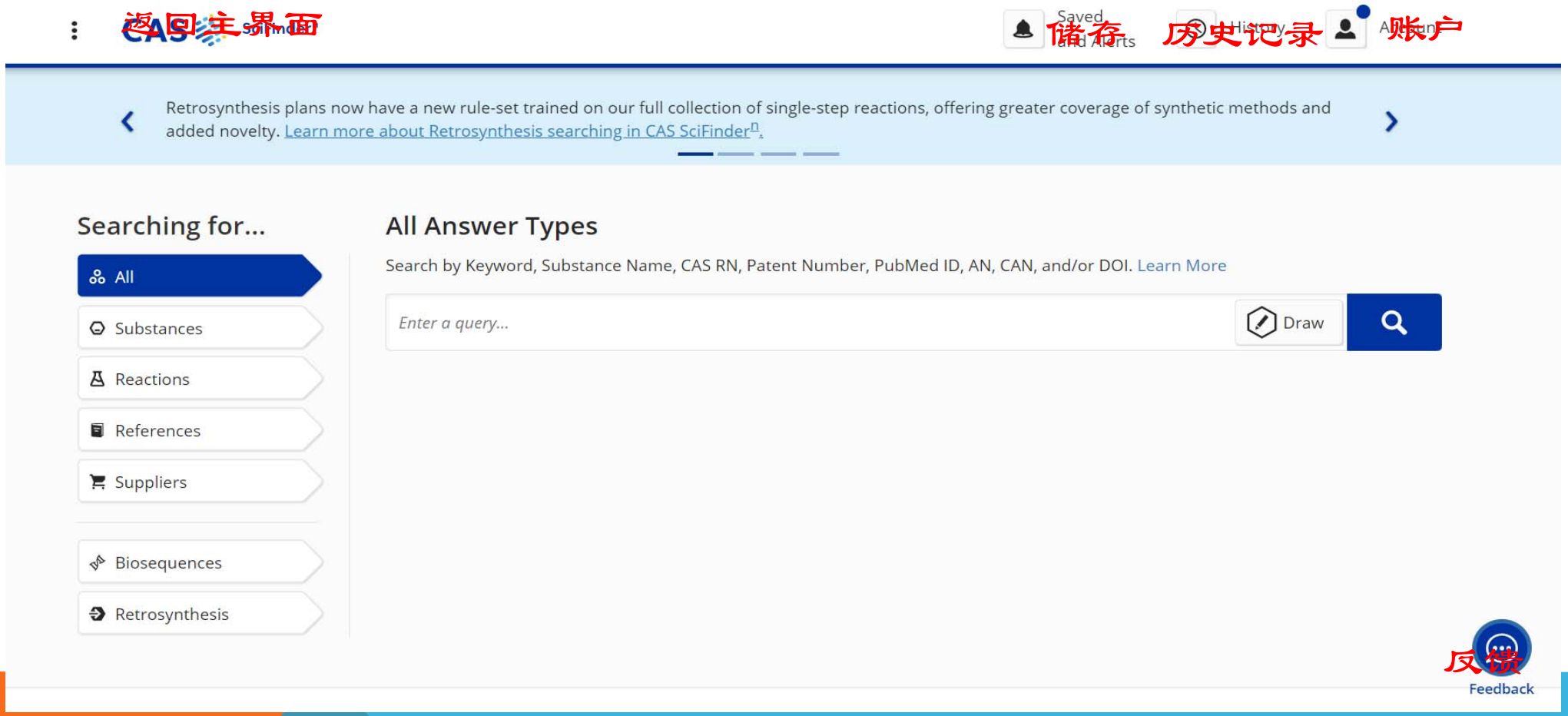
MAIN MENU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Retrosynthesis plans now have a new rule-set trained on our full collection of single-step reactions, offering greater coverage of synthetic methods and added novelty. Learn more about Retrosynthesis searching in CAS SciFinder.
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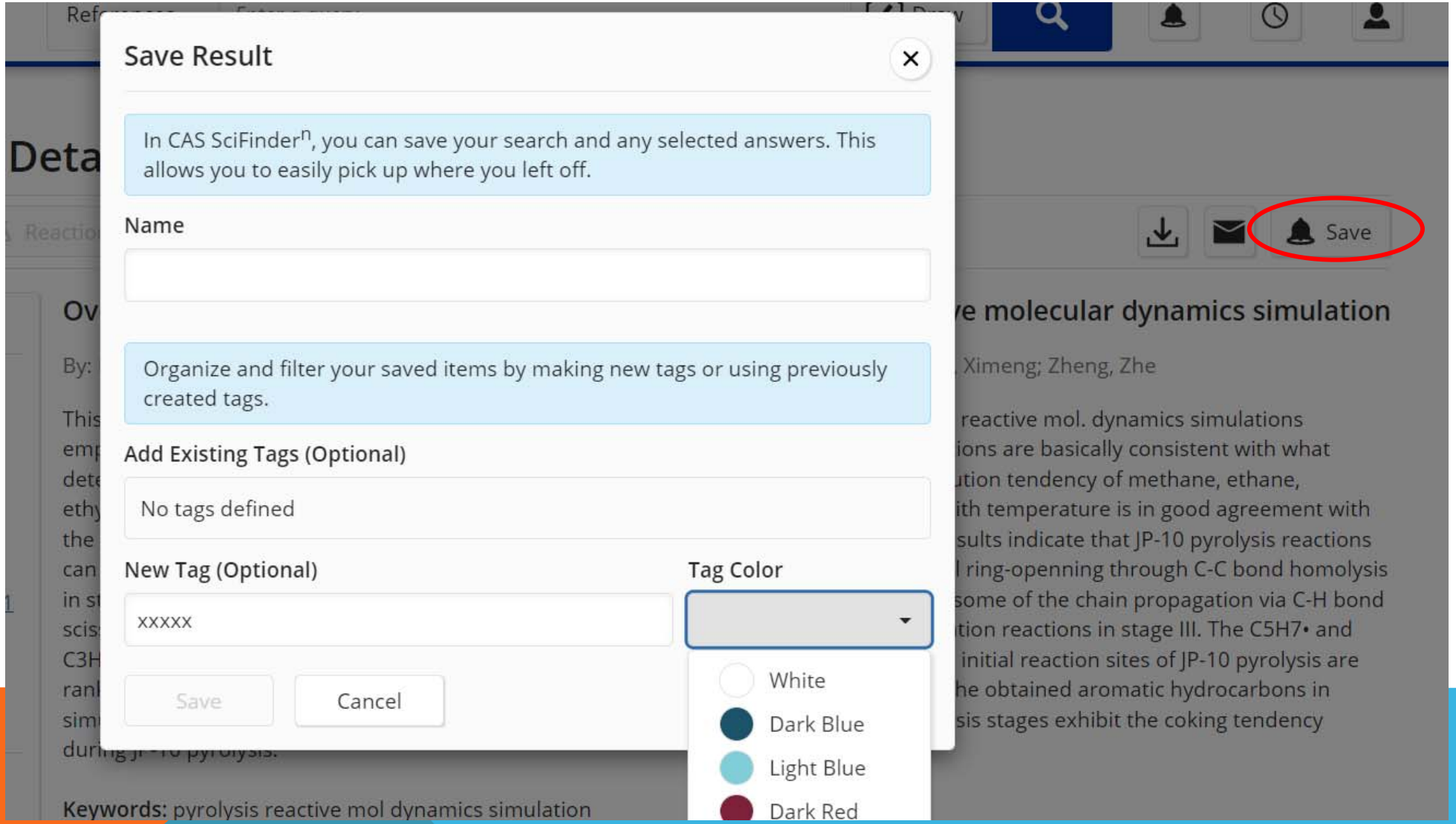

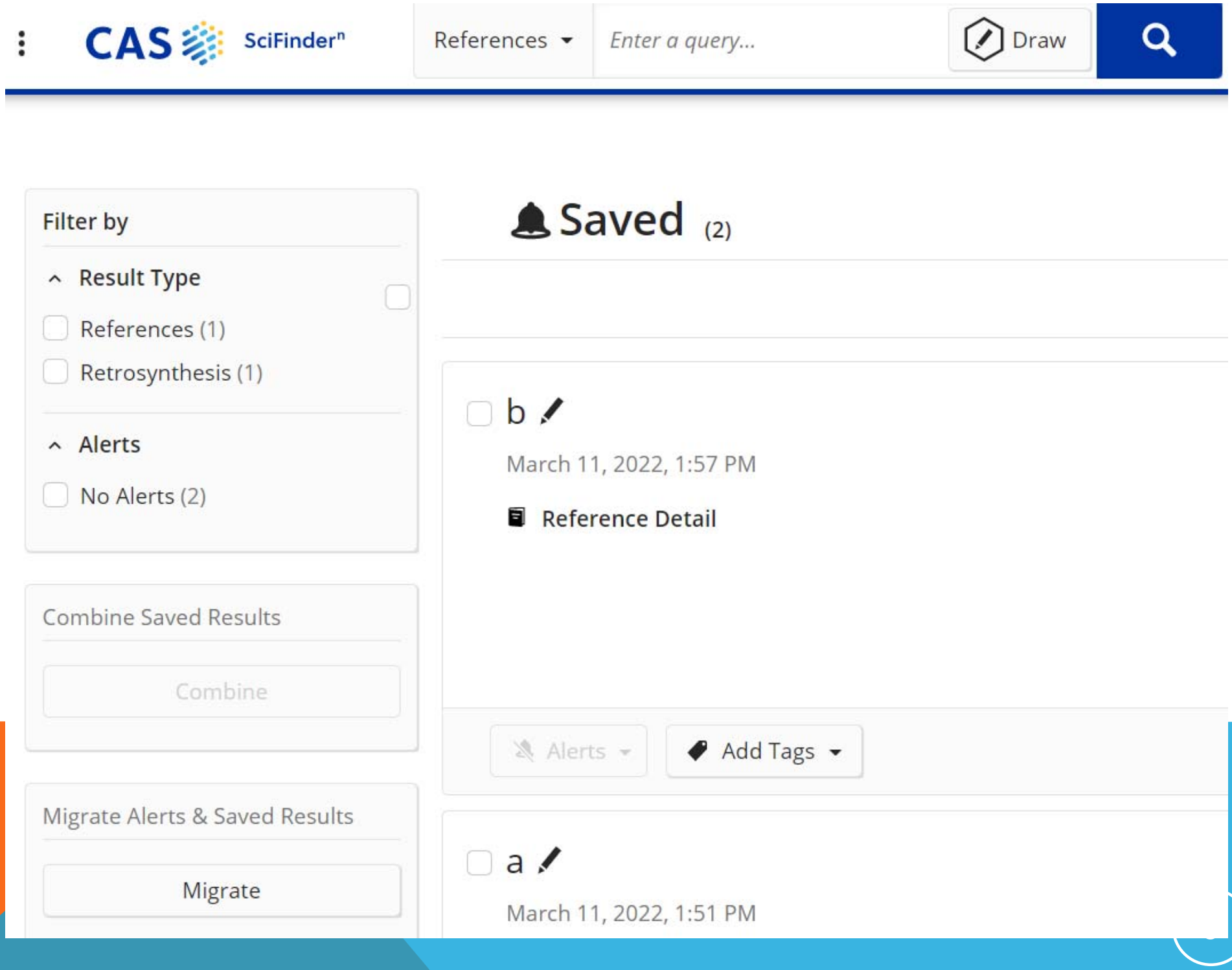
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References
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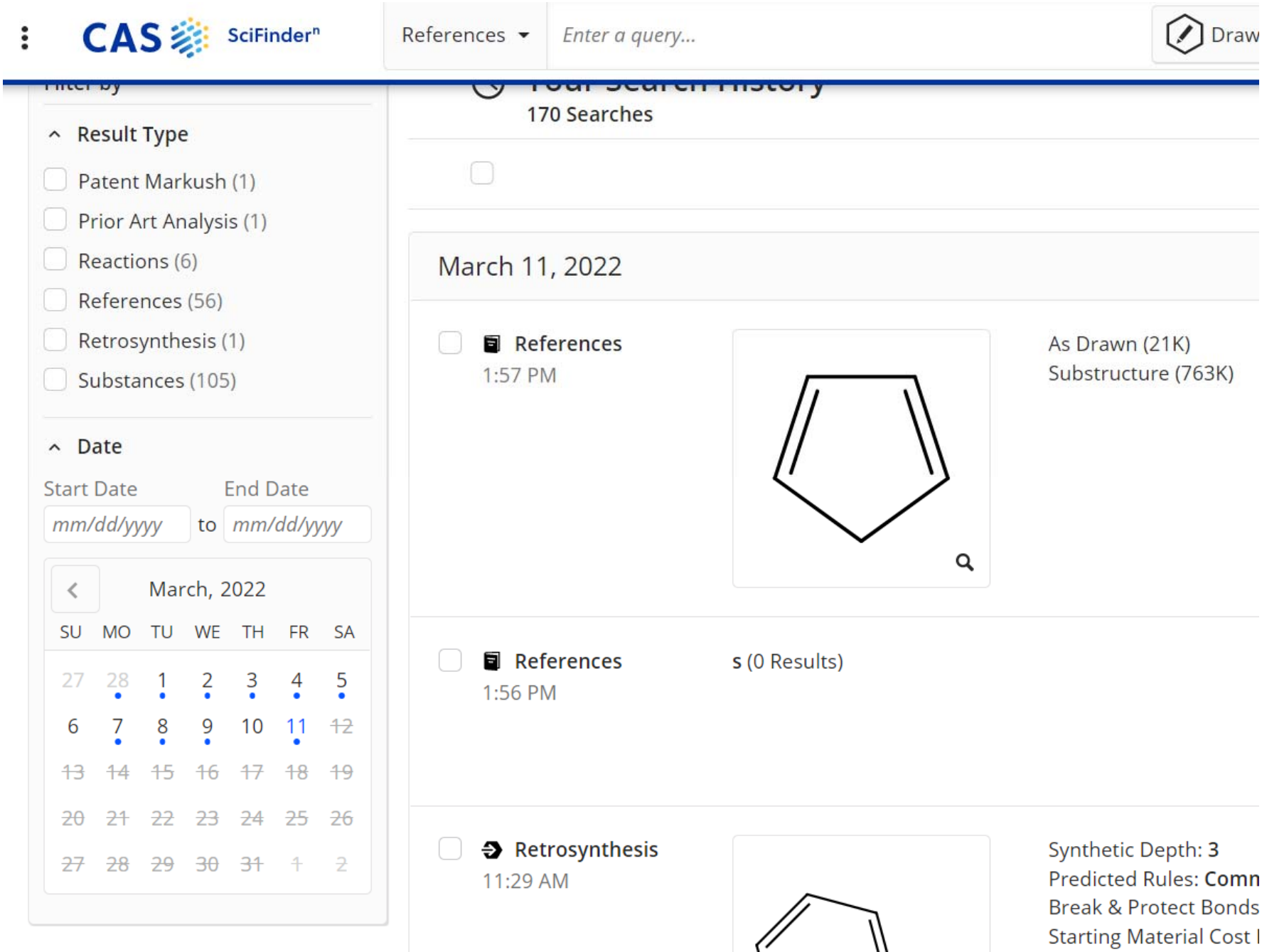
Filter by
Result Type
References (1)
Retrosynthesis (1)
Alerts
No Alerts (2)
Combine Saved Results
Combine
Migrate Alerts & Saved Results
Migrate
Saved (2)
b
March 11, 2022, 1:57 PM
Reference Detail
Alerts
Add Tags
a
March 11, 2022, 1:51 PM

History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Patent Markush (1)
Prior Art Analysis (1)
Reactions (6)
References (56)
Retrosynthesis (1)
Substances (105)
Date
Start Date
End Date
mm/dd/yyyy
to
mm/dd/yyyy
March, 2022
SU MO TU WE TH FR SA
170 Searches
March 11, 2022
References
1:57 PM
As Drawn (21K)
Substructure (763K)
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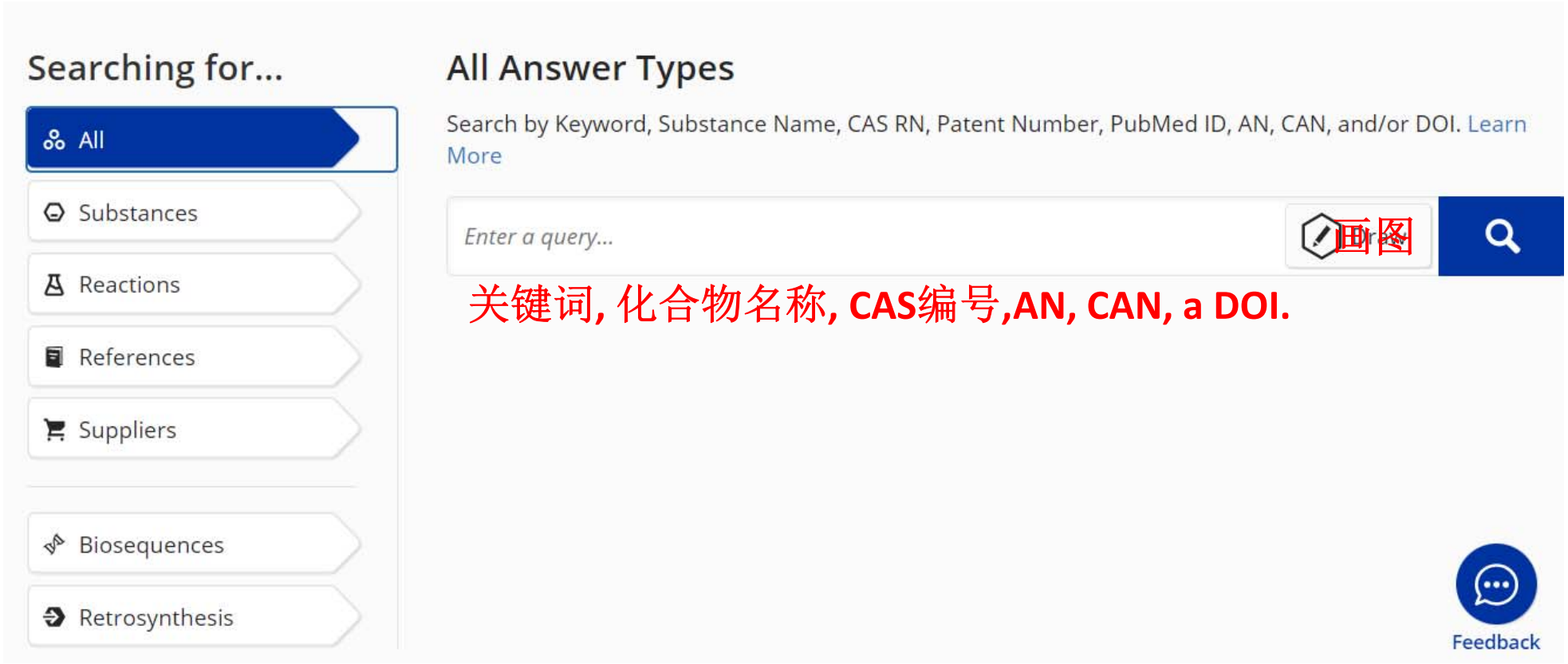
1:56 PM
s (0 Results)
Retrosynthesis
11:29 AM
Synthetic Depth: 3
Predicted Rules: Comn
Break & Protect Bonds
Starting Material Cost

All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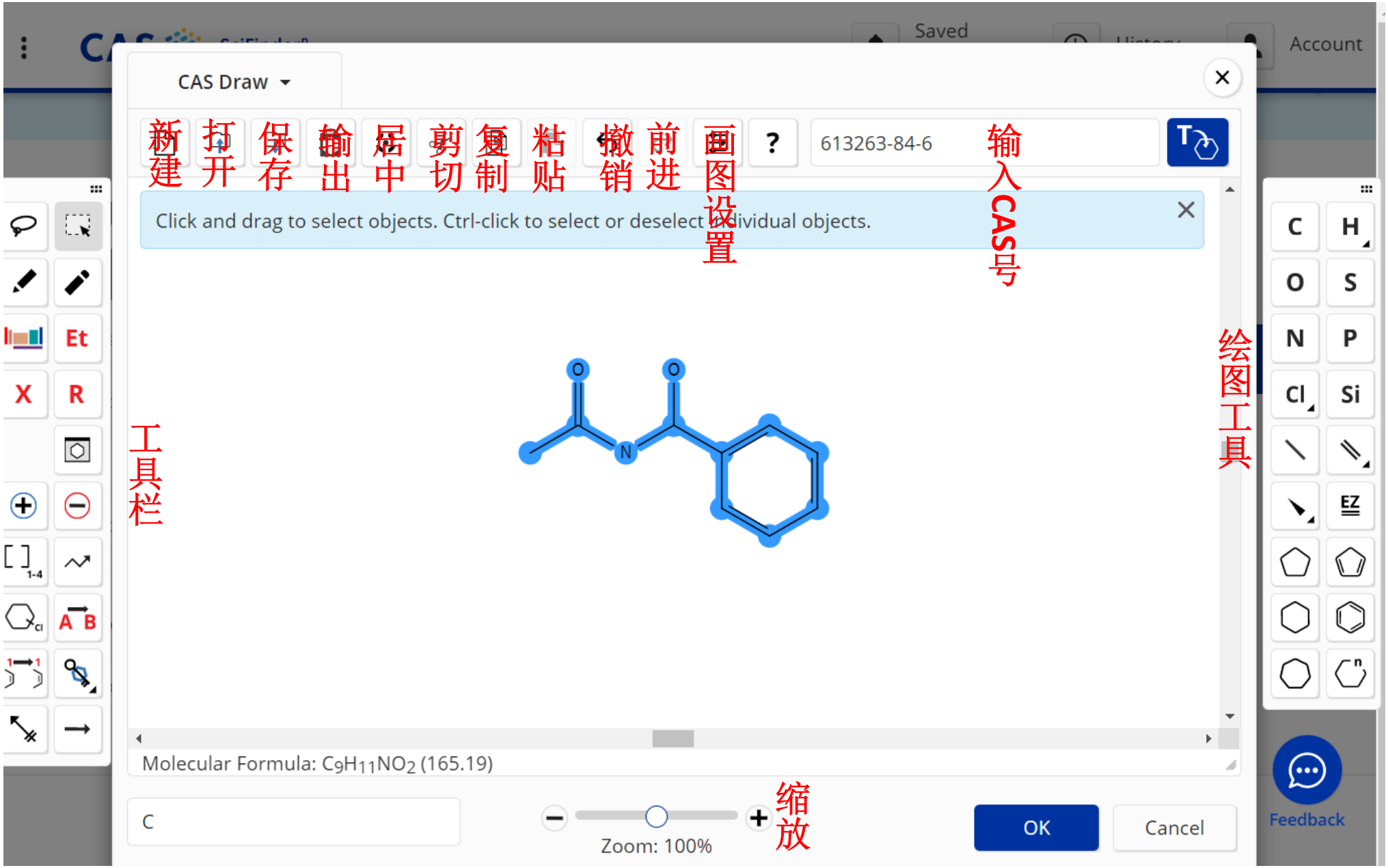
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剪切
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前进
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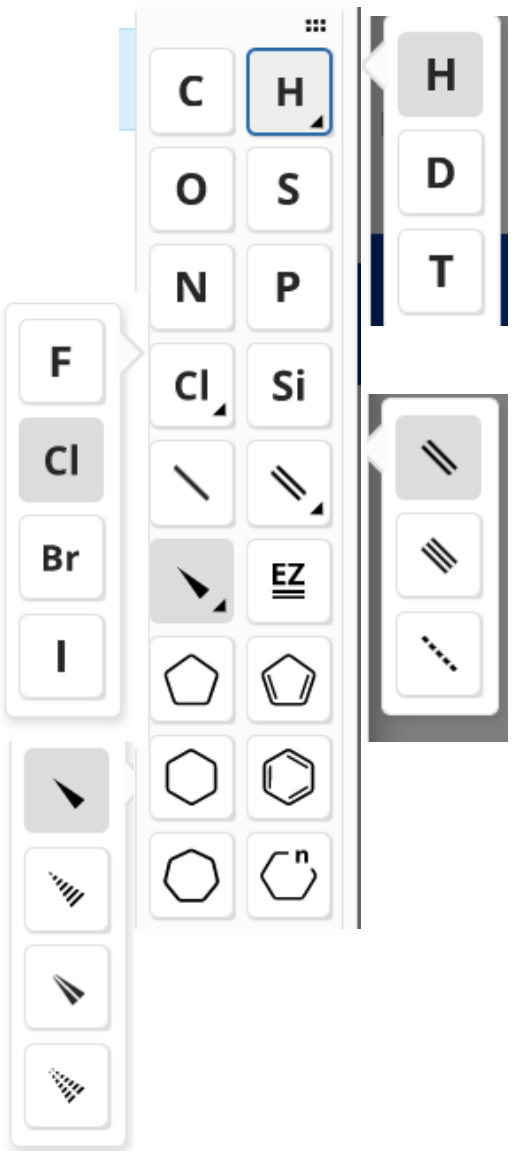
?
613263-84-6
输入CAS号
Click and drag to select objects. Ctrl-click to select or deselect individual objects.
工具栏
绘图工具
Molecular Formula: C9H11NO2 (165.19)
C
Zoom: 100%
缩放
OK
Cancel
Feedback
Saved
Account

draw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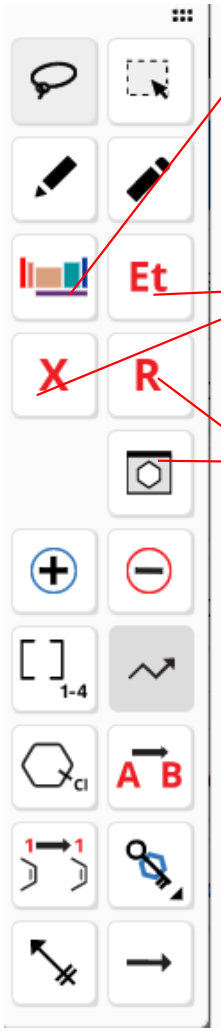
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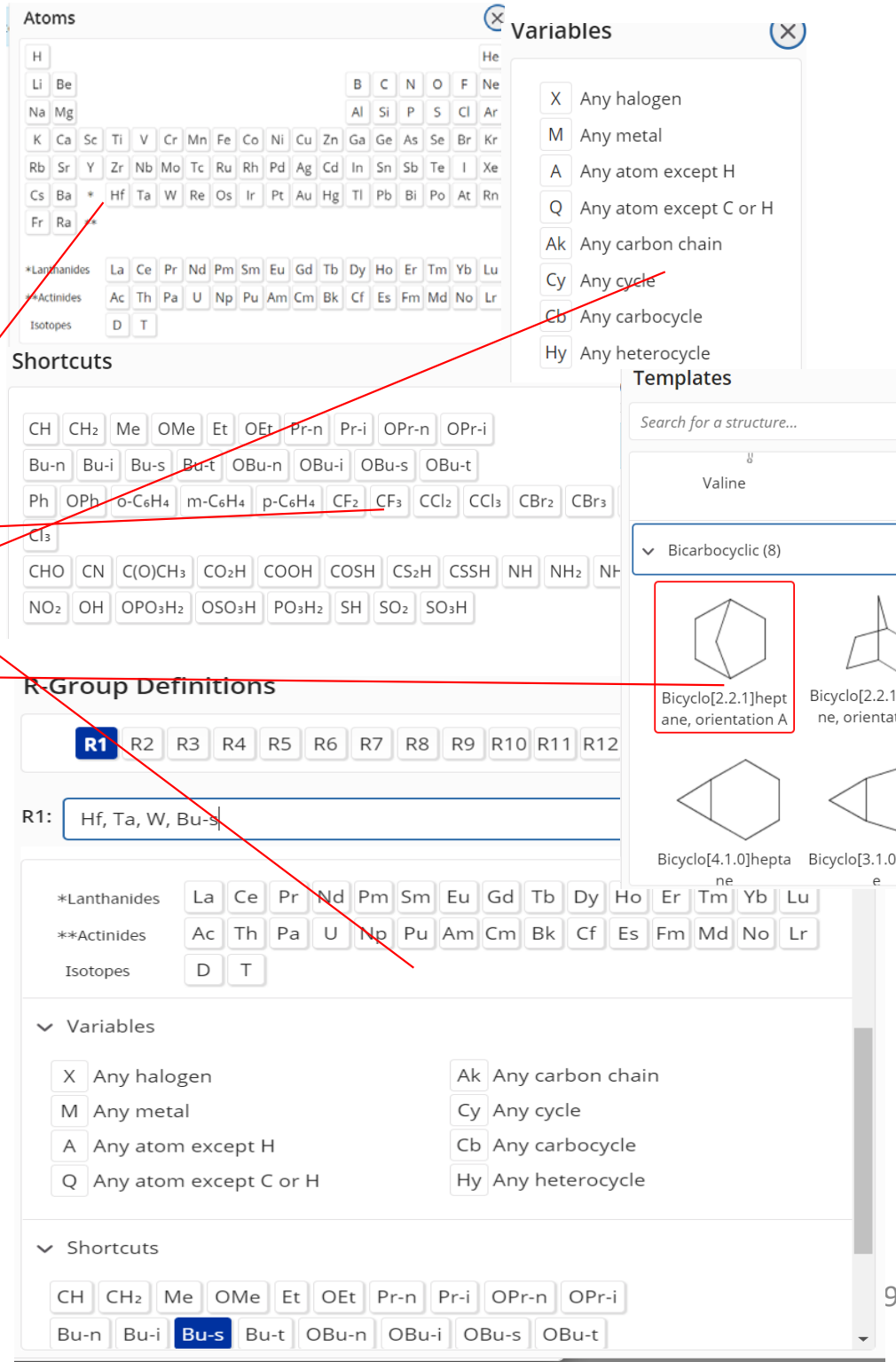
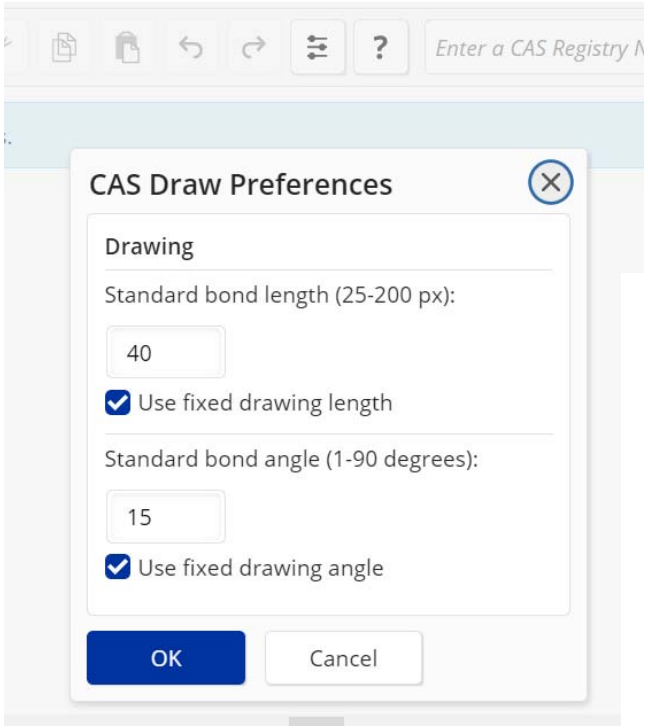
1-4
A B


Atoms
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Shortcuts
CH CH₂ Me OMe Et OEt Pr-n Pr-i OPr-n OPr-i
Bu-n Bu-i Bu-s Bu-t OBu-n OBu-i OBu-s OBu-t
Ph OPh o-C6H4 m-C6H4 p-C6H4 CF2 CF3 CCl2 CCl3 CBr2 CBr3
CHO CN C(O)CH3 CO2H COOH COSH CS2H CSSH NH NH2
NO2 OH OPO3H2 OSO3H PO3H2 SH SO2 SO3H
Templates
Search for a structure...
Valine
Bicarbocyclic (8)
Bicyclo[2.2.1]heptane, orientation A
Bicyclo[2.2.1]heptane, orientation B
Bicyclo[4.1.0]heptane
Bicyclo[3.1.0]hexane
R-Group Definitions
R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12
R1: Hf, Ta, W, Bu-s
*Lanthanides La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
**Actinides Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr
Isotopes D T
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Shortcuts
CH CH₂ Me OMe Et OEt Pr-n Pr-i OPr-n OPr-i
Bu-n Bu-i Bu-s Bu-t OBu-n OBu-i OBu-s OBu-t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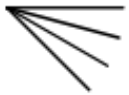
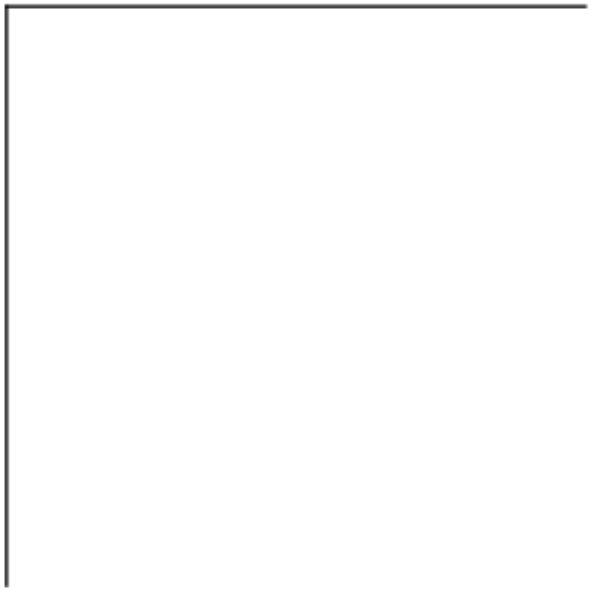
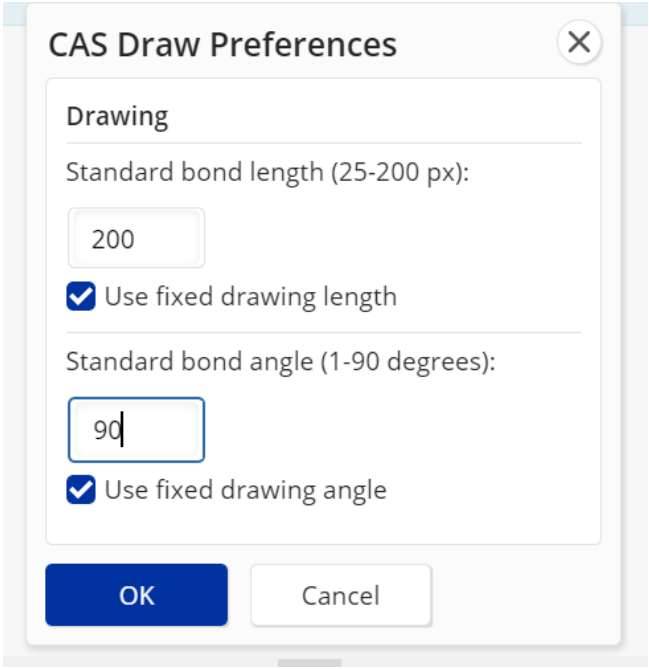
40
Use fixed drawing length
Standard bond angle (1-90 degrees):
15
Use fixed drawing angle
OK
Cancel






CAS Draw Preferences
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Standard bond angle (1-90 degrees):
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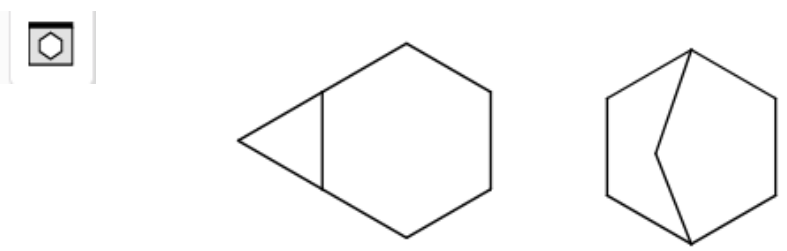
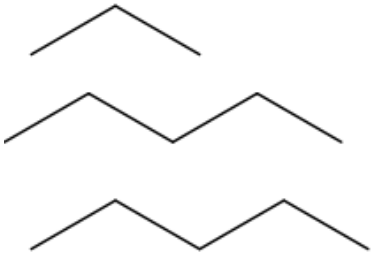
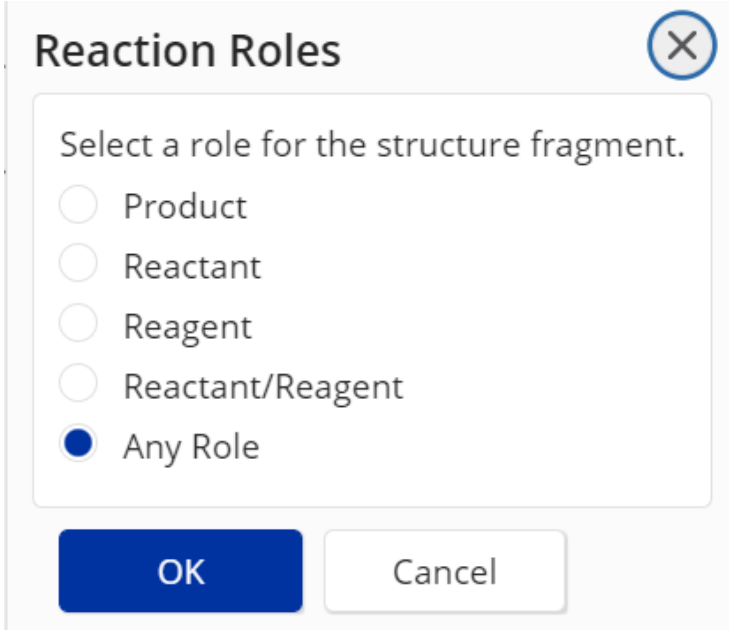
OK
Cancel



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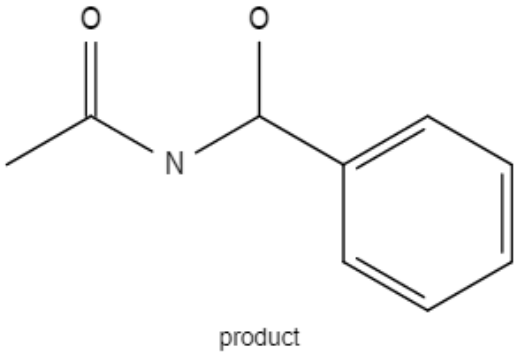
Select a role for the structure fragment.
Product
Reactant
Reagent
Reactant/Reagent
Any Role
OK
Cancel


O
O
N
product

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Show only

Substances (1)

Reactions (2)

References (4)

Suppliers (2)

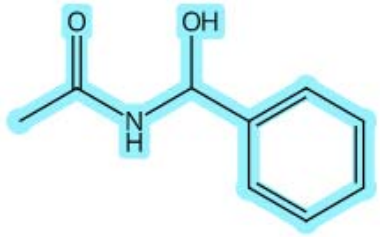
All Answer Types

Top two answers by relevance from each answer type.

Substances (1)

1

613263-84-6



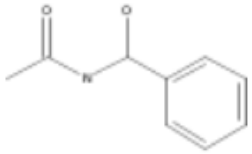
$C_9H_{11}NO_2$

N-(Hydroxyphenylmethyl)acetamide

4 References | 2 Reactions | 2 Suppliers

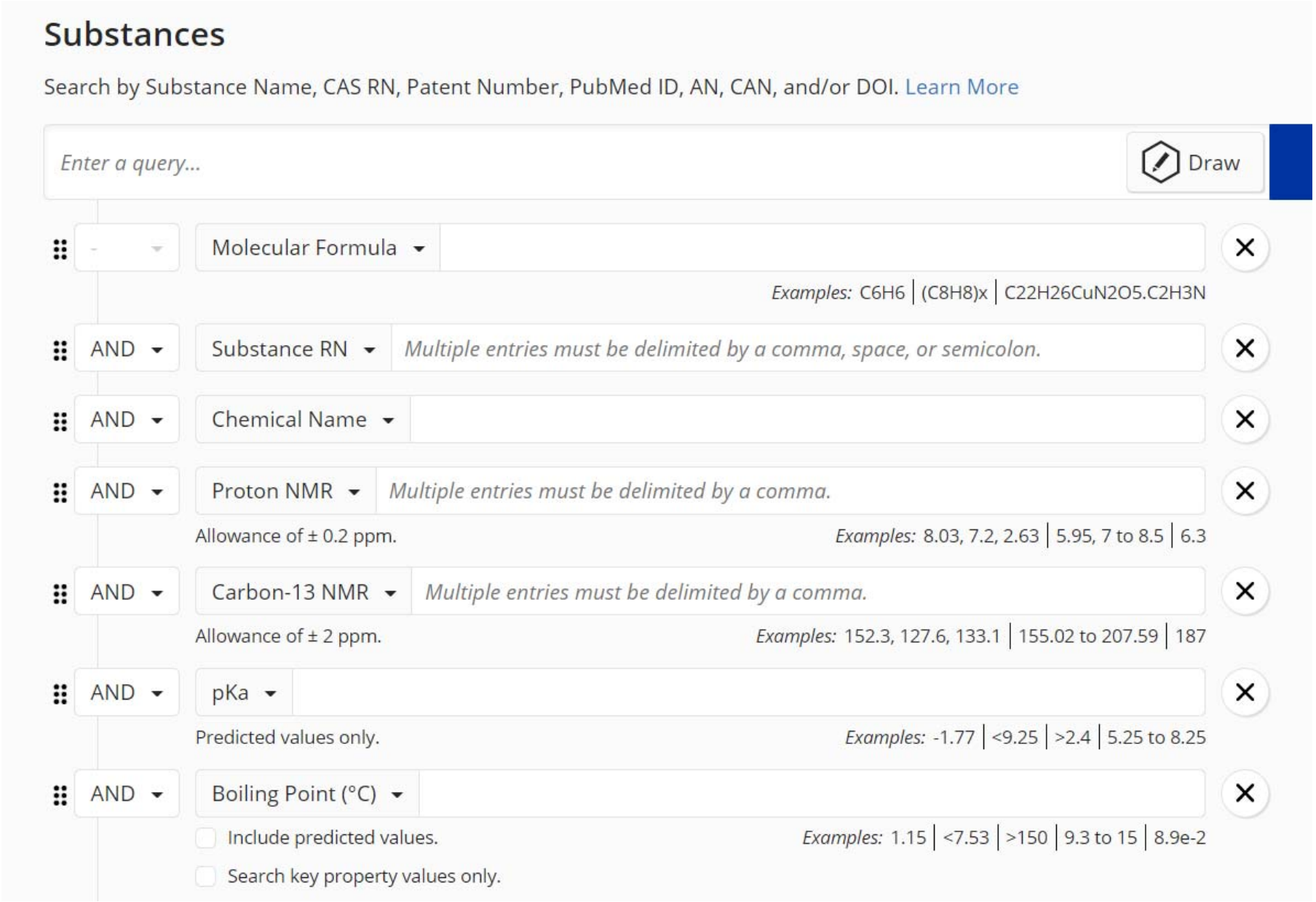
View All Substances

Edit



Edit Drawing Remove

Substances


Substances
Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More
Enter a query...
Draw
Molecular Formula
Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N
AND
Substance RN
Multiple entries must be delimited by a comma, space, or semicolon.
AND
Chemical Name
AND
Proton NMR
Multiple entries must be delimited by a comma.
Allowance of ± 0.2 ppm.
Examples: 8.03, 7.2, 2.63 | 5.95, 7 to 8.5 | 6.3
AND
Carbon-13 NMR
Multiple entries must be delimited by a comma.
Allowance of ± 2 ppm.
Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187
AND
pKa
Predicted values only.
Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25
AND
Boiling Point (°C)
Include predicted values.
Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2
Search key property values only.

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID

Enter a query...

- Molecular Formula: C9H11NO2
- AND — Boiling Point (°C): 390
  - [x] Include predicted values.
  - [ ] Search key property values only.
- AND — Melting Point (°C): 159

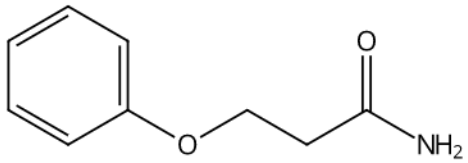
Substances (3)

Sort: Relevance View: Partial

References | Reactions | Suppliers | Save And Alerts

1

22409-37-6



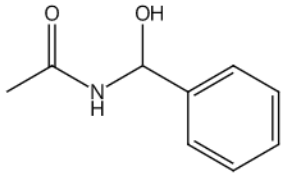
$C_9H_{11}NO_2$

3-Phenoxypropanamide

23 References | 13 Reactions | 14 Suppliers

2

613263-84-6



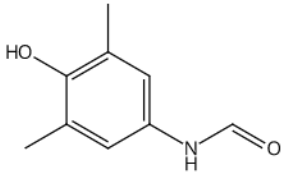
$C_9H_{11}NO_2$

N-(Hydroxyphenylmethyl)acetamide

4 References | 2 Reactions | 2 Suppliers

3

109942-08-7

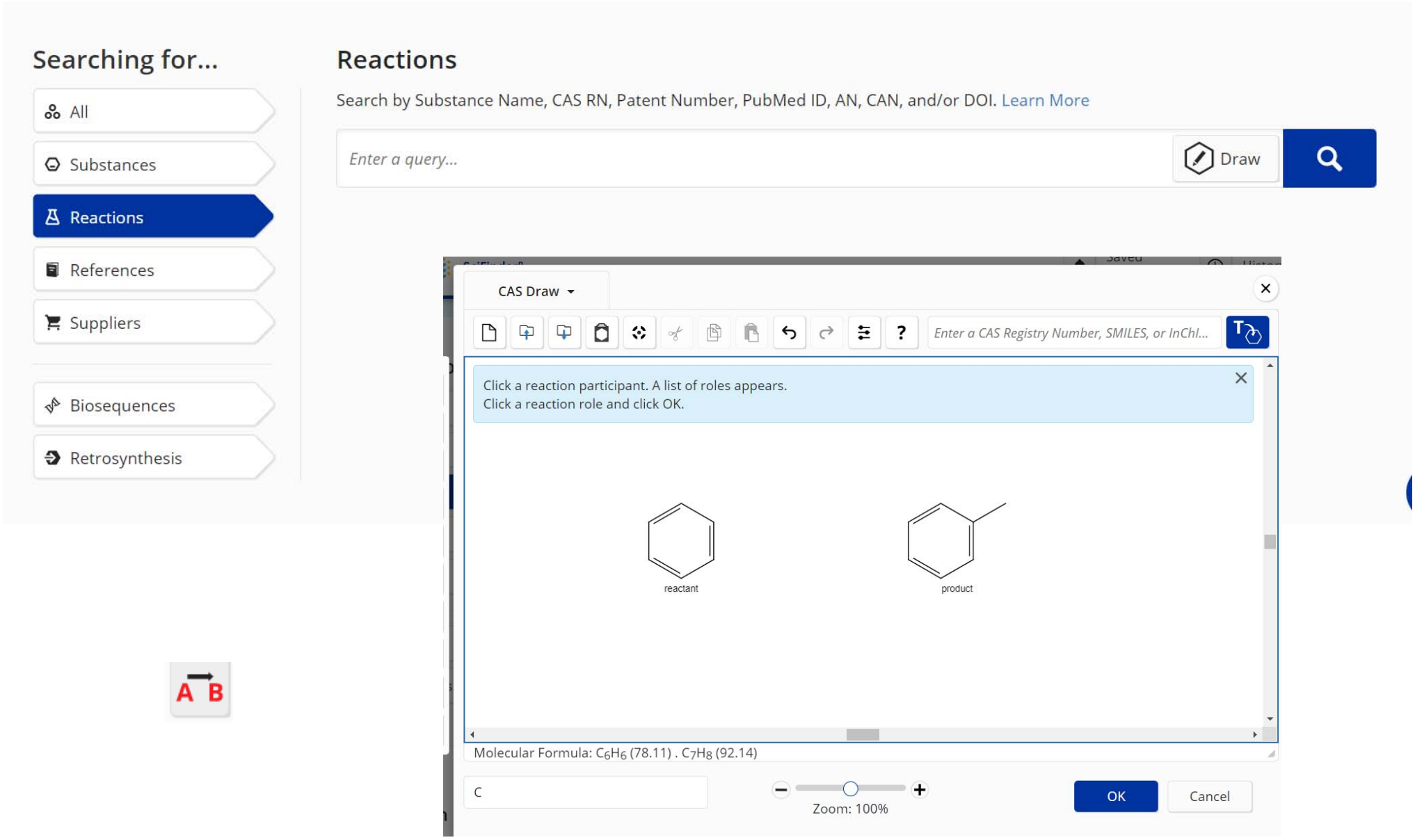


$C_9H_{11}NO_2$

N-(4-Hydroxy-3,5-dimethylphenyl) formamide

1 Reference | 0 Reactions | 4 Suppliers

Reactions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Enter a query...
Draw
CAS Draw
Enter a CAS Registry Number, SMILES, or InChI...
Click a reaction participant. A list of roles appears.
Click a reaction role and click OK.
reactant
product
Molecular Formula: C6H6 (78.11) . C7H8 (92.14)
C
Zoom: 100%
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Structure Match

As Drawn (437)

Substructure (70.7M)

Similarity (14K)

Filter Behavior

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Yield

- 90-100% (14)
- 80-89% (8)
- 70-79% (4)
- 50-69% (16)
- 30-49% (14)

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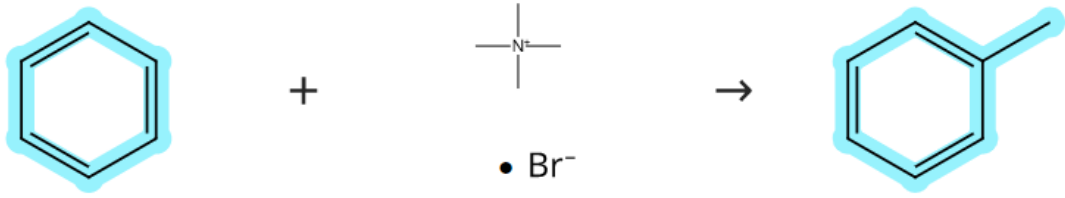
Reactions (437)

Group: By Scheme View: Expanded

References Save And Alerts

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%



Suppliers (167) Suppliers (65) Suppliers (248)

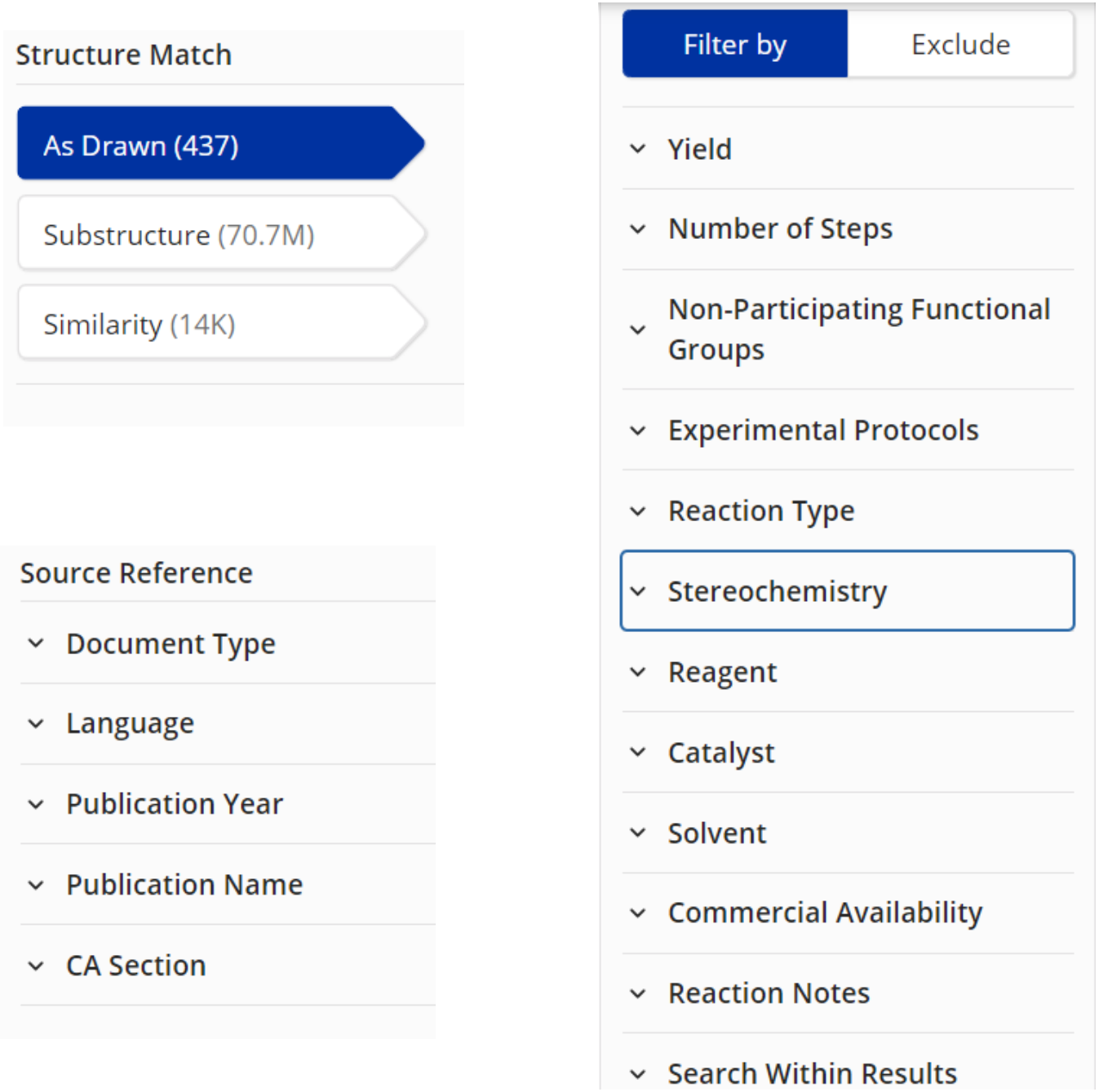
Reaction Summary Steps: 1 Yield: 100%

1.1 Catalysts: Carbon nitride (C_3N_4)
Solvents: Benzene; 24 h, 150 °C

Metal-free catalysis of sustainable Friedel-Crafts reactions: direct activation of benzene by carbon nitrides to avoid the use of chlorides and halogenated compounds

Feedback

By: Goettmann, Frederic; et al
Chemical Communications (Cambridge,


Structure Match
As Drawn (437)
Substructure (70.7M)
Similarity (14K)
Source Reference
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Publication Year
Publication Name
CA Section
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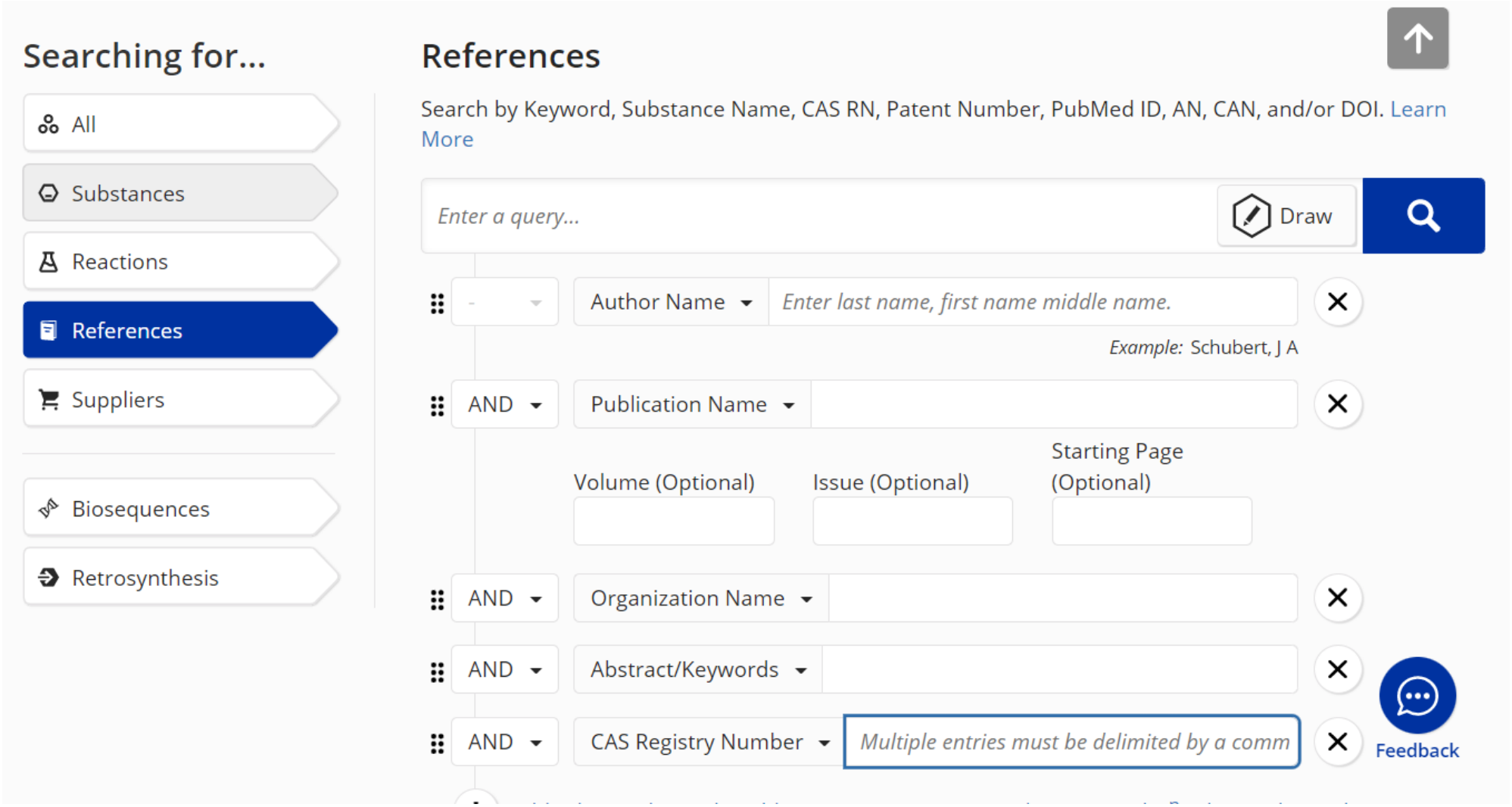
Yield
Number of Steps
Non-Participating Functional Groups
Experimental Protocols
Reaction Type
Stereochemistry
Reagent
Catalyst
Solvent
Commercial Availability
Reaction Notes
Search Within Results

References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Enter last name, first name middle name.
Example: Schubert, J A
AND
Publication Name
Volume (Optional)
Issue (Optional)
Starting Page (Optional)
AND
Organization Name
AND
Abstract/Keywords
AND
CAS Registry Number
Multiple entries must be delimited by a comm
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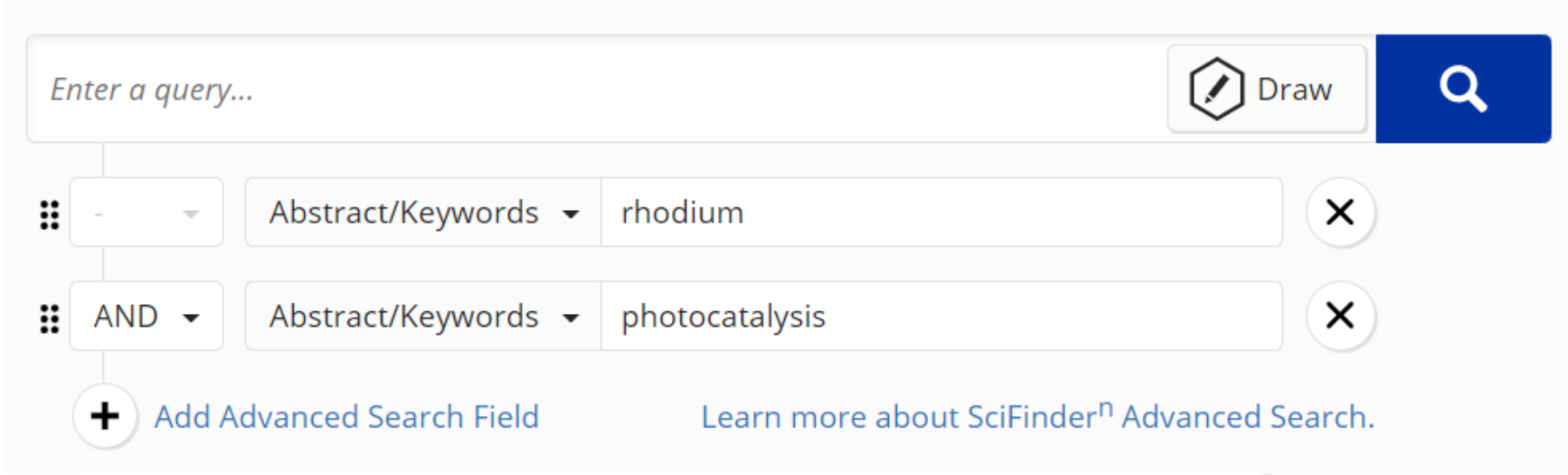
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rhodium
AND
Abstract/Keywords
photocatalysis
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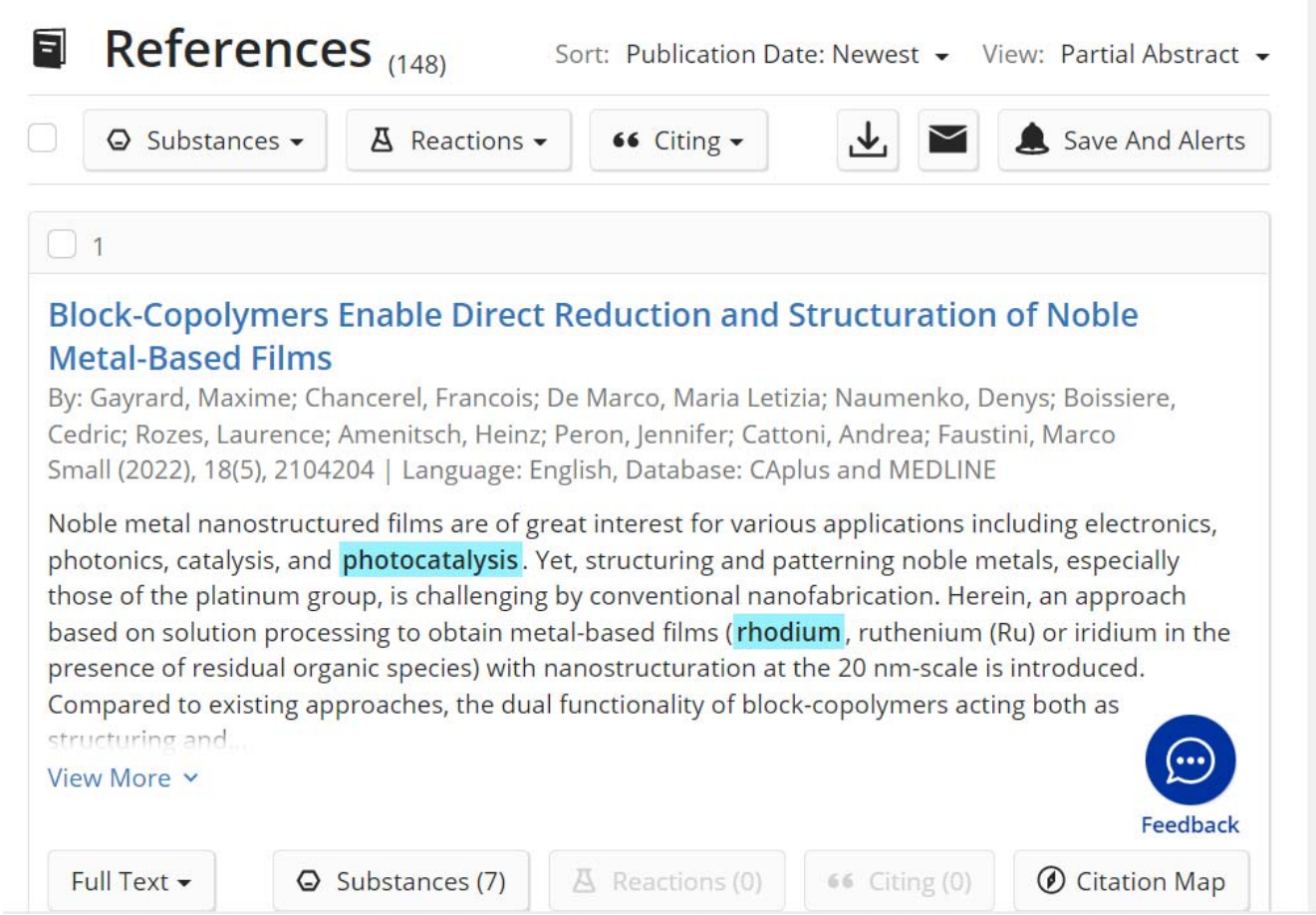
References (148)
Sort: Publication Date: Newest
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1
Block-Copolymers Enable Direct Reduction and Structuration of Noble Metal-Based Films
By: Gayrard, Maxime; Chancerel, Francois; De Marco, Maria Letizia; Naumenko, Denys; Boissiere, Cedric; Rozes, Laurence; Amenitsch, Heinz; Peron, Jennifer; Cattoni, Andrea; Faustini, Marco
Small (2022), 18(5), 2104204 | Language: English, Database: CAplus and MEDLINE
Noble metal nanostructured films are of great interest for various applications including electronics, photonics, catalysis, and photocatalysis. Yet, structuring and patterning noble metals, especially those of the platinum group, is challenging by conventional nanofabrication. Herein, an approach based on solution processing to obtain metal-based films (rhodium, ruthenium (Ru) or iridium in the presence of residual organic species) with nanostructuration at the 20 nm-scale is introduced. Compared to existing approaches, the dual functionality of block-copolymers acting both as structuring and...
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Reactions (0)
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Document Type

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- Patent (13)
- Review (5)
- Conference (8)
- Preprint (1)
- Report (1)

Language

- English (136)
- Chinese (10)
- Japanese (2)

Publication Year

Author

- Brewer, Karen J. (8)
- Kudo, Akihiko (8)
- Arachchige, Shamindri M. (7)
- Saito, Yasukazu (7)
- Domen, Kazunari (6)

View All

Organization

- Tokyo University of Science (8)
- Univ. Tokyo (7)
- Duke University (5)
- Chinese Academy of Sciences (4)
- The University of Tokyo (4)

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Publication Name

Concept

- Photocatalysis (54)
- Photolysis catalysts (50)
- Photocatalysts (39)
- Photolysis (31)
- Band gap (16)

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THE YANG
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