Vinit Kunte
Dr. Jyoti Singh
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SciFinder n
A CAS SOLUTION

Agenda

- Introduction of CAS
- What is SciFinder^{n}?
- Content and Coverage in SciFinder^{n}
- A few online Case studies – General interest
  - Substance searching
  - Reference searching and PatentPak
  - Reaction searching and MethodsNow Synthesis
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

SciFinder^{n}
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Chemical Abstract Service

- More than 2,500 scientists, engineers are behind creation of SciFinder^{n}.
- They intellectually analyze published articles, patents and “structure” them with standard concepts/ keywords for easy retrieval.

SciFinder^{n}
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Value added Indexing

(12) 发明专利申请

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A61K 49/22 (2006.01)
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A61K 47/34 (2006.01)
A61P 35/00 (2006.01)

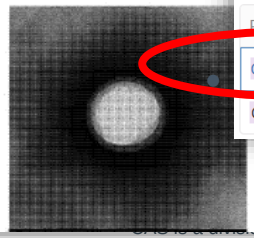
权利要求书 2 页 说明书 11 页 附图

(54) 发明名称

体内相转变肿瘤靶向纳米泡及其制备方法和用途

(57) 摘要

本发明属于生物医药技术领域，具体为一种体内相转变肿瘤靶向纳米泡及其制备方法和用途。纳米泡以偶联肿瘤靶向因子的聚磷酸酯－聚酯共聚物为包膜材料，以可在体内发生液－气相转变的全氟戊烷为泡心填充物质，采用预复乳－中空膜管乳化方法制备。纳米泡进入体内后，液态全氟戊烷在体温下发生液－气相转变，形成含气纳米泡，通过靶向因子与肿瘤细胞的特异性结合，纳米泡富集在肿瘤病灶部位，从而改善肿瘤



Preparation method of in-vivo phase-transition tumor targeting nanobubble and its application

By: Liu, Wei; Xu, Haibo; Chen, Yunchao; Yang, Xiangliang; Cheng, Xin; Li, Huan; Luo, Binhua; Wan, Jiangling; Zhou, Xiaoshun

Abstract: The title nanobubble comprises filling material with perfluoropentane as core, which can have liquid-gas phase transition in vivo, and tumor targeted factor modified biodegradable polyphosphate-polyester copolymer as coating material, and the nanobubble contains polyphosphate-polyester copolymer 1-30%, tumor targeted factor 0.1-10%, liquid perfluoropentane 0.1-5% and pure water. The polyphosphate-polyester copolymer (average mol. weight 2000-60000, polyphosphate:polyester 1:5-5:1) has chem. structure as in patent. The particle size of nanobubble (PDI ≤ 0.35) is 30-1000 nm. The polyphosphate is polyethyl alkyl phosphate (C_1-C_1 alkyl) or polypropyl alkyl phosphate (C_1-C_1 alkyl). The polyester is D,L-lactide, poly L-lactide or the like. The tumor targeted factor includes folic acid, lactoferrin or the like. The preparation method consists of dissolving polyphosphate-polyester copolymer in mixture of Et acetate and THF to obtain oil phase 1, using liquid perfluoropentane as oil phase 2, mixing oil phases by high shear(5000-30000 rpm) in ice bath, dripping oil phase into water phase by magnetic stirring in ice bath to obtain $O_2/O_1/W$, pushing mixture through hollow-membrane tube, pouring mixture into normal saline, stirring at 25°C by magnetic force, removing organic solvent by extraction The hollow-membrane tube is prepared with polyethylene, polypropylene or the like. The MRI contrast agent (0.01-3%) is added into nanobubble. The title nanobubble is used for delivery of anti-cancer drugs, which include paclitaxel, docetaxel or the like.

PATENTPAK PDF | Full Text

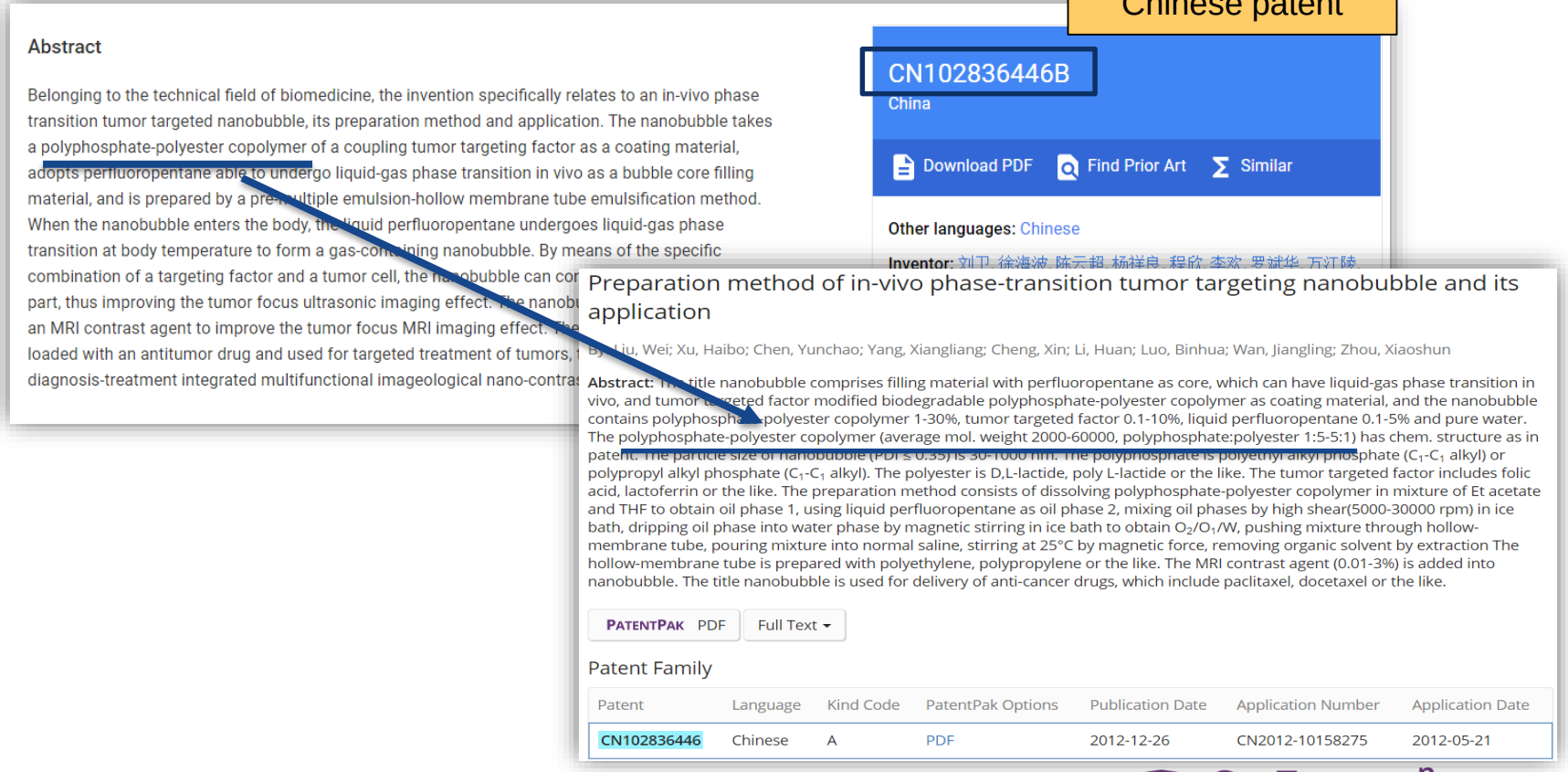
Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN102836446	Chinese	A	PDF	2012-12-26	CN2012-10158275	2012-05-21
CN102836446	Chinese	B	PDF	2014-08-27	CN2012-10158275	2012-05-21

SCIFINDER^n A CAS SOLUTION

Value added Indexing

Chinese patent



Abstract

Belonging to the technical field of biomedicine, the invention specifically relates to an in-vivo phase transition tumor targeted nanobubble, its preparation method and application. The nanobubble takes a polyphosphate-polyester copolymer of a coupling tumor targeting factor as a coating material, adopts perfluoropentane able to undergo liquid-gas phase transition in vivo as a bubble core filling material, and is prepared by a pre-[illegible]ultiple emulsion-hollow membrane tube emulsification method. When the nanobubble enters the body, the liquid perfluoropentane undergoes liquid-gas phase transition at body temperature to form a gas-cont[illegible]ining nanobubble. By means of the specific combination of a targeting factor and a tumor cell, the [illegible]anobubble can cor[illegible] part, thus improving the tumor focus ultrasonic imaging effect. The nanobu[illegible] an MRI contrast agent to improve the tumor focus MRI imaging effect. The[illegible] loaded with an antitumor drug and used for targeted treatment of tumors, [illegible] diagnosis-treatment integrated multifunctional imageological nano-contras[illegible]

CN102836446B

China

Download PDF | Find Prior Art | Similar

Other languages: Chinese

Inventor: 刘卫; 徐海波; 陈云超; 杨祥良; 程欣; 李欢; 罗斌华; 万江陵;

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CN102836446	Chinese	A	PDF	2012-12-26	CN2012-10158275	2012-05-21

SciFinder^n A CAS SOLUTION

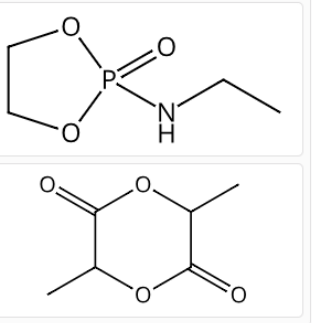
Concepts

- **Antibodies and Immunoglobulins**
  Role: Biological Use, Unclassified
- **Antitumor agents**
- **Ceramics**
- **Dissolution**
- **Extraction**
- **Fluoropolymers**
  Role: Other Use, Unclassified
- **Imaging agents**
- **Lactoferrins**
  Role: Reactant
- **Liver neoplasm**
- **Microstructure**
- **NMR imaging**
- **NMR imaging agents**
- **Particle size**
- **Particle size distribution**
- **Physiological saline solutions**
- **Polycarbonates**
  Role: Other Use, Unclassified
- **Polysulfones**
  Role: Other Use, Unclassified
- **Stability**
- **Transferrins**
  Role: Reactant
- **Zeta potential**

Substances

Substances (33)

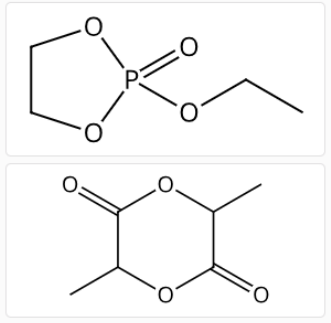
1417421-76-1



$(C_6H_8O_4.C_4H_{10}NO_3P)_x$
1,4-Dioxane-2,5-dione, 3,6-dimethyl-, polymer with *N*-ethyl-1,3,2-dioxaphospholan...

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

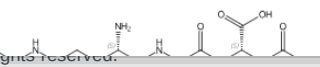
326604-67-5



$(C_6H_8O_4.C_4H_9O_4P)_x$
1,4-Dioxane-2,5-dione, 3,6-dimethyl-, polymer with 2-ethoxy-1,3,2-dioxaphosphola...

Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

99896-85-2



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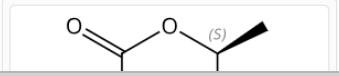

Content and coverage

Reference

- >48M references available
- Patents from 63 patent issuing authorities
- 10,000+ Journal Publications
- ***PatentPak***

Substances

- >148M substances
- >7.6BProperty values
- >1M Markush structures
- Back referencing for substances till 1800

Reactions

- >116M reactions available
- ***MethodsNow Synthesis***
- ***CAS Retrosynthesis planner***

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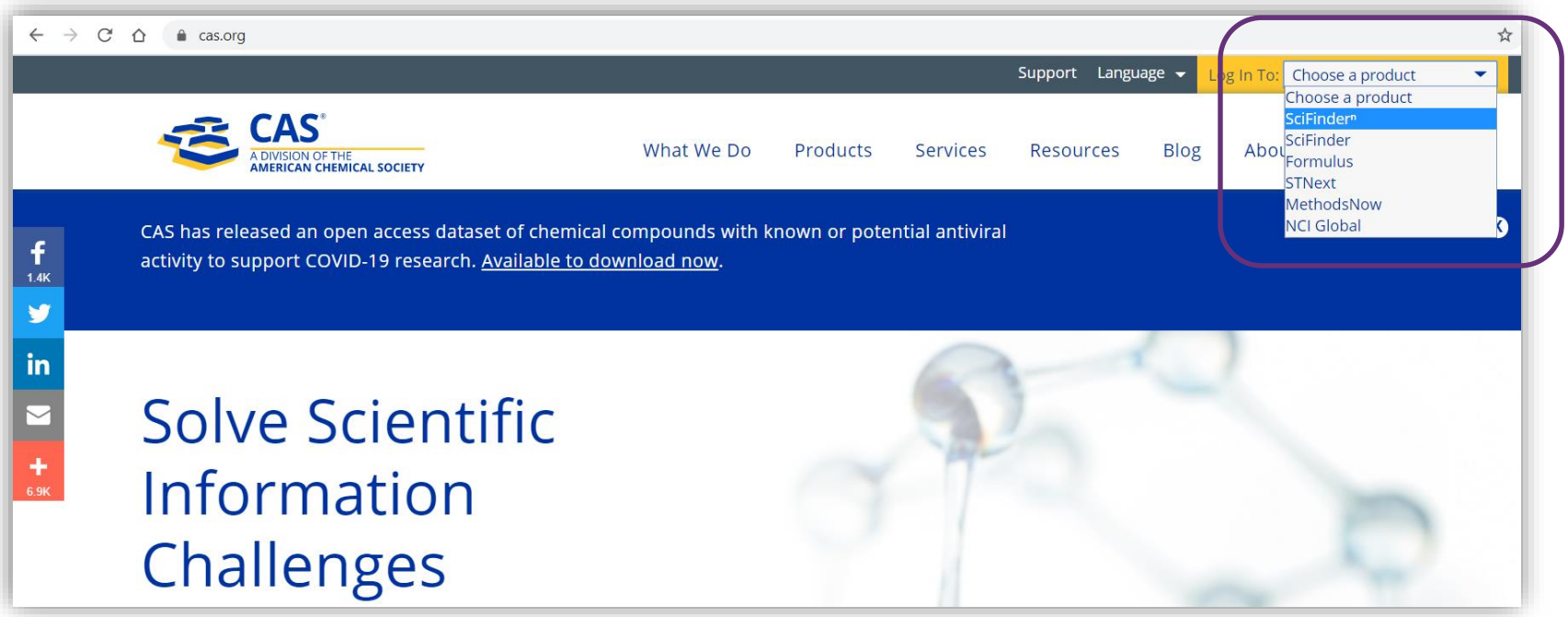
How to Log in into SciFinder-n

1. Go to https://www.cas.org/ > Login to > SciFinder-n



SciFinderⁿ
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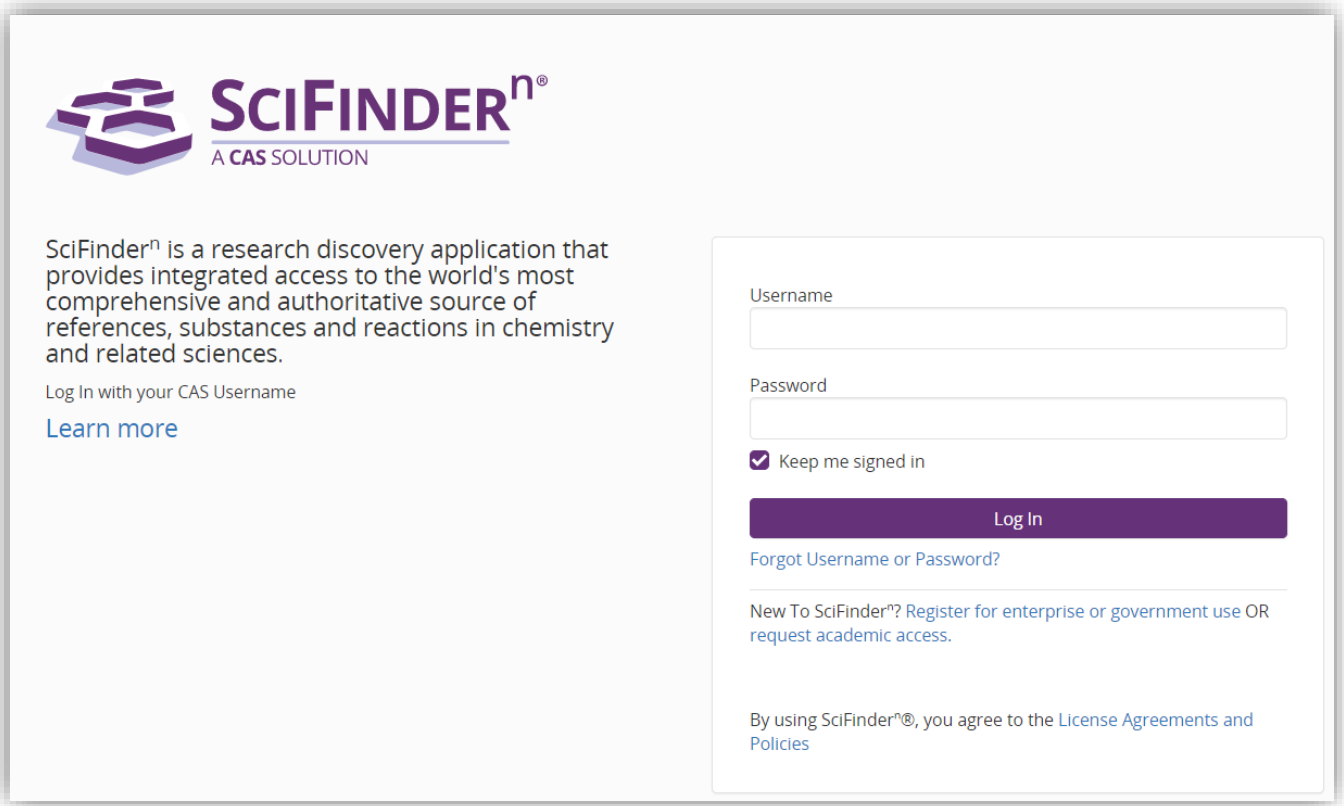
Enter your Login credentials



SciFinder n
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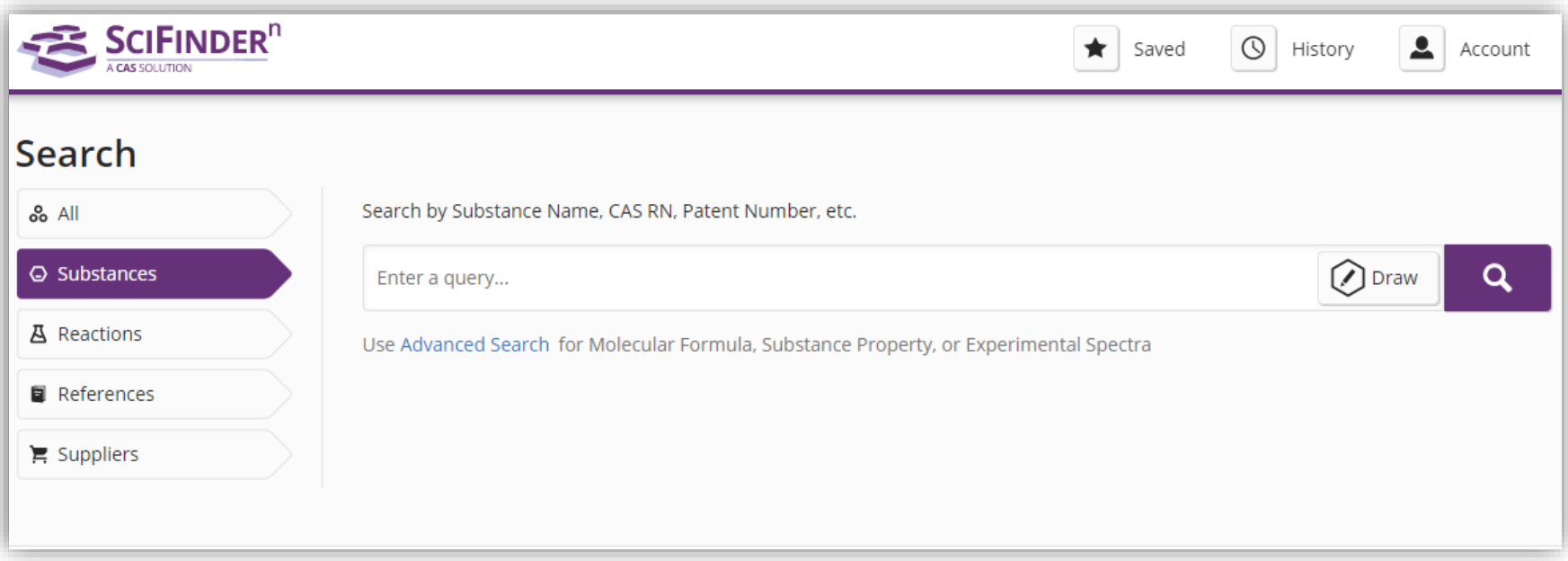
SciFinder-n interface



SCIFINDER n
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Agenda

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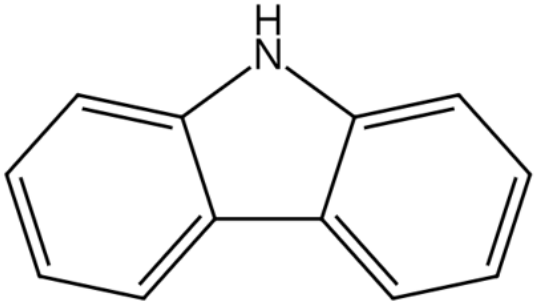
- What is SciFinder^{n}?
- Content and Coverage searchable in SciFinder^{n}
- A few online Case studies – General interest
  - **Substance searching**
  - Reference searching and PatentPak
  - Reaction searching
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

SciFinder^{n}
A CAS SOLUTION

Substance searching



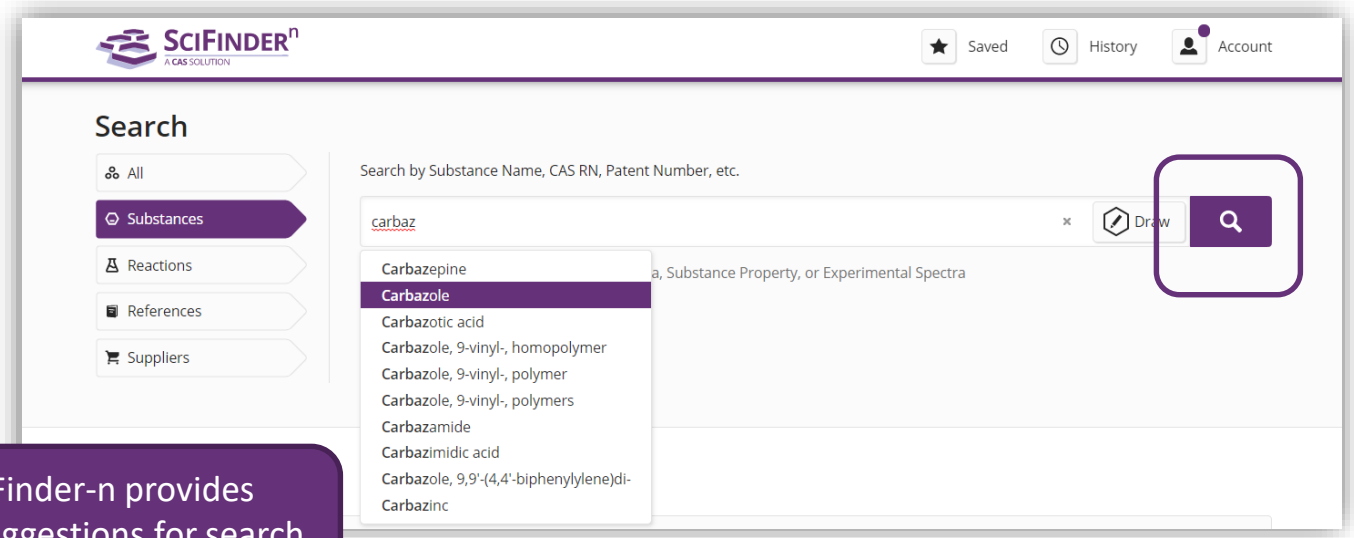
- Search substance query: ***Carbazole***

1. Search substance by name (Commercial name, IUPAC name or CAS registry number)

2. Search substance using structure

SciFinder^n
A CAS SOLUTION

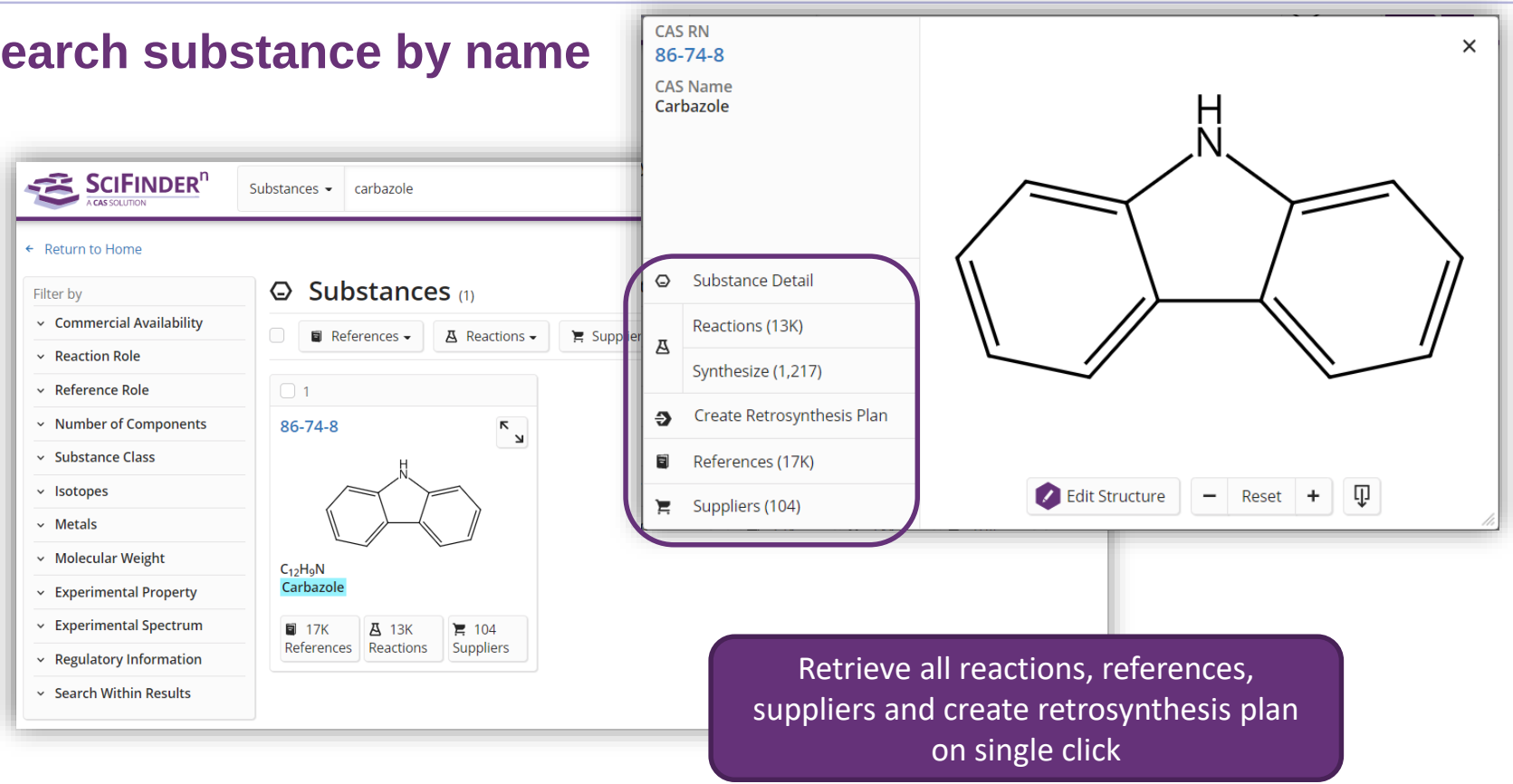
1. Search substance by name



SciFinder-n provides autosuggestions for search query

SciFinder n
A CAS SOLUTION

Search substance by name



Retrieve all reactions, references, suppliers and create retrosynthesis plan on single click

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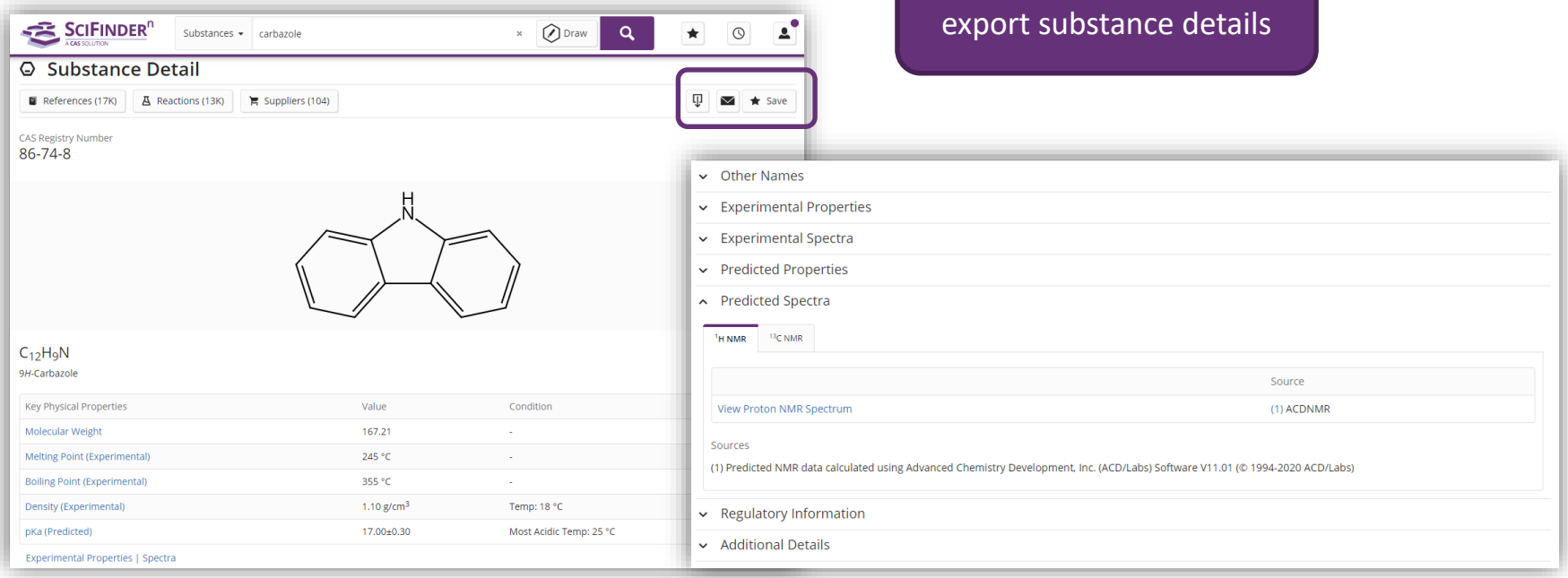
Substance details

Download, share and export substance details



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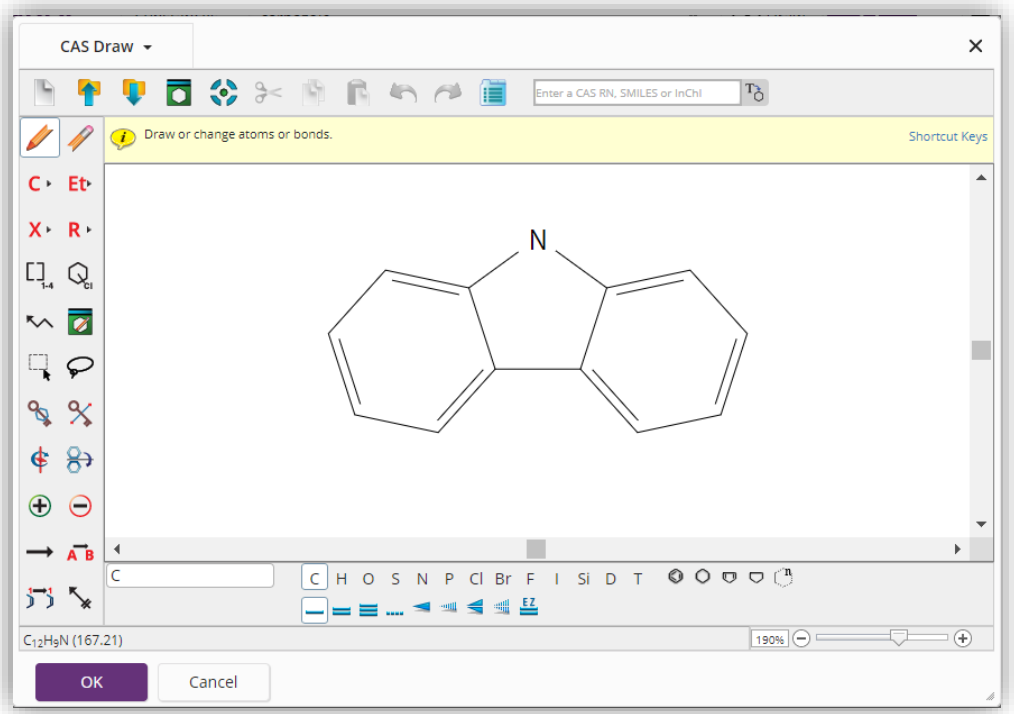
2. Search substance using structure



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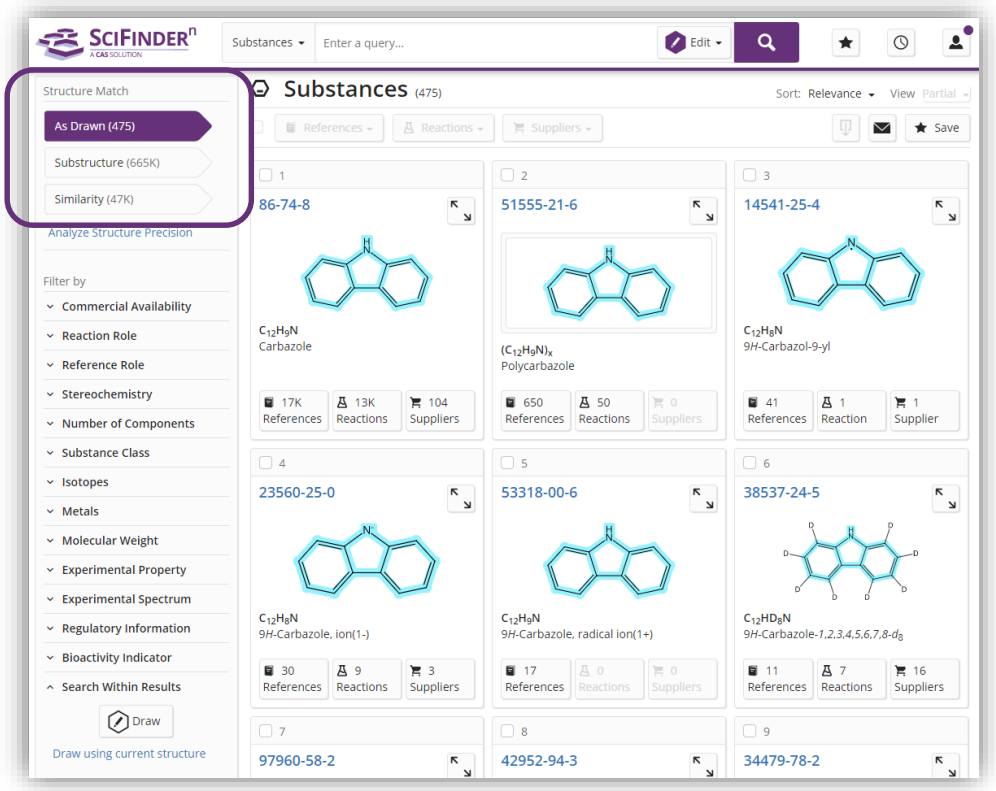
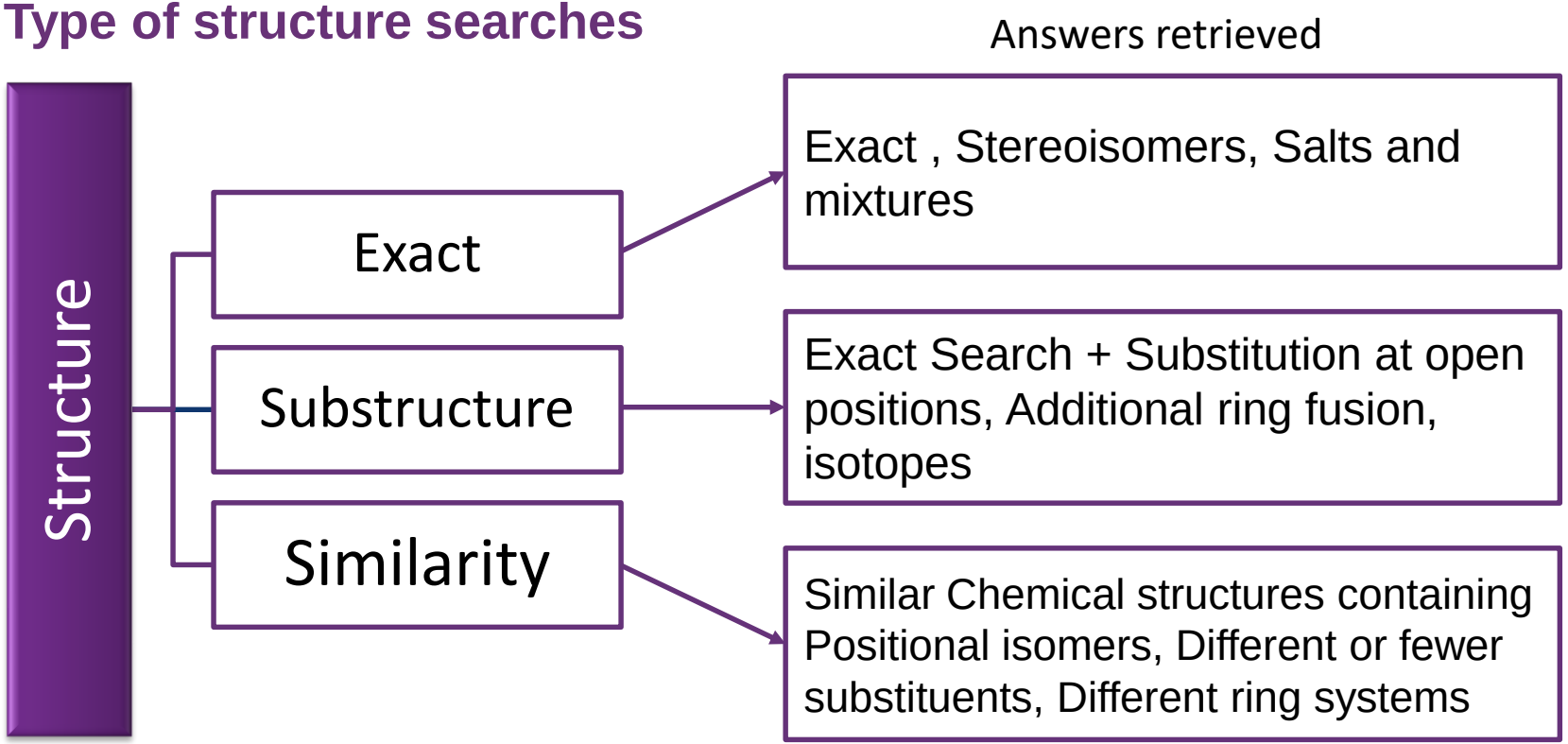
A CAS SOLUTION

Substance search



SciFinder A CAS SOLUTION

Type of structure searches



SciFinder^n
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Case study

Search references for Shape memory polymers

1. Search for ***Shape memory polymer*** as a keyword
2. Retrieve all references and filter all references by document type Patent
3. Explore all other refinement options

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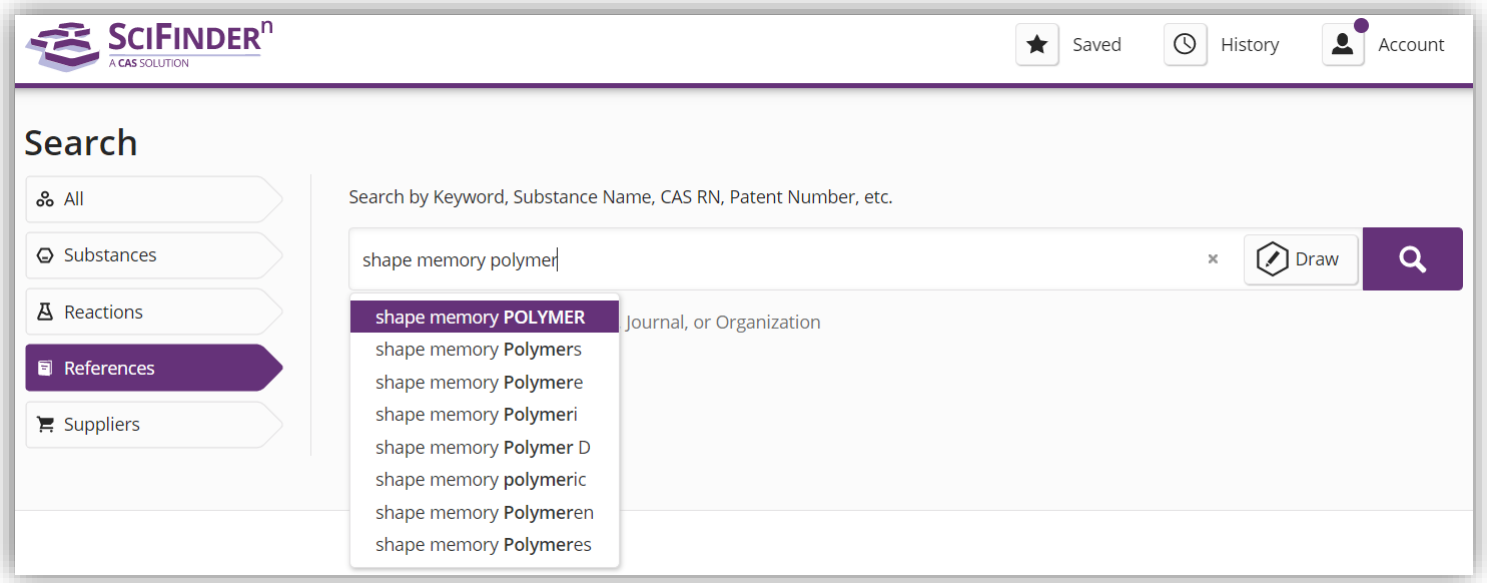
Key word search



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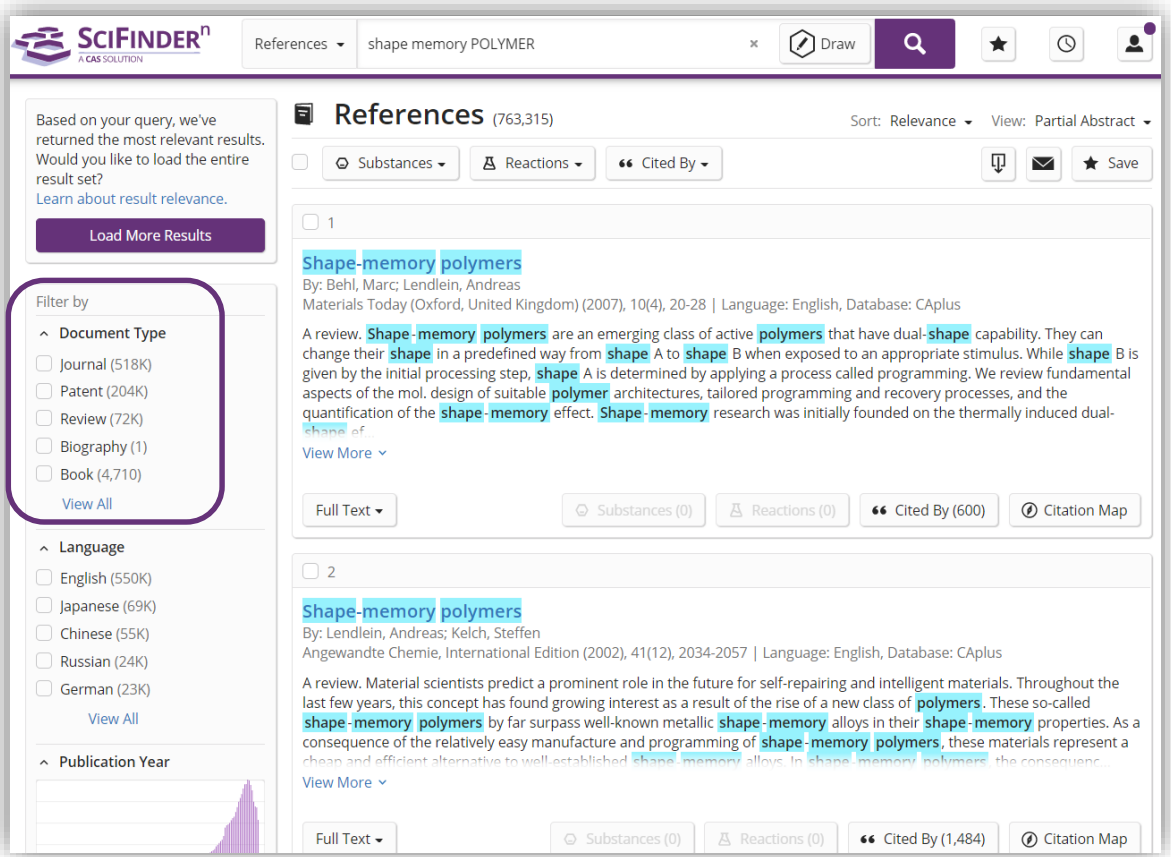
References retrieved

A new, proprietary algorithm presents the most relevant answers for your immediate review and evaluation alongside other important criteria



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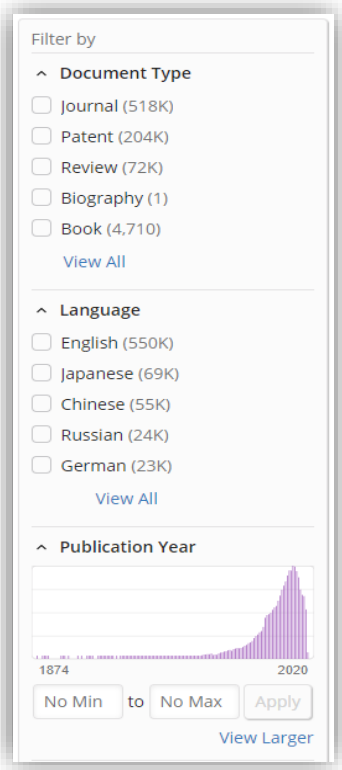
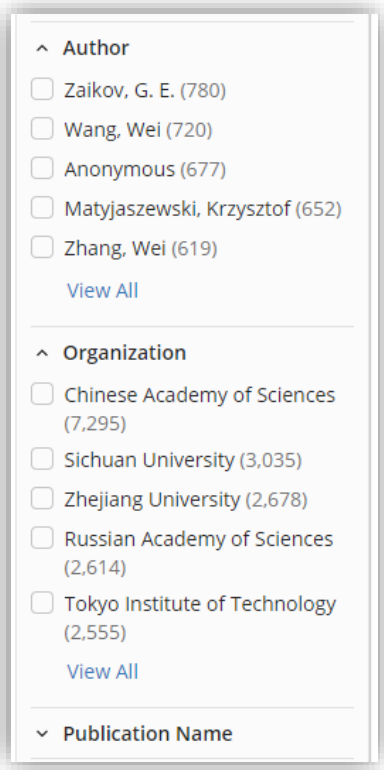
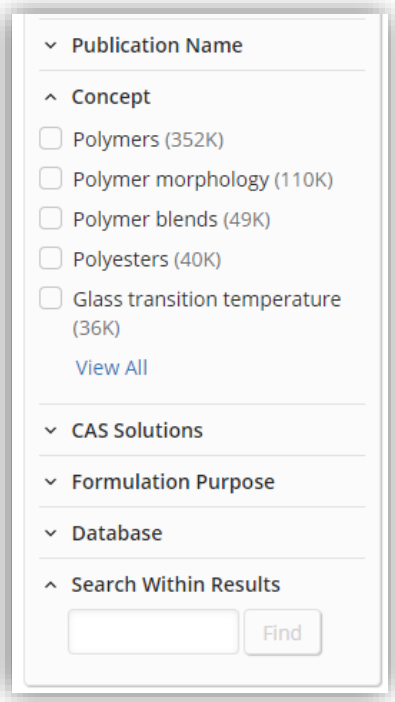
Different filtration options







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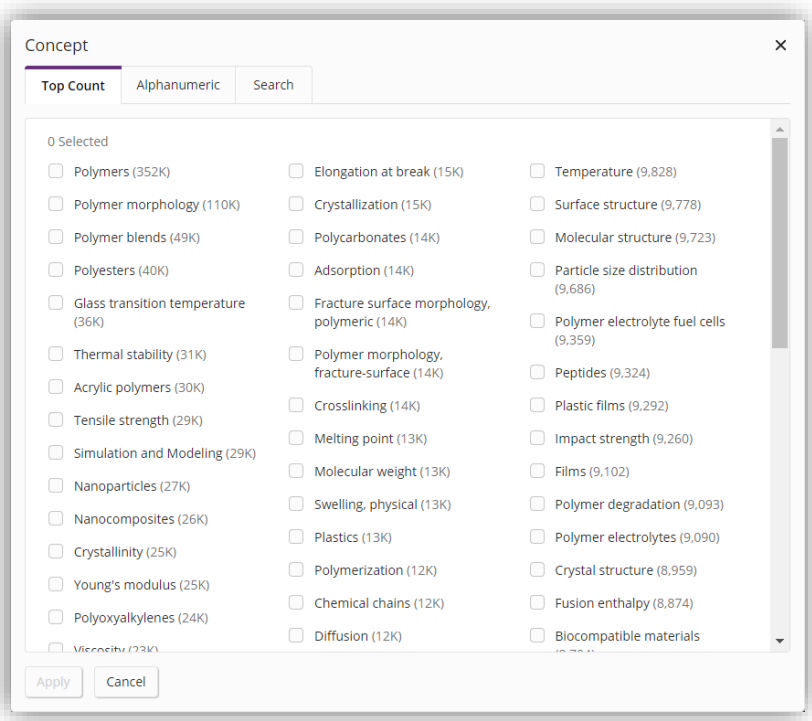
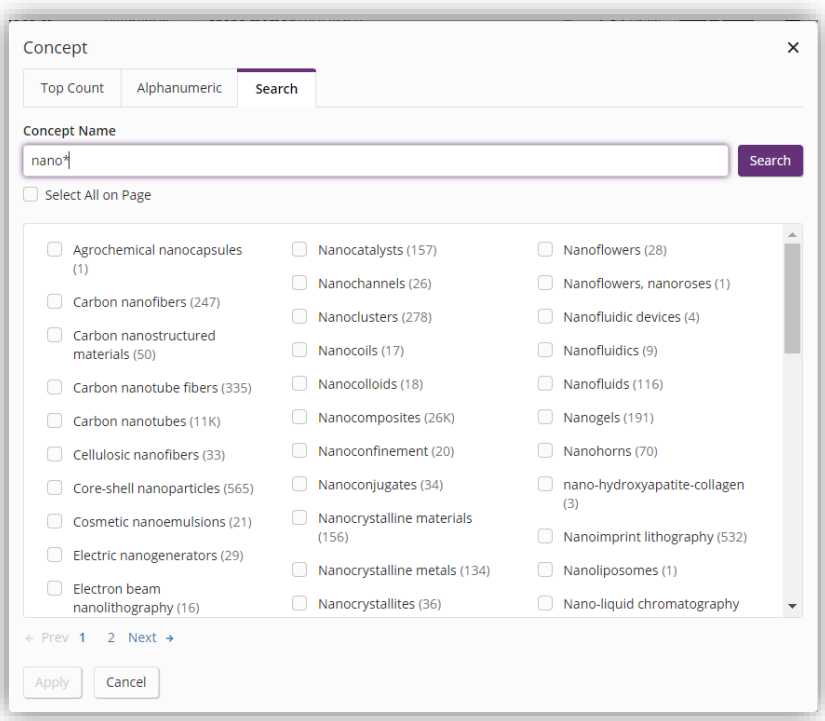
Refine references using concept titles





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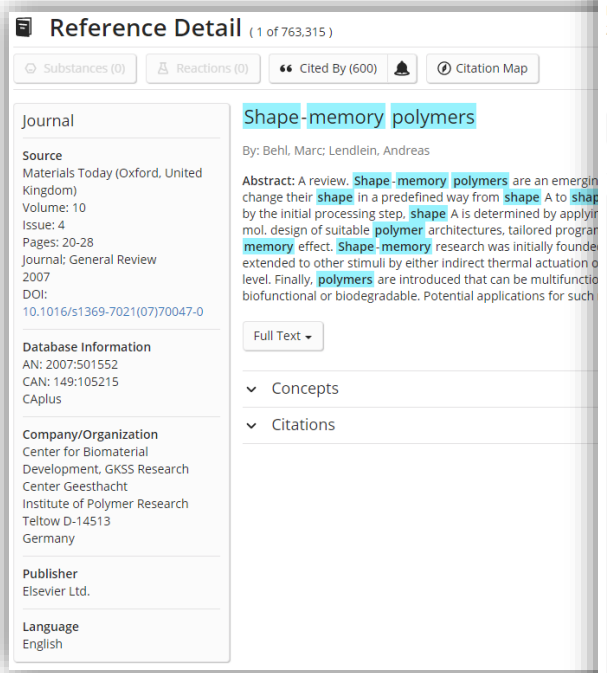
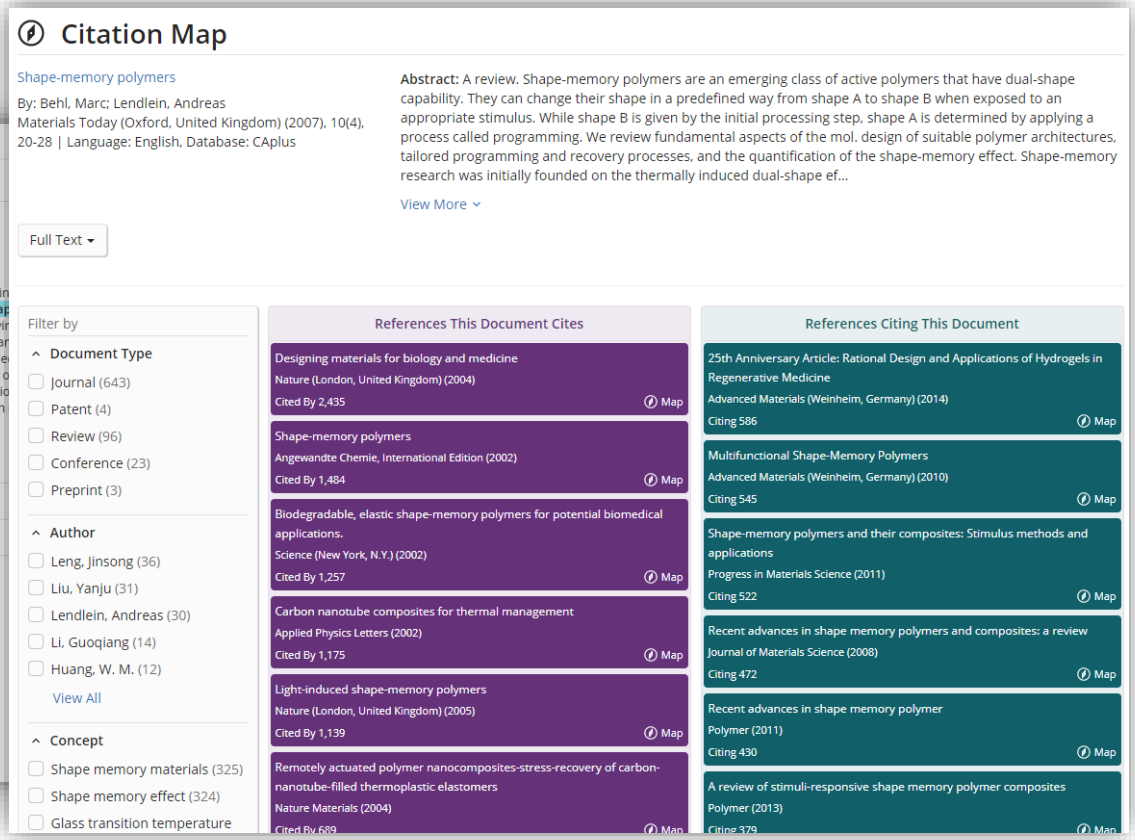
Citation Map





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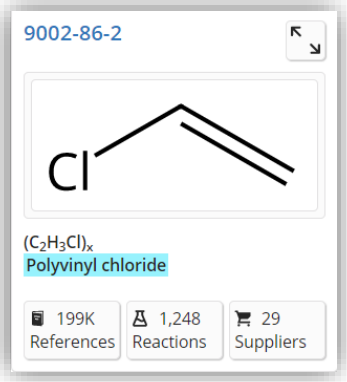
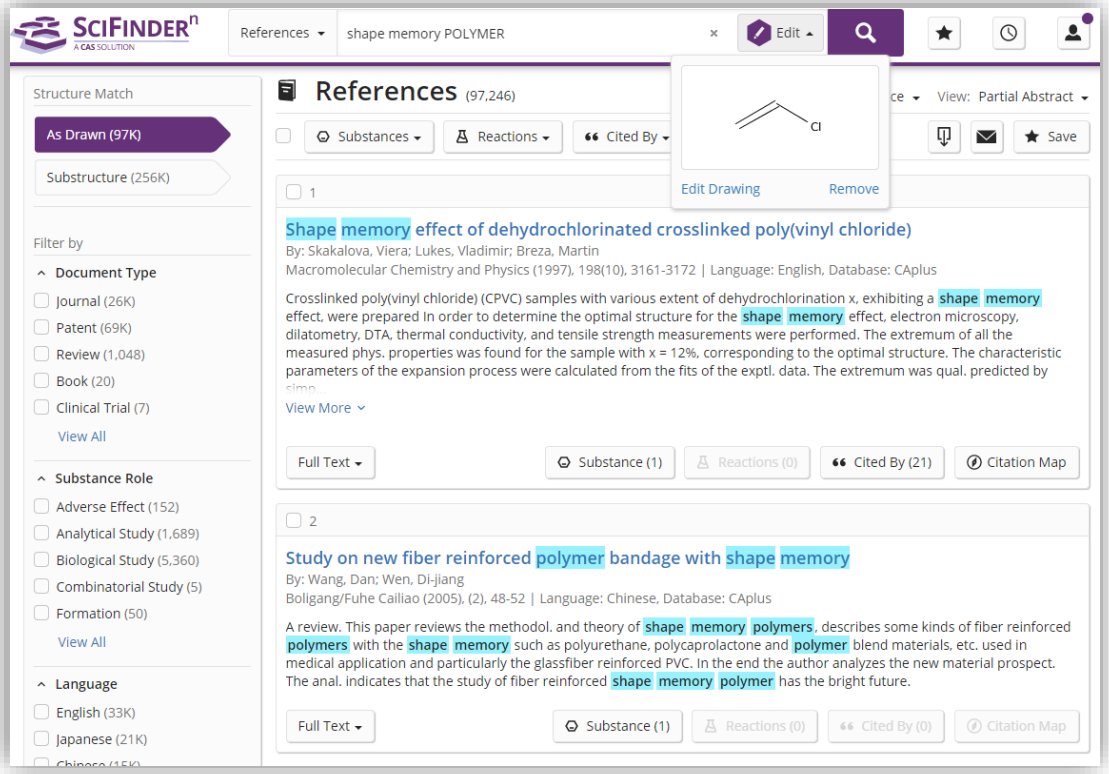
Combine text and structure searching

Draw structure within ‘Draw” option available to combine Keyword and structure query





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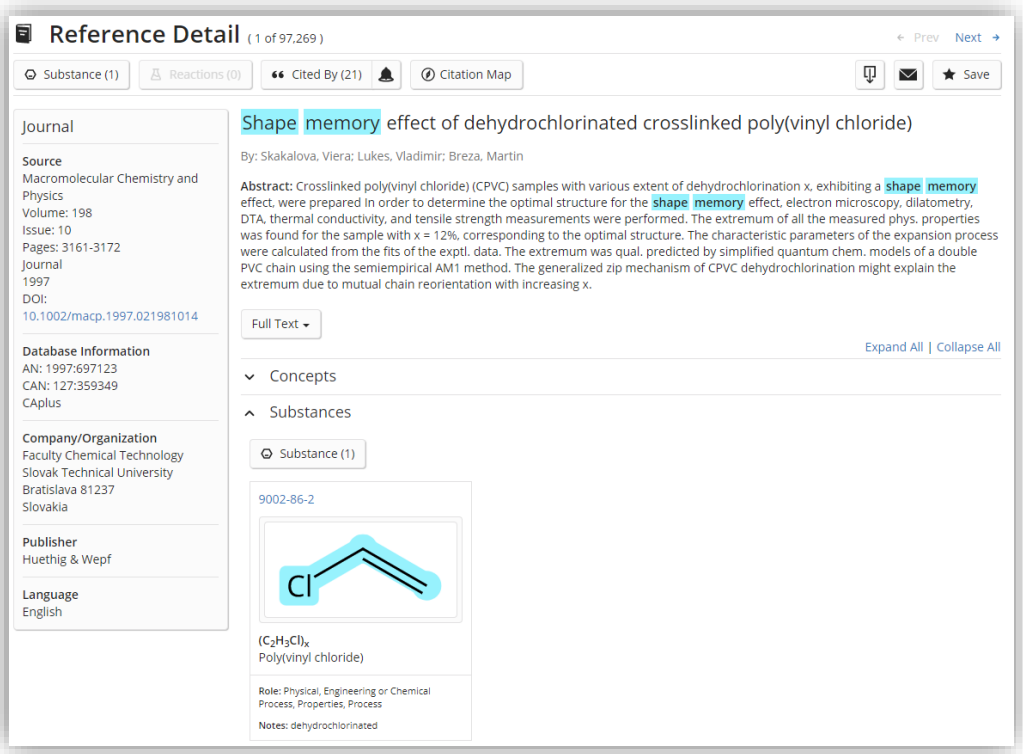
One of the reference



SciFinder^n
A CAS SOLUTION

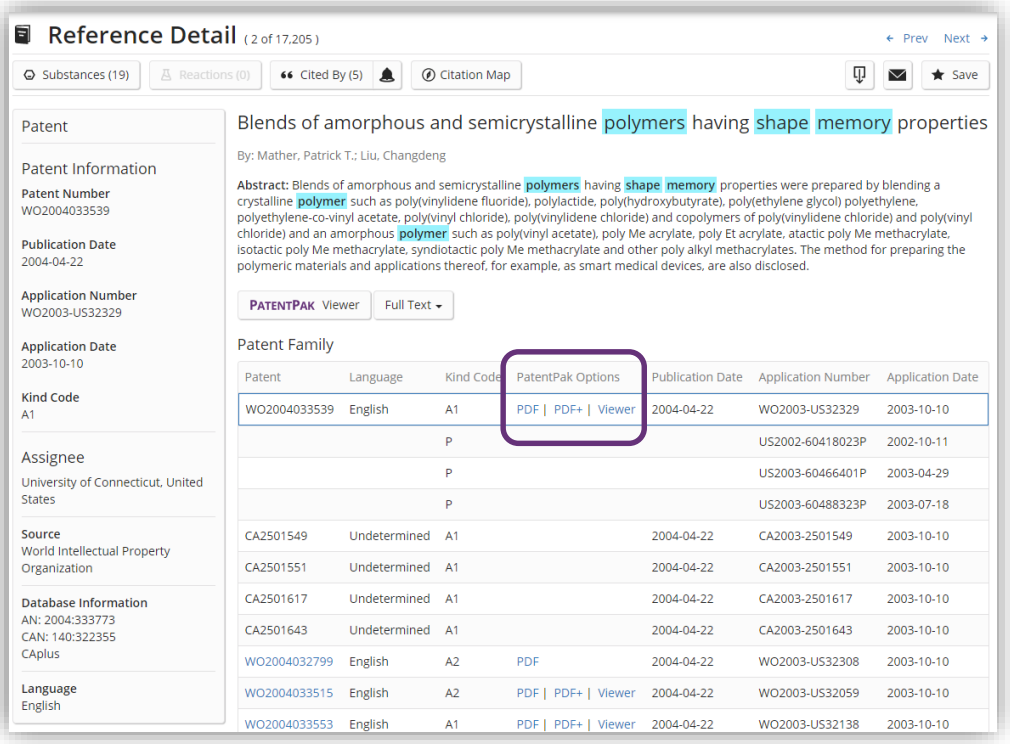
PatentPak is a CAS solution to ease the substance search in patents

- Types of issues & challenges faced in day-today while searching patents
- What is PatentPak? And how does it work?
- Coverage and Content of PatentPak
- What if an important Patent is not in English?
- Conclusion

SCIFINDER^n
A CAS SOLUTION

Search patented references published in English language

Explore patent in PatentPak



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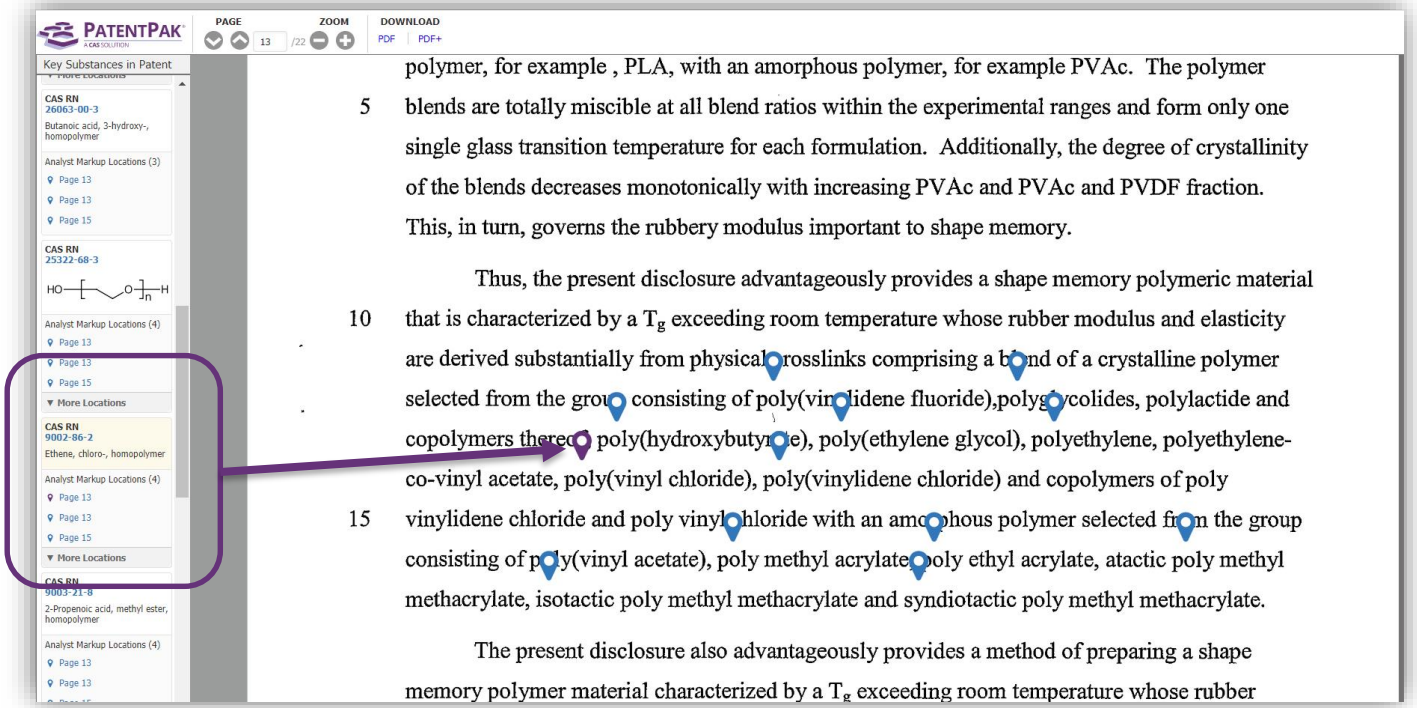
PatentPak viewer



polymer, for example , PLA, with an amorphous polymer, for example PVAc. The polymer blends are totally miscible at all blend ratios within the experimental ranges and form only one single glass transition temperature for each formulation. Additionally, the degree of crystallinity of the blends decreases monotonically with increasing PVAc and PVAc and PVDF fraction. This, in turn, governs the rubbery modulus important to shape memory.

Thus, the present disclosure advantageously provides a shape memory polymeric material that is characterized by a T_g exceeding room temperature whose rubber modulus and elasticity are derived substantially from physical crosslinks comprising a blend of a crystalline polymer selected from the group consisting of poly(vinylidene fluoride),polyglycolides, polylactide and copolymers thereof, poly(hydroxybutyrate), poly(ethylene glycol), polyethylene, polyethylene-co-vinyl acetate, poly(vinyl chloride), poly(vinylidene chloride) and copolymers of poly vinylidene chloride and poly vinyl chloride with an amorphous polymer selected from the group consisting of poly(vinyl acetate), poly methyl acrylate, poly ethyl acrylate, atactic poly methyl methacrylate, isotactic poly methyl methacrylate and syndiotactic poly methyl methacrylate.

The present disclosure also advantageously provides a method of preparing a shape memory polymer material characterized by a T_g exceeding room temperature whose rubber

SciFinder^n
A CAS SOLUTION

Situation 1: Patent disclosed substances only by IUPAC name

vacuo and collected in EtOH, azeotroping to dryness to afford the title compound.

Step 2: 5-Amino-2-fluoro-4-methylbenzoic acid

2-Fluoro-4-methyl-5-nitrobenzoic acid (900 mg, 4.52 mmol) in MeOH (70 ml) was treated with ammonium formate 1(425 mg, 22.60 mmol) and Pd (Carbon) (144 mg, 1.356 mmol). The mixture was degassed thoroughly refilling with nitrogen and heated to 60 °C for 2 hrs. The mixture was filtered through silic

The filtrate was passed through SCX-2 resin (30g 0.67

(250 ml) followed by 2M ammonia in MeOH (250 ml). T

were evaporated to dryness and the resulting crude re

recrystallisation from MeOH to afford the title compound;

LC-MS: Rt 0.53 mins; MS m/z 170 $\{M+H\}^+$; Method 10minLC_v003

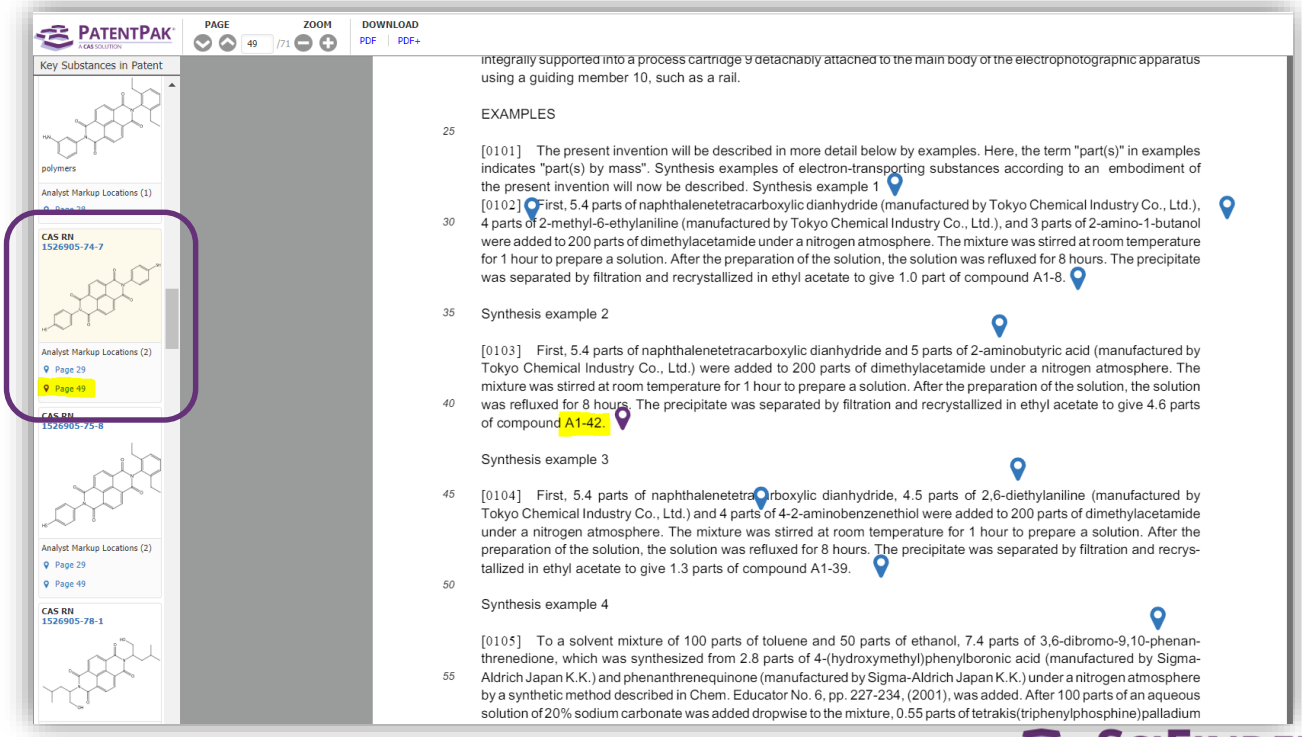
Step 3: 5-Amino-2-fluoro-4-methyl-N-(2-(4-methylpiperazin-1-yl)benzyl)benzamide

A mixture comprising (2-(4-methylpiperazin-1-yl)phenyl)methanamine (413 mg, 2.010 mmol) and 5-amino-2-fluoro-4-methylbenzoic acid (step 2)(340 mg, 2.010 mmol) in DMF (3 ml) was treated with DIPEA (0.351 ml, 2.010 mmol) followed by HATU (764 mg, 2.010 mmol) and stirred at 25 °C for 24 hrs. The mixture was partitioned between water and EtOAc. The organic portion was washed with sat. aq. $NaHCO_3$, 0.5 M LiCl and brine (each back extracted with EtOAc). The combined organic layers were dried ($MgSO_4$), filtered and evaporated to dryness to give a pink oil. Purification

If the patent is big, it is difficult to find the substance by just its name……..

SciFinder^n
A CAS SOLUTION

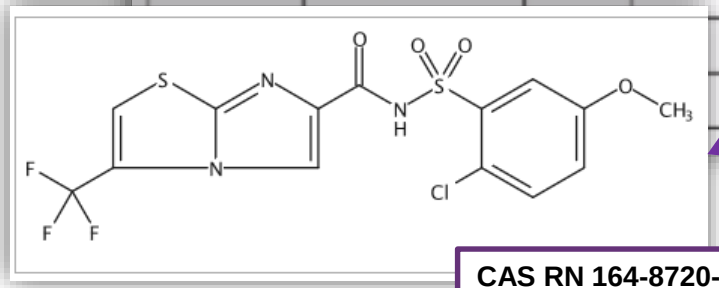
Situation 2: Name or structure not given - Only data is available.



SciFinder^n
A CAS SOLUTION

Situation 3: Disclosed/Claimed compounds are in tabular form.

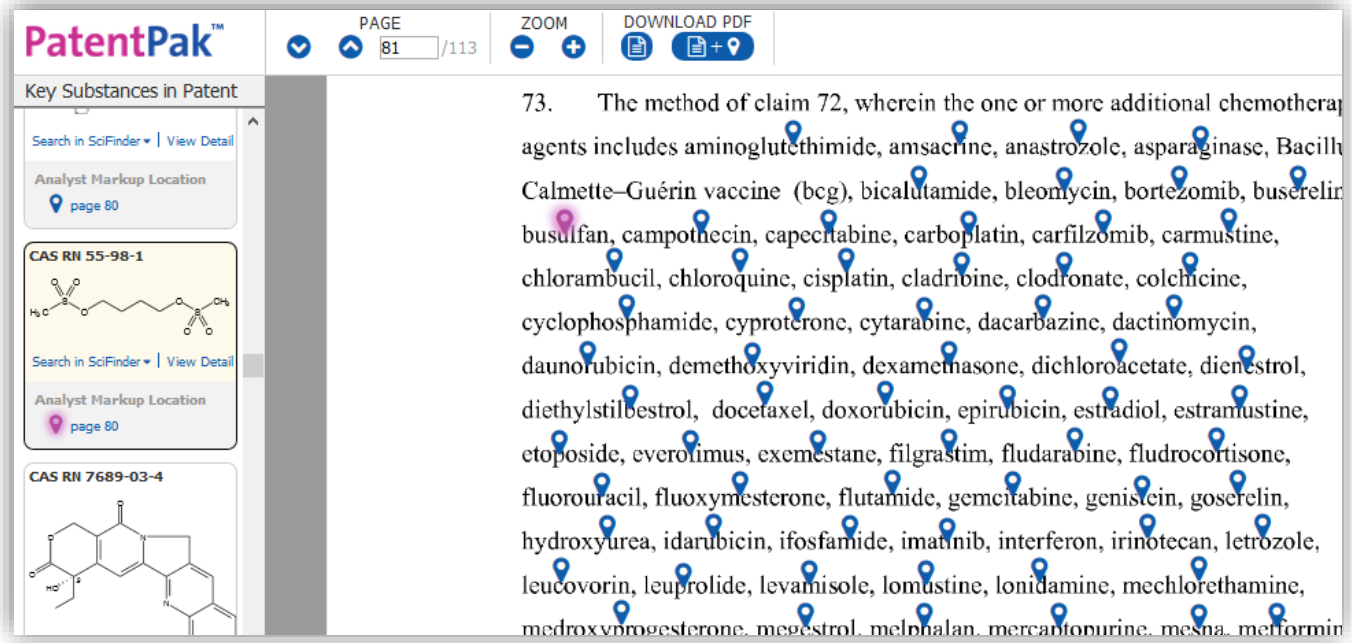
Example	R^1	n	A	R^a	R^b	R^c	R^d	R^e	Remarks
I-1-28	2-CF_3	1	CH	CH_3	H	H	Cl	H	
I-1-29	3-CF_3	1	C-R^1	Cl	H	H	OMe	H	NMR
I-1-30	3-CF_3	1	C-R^1	Cl	H	H	H	Cl	NMR
I-1-31	3-CF_3	1	C-R^1	Cl	H	H	Cl	H	NMR
I-1-32	3-CF_3	1	C-R^1	Cl	H	H	CH_3	H	
				Cl	H	H	Et	H	
				CH_3	H	H	Cl	H	
				C	H	H	OMe	H	



CAS RN 164-8720-97-1 assigned by Chemical Abstract Service

SciFinder^n
A CAS SOLUTION

Situation 4: Disclosed/Claimed compounds have a different common name (which you are not aware)

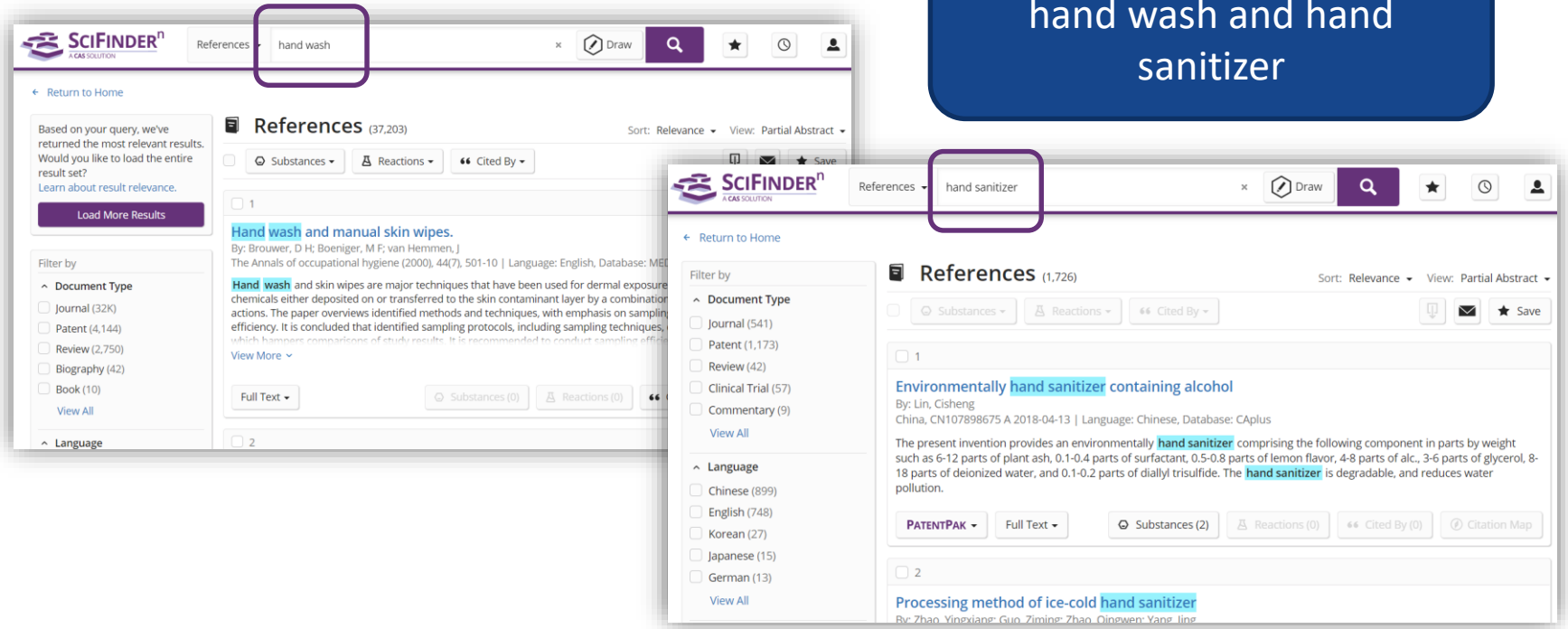


We had searched by "Sulfabutin" and were not aware that it's also called "busulfan"

SciFinder^n
A CAS SOLUTION

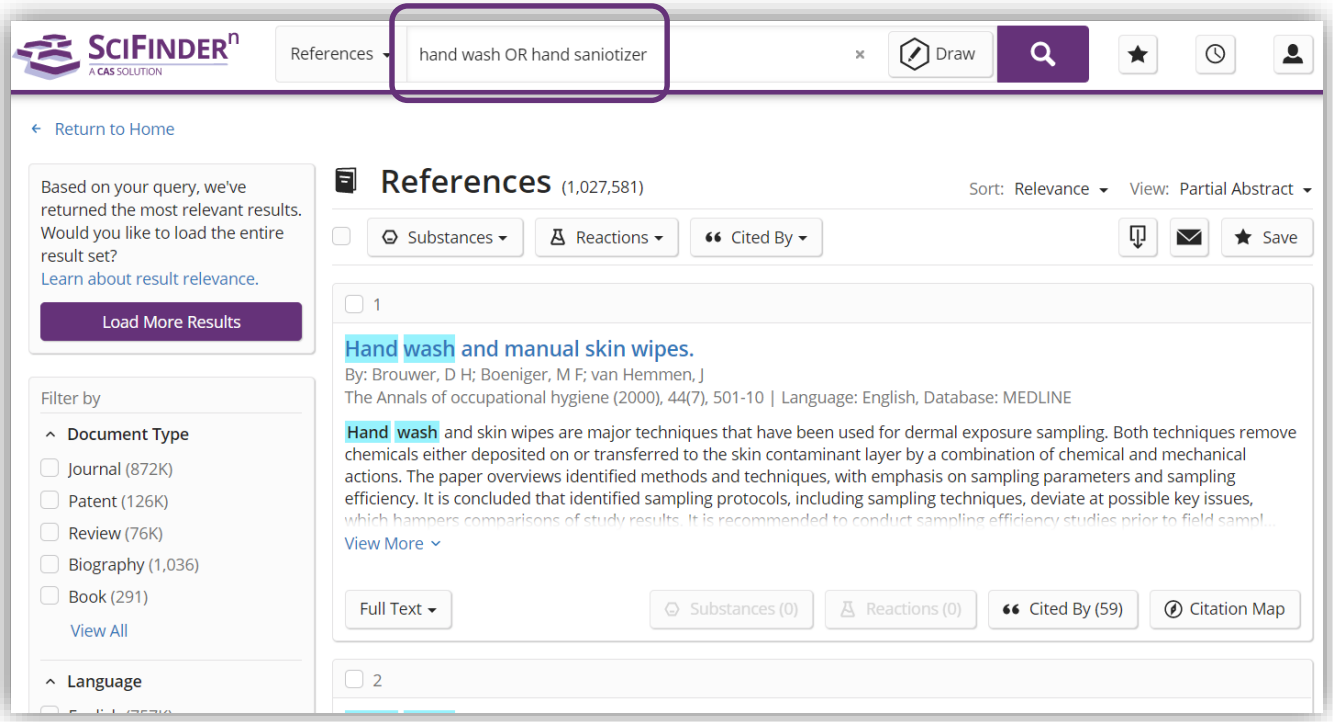
How to use Boolean operators

Separate keyword search for hand wash and hand sanitizer



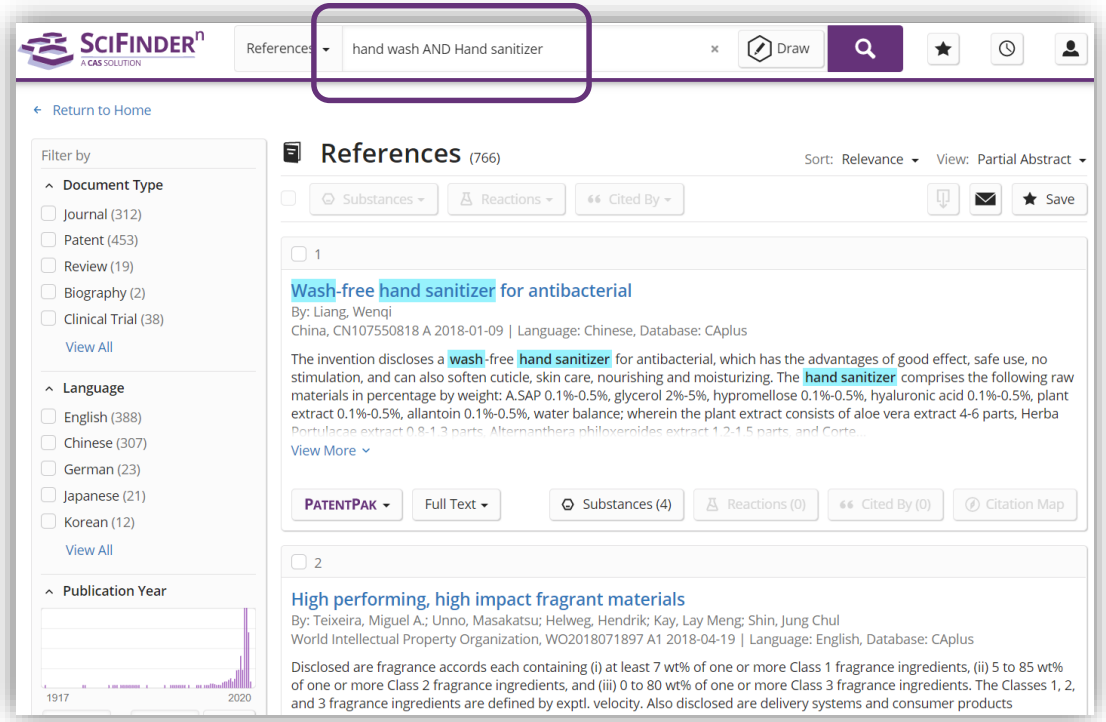
SciFinder
A CAS SOLUTION

Use ‘OR’ Boolean operator to get combined search for both keywords



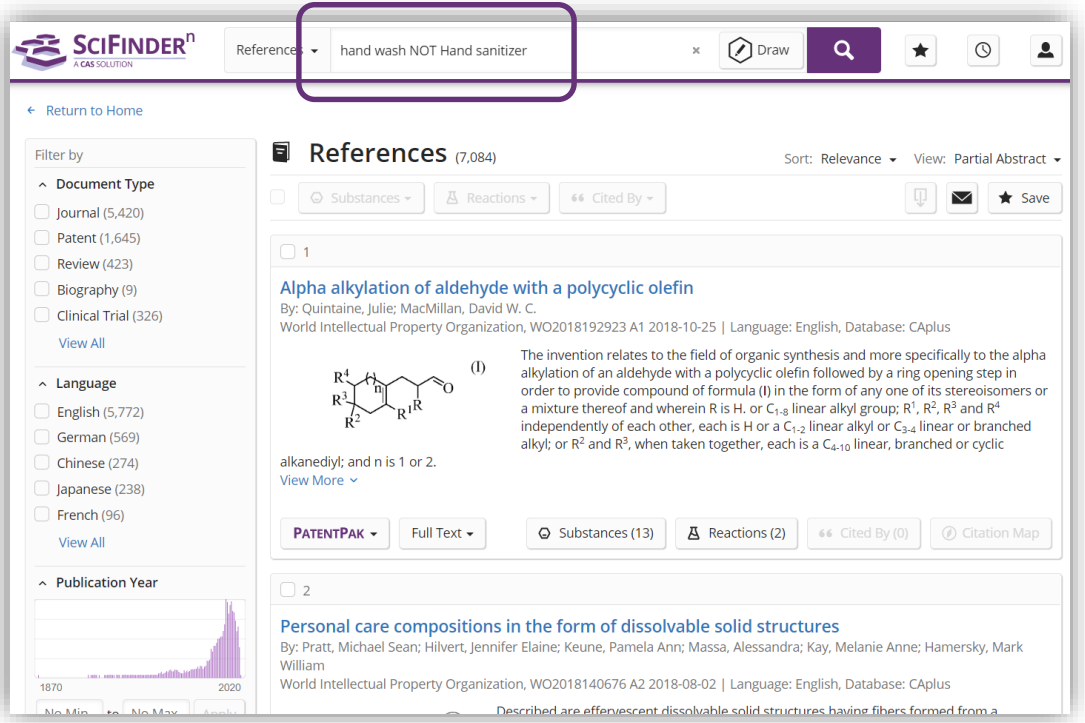
SCIFINDER n
A CAS SOLUTION

Use of ‘AND’ Boolean operator to get references containing both keywords/ concepts in same reference



SciFinder n
A CAS SOLUTION

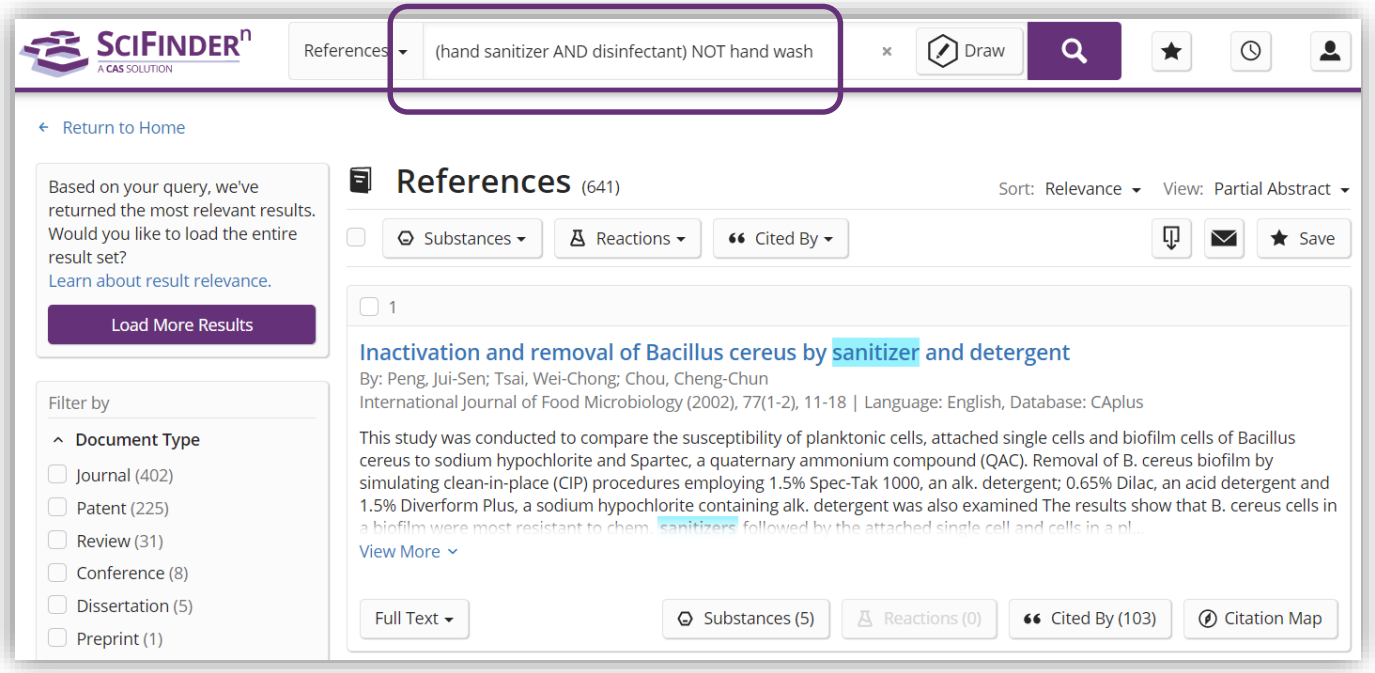
Use of ‘NOT’ Boolean operator to exclude one of the keyword from main search



SciFinder n
A CAS SOLUTION

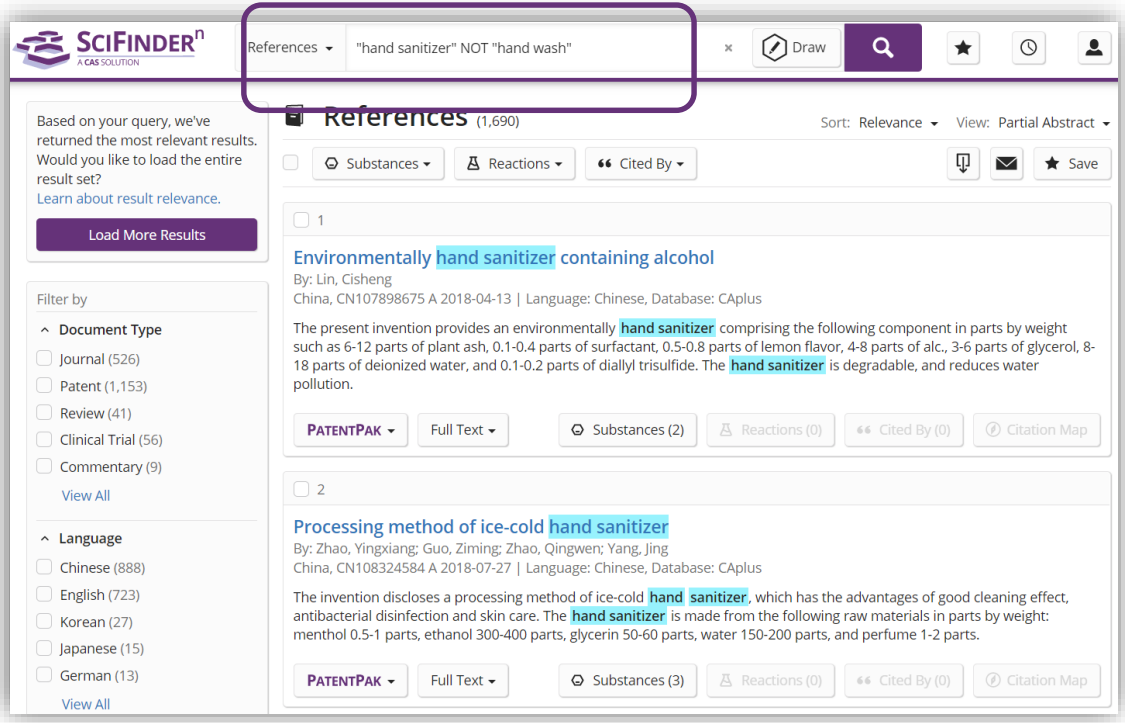
Use of parenthesis with Boolean operators

This will search references in which keyword/concept of Hand sanitizer and disinfectant is mentioned together but not Hand wash



SciFinder n
A CAS SOLUTION

Use of quotation marks to search exact phrase along with Boolean operator

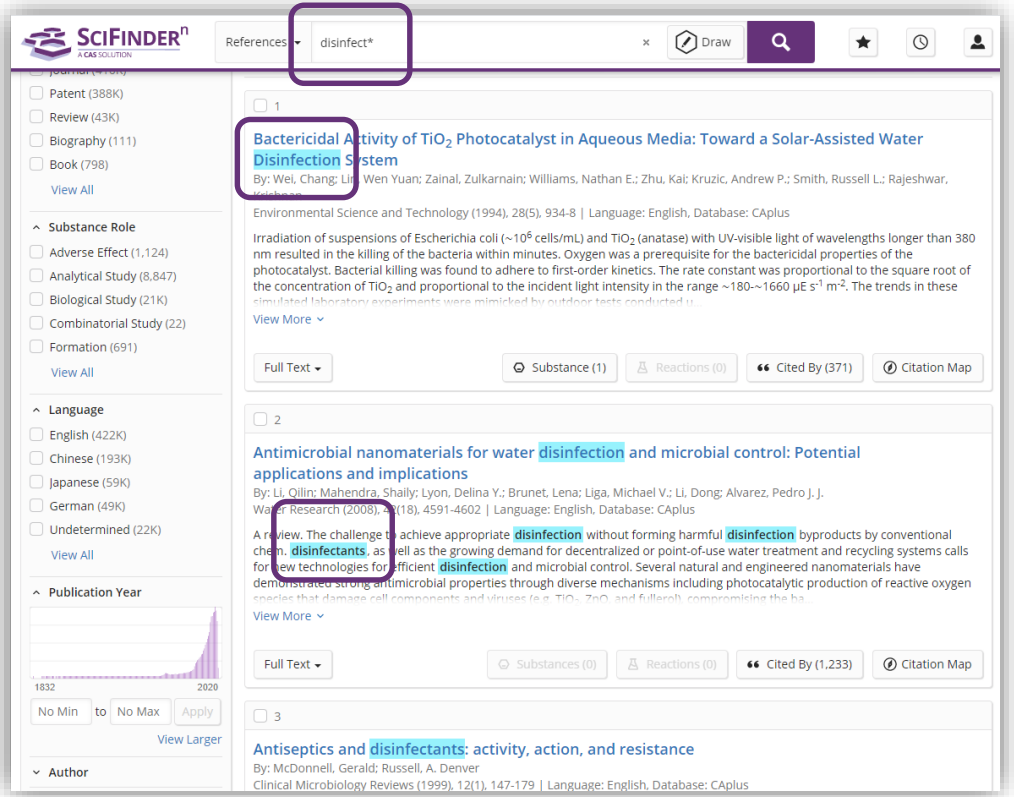


SciFinder n
A CAS SOLUTION

Special characters and wildcard searching

- ***Use of Asterisk (*) mark***

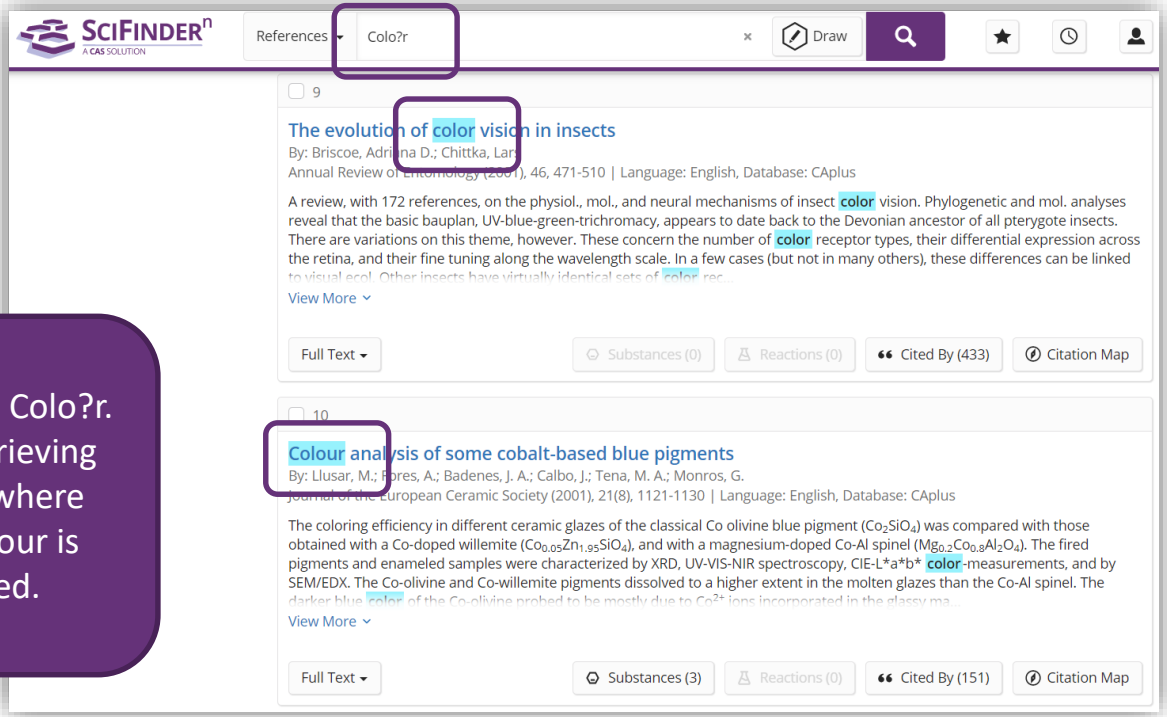
Query Disinfect* will match Disinfectant, disinfection, disinfecting, disinfected etc.



SciFinder n
A CAS SOLUTION

Special characters and wildcard searching

- ***Use of question mark (?)***



Search query: Colo?r. it helped retrieving references where color or colour is mentioned.

SciFinder n
A CAS SOLUTION

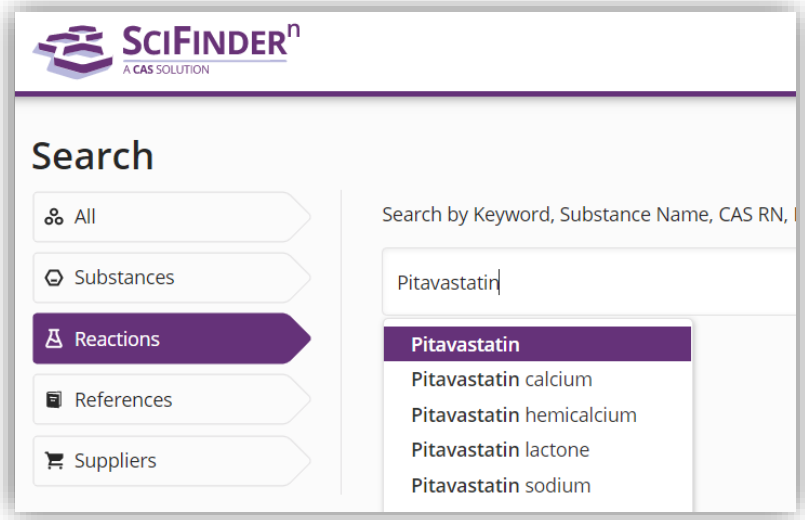
Agenda

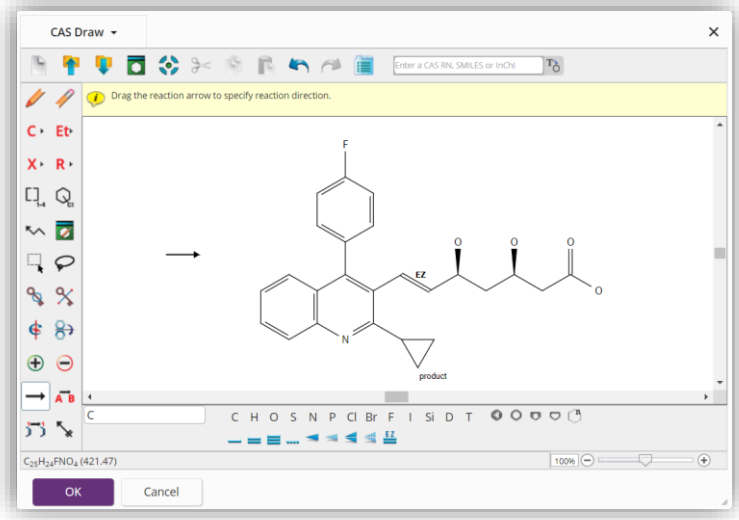
- Introduction of CAS
- What is SciFinder^{n}?
- Content and Coverage searchable in SciFinder^{n}
- A few online Case studies – General interest
  - Substance searching
  - Reference searching and PatentPak
  - **Reaction searching**
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

SciFinder^{n}
A CAS SOLUTION

Reaction searching

- Search reactions for Pitavastatin

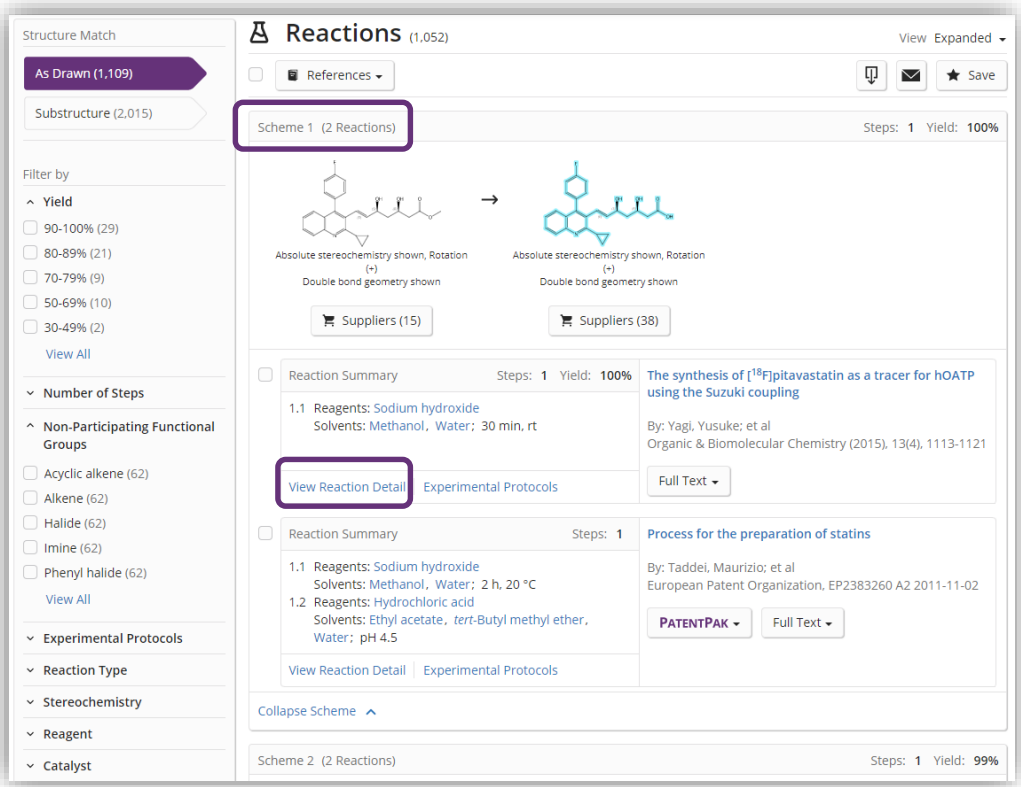


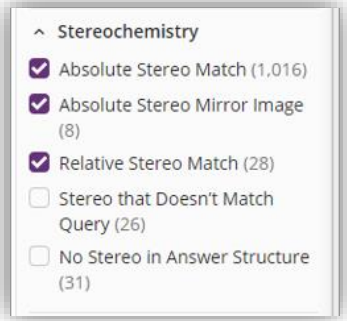


SciFinder n
A CAS SOLUTION

Synthetic reactions for Pitavastatin

Selecting all required refinement options, available reactions

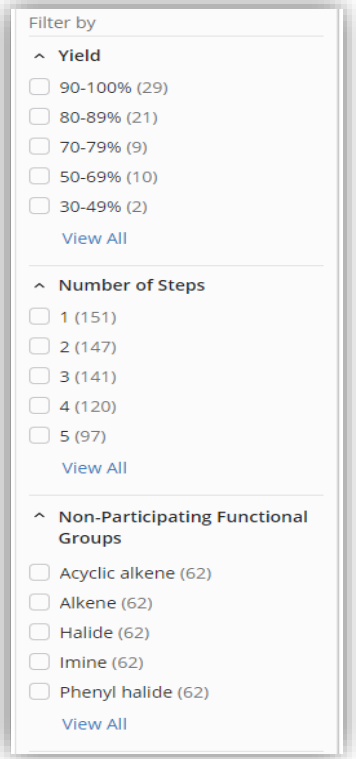


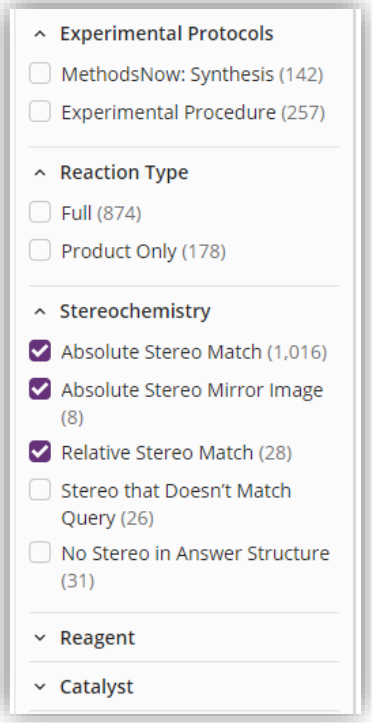


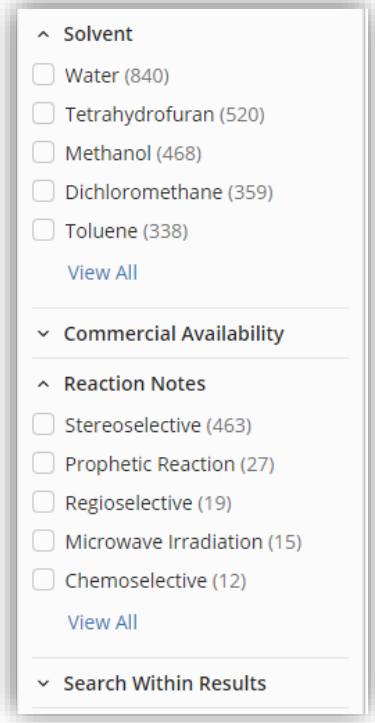
SciFinder-n will consider sterio-structures. We can select required stereochemistry

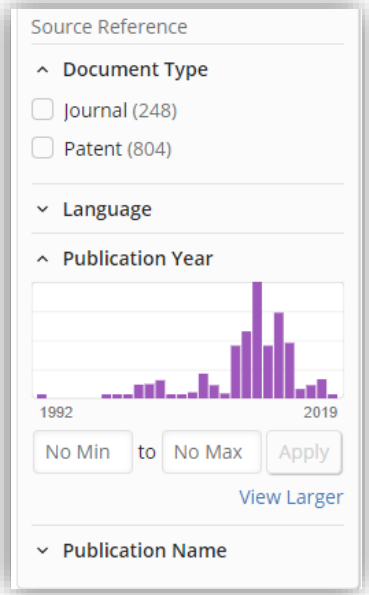
SCIFINDER^n
A CAS SOLUTION

Search for exact reaction using various refinement options available



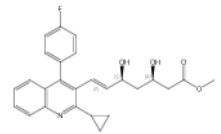






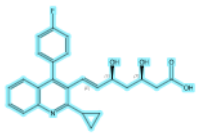
SciFinder^n
A CAS SOLUTION

Exploring one of the reaction Scheme



Absolute stereochemistry shown,
Rotation (+)
Double bond geometry shown

Suppliers (15)



Absolute stereochemistry shown,
Rotation (+)
Double bond geometry shown

Suppliers (38)

Step 1

Alternative Steps (1)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Sodium hydroxide	-	Methanol Water	2 h, 20 °C
2	Hydrochloric acid	-	Ethyl acetate *tert*-Butyl methyl ether Water	pH 4.5

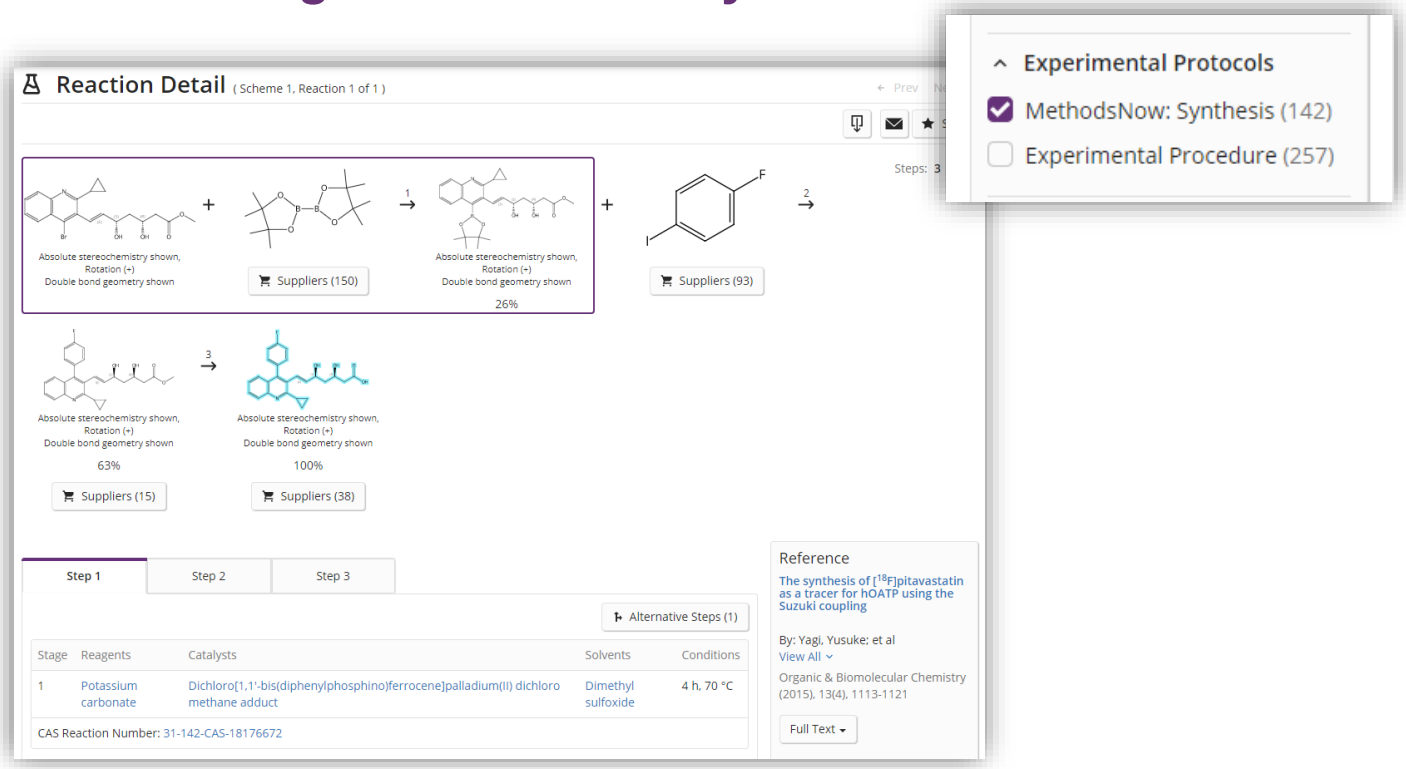
SciFinder^n
A CAS SOLUTION

MethodsNow Synthesis

- MethdsNow provides detailed description of the synthetic experimental procedures utilized in the lab.
- Finding these methods and protocols in the literature is time consuming.
- MethodsNow® is a single source for searching the latest published scientific methods by featuring step-by-step instructions that you can take right to the lab and synthesize the compound.

SciFinder^n
A CAS SOLUTION

Experimental details using MethodsNow synthesis



SciFinder^n A CAS SOLUTION

Experimental details using MethodsNow synthesis

Experimental Protocols

MethodsNow™

Products	6-Heptenoic acid, 7-[2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-quinolinyl]-3,5-dihydroxy-, methyl ester, (3*R*,5*S*,6*E*)-, Yield: 26%
Reactants	Bis(pinacolato)diborane 6-Heptenoic acid, 7-(4-bromo-2-cyclopropyl-3-quinolinyl)-3,5-dihydroxy-, methyl ester, (3*R*,5*S*,6*E*)-
Reagents	Potassium carbonate
Catalysts	Dichloro[1,1'-bis(diphenylphosphino)ferrocene]palladium(II) dichloromethane adduct
Solvents	Dimethyl sulfoxide
Procedure	1. Stir a of methyl (3R,5S,6E)-7-(4-bromo-2-cyclopropylquinolin-3-yl)-3,5-dihydroxyhept-6-enoate (1.00 g, 2.40 mmol), bis(pinacolato)- diboron (12) (0.790 g, 3.12 mmol) and K_2CO_3 (1.00 g, 7.20 mmol) in DMSO (40.0 mL) under an argon atmosphere. 2. Add $Pdcl_2(dppf)CH_2Cl_2$ (0.19 g, 0.240 mmol) to the above reaction mixture. 3. Stir the resulting mixture for 4 hours at 70 °C. 4. Add silica gel to the reaction and filter the resulting mixture through celite. 5. Extract the filtrate with EtOAc and wash the organic layer with water and brine. 6. Dry the reaction mixture over Na_2SO_4. 7. Concentrate the solvent under reduced pressure to obtain a residue. 8. Subject the residue to azeotropic dehydration with MeCN and purify by by HPLC to obtain a brown oil. 9. Powder the resulting oil with a 1 : 1 (v/v) mixture of diisopropyl ether and n-heptane to obtain methyl (3R,5S,6E)-7-(2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3-dioxabolan-2-yl)quinolin-3-yl)-3,5-dihydroxyhept-6-enoate.
Transformation	Preparation of Borates and Boronic Acids
Scale	gram

Characterization Data

6-Heptenoic acid, 7-[2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-quinolinyl]-3,5-dihydroxy-, methyl ester, (3*R*,5*S*,6*E*)-

Proton NMR Spectrum	(500 MHz, $CDCl_3$) δ: 7.91 (d, *J* = 9.2 Hz, 1H), 7.89 (d, *J* = 9.2 Hz, 1H), 7.56 (t, *J* = 9.2 Hz, 1H), 7.40 (t, *J* = 9.2 Hz, 1H), 7.19 (dd, *J* = 16.0, 1.4 Hz, 1H), 6.03 (dd, *J* = 16.0, 5.4 Hz, 1H), 4.66 (br, 1H), 4.38 (br, 1H), 3.75 (br, 1H), 3.73 (s, 3H), 3.32 (br, 1H), 2.56 (d, *J* = 3.4 Hz, 1H), 2.54 (s, 1H), 2.28 (tt, *J* = 8.0, 4.6 Hz, 1H), 1.87-1.78 (m, 2H), 1.46 (s, 12H), 1.25-1.20 (m, 2H), 0.98 (dd, *J* = 8.0, 3.1 Hz, 2H)
Carbon-13 NMR	(125 MHz, $CDCl_3$): δ 172.9, 159.6, 146.3, 138.2, 135.6, 129.2, 128.9 (2C), 128.4, 127.2 (2C), 125.4, 84.7 (2C), 72.4, 68.5, 51.9, 42.7, 41.3, 25.3 (2C), 25.2 (2C), 15.4, 9.5, 9.3
Optical Rotatory Power	$[\alpha]^{20}{}_D$: +22.932 (*c* 1.00, MeOH)
HRMS	calcd for $C_{26}H_{34}BNO_6$ (M^+): 467.2479, found 467.2481
Mass Spectrum	MS (EI): 467 (M+, 6.8), 346 (100), 322 (80), 220 (92), 206 (57)
State	pale yellow solid

SciFinder^n A CAS SOLUTION

Agenda

- Introduction of CAS
- What is SciFinder^{n}?
- Content and Coverage searchable in SciFinder^{n}
- A few online Case studies – General interest
  - Substance searching
  - Reference searching and PatentPak
  - Reaction searching
- **CAS Retrosynthesis planner**
- Markush structure searching
- Questions and Answers

SciFinder^{n}
A CAS SOLUTION

CAS Retrosynthesis Planner

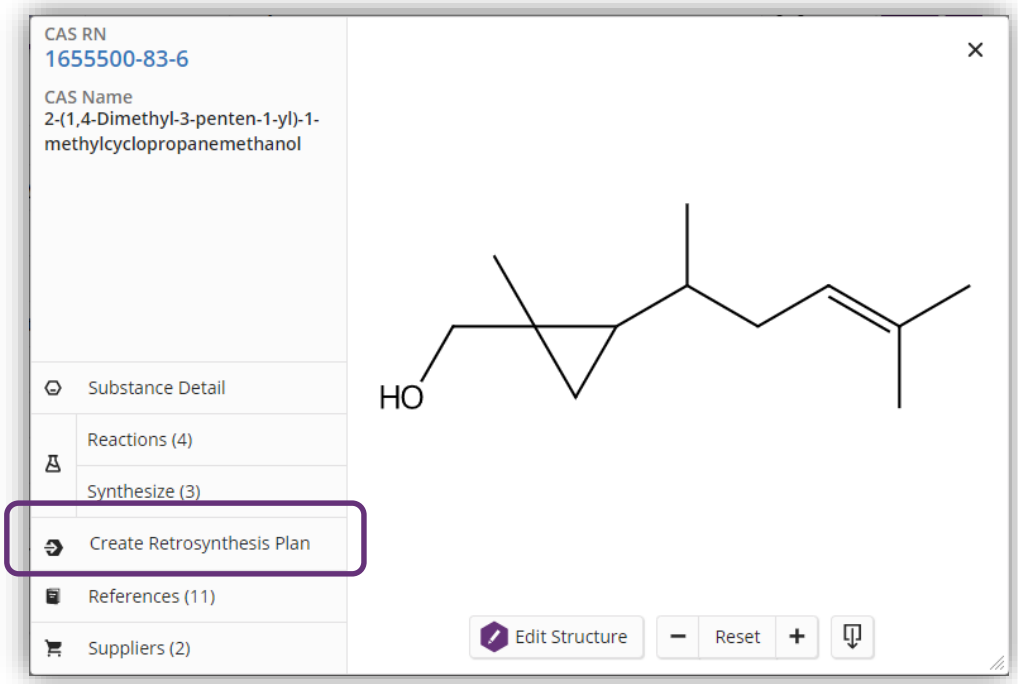
- For new or known molecules, SciFinder^n will perform a full retrosynthetic analysis utilizing the renowned CAS collection of reactions, presenting results in a highly intuitive and interactive synthesis plan.

- It will help,
  - Synthesizing new molecular innovations
  - Process development and scale up
  - Evaluating new synthetic options
  - Identifying opportunities for new breakthroughs in methods development

SciFinder^n
A CAS SOLUTION

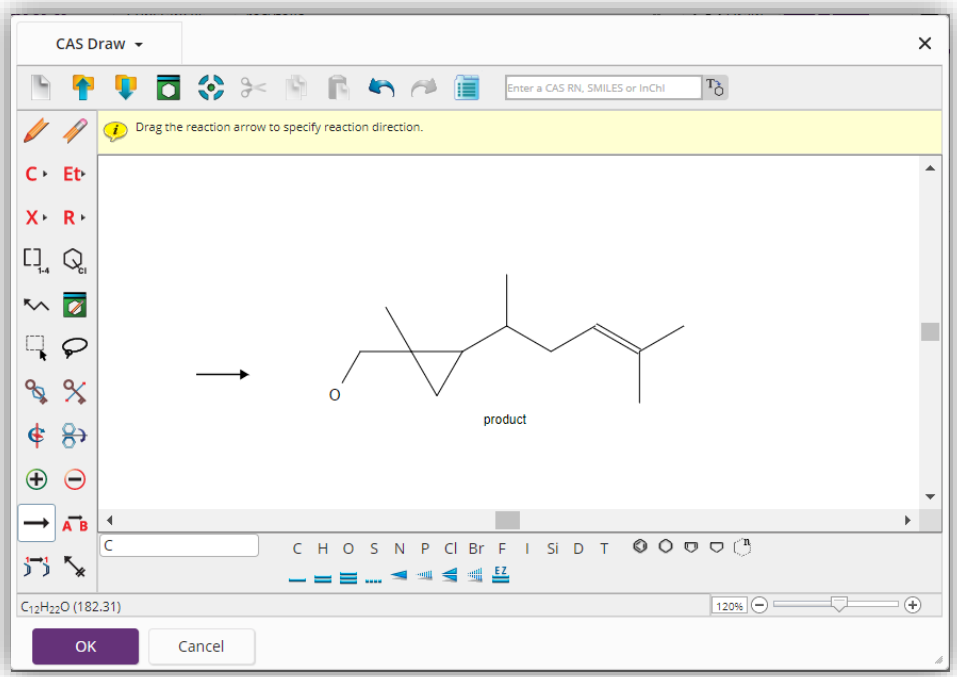
Creating retrosynthetic plan for required compound

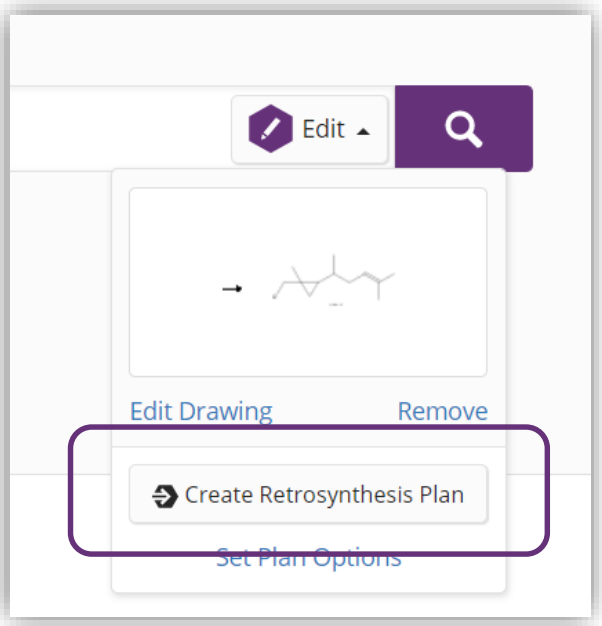
- Built retrosynthetic plan for ***Rosyfolia***



SciFinder^n
A CAS SOLUTION

Creating retrosynthetic plan for required compound





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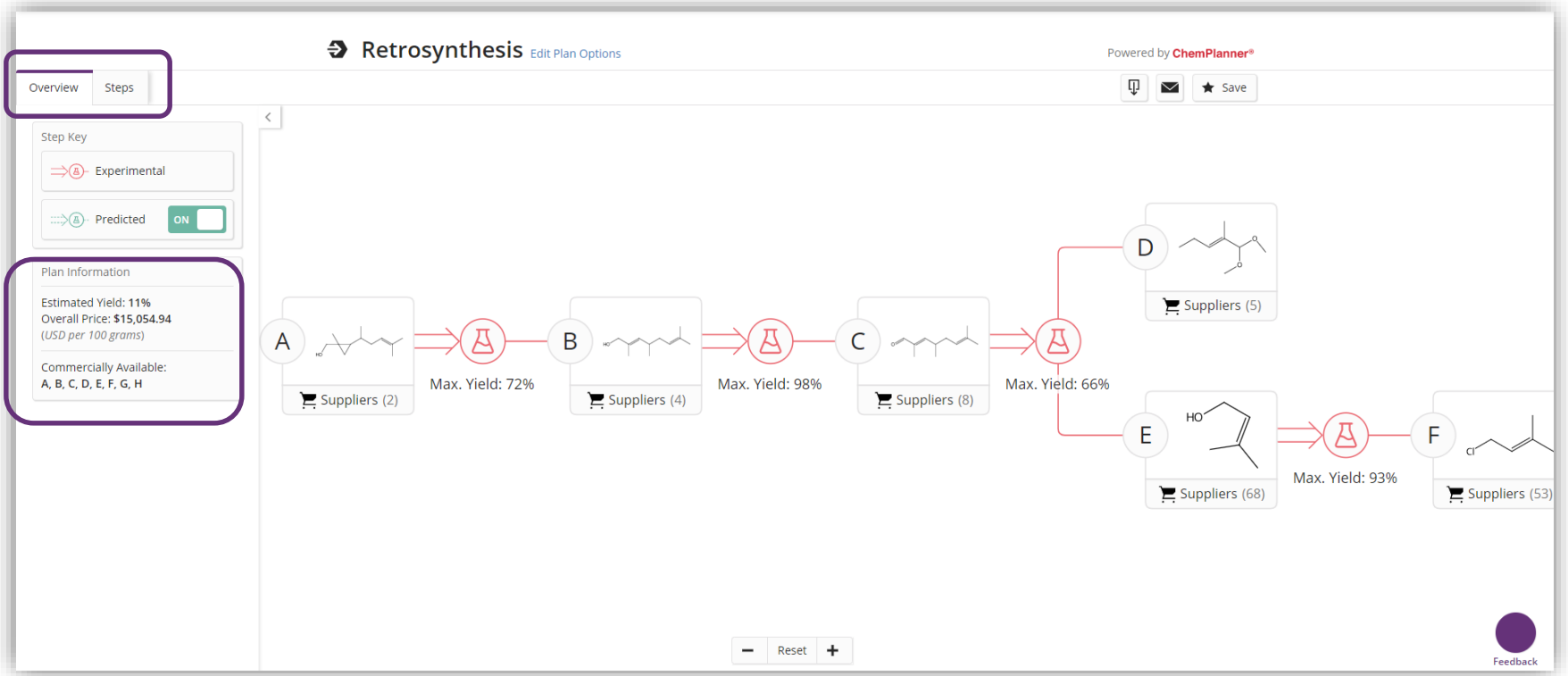
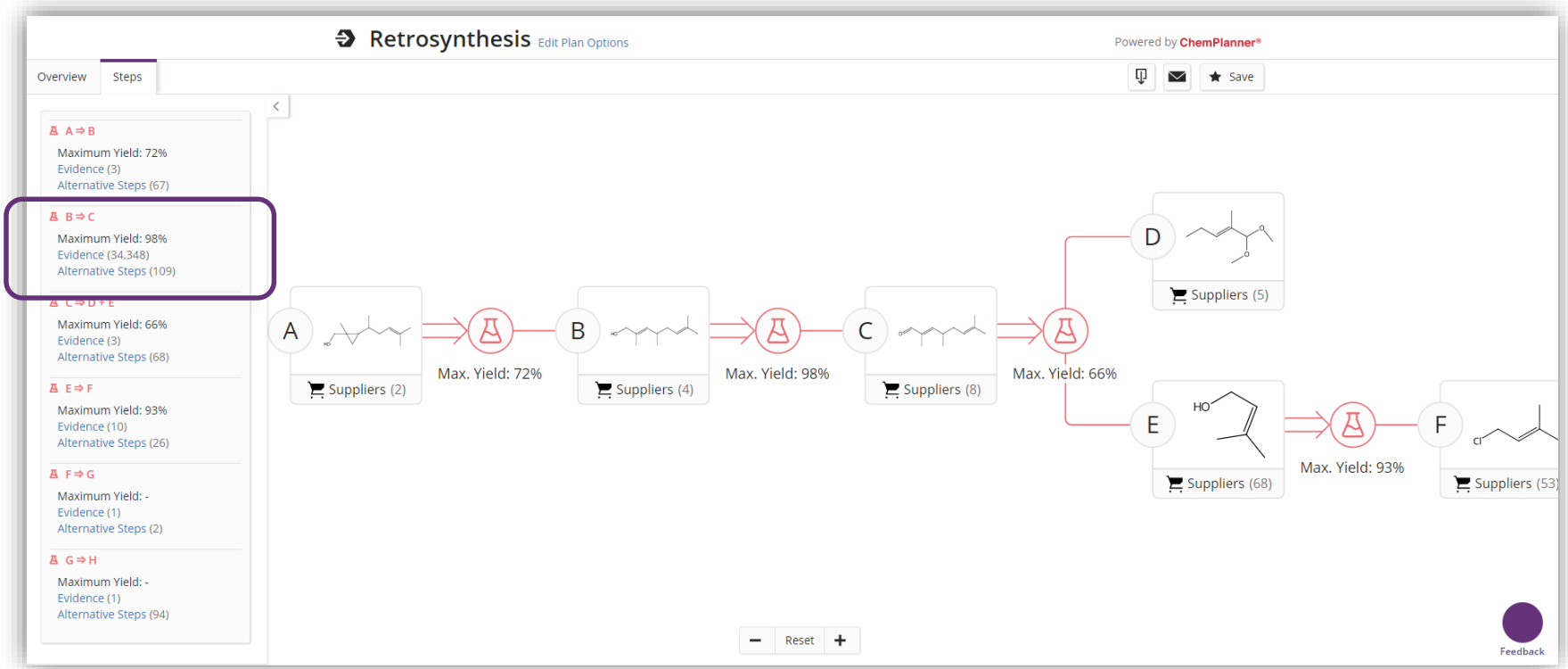
A CAS SOLUTION

Retrosynthesis plan



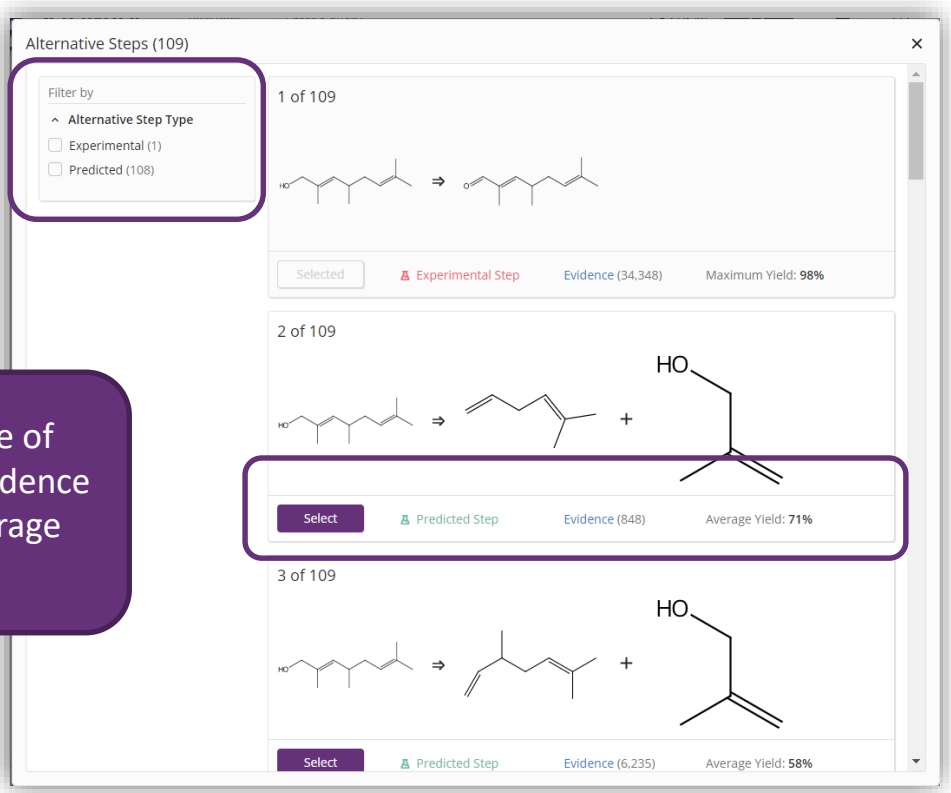
SciFinder^n
A CAS SOLUTION

Searching alternative step



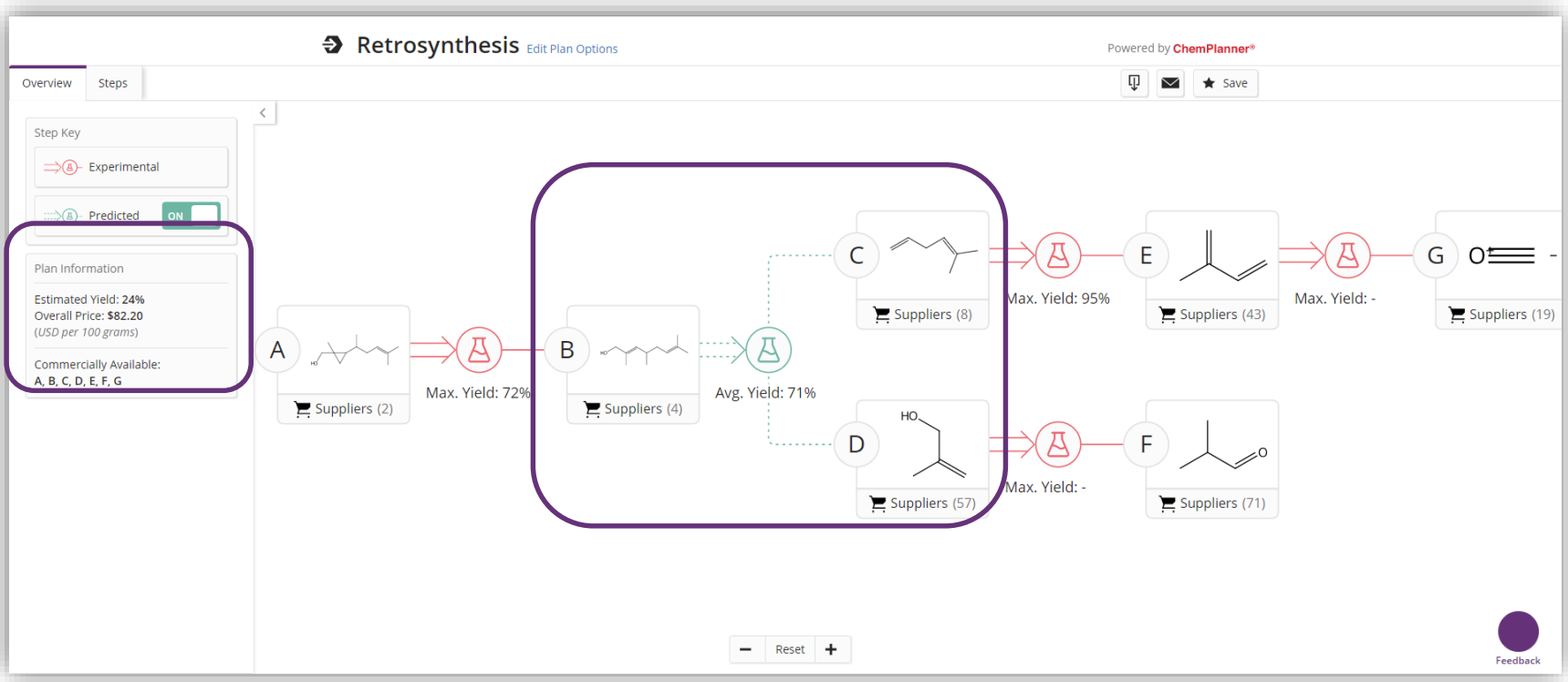
SciFinder^n
A CAS SOLUTION

Alternative steps (Experimental and Predictive)



Check for the type of alternative step, evidence reactions and average yield

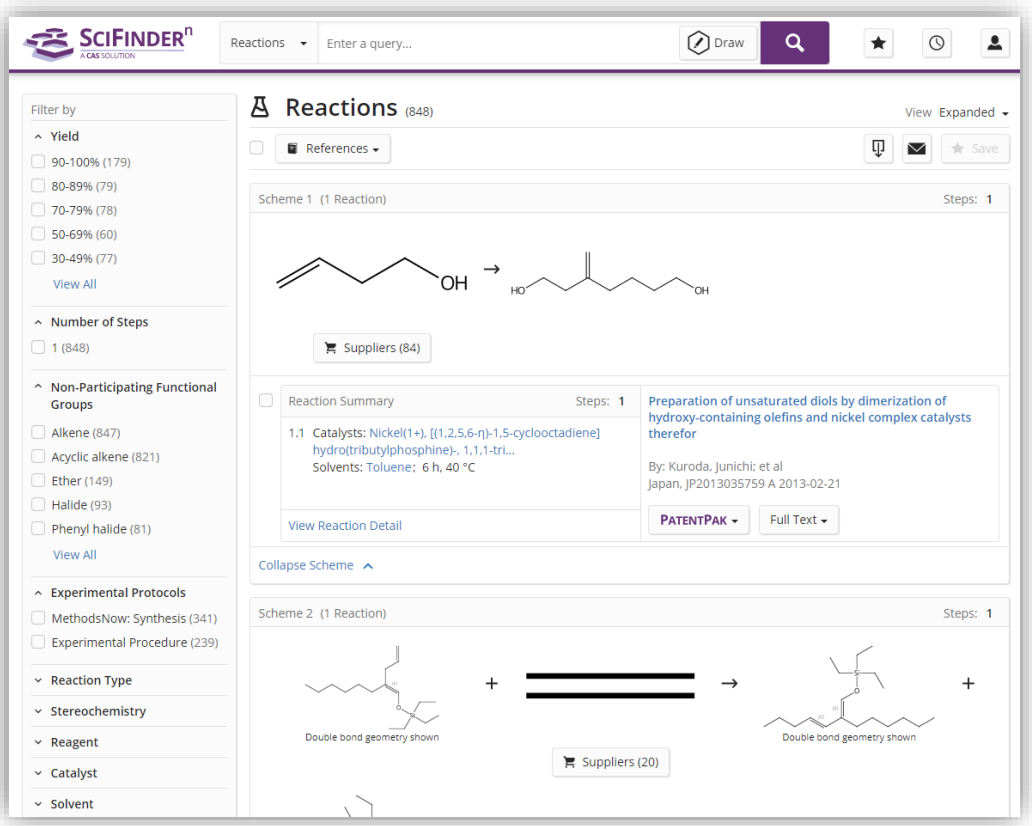
Incorporating predictive step



SciFinder^n
A CAS SOLUTION

Evident reactions

Retrieves all published reactions discussing same type of chemical transformation



SciFinder A CAS SOLUTION

Edit Plan Options

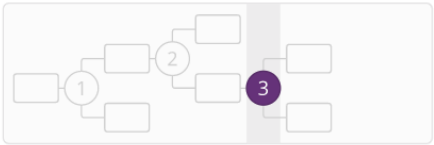
Plan Options

Powered by ChemPlanner®

Select Synthetic Depth

Synthetic depth restricts the number of steps generated in the plan. Learn More.

- 1
- 2
- 3
- 4



Set Rules Supporting Predicted Reactions

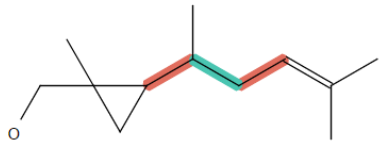
Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. Learn More.

- Common
- Uncommon (includes Common Rules)
- Rare (includes Common and Uncommon Rules)

Break and Protect Bonds

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. Learn More.

Break Bond | Protect Bond | Clear All Bond Selections



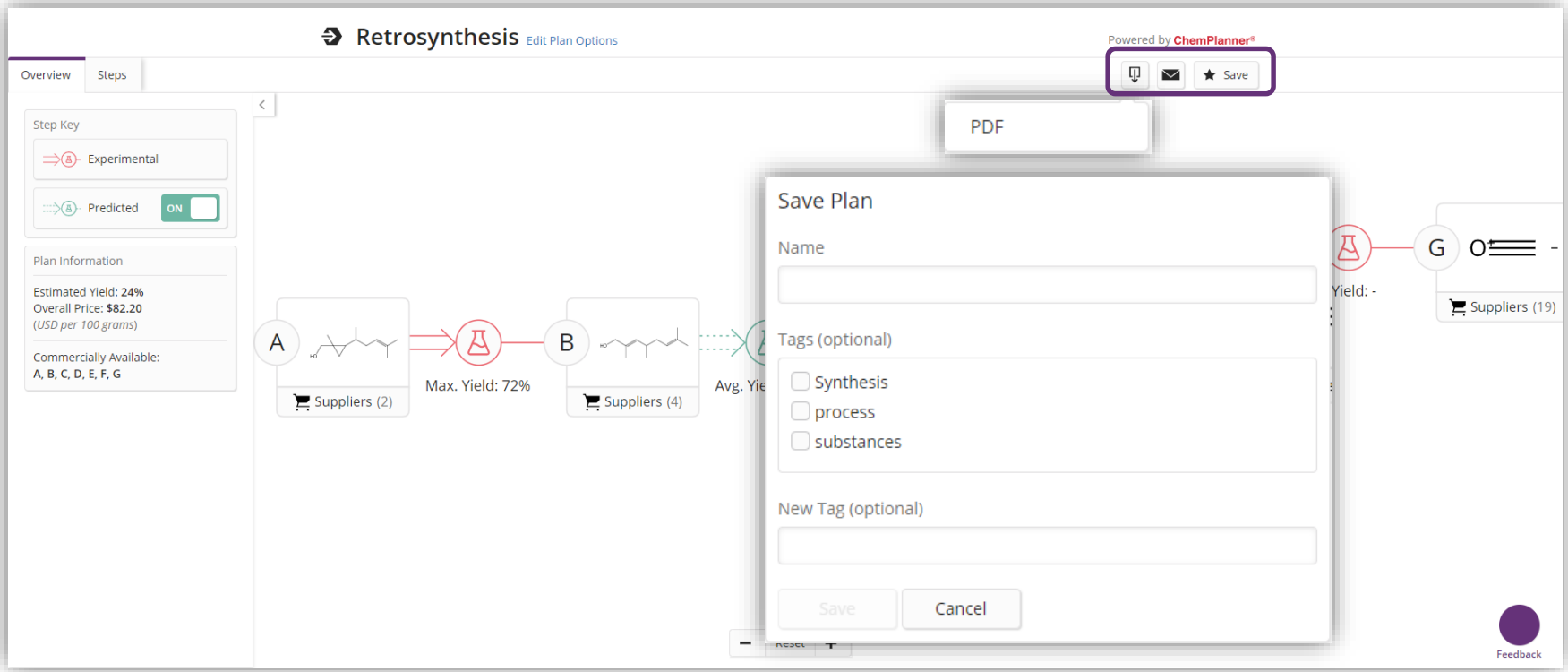
Create Retrosynthesis Plan

Break Bond

Protect Bond

SciFinder^n A CAS SOLUTION

Export, Share and Save retrosynthesis plan



SciFinder^n
A CAS SOLUTION

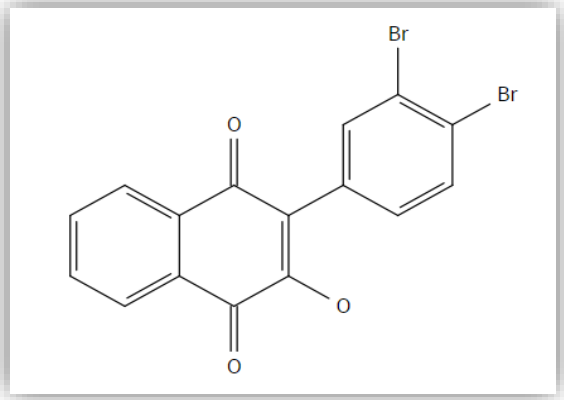
Agenda

- Introduction of CAS
- What is SciFinder^{n}?
- Content and Coverage searchable in SciFinder^{n}
- A few online Case studies – General interest
  - Substance searching
  - Reference searching and PatentPak
  - Reaction searching
- CAS Retrosynthesis planner
- **Markush structure searching**
- Questions and Answers

SciFinder^{n}
A CAS SOLUTION

Difficult to find some substances?

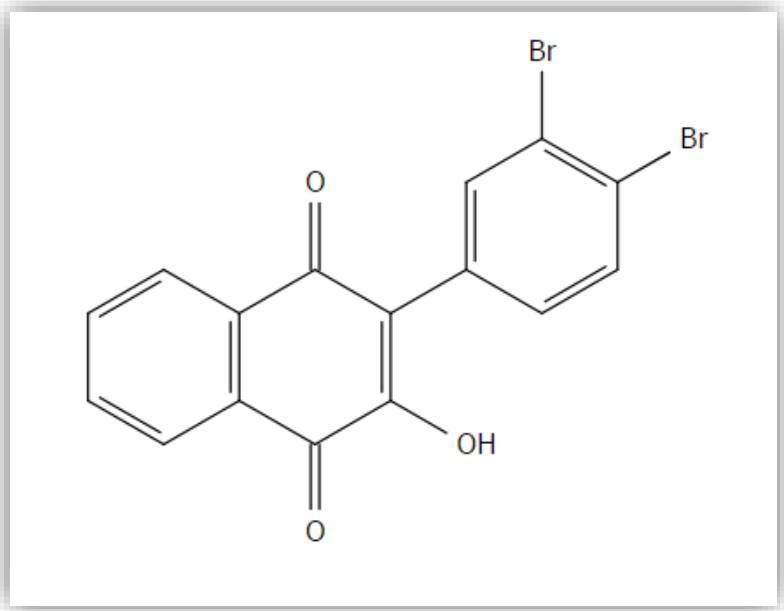
- Whether the substance I prepared is novel?
- Is the below substance claimed generically in any patent?

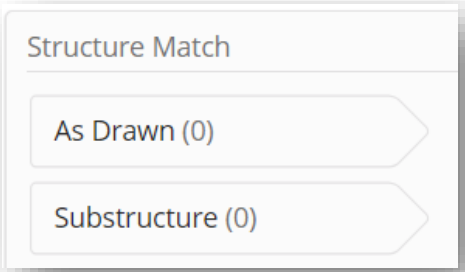


Find it with Markush search

SciFinder^n
A CAS SOLUTION

Is this substance indexed?





So is this substance is a novel substance?

SciFinder^n
A CAS SOLUTION

Indexing substances in patent

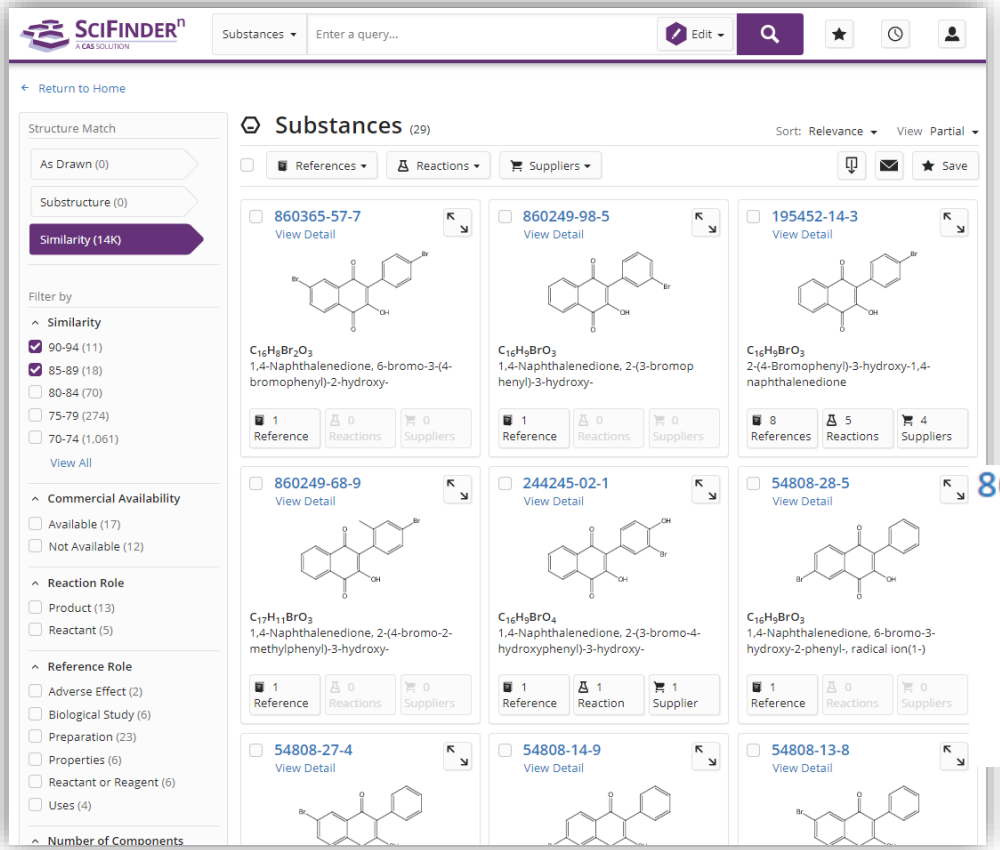
There are generally two types of substance indexing when it come to indexing in patent.

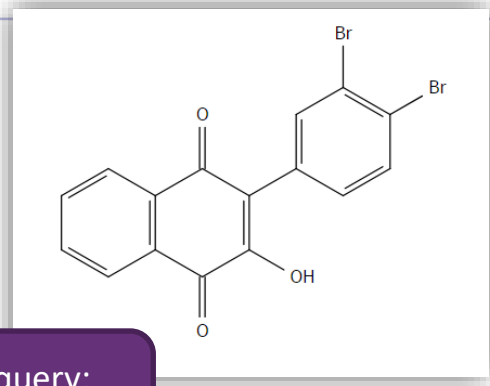
1. Specific substances: Represented with an exact structure and name. these substances also get CAS Registry number.

2. Generic substances: Represented with general or generic structure. So a single generic structure can represent hundreds of substances at once.

SciFinder^n
A CAS SOLUTION

Similar compounds available

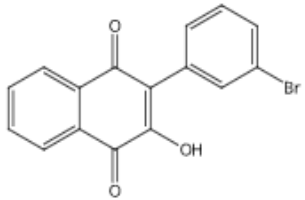


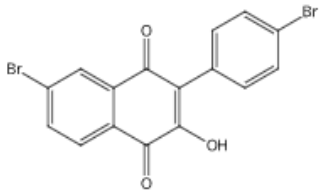


Searched query:
Similar substances:

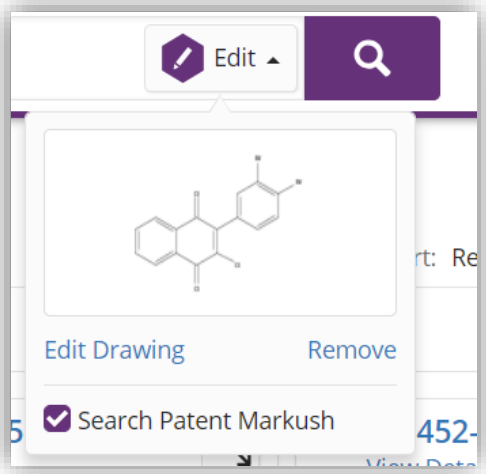
860365-57-7

860249-98-5

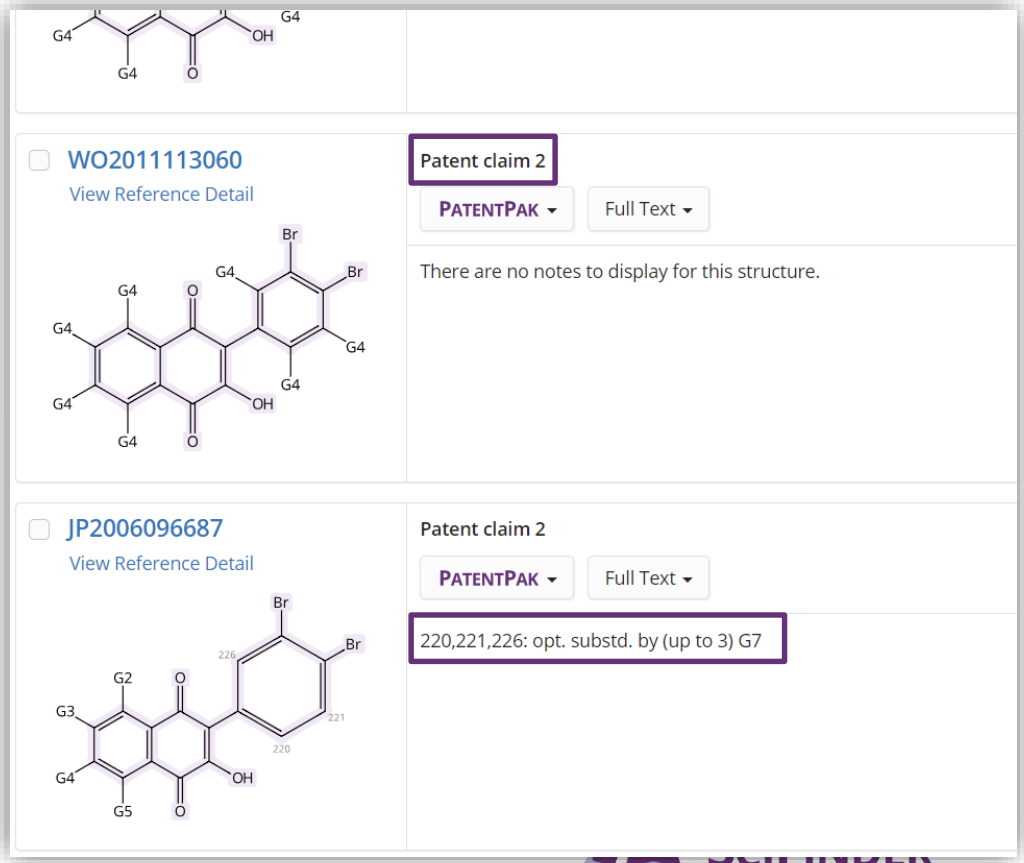




SciFinder n
A CAS SOLUTION



Know exact location of substance using PatentPak



Patent

Patent Information

Patent Number
JP2006096687

Publication Date
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Application Number
JP2004-282855

Application Date
2004-09-28

Kind Code
A

Assignee

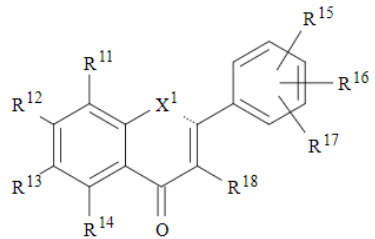
Riron Soyaku Kenkyusho K. K., Japan

Source
Japan

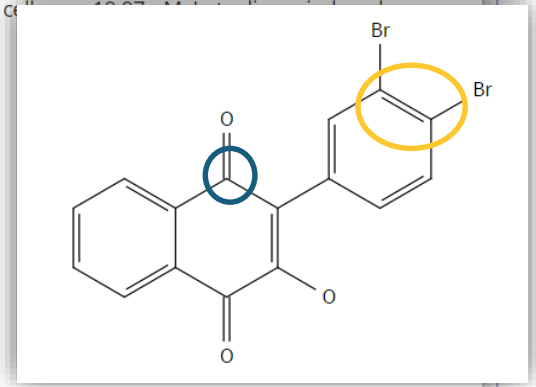
Glyoxalase I inhibitors containing compounds characterized by specific pharmacophores and screening of compounds showing glyoxalase I inhibiting or apoptosis inducing activity

By: Tanuma, Seiichi; Yoshimori, Atsushi

Abstract: Glyoxalase I (**I**) inhibitors, which induce apoptosis because of accumulation of methylglyoxal, contain ≥1 selected from compounds characterized by specific pharmacophores (a figure is given) and their glycosides. The compounds may be flavones or their analogs **I** [R^{11} = H, C_{1-6} alkoxy; R^{12} = H, OH, C_{1-6} alkoxy, aryl, aryl, aryloxy, halo, etc.; R^{13} = H, OH, c_{1-6} alkoxy, halo; R^{14} = H, OH; R^{15}-R^{17} = H, OH, C_{1-6} alkoxy, aryl, halo, etc.; R^{18} = H, OH, etc.; dotted line = direct bond or none; when dotted line is direct bond, then X^1 = O, S, CO, SO, SO_2, NR^{19} (R^{19} = H, C_{1-6} alkyl); when dotted line is none, then X^1 = H, OH, C_{1-6} alkoxy, amino, C_{1-6} alkylcarbonyl, etc.; X^2 = O, S, CO, SO, SO_2, NR^{19}], etc. Method for screening compounds which inhibit **I** or induce apoptosis, useful as antitumor agents, involves (1) a step to analyze pharmacophores of test compounds, (2) a step to examine whether or not the pharmacophores agree the above specific pharmacophores, and (3) a step to measure **I**-inhibiting activity. Thus, IC_{50} of luteolin on **I** derived from HL-60 c… apoptosis of HL-60 cells with ED_{50} 28.3 μM.



I

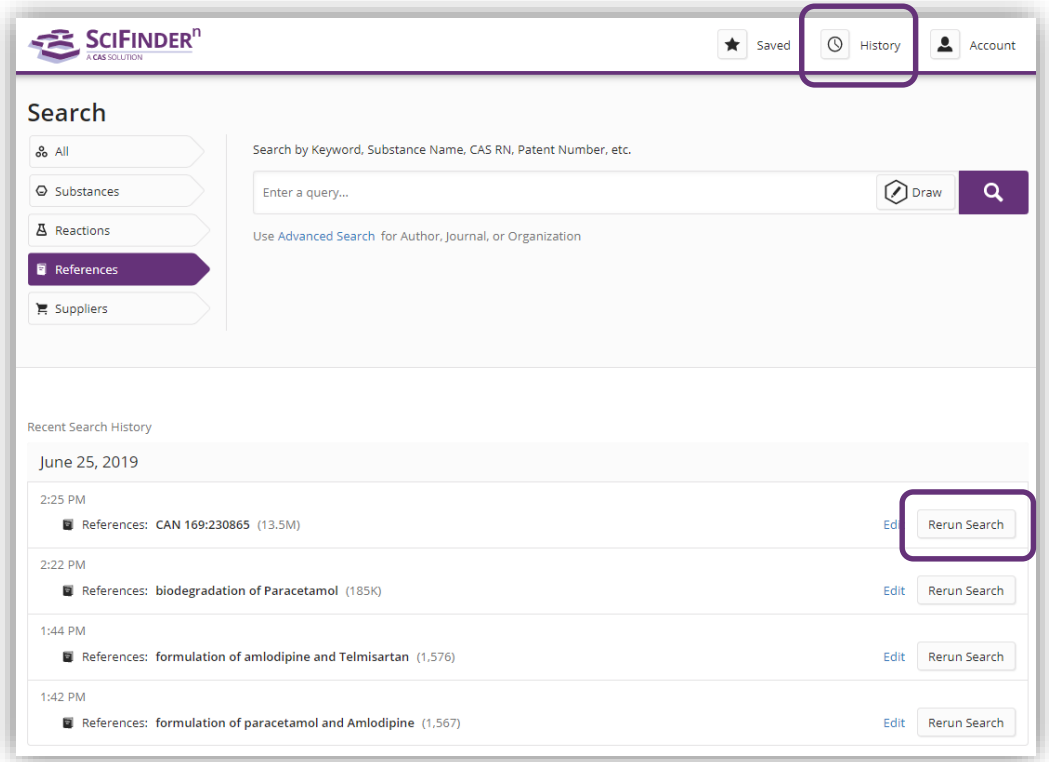


PATENTPAK PDF | Full Text

SCIFINDER^n A CAS SOLUTION

Search history

Rerun the resent search.

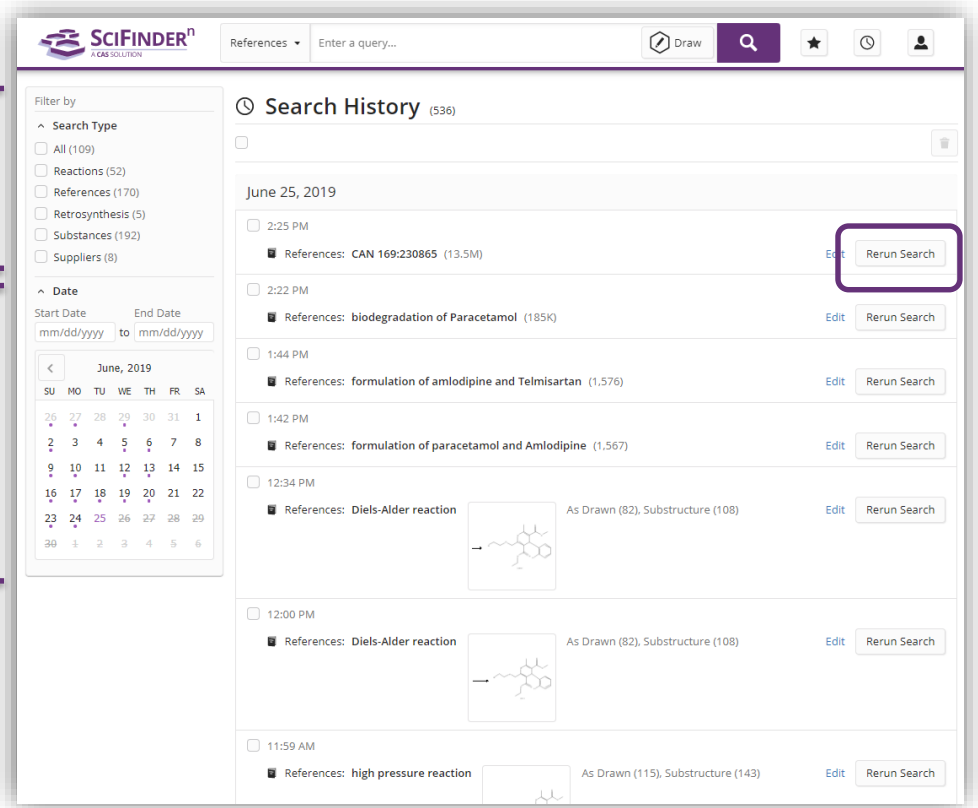


SciFinder n
A CAS SOLUTION

Search history

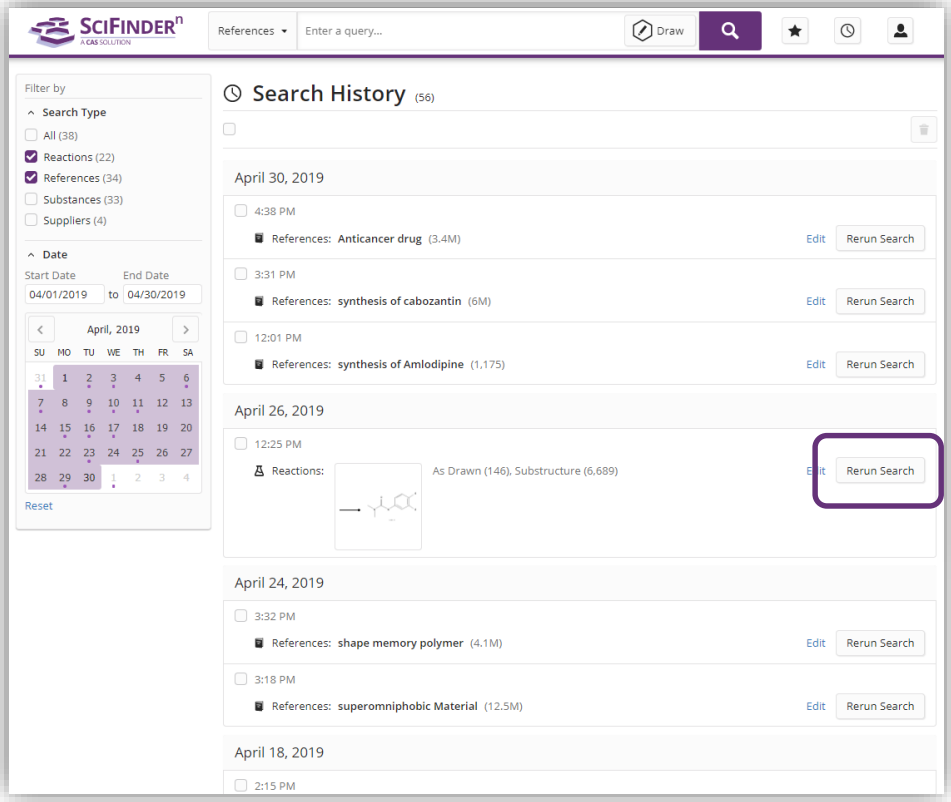
Handpick a type of search from search history

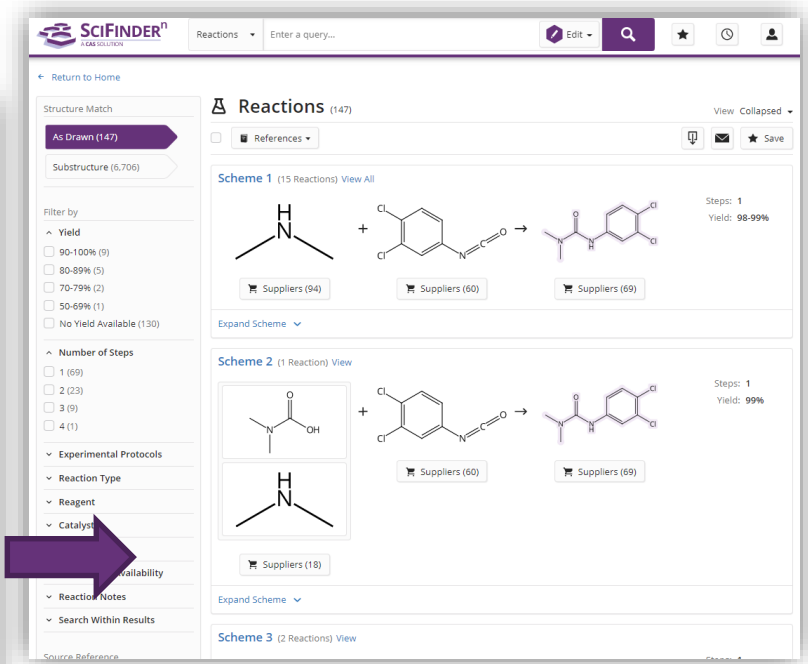
Assign a range of dates or select a particular month to search the history and rerun the search to get all previously viewed data.



SciFinder n
A CAS SOLUTION

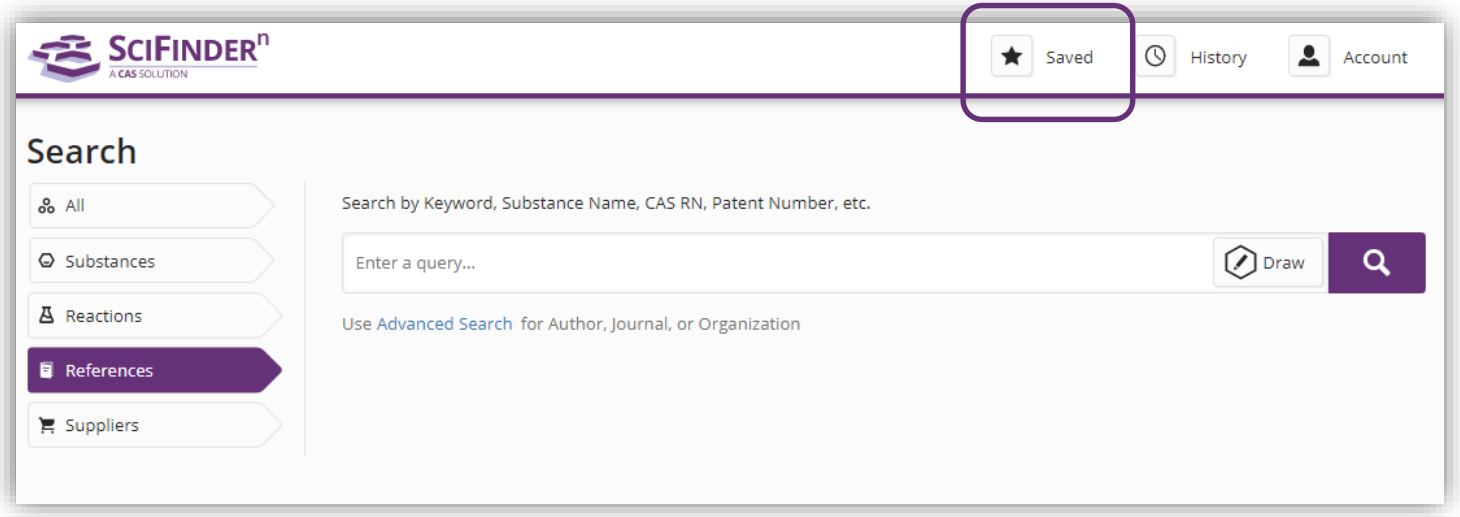
For example





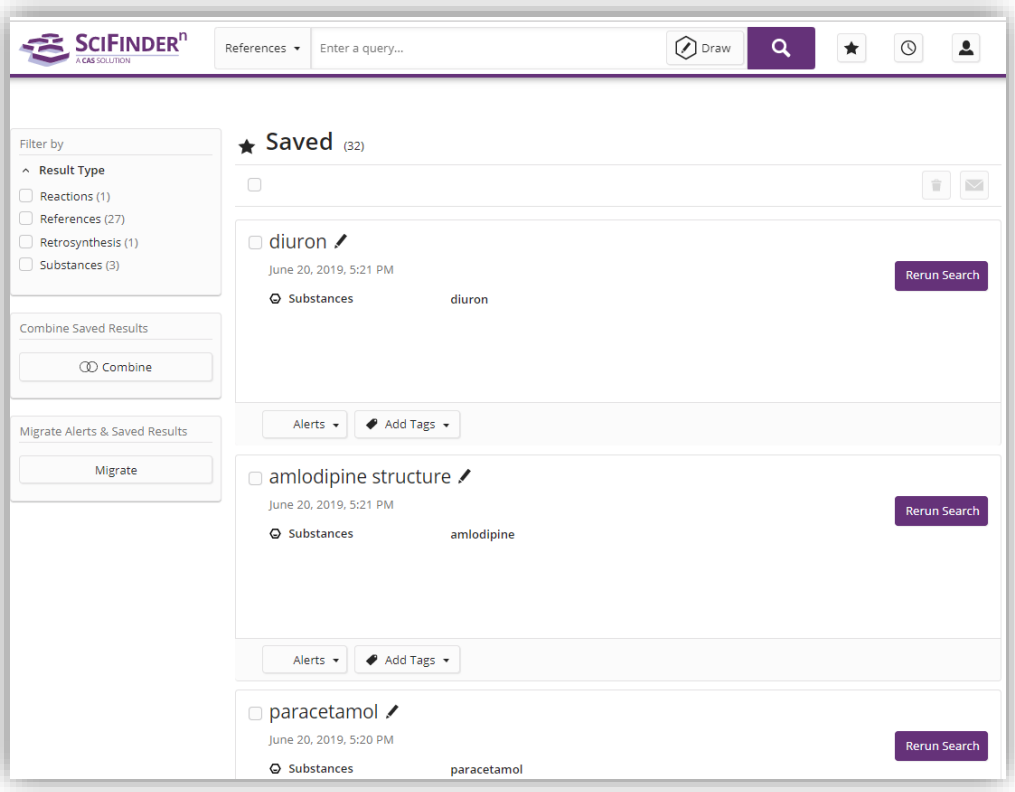
SciFinder A CAS SOLUTION

Access all saved answer sets



SciFinder n
A CAS SOLUTION

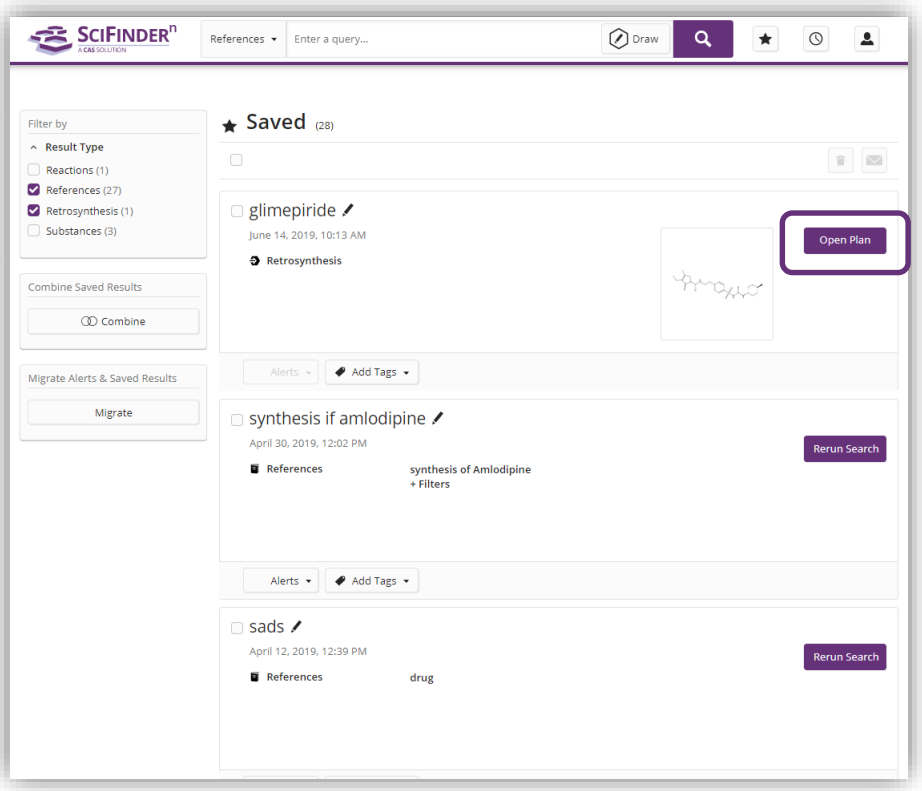
Overview



SciFinder n
A CAS SOLUTION

Search according to result type

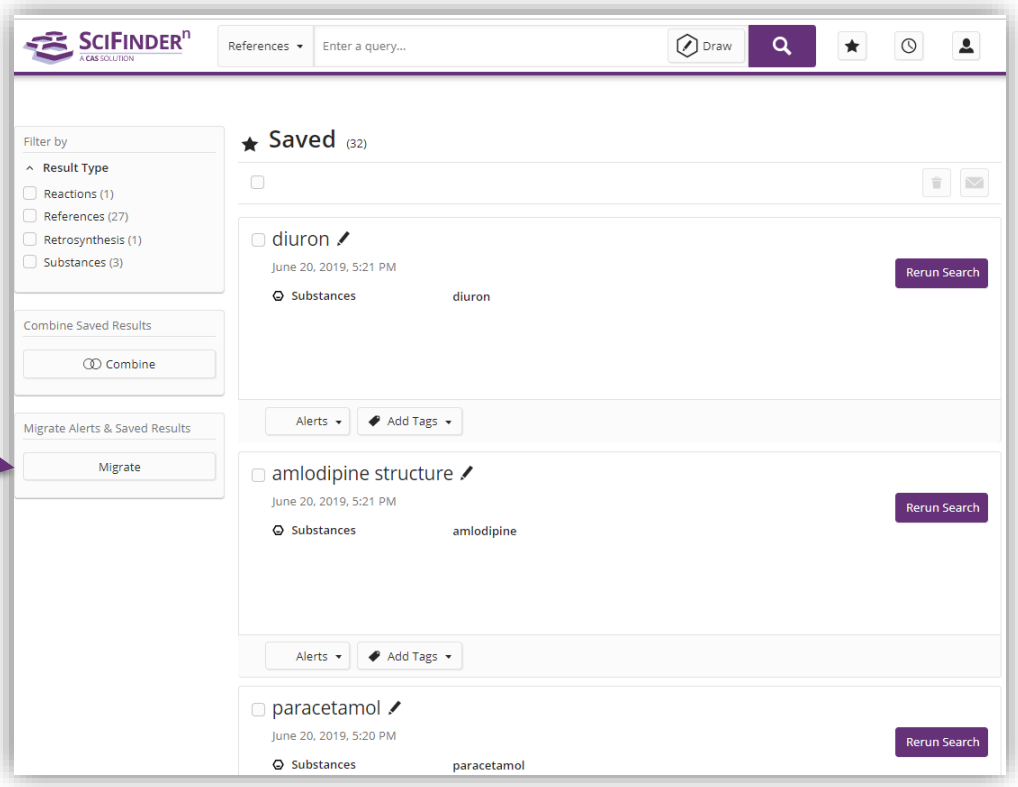
Select any result type and rerun the search



SciFinder^n
A CAS SOLUTION

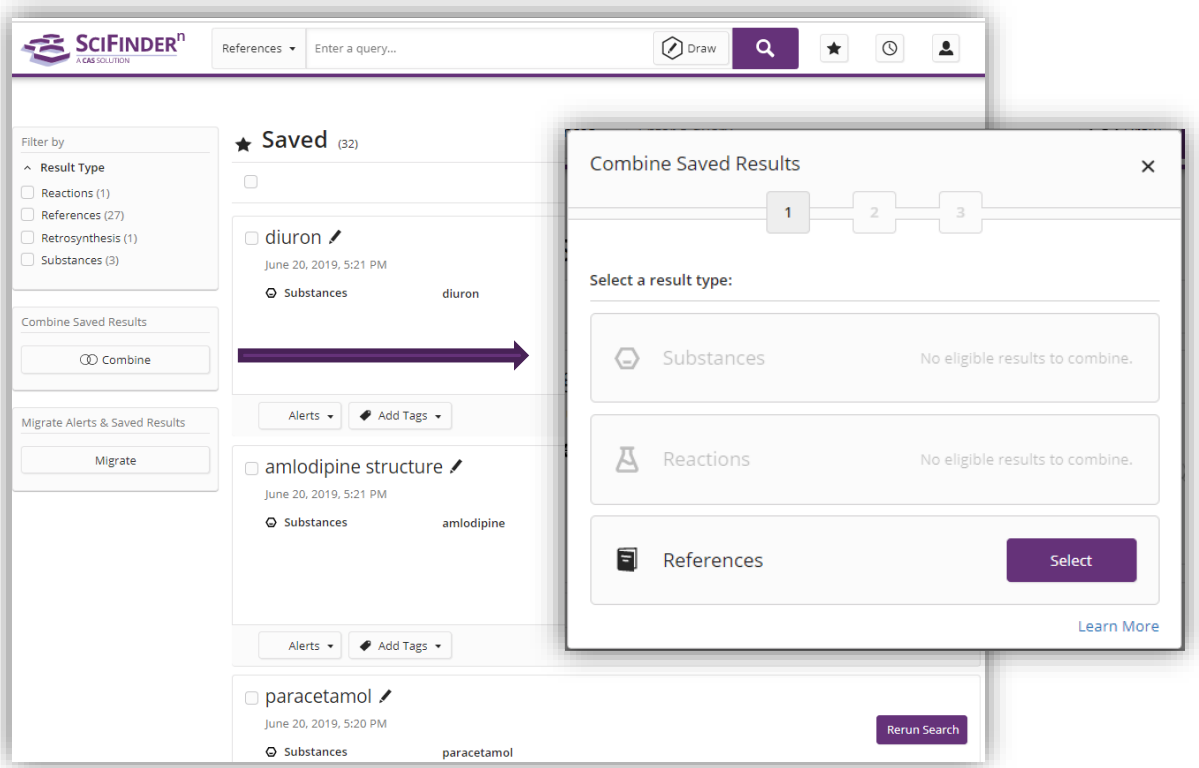
Migrate from SciFinder

Migrate all saved references, substances or Keep me posted alerts from SciFinder if any



SciFinder n
A CAS SOLUTION

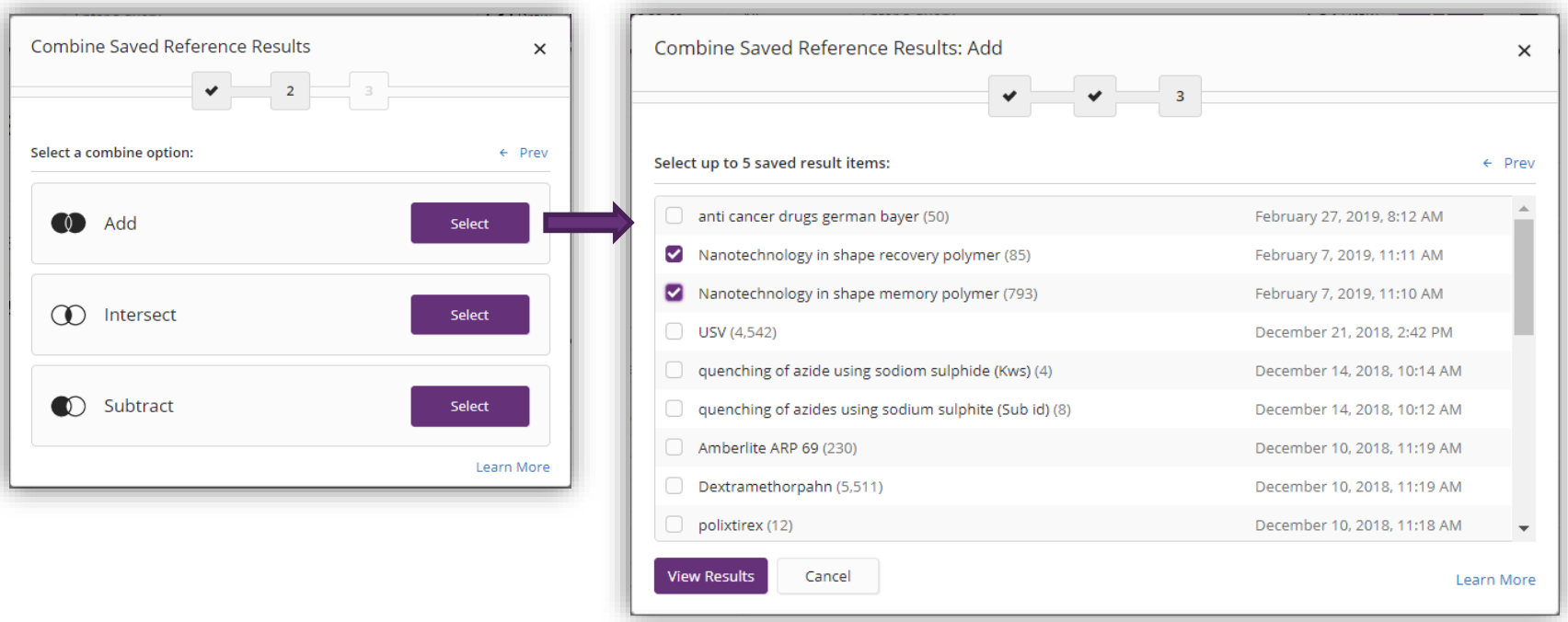
Combine option



Saved reference sets can be combined, intersected or excluded to get expected set of references

SciFinder n
A CAS SOLUTION

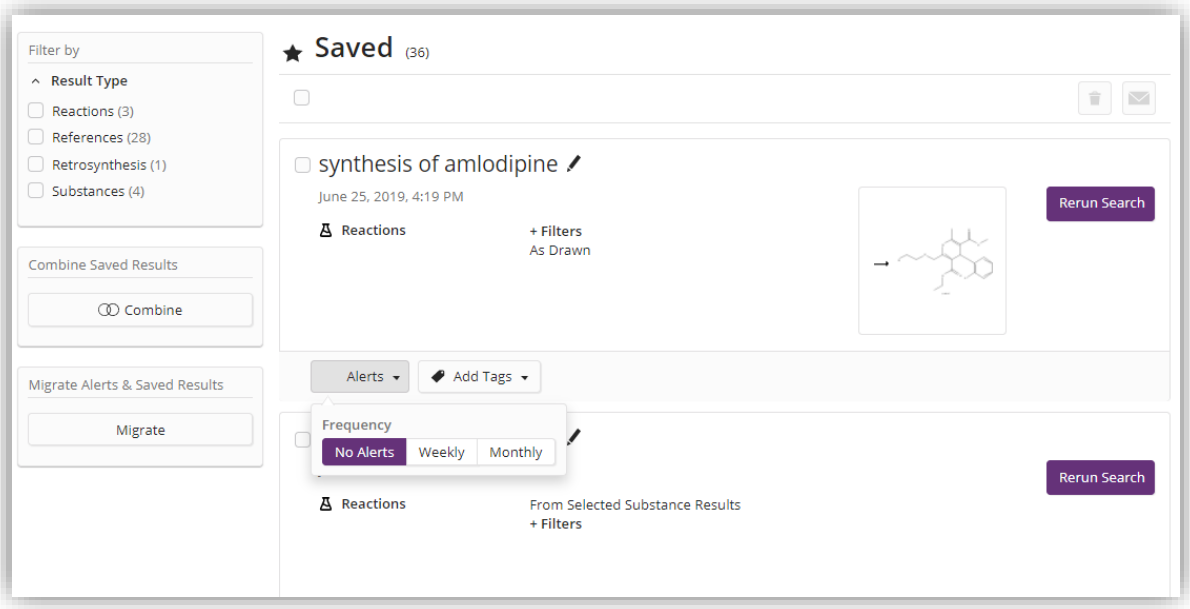
Select sets of references to run desired combine option



SciFinder^{n}
A CAS SOLUTION

Stay updated

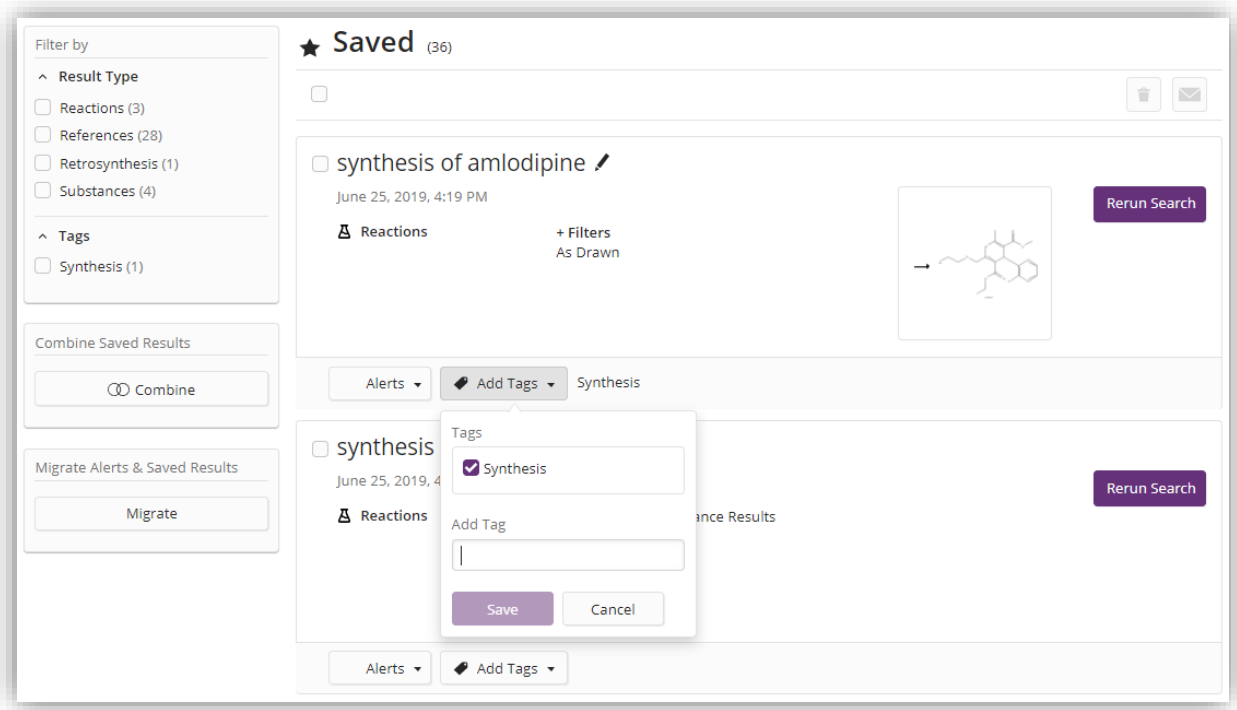
Assign alerts with required frequency to stay updated



SciFinder^n
A CAS SOLUTION

Add tags

Add a pre-saved tag or assign a new tag to saved answer



SciFinder^n
A CAS SOLUTION

Thank You!

For any additional information, please contact us at

info@acs-i.org

SciFinder^n
A CAS SOLUTION