Vinit Kunte

Application Spacilist

vkunte@acs-i.org

7738818353

CAS is a division of the American Chemical Society.
Copyright 2017 American Chemical Society. All rights reserved.

SciFinder®
A CAS SOLUTION

What are we going to discuss

- Introduction to CAS
- Introduction to SciFinder
- Contents available in SciFinder
- Examples and case study
- Advantages
- New enhancements
- Questions and answers

CAS is a division of the American Chemical Society.
Copyright 2017 American Chemical Society. All rights reserved.

SciFinder®
A CAS SOLUTION

Chemical Abstract Service

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

SciFinder®
A CAS SOLUTION

Value added Indexing

(12) 发明专利申请

(10) 申请公布号 CN 102836446 A
(43) 申请公布日 2012.12.26

(21) 申请号 201210158275.9

(22) 申请日 2012.05.21

(71) 申请人 华中科技大学
地址 430074 湖北省武汉市洪山区珞瑜路 1037 号

(72) 发明人 刘卫 徐海波 陈云超 杨祥良 程欣 李欢 罗斌华 万江陵 周小顺

(74) 专利代理机构 华中科技大学专利中心 42201
代理人 曹葆青

(51) Int. Cl.
A61K 49/18 (2006.01)
A61K 49/22 (2006.01)
A61K 9/10 (2006.01)
A61K 45/00 (2006.01)
A61K 47/34 (2006.01)
A61P 35/00 (2006.01)

权利要求书

(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

27. 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
Assignee: Huazhong University of Science and Technology, Peop. Rep. China

The title nanobubble comprises filling material with perfluoropentane as core, which can have liq.-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%, liq. perfluoropentane 0.1-5% and pure water. The polyphosphate-polyester copolymer (av. mol. wt. 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 prepn. method consists of dissolving polyphosphate-polyester copolymer in mixt. of Et acetate and THF to obtain oil phase 1, using liq. 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 mixt. through hollow-membrane tube, pouring mixt. into normal saline, stirring at 25°C by magnetic force, removing org. solvent by extn. The hollow-membrane tube is prepd. 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.

Patent Information

Patent No.	Kind	Date	Application No.	Date
CN 102836446	A	Dec 26, 2012	CN 2012-10158275	May 21, 2012

Value added indexing

Chinese patent

Abstract of CN102836446 (A)

Translate this text into

Bulgarian

patenttranslate powered by EPO and Google

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-multiple 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-containing nanobubble. By means of the specific combination of a targeting factor and a tumor cell, the nan
focus ultrasonic imaging effect. The nanobubble can be loaded wi
The nanobubble can also be loaded with an antitumor drug and u
treatment integrated multifunctional imageological nano-contrast

27. 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
Assignee: Huazhong University of Science and Technology, Peop. Rep. China

The title nanobubble comprises filling material with perfluoropentane as core, which can have liq.-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%, liq. perfluoropentane 0.1-5% and pure water. The polyphosphate-polyester copolymer (av. mol. wt. 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 prepn. method consists of dissolving polyphosphate-polyester copolymer in mixt. of Et acetate and THF to obtain oil phase 1, using liq. 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 mixt. through hollow-membrane tube, pouring mixt. into normal saline, stirring at 25°C by magnetic force, removing org. solvent by extn. The hollow-membrane tube is prepd. 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.

Patent Information

Patent No.	Kind	Date	Application No.	Date
CN 102836446	A	Dec 26, 2012	CN 2012-10158275	May 21, 2012

Concepts

Antitumor agents
Ceramics
Dissolution
Extraction
Imaging agents
Liver, neoplasm
Microstructure
NMR imaging
NMR imaging agents
Particle size
Particle size distribution
Physiological saline solutions
Stability
Zeta potential

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

Biological use, unclassified; Biological study; Uses

Fluoropolymers
Polycarbonates
Polysulfones

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

Other use, unclassified; Uses

Lactoferrins
Transferrins

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

Reactant; Reactant or reagent

Substances

1317-61-9P Ferroferric oxide, biological studies

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

Diagnostic use; Properties; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses

50-18-0 Cyclophosphamide
51-21-8 5-Fluorouracil
59-05-2 Methotrexate
147-94-4 Cytarabine
1404-00-8 Mitomycin
10540-29-1 Tamoxifen
25316-40-9 Adriamycin
33069-62-4 Paclitaxel
114977-28-5 Docetaxel

Roles

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

Pharmacokinetics; Therapeutic use; Biological study; Uses

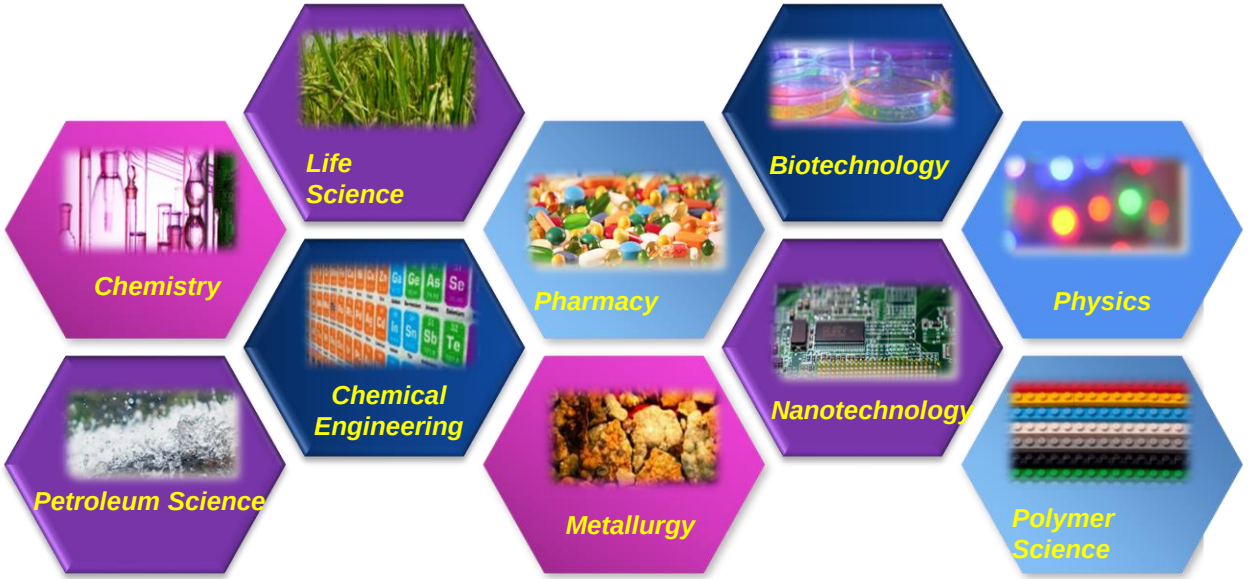
326604-67-5P

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

Properties; Reactant; Synthetic preparation; Preparation; Reactant or reagent

59-30-3 Folic acid, reactions
64-17-5 Ethanol, reactions
67-63-0 Isopropanol, reactions
111-27-3 n-Hexanol, reactions

Comprehensive coverage



Helps you explore vast research areas !!

Find application of your research in inter-disciplinary areas

SciFinder®
A CAS SOLUTION

SciFinder covers 80 different sections

Toxicology

1. Pharmacology
2. Mammalian Hormones
3. Biochemical Genetics
4. Toxicology
5. Agrochemical Bioregulators
6. General Biochemistry
7. Enzymes

Biochemistry

8. Radiation Biochemistry
9. Biochemical Methods
10. Microbial, Algal, and Fungal Biochemistry
11. Plant Biochemistry
12. Nonmammalian Biochemistry
13. Mammalian Biochemistry
14. Mammalian Pathological Biochemistry
15. Immunochemistry
16. Fermentation and Bioindustrial Biochemistry
17. Food and Feed Chemistry
18. Animal Nutrition
19. Fertilizers, Soils, and Plant Nutrition
20. History, Education, and Documentation

Organic

21. General Organic Chemistry
22. Physical Organic Chemistry
23. Aliphatic Compounds
24. Alicyclic Compounds
25. Benzene, Its Derivatives, and Condensed Benzenoid Compounds
26. Biomolecules and Their Synthetic Analogs
27. Heterocyclic Compounds (One Hetero Atom)
29. Organometallic and Organometalloidal

Natural Products

30. Terpenes and Terpenoids
31. Alkaloids
32. Steroids
33. Carbohydrates

Polymers

34. Amino Acids, Peptides, and Proteins
35. Chemistry of Synthetic High Polymers
36. Physical Properties of Synthetic High Polymers
37. Plastics Manufacture and Processing
38. Plastics Fabrication and Uses

macromolecular

39. Synthetic Elastomers and Natural Rubber
40. Textiles and Fibers
41. Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers

Physical, Nuclear

47. Apparatus and Plant Equipment
48. Unit Operations and Processes
49. Industrial Inorganic Chemicals
50. Propellants and Explosives
51. Fossil Fuels, Derivatives, and Related Products

Material

52. Electrochemical, Radiational, and Thermal Energy Technology
53. Mineralogical and Geological Chemistry
54. Extractive Metallurgy
55. Ferrous Metals and Alloys
56. Nonferrous Metals and Alloys
57. Ceramics
58. Cement, concrete, and Related Building Materials

Environmental

59. Air Pollution and Industrial Hygiene
60. Waste Treatment and Disposal
61. Water

Pharma

62. Essential Oils and Cosmetics
63. Pharmaceuticals
64. Pharmaceutical Analysis

SciFinder® A CAS SOLUTION

And Many More…….

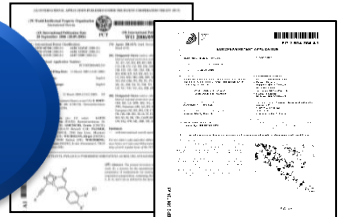
Content & Coverage- References

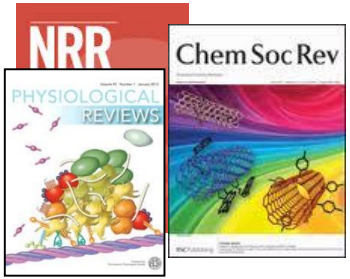
Worldwide coverage of references for many scientific disciplines all in one source

Updated Daily

>48M
Journal Articles, Patents & Dissertations
Covered till early 1800

63 Patent issuing authorities



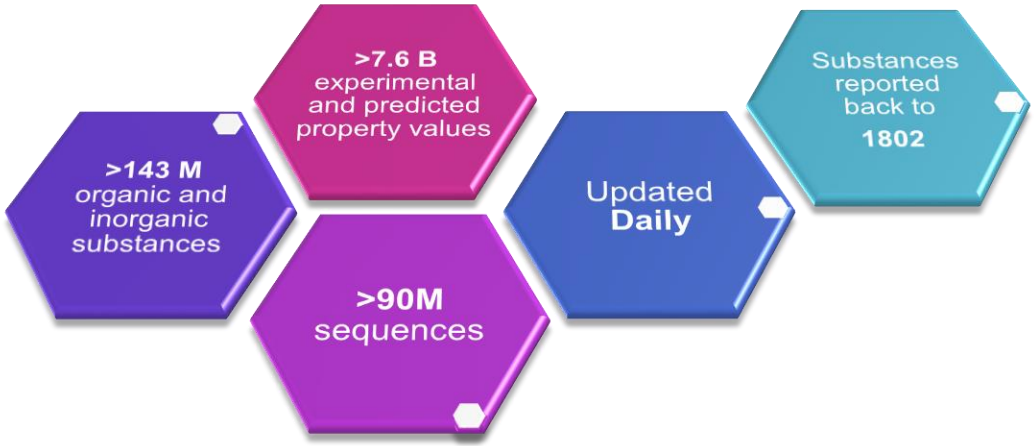


>10,000 Journals publications

Document Types		
	☐ Biography	☐ Historical
	☐ Book	☐ Journal
	☐ Clinical Trial	☐ Letter
	☐ Commentary	☐ Patent
	☐ Conference	☐ Preprint
	☐ Dissertation	☐ Report
	☐ Editorial	☐ Review

Content & Coverage- Substances

SciFinder has the world's Largest collection of substance-the gold standard for chemical substance information



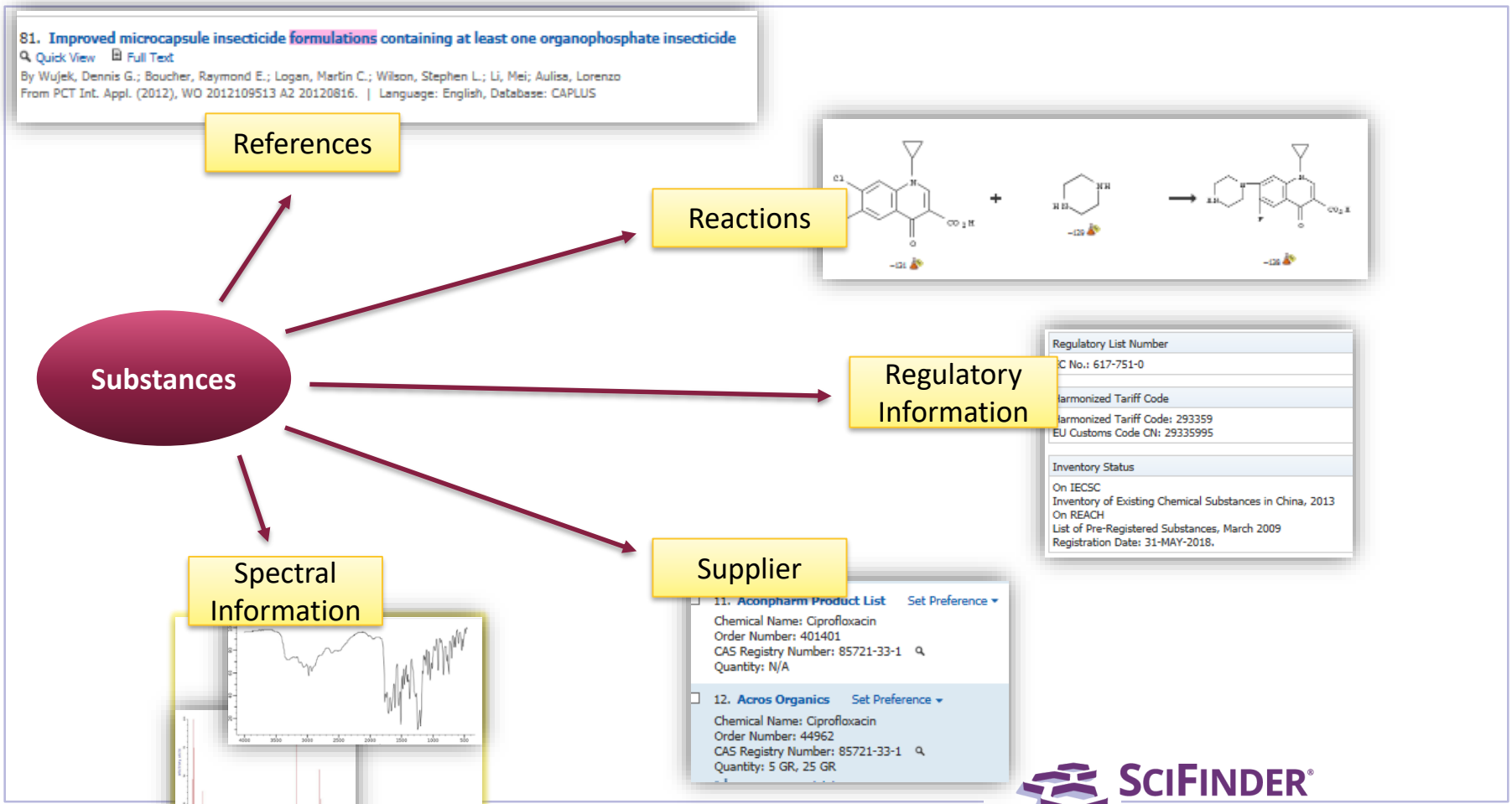
SciFinder®
A CAS SOLUTION

CAS is a division of the American Chemical Society.
Copyright 2018 American Chemical Society. All rights reserved.

Exploring Substance related Information on SciFinder

Types of substances:

- Organic compounds
- Inorganic compounds
- Coordination compounds
- Sequences
- Small Biologicals (Enzymes, Immunoglobulins)
- Polymers
- Compounds referred to by designation(eg.,lab code)
- Salts
- Hydrates
- Mixtures



CAS is a division of the American Chemical Society.
Copyright 2018 American Chemical Society. All rights reserved.

SciFinder® A CAS SOLUTION

Case Study

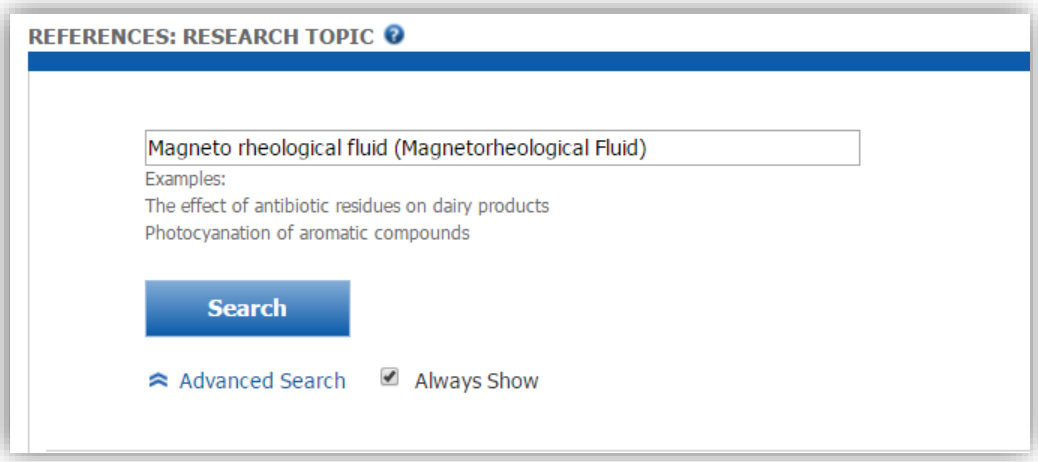
- Locate references since 2012 discussing Magneto-rheological fluids.
- Locate the top organizations working on the same

Search Strategy:-

a) Explore by Research Topic
b) Refine by Publication year

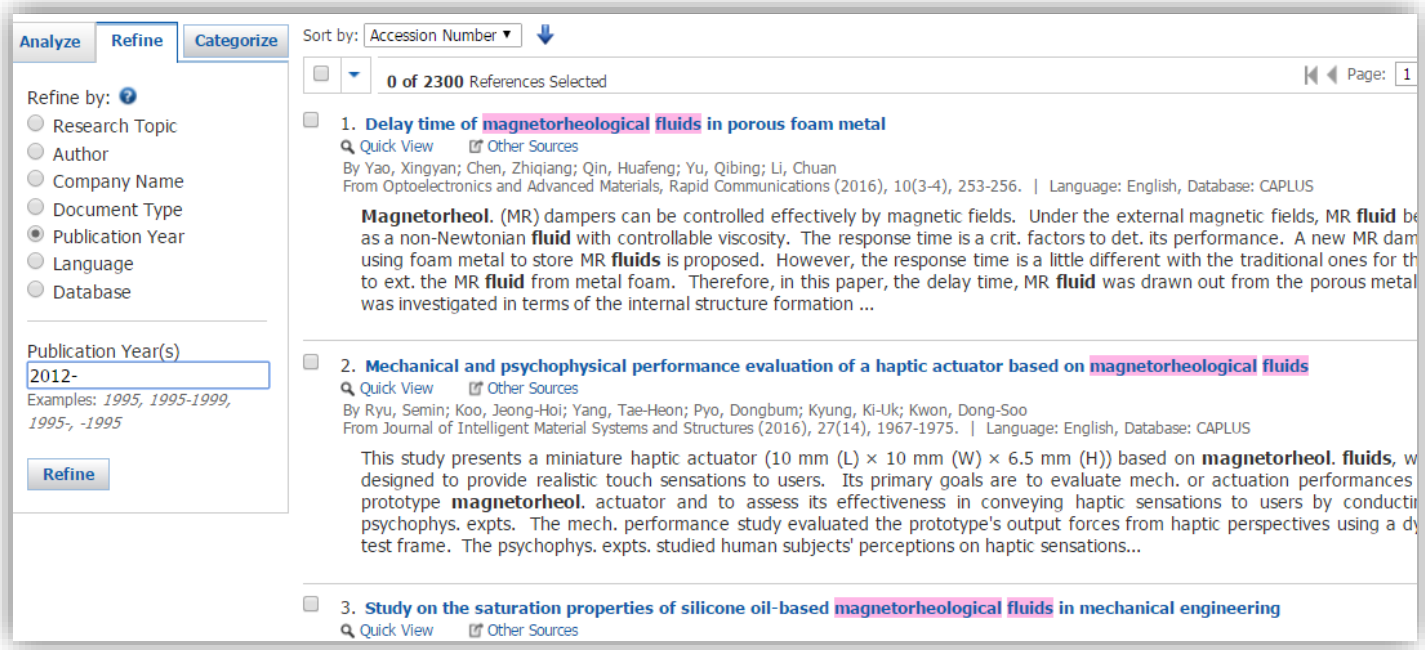
SciFinder®
A CAS SOLUTION

Search by Keyword



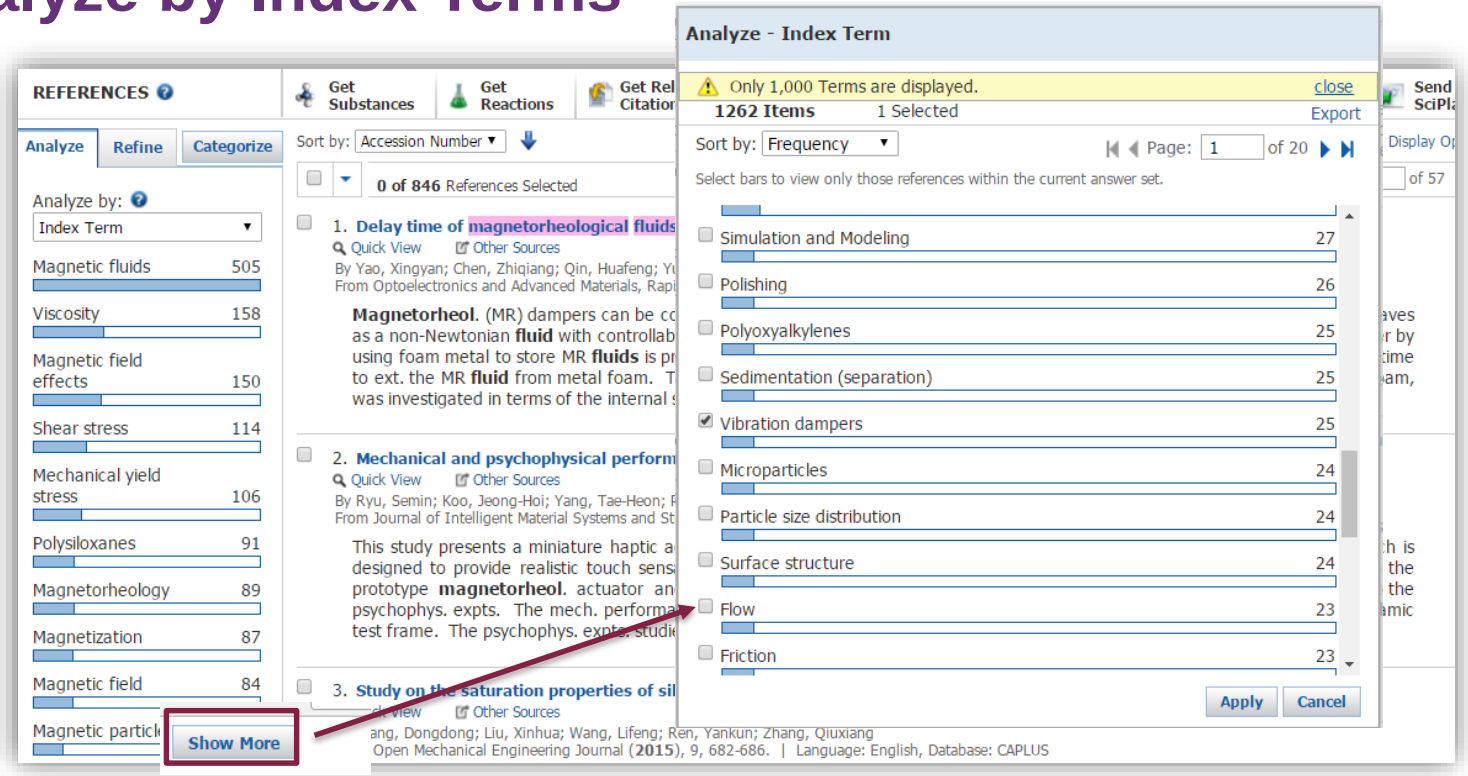
SciFinder®
A CAS SOLUTION

Refine by Publication year



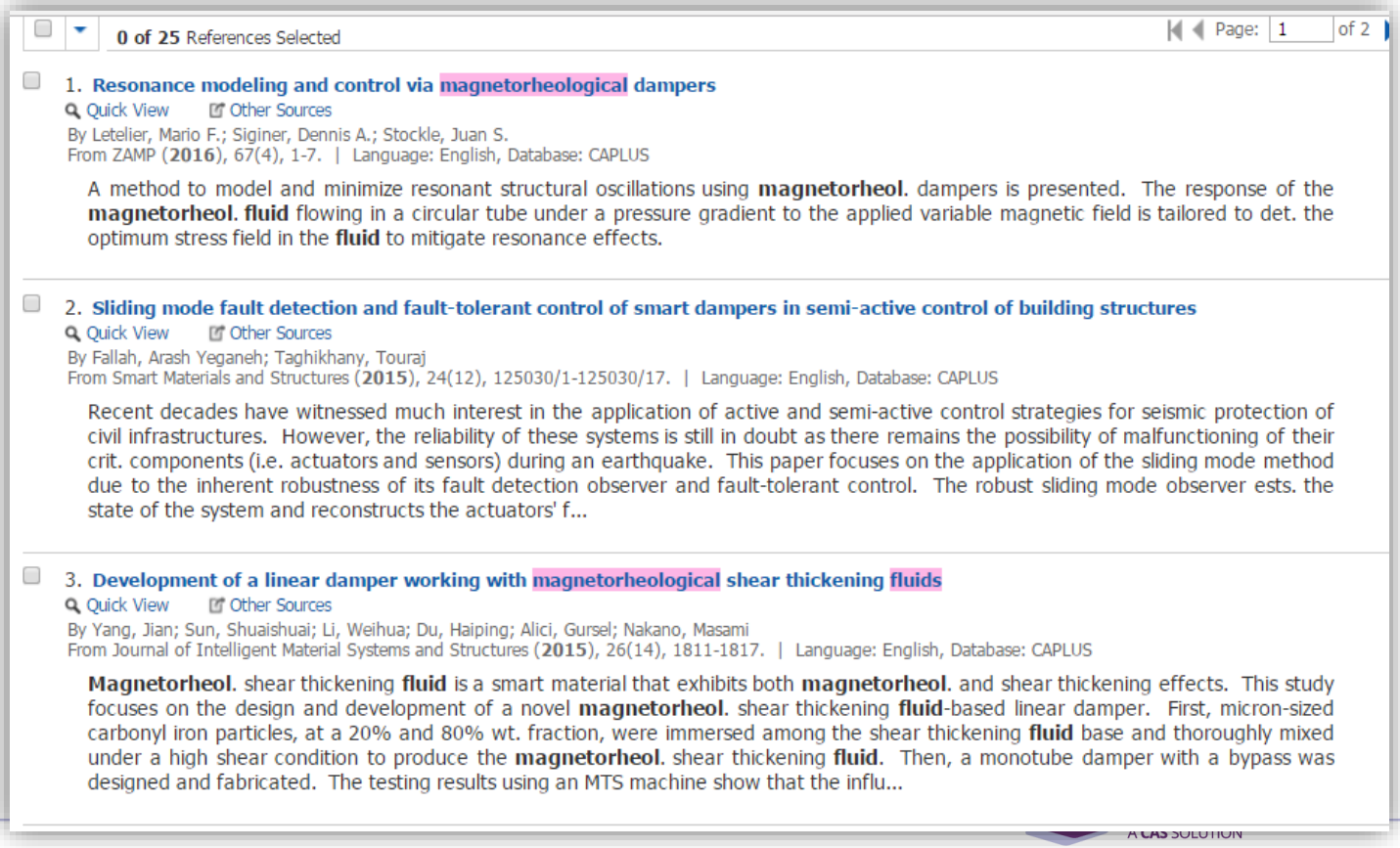
SciFinder®
A CAS SOLUTION

Analyze by Index Terms



SciFinder®
A CAS SOLUTION

Results



0 of 25 References Selected

Page: 1 of 2

1. **Resonance modeling and control via magnetorheological dampers**

Quick View Other Sources

By Letelier, Mario F.; Siginer, Dennis A.; Stockle, Juan S.
From ZAMP (**2016**), 67(4), 1-7. | Language: English, Database: CAPLUS

A method to model and minimize resonant structural oscillations using **magnetorheol**. dampers is presented. The response of the **magnetorheol**. **fluid** flowing in a circular tube under a pressure gradient to the applied variable magnetic field is tailored to det. the optimum stress field in the **fluid** to mitigate resonance effects.

2. **Sliding mode fault detection and fault-tolerant control of smart dampers in semi-active control of building structures**

Quick View Other Sources

By Fallah, Arash Yeganeh; Taghikhany, Touraj
From Smart Materials and Structures (**2015**), 24(12), 125030/1-125030/17. | Language: English, Database: CAPLUS

Recent decades have witnessed much interest in the application of active and semi-active control strategies for seismic protection of civil infrastructures. However, the reliability of these systems is still in doubt as there remains the possibility of malfunctioning of their crit. components (i.e. actuators and sensors) during an earthquake. This paper focuses on the application of the sliding mode method due to the inherent robustness of its fault detection observer and fault-tolerant control. The robust sliding mode observer ests. the state of the system and reconstructs the actuators' f...

3. **Development of a linear damper working with magnetorheological shear thickening fluids**

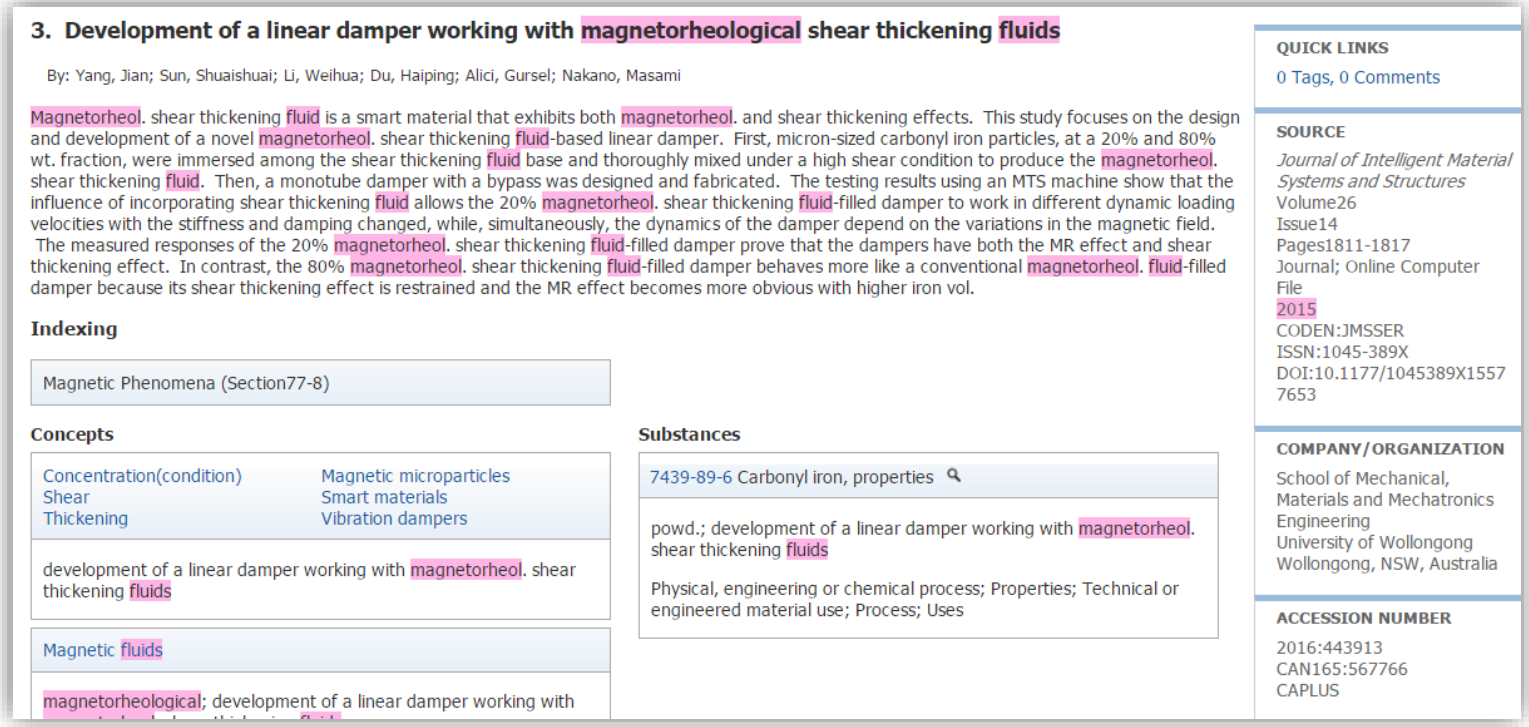
Quick View Other Sources

By Yang, Jian; Sun, Shuaishuai; Li, Weihua; Du, Haiping; Alici, Gursel; Nakano, Masami
From Journal of Intelligent Material Systems and Structures (**2015**), 26(14), 1811-1817. | Language: English, Database: CAPLUS

Magnetorheol. shear thickening **fluid** is a smart material that exhibits both **magnetorheol**. and shear thickening effects. This study focuses on the design and development of a novel **magnetorheol**. shear thickening **fluid**-based linear damper. First, micron-sized carbonyl iron particles, at a 20% and 80% wt. fraction, were immersed among the shear thickening **fluid** base and thoroughly mixed under a high shear condition to produce the **magnetorheol**. shear thickening **fluid**. Then, a monotube damper with a bypass was designed and fabricated. The testing results using an MTS machine show that the influ...

A CAS SOLUTION

One of the results



3. Development of a linear damper working with magnetorheological shear thickening fluids

By: Yang, Jian; Sun, Shuaishuai; Li, Weihua; Du, Haiping; Alici, Gursel; Nakano, Masami

Magnetorheol. shear thickening fluid is a smart material that exhibits both magnetorheol. and shear thickening effects. This study focuses on the design and development of a novel magnetorheol. shear thickening fluid-based linear damper. First, micron-sized carbonyl iron particles, at a 20% and 80% wt. fraction, were immersed among the shear thickening fluid base and thoroughly mixed under a high shear condition to produce the magnetorheol. shear thickening fluid. Then, a monotube damper with a bypass was designed and fabricated. The testing results using an MTS machine show that the influence of incorporating shear thickening fluid allows the 20% magnetorheol. shear thickening fluid-filled damper to work in different dynamic loading velocities with the stiffness and damping changed, while, simultaneously, the dynamics of the damper depend on the variations in the magnetic field. The measured responses of the 20% magnetorheol. shear thickening fluid-filled damper prove that the dampers have both the MR effect and shear thickening effect. In contrast, the 80% magnetorheol. shear thickening fluid-filled damper behaves more like a conventional magnetorheol. fluid-filled damper because its shear thickening effect is restrained and the MR effect becomes more obvious with higher iron vol.

Indexing

Magnetic Phenomena (Section77-8)

Concepts

Concentration(condition)
Shear
Thickening
Magnetic microparticles
Smart materials
Vibration dampers

development of a linear damper working with magnetorheol. shear thickening fluids

Magnetic fluids

magnetorheological; development of a linear damper working with

Substances

7439-89-6 Carbonyl iron, properties

powd.; development of a linear damper working with magnetorheol. shear thickening fluids

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Journal of Intelligent Material Systems and Structures
Volume26
Issue14
Pages1811-1817
Journal; Online Computer File
2015
CODEN:JMSSER
ISSN:1045-389X
DOI:10.1177/1045389X15577653

COMPANY/ORGANIZATION

School of Mechanical, Materials and Mechatronics Engineering
University of Wollongong
Wollongong, NSW, Australia

ACCESSION NUMBER

2016:443913
CAN165:567766
CAPLUS

SciFinder®
A CAS SOLUTION

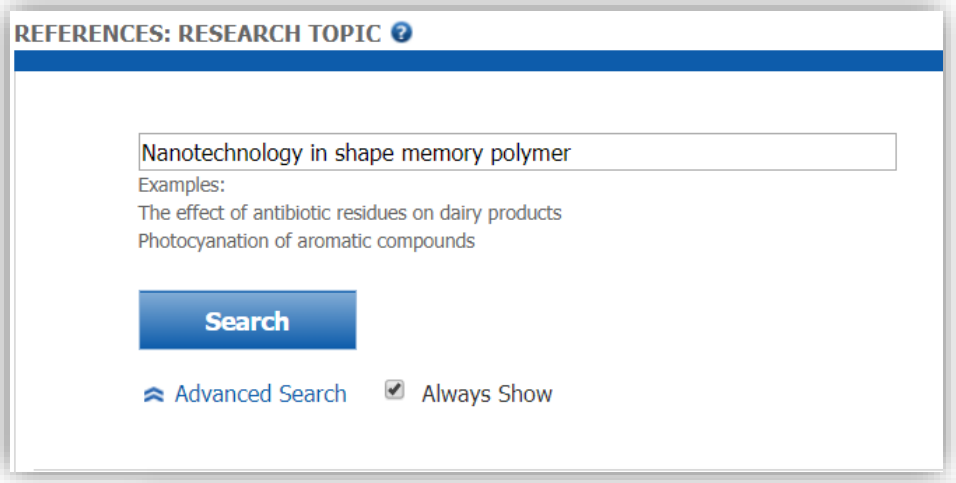
Case study

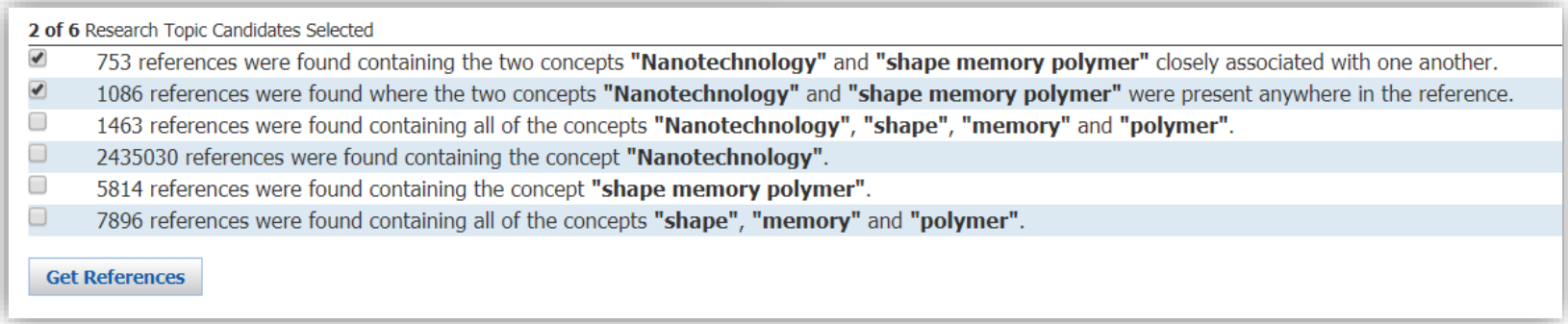
- Nanotechnology in shape memory polymers and find maximum number of references related in term of patents and find products related to it

- Search for ‘Nanotechnology in shape memory polymer’
- Refine using document type to Patents
- Categorize search to products in term of Shape memory polymer

SciFinder® A CAS SOLUTION

CAS is a division of the American Chemical Society.
Copyright 2017 American Chemical Society. All rights reserved.





SciFinder®
A CAS SOLUTION

CAS is a division of the American Chemical Society.
Copyright 2017 American Chemical Society. All rights reserved.

Refine search topics with document type to patent

Research Topic "Nanotechnology in shape memory..." > **references (993)**

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 993 References Selected

Analyze by: Author Name

Leng Jinsong	72
Liu Yanju	56
Lu Haibao	46
Gou Jihua	24
Lendlein Andreas	22
Luo Hongsheng	22
Jana Sadhan C	21
Du Shanyi	20
Cho Jae Whan	18
Yi Guobin	17

Show More

1. **Design of shape-memory materials based on sea-island structured EPDM/PP TPVs via in-situ compatibilization of methacrylic acid and excess zinc**

Quick View | Other Sources

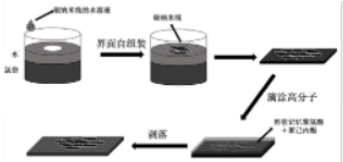
By Xu, Chuanhui; Wu, Wenchao; Zheng, Zhongjie; Wang, Zhiwei; Nie, Jiada
From Composites Science and Technology (2018), 167, 431-439. | Language: English, Database: CAPLUS

It is a challenge to achieve considerable **shape-memory** (SM) effect for typical sea-island structured **polymer** blends. In this paper, we succ propylene-diene rubber/polypropylene (EPDM/PP) thermoplastic vulcanizates (TPVs) through a strong rubber/plastic interface compatibilized by in-si methacrylic acid (MAA) and excess zinc oxide (ZnO) **nanoparticles**. With MAA/ZnO, the av. size of EPDM particles reduced to 400-500 nm, which sig T...

2. **Based on ordered conductive network structure for self-healing sensing polymer composite material and preparation method thereof [Machine Tra**

Quick View | PATENTPAK

By Luo, Hongsheng; Zhou, Huankai; Zhang, Yihang; Yi, Guobin; Zhou, Xingdong; Wang, Huaquan
From Faming Zhuanli Shenqing (2018), CN 108485234 A 20180904. | Language: Chinese, Database: CAPLUS



[Machine Translation of Descriptors]. The invention discloses a kind of ordered based on conductive netw material and prepn. method thereof, it adopts interface self-assembly of the **nano** silver wire ordered, co self-healing polycaprolactone and **shape-memory** polyurethane **polymer** blend evenly to obtain mixed to spin coating or dip coating ordered **nano** silver conductive line film surface; carry out heat treatment t

3. **Preparation method of novel shape memory liquid crystal novel material**

Quick View | PATENTPAK

By Zhang, Yunwei; Wang, Weixin; Zheng, Chunying; Li, Shougang
From Faming Zhuanli Shenqing (2018), CN 108424587 A 20180821. | Language: Chinese, Database: CAPLUS

Analyze | Refine | Categorize

Refine by:
- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)
- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

Copyright 2017 American Chemical Society. All rights reserved.

Use categorize to hand pick required index terms

Research Topic "Nanotechnology in shape memory..." > references (993) > **refine "Patents only" (195)**

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

Sort by: Accession Number

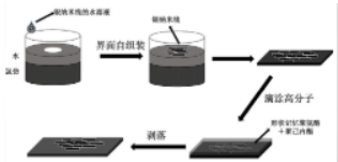
0 of 195 References Selected

Analyze by: Author Name

Liu Yanju	17
Leng Jinsong	13
Luo Hongsheng	11
Yi Guobin	11
Wang Huaquan	10
Zhou Xingdong	10
Maitland Duncan J	7
Wilson Thomas S	7
Lendlein Andreas	6
Behl Marc	5

Show More

1. **Based on ordered conductive network structure for self-healing sensing polymer composite material and preparation method thereof [Machine Translation].**
Quick View PATENTPAK
By Luo, Hongsheng; Zhou, Huankai; Zhang, Yihang; Yi, Guobin; Zhou, Xingdong; Wang, Huaquan
From Faming Zhuanli Shenqing (2018), CN 108485234 A 20180904. | Language: Chinese, Database: CAPLUS



[Machine Translation of Descriptors]. The invention discloses a kind of ordered based on conductive network structur material and prepn. method thereof, it adopts interface self-assembly of the **nano** silver wire ordered, constructing o self-healing polycaprolactone and **shape-memory** polyurethane **polymer** blend evenly to obtain mixed soln., Adop to spin coating or dip coating ordered **nano** silver conductive line film surface; carry out heat treatment to remove or

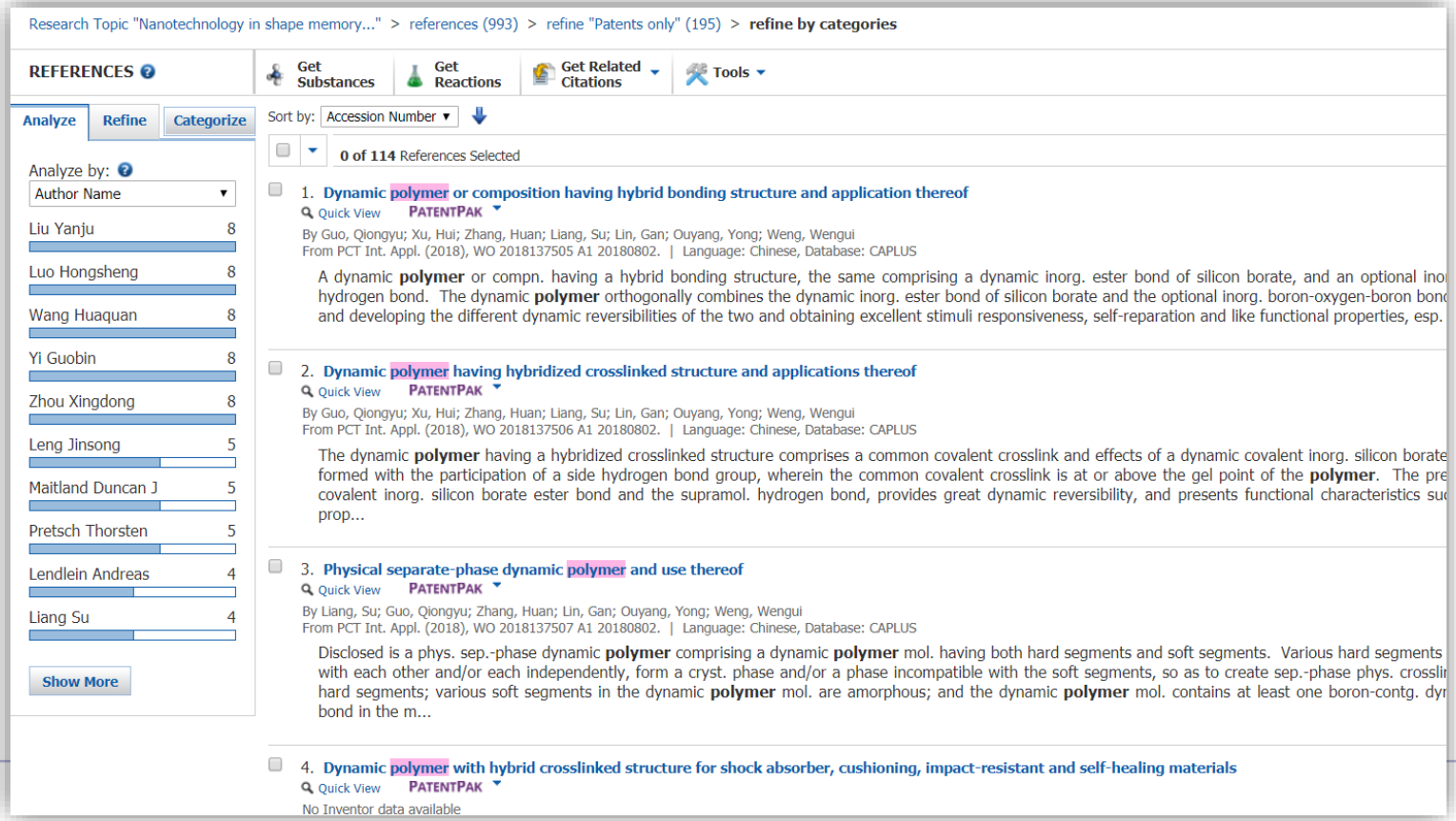
2. **Preparation method of novel shape memory liquid crystal novel material**
Quick View PATENTPAK
By Zhang, Yunwei; Wang, Weixin; Zheng, Chunying; Li, Shougang
From Faming Zhuanli Shenqing (2018), CN 108424587 A 20180821. | Language: Chinese, Database: CAPLUS

A prepn. method of a novel **shape memory** liq. crystal novel material having improved mech. properties, **shape memory** recovery stress and **shape memo** application prospects is provided. The method comprises the following steps: (1) adding vinyl terephthalate into a completely-dried polymn. kettle, then vacuuming, and using high-purity nitrogen for replacing air in the reaction kettle, filling nitrogen for protection, heating the reaction system, reacting for 4-9 h reac...

3. **Dynamic polymer or composition having hybrid bonding structure and application thereof**
Quick View PATENTPAK
By Guo, Qiongyu; Xu, Hui; Zhang, Huan; Liang, Su; Lin, Gan; Ouyang, Yong; Weng, Wengui
From PCT Int. Appl. (2018), WO 2018137505 A1 20180802. | Language: Chinese, Database: CAPLUS

A dynamic **polymer** or compn. having a hybrid bonding structure, the same comprising a dynamic inorg. ester bond of silicon borate, and an optional inorg. hydrogen bond. The dynamic **polymer** orthogonally combines the dynamic inorg. ester bond of silicon borate and the optional inorg. boron-oxygen-boron bond

Probable answer set



Research Topic "Nanotechnology in shape memory..." > references (993) > refine "Patents only" (195) > **refine by categories**

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 114 References Selected

Analyze by: Author Name

Liu Yanju	8
Luo Hongsheng	8
Wang Huaquan	8
Yi Guobin	8
Zhou Xingdong	8
Leng Jinsong	5
Maitland Duncan J	5
Pretsch Thorsten	5
Lendlein Andreas	4
Liang Su	4

Show More

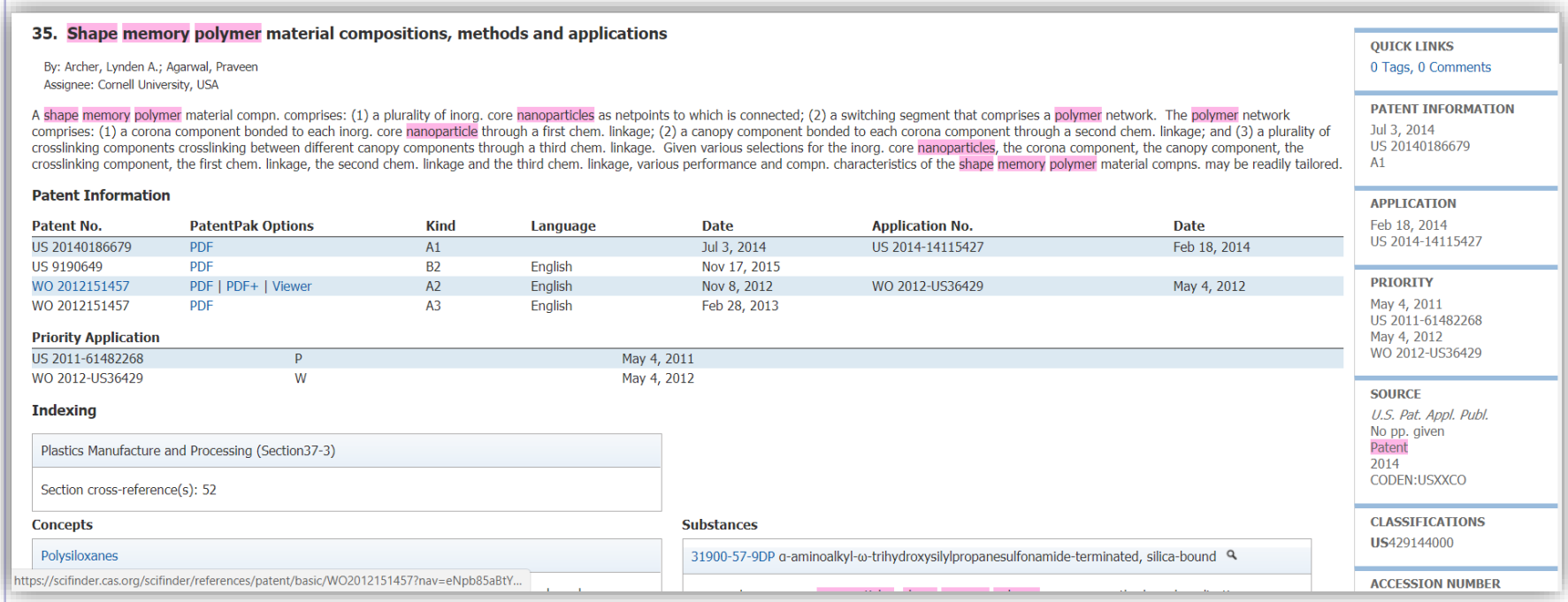
1. **Dynamic polymer or composition having hybrid bonding structure and application thereof**
   Quick View | PATENTPAK
   By Guo, Qiongyu; Xu, Hui; Zhang, Huan; Liang, Su; Lin, Gan; Ouyang, Yong; Weng, Wengui
   From PCT Int. Appl. (2018), WO 2018137505 A1 20180802. | Language: Chinese, Database: CAPLUS
   A dynamic **polymer** or compn. having a hybrid bonding structure, the same comprising a dynamic inorg. ester bond of silicon borate, and an optional ino hydrogen bond. The dynamic **polymer** orthogonally combines the dynamic inorg. ester bond of silicon borate and the optional inorg. boron-oxygen-boron bon and developing the different dynamic reversibilities of the two and obtaining excellent stimuli responsiveness, self-reparation and like functional properties, esp.

2. **Dynamic polymer having hybridized crosslinked structure and applications thereof**
   Quick View | PATENTPAK
   By Guo, Qiongyu; Xu, Hui; Zhang, Huan; Liang, Su; Lin, Gan; Ouyang, Yong; Weng, Wengui
   From PCT Int. Appl. (2018), WO 2018137506 A1 20180802. | Language: Chinese, Database: CAPLUS
   The dynamic **polymer** having a hybridized crosslinked structure comprises a common covalent crosslink and effects of a dynamic covalent inorg. silicon borate formed with the participation of a side hydrogen bond group, wherein the common covalent crosslink is at or above the gel point of the **polymer**. The pre covalent inorg. silicon borate ester bond and the supramol. hydrogen bond, provides great dynamic reversibility, and presents functional characteristics su prop...

3. **Physical separate-phase dynamic polymer and use thereof**
   Quick View | PATENTPAK
   By Liang, Su; Guo, Qiongyu; Zhang, Huan; Lin, Gan; Ouyang, Yong; Weng, Wengui
   From PCT Int. Appl. (2018), WO 2018137507 A1 20180802. | Language: Chinese, Database: CAPLUS
   Disclosed is a phys. sep.-phase dynamic **polymer** comprising a dynamic **polymer** mol. having both hard segments and soft segments. Various hard segments with each other and/or each independently, form a cryst. phase and/or a phase incompatible with the soft segments, so as to create sep.-phase phys. crosslin hard segments; various soft segments in the dynamic **polymer** mol. are amorphous; and the dynamic **polymer** mol. contains at least one boron-contg. dyn bond in the m...

4. **Dynamic polymer with hybrid crosslinked structure for shock absorber, cushioning, impact-resistant and self-healing materials**
   Quick View | PATENTPAK
   No Inventor data available

Probable answer, concepts and substances mentioned in it!



35. Shape memory polymer material compositions, methods and applications

By: Archer, Lynden A.; Agarwal, Praveen
Assignee: Cornell University, USA

A shape memory polymer material compn. comprises: (1) a plurality of inorg. core nanoparticles as netpoints to which is connected; (2) a switching segment that comprises a polymer network. The polymer network comprises: (1) a corona component bonded to each inorg. core nanoparticle through a first chem. linkage; (2) a canopy component bonded to each corona component through a second chem. linkage; and (3) a plurality of crosslinking components crosslinking between different canopy components through a third chem. linkage. Given various selections for the inorg. core nanoparticles, the corona component, the canopy component, the crosslinking component, the first chem. linkage, the second chem. linkage and the third chem. linkage, various performance and compn. characteristics of the shape memory polymer material compns. may be readily tailored.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
US 20140186679	PDF	A1		Jul 3, 2014	US 2014-14115427	Feb 18, 2014
US 9190649	PDF	B2	English	Nov 17, 2015		
WO 2012151457	PDF | PDF+ | Viewer	A2	English	Nov 8, 2012	WO 2012-US36429	May 4, 2012
WO 2012151457	PDF	A3	English	Feb 28, 2013		

Priority Application

US 2011-61482268	P	May 4, 2011
WO 2012-US36429	W	May 4, 2012

Indexing

Plastics Manufacture and Processing (Section37-3)

Section cross-reference(s): 52

Concepts

Polysiloxanes

Substances

31900-57-9DP α-aminoalkyl-ω-trihydroxysilylpropanesulfonamide-terminated, silica-bound

https://scifinder.cas.org/scifinder/references/patent/basic/WO2012151457?nav=eNpb85aBtY...

QUICK LINKS
0 Tags, 0 Comments

PATENT INFORMATION
Jul 3, 2014
US 20140186679
A1

APPLICATION
Feb 18, 2014
US 2014-14115427

PRIORITY
May 4, 2011
US 2011-61482268
May 4, 2012
WO 2012-US36429

SOURCE
U.S. Pat. Appl. Publ.
No pp. given
Patent
2014
CODEN:USXXCO

CLASSIFICATIONS
US429144000

ACCESSION NUMBER

SciFinder® A CAS SOLUTION

CAS is a division of the American Chemical Society.
Copyright 2017 American Chemical Society. All rights reserved.

Indexing

Plastics Manufacture and Processing (Section37-3)

Section cross-reference(s): 52

Concepts

Polysiloxanes

amine-terminated, silica nanoparticle-bound; shape memory polymer compns., methods and applications

Industrial manufacture; Reactant; Technical or engineered material use; Preparation; Uses; Reactant or reagent

Polyoxyalkylenes

amino-terminated, silica nanoparticle-bound; shape memory polymer compns., methods and applications

Industrial manufacture; Reactant; Technical or engineered material use; Preparation; Uses; Reactant or reagent

Alloys
Borides
Fluorides
Hydroxides(inorganic)
Metals
Nitrides
Oxides(inorganic)
Oxynitrides
Sulfides

nanoparticles; shape memory polymer compns., methods and applications

Technical or engineered material use; Uses

Battery electrolytes
Lithium primary batteries
Lithium-ion secondary batteries
Nanoparticles
Polymer brushes
Polymer electrolytes
Primary battery separators
Secondary battery separators
Shape memory materials

shape memory polymer compns., methods and applications

Substances

31900-57-9DP α-aminoalkyl-ω-trihydroxysilylpropanesulfonamide-terminated, silica-bound

assumed monomers, nanoparticles; shape memory polymer compns., methods and applications

Industrial manufacture; Reactant; Preparation; Reactant or reagent

822-06-0

linking agent; shape memory polymer compns., methods and applications

Reactant; Reactant or reagent

7631-86-9 Silica, miscellaneous

nanoparticles, Ludox SM 30; shape memory polymer compns., methods and applications

Reactant; Reactant or reagent

9016-00-6DP Poly[oxy(dimethylsilylene)], α-aminoalkyl-ω-trihydroxysilylpropanesulfonamide-terminated, silica-bound
1404117-09-4DP silica-bound

nanoparticles; shape memory polymer compns., methods and applications

Industrial manufacture; Reactant; Preparation; Reactant or reagent

70942-24-4D silica-bound

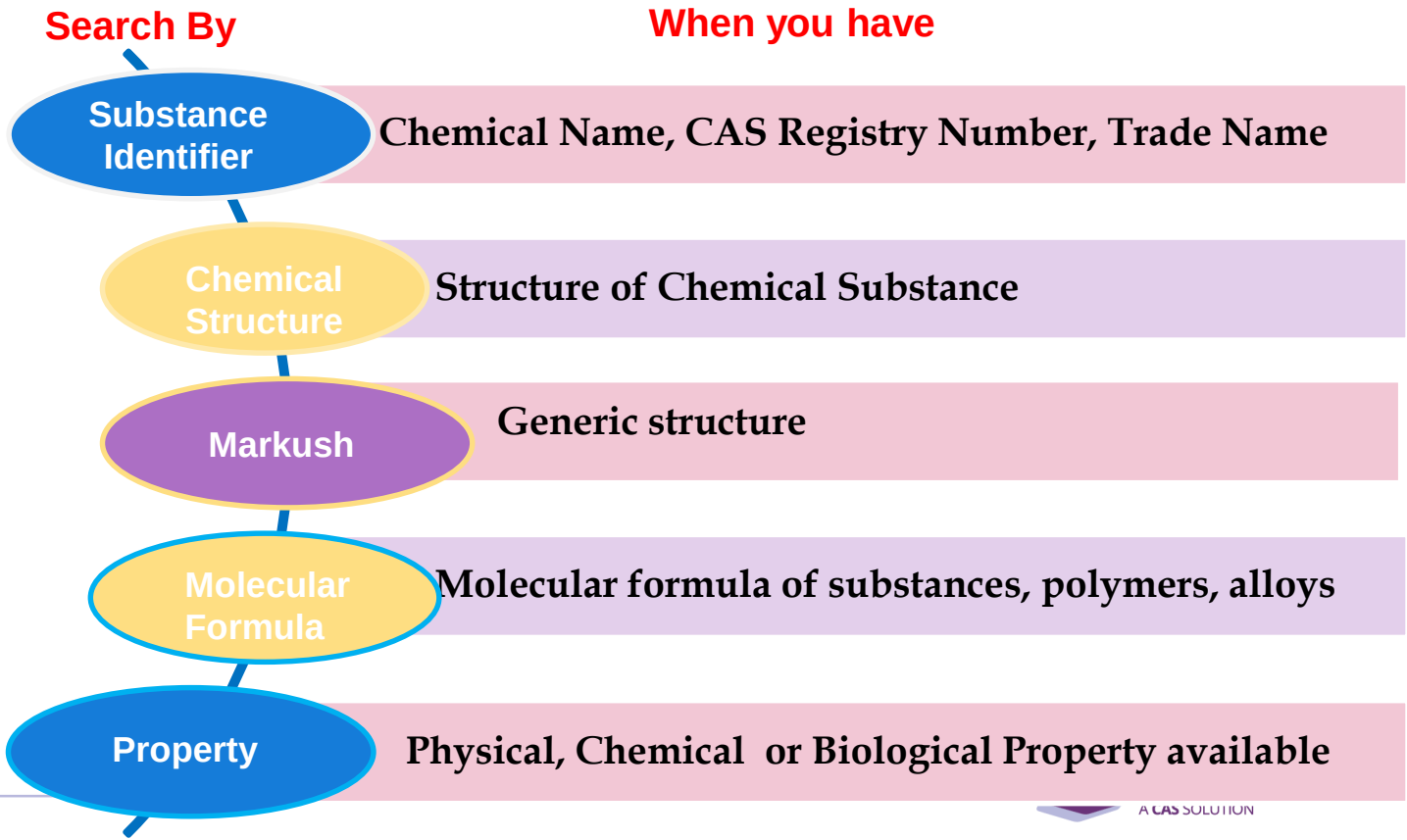
nanoparticles; shape memory polymer compns., methods and applications

Reactant; Reactant or reagent

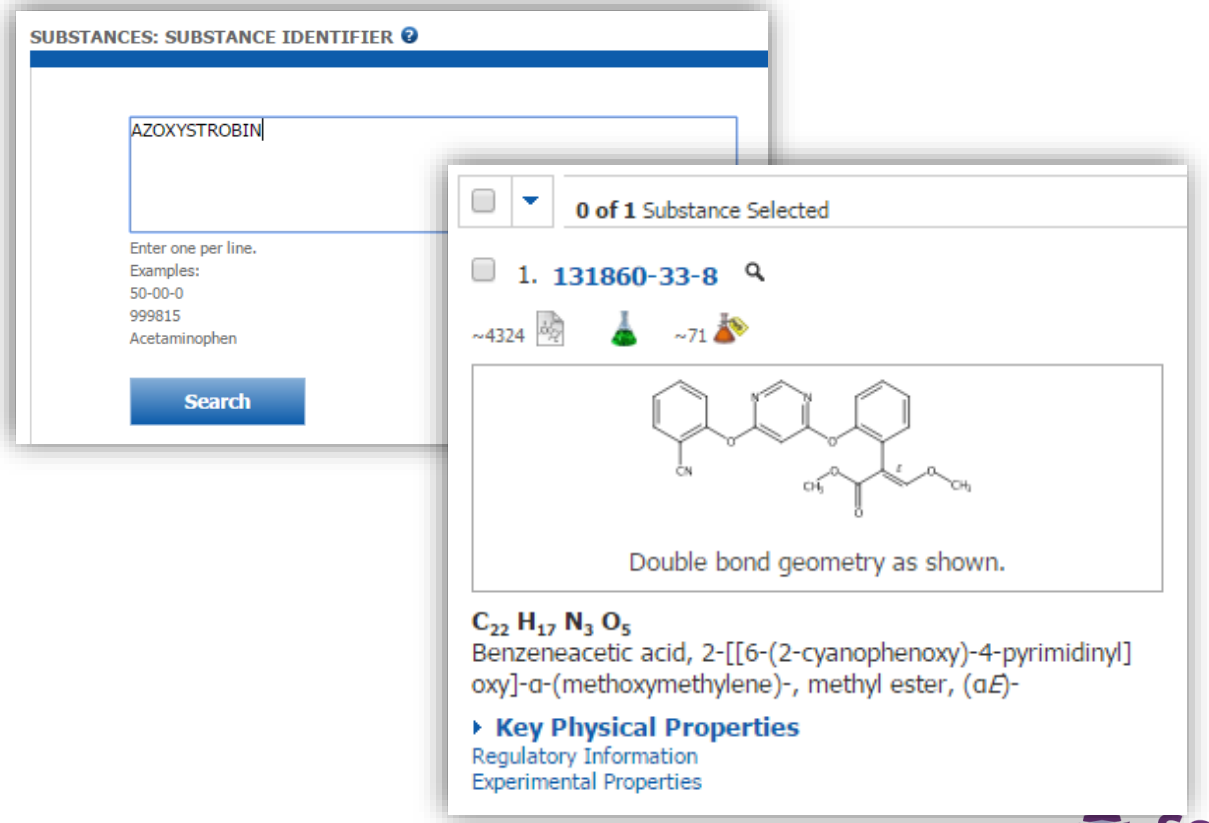
7439-93-2D Lithium, polyoxyalkylene complexes, silica-bound

Copyright 2017 American Chemical Society. All rights reserved.

Explore Substance

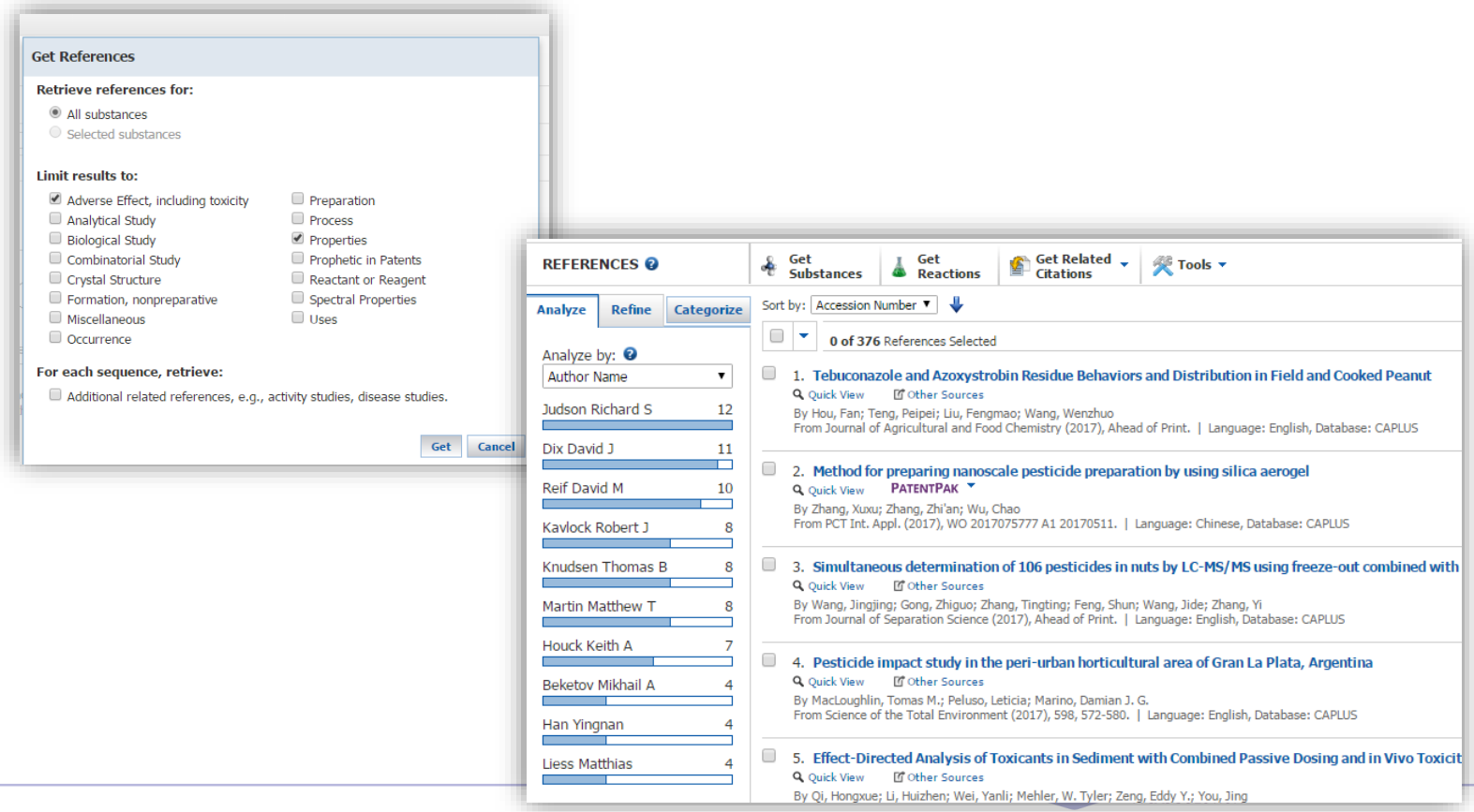


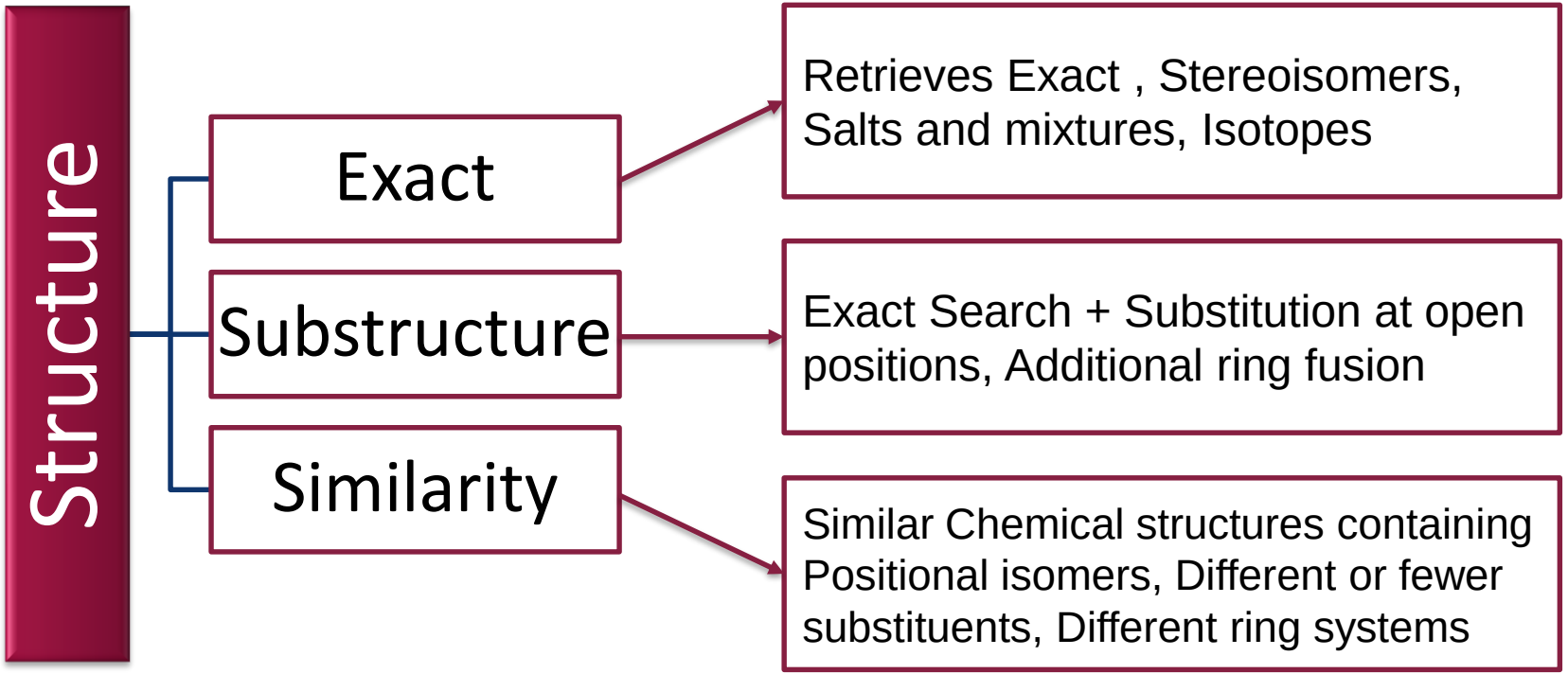
Case Study – Azoxystrobin



SciFinder®
A CAS SOLUTION

Related References



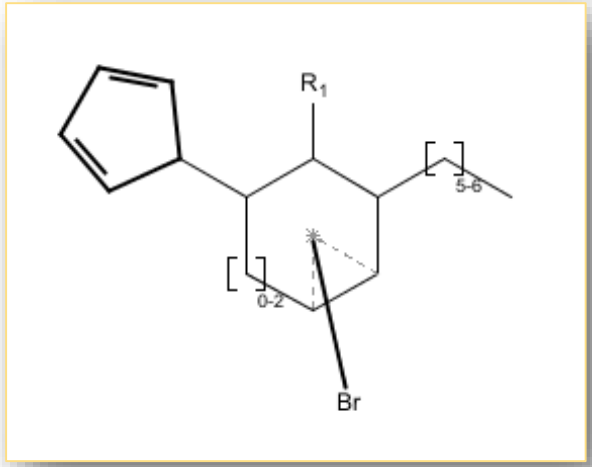


SciFinder® A CAS SOLUTION

CAS is a division of the American Chemical Society.
Copyright 2018 American Chemical Society. All rights reserved.

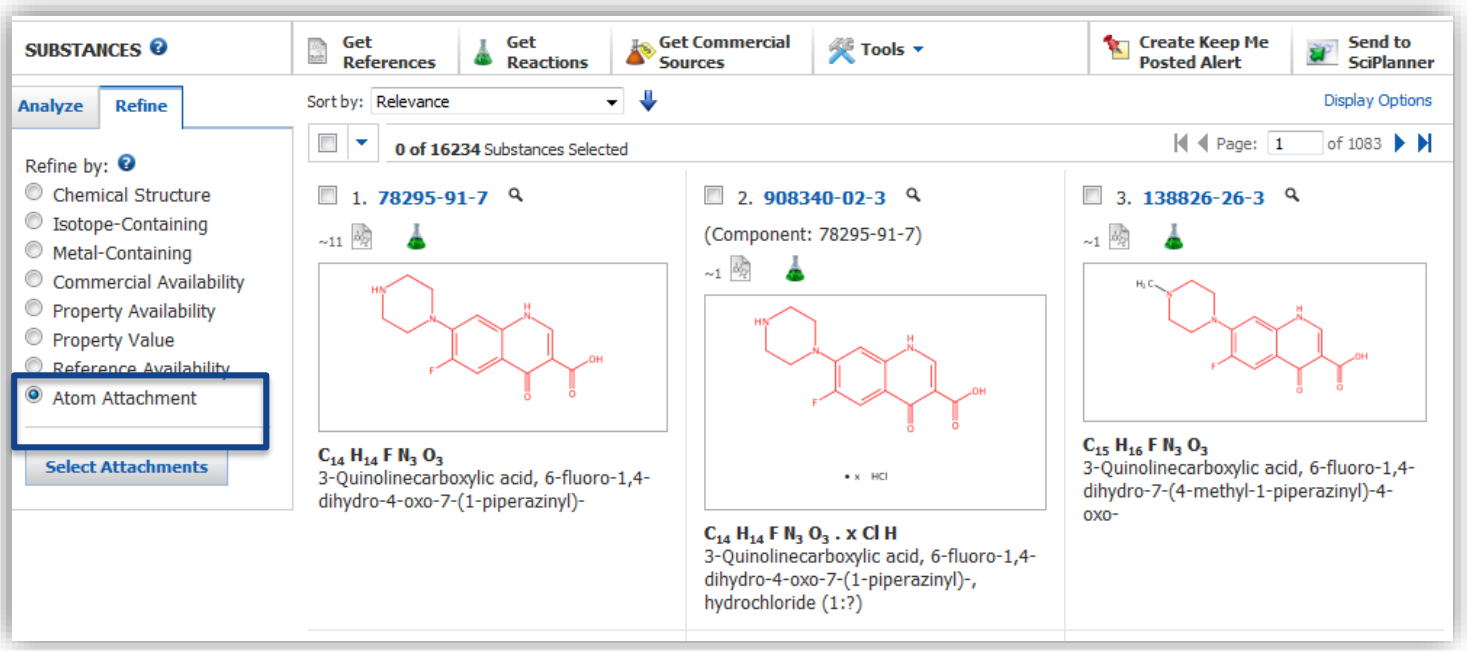
Advanced structure searching tips

1. R groups.
2. Repeating units
3. Variable point of attachments (VPA)
4. Ring expansion
5. Ring block and Node block
6. Charges
7. Undefined bonds
8. Refine by atom attachment



SciFinder®
A CAS SOLUTION

Refine by Atom Attachment



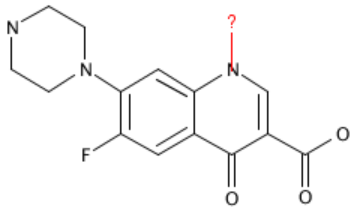
SciFinder®
A CAS SOLUTION

Refine by Atom Attachment

1. Click an atom to display the attachments present at that site.

2. Select attachment(s) of interest.

Substructure



Atom Attachments

Select All Deselect All

H or None	58
C	15753
N	367
O	9
S	4
F	2
Other	43
A - Any (not H)	16155
Cb - Carbocycle	8016
Ak - Alkyl chain	5304
Q - Any (not C,H)	382
Hy - Heterocycle	331
X - Halogen	2

? = Cb

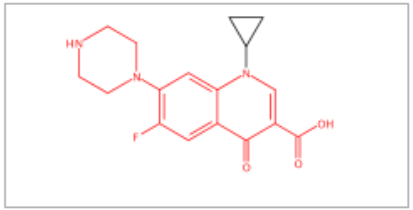
Refine Cancel

IDER®

Results

1. **85721-33-1**

~33256 ~164

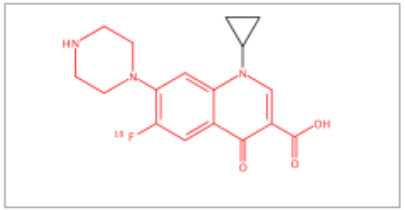


$C_{17}H_{18}FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-

Regulatory Information
Spectra
Experimental Properties

2. **637328-09-7**

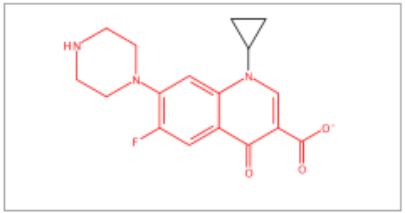
~6



$C_{17}H_{18}FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-6-(fluoro-^{18}F)-1,4-dihydro-4-oxo-7-(1-piperazinyl)- (9CI)

3. **234086-32-9**

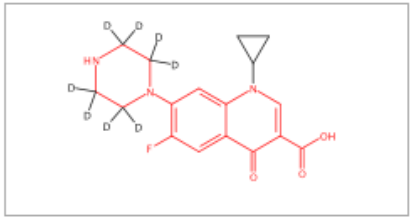
~4



$C_{17}H_{17}FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-, ion(1-)

4. **1130050-35-9**

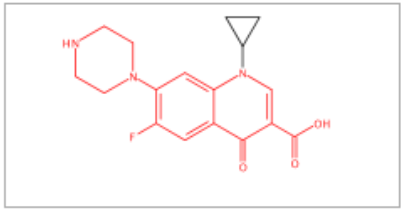
~4 ~4



$C_{17}H_{10}D_8FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-

5. **432015-55-9**

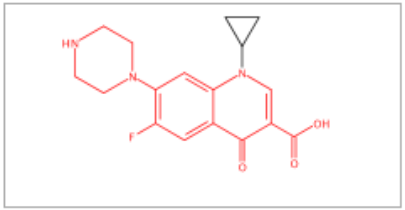
~2



$C_{17}H_{18}FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-

6. **438571-51-8**

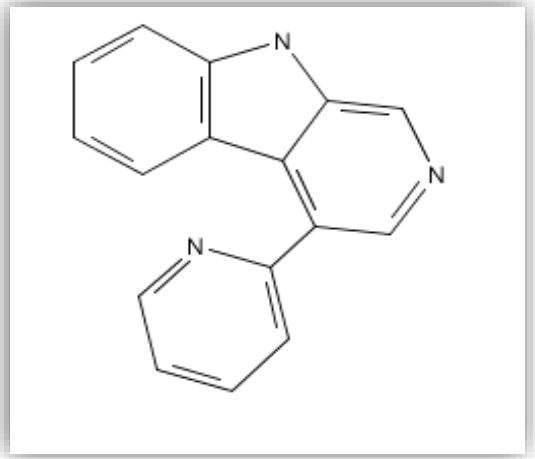
~2



$C_{17}H_{18}FN_3O_3$
3-Quinolinecarboxylic acid, 1-cyclopropyl-

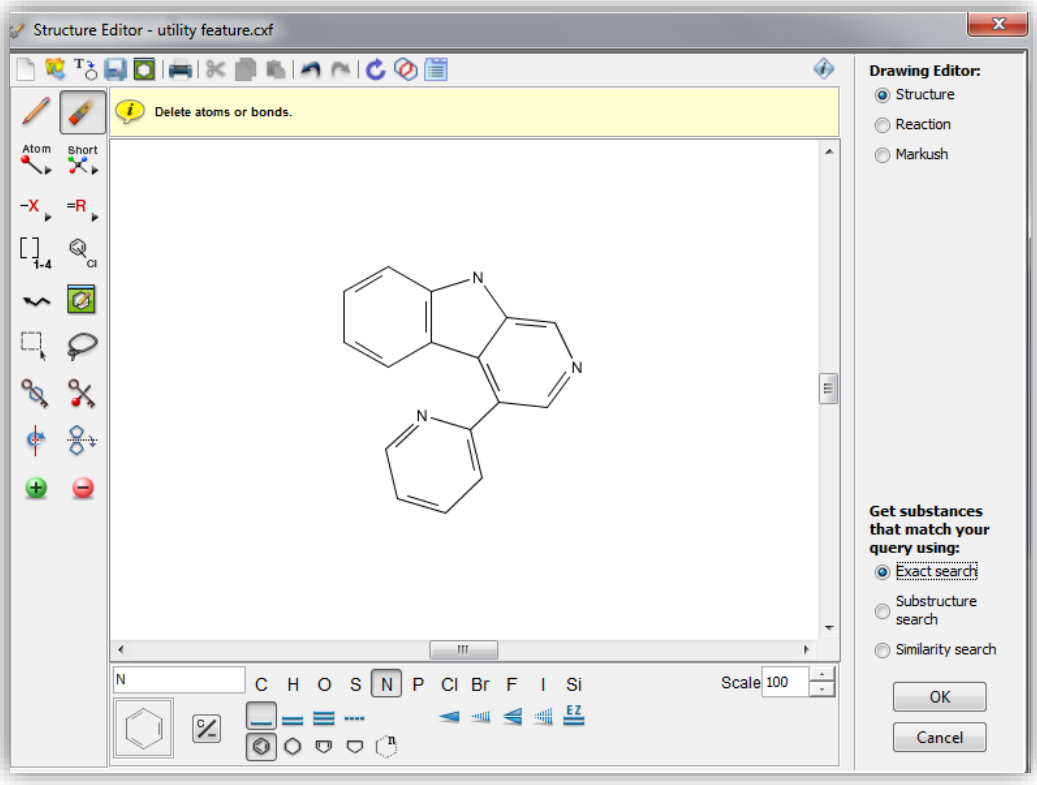
Case Study

Can I locate process to prepare below moiety?

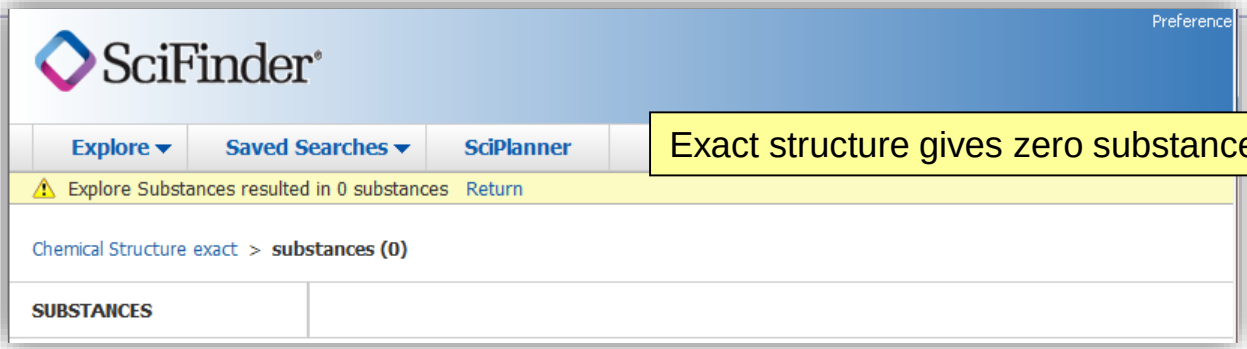


Showcasing the utility of similarity searching

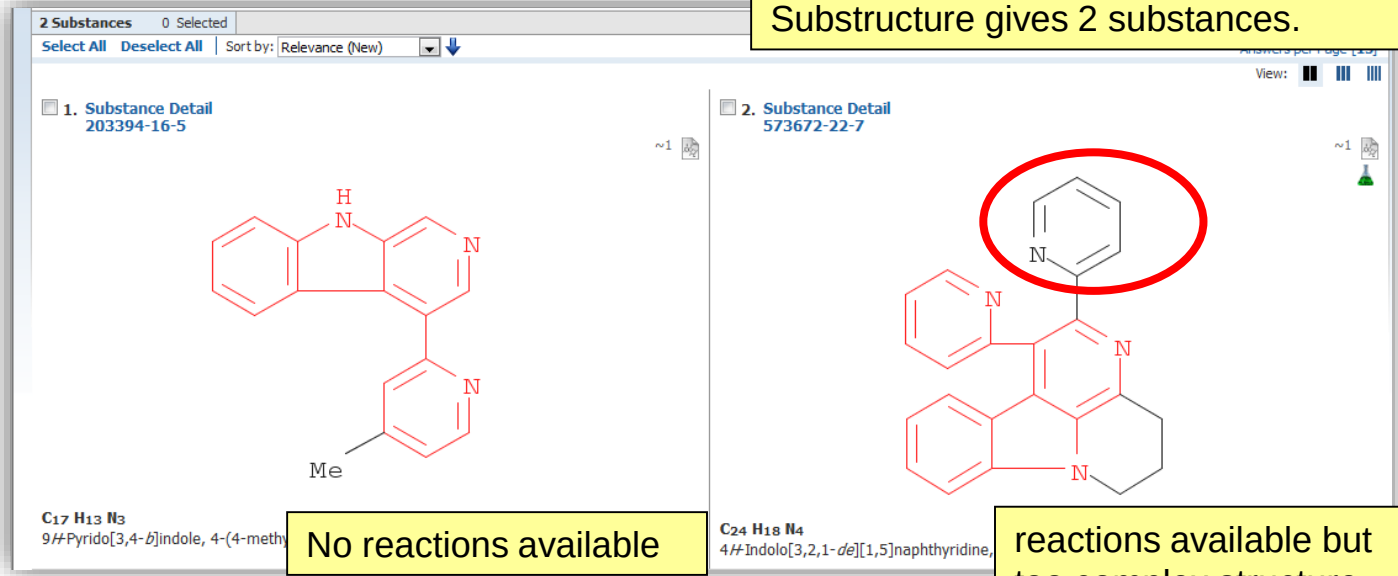
SciFinder®
A CAS SOLUTION



SciFinder®
A CAS SOLUTION



Exact structure gives zero substance



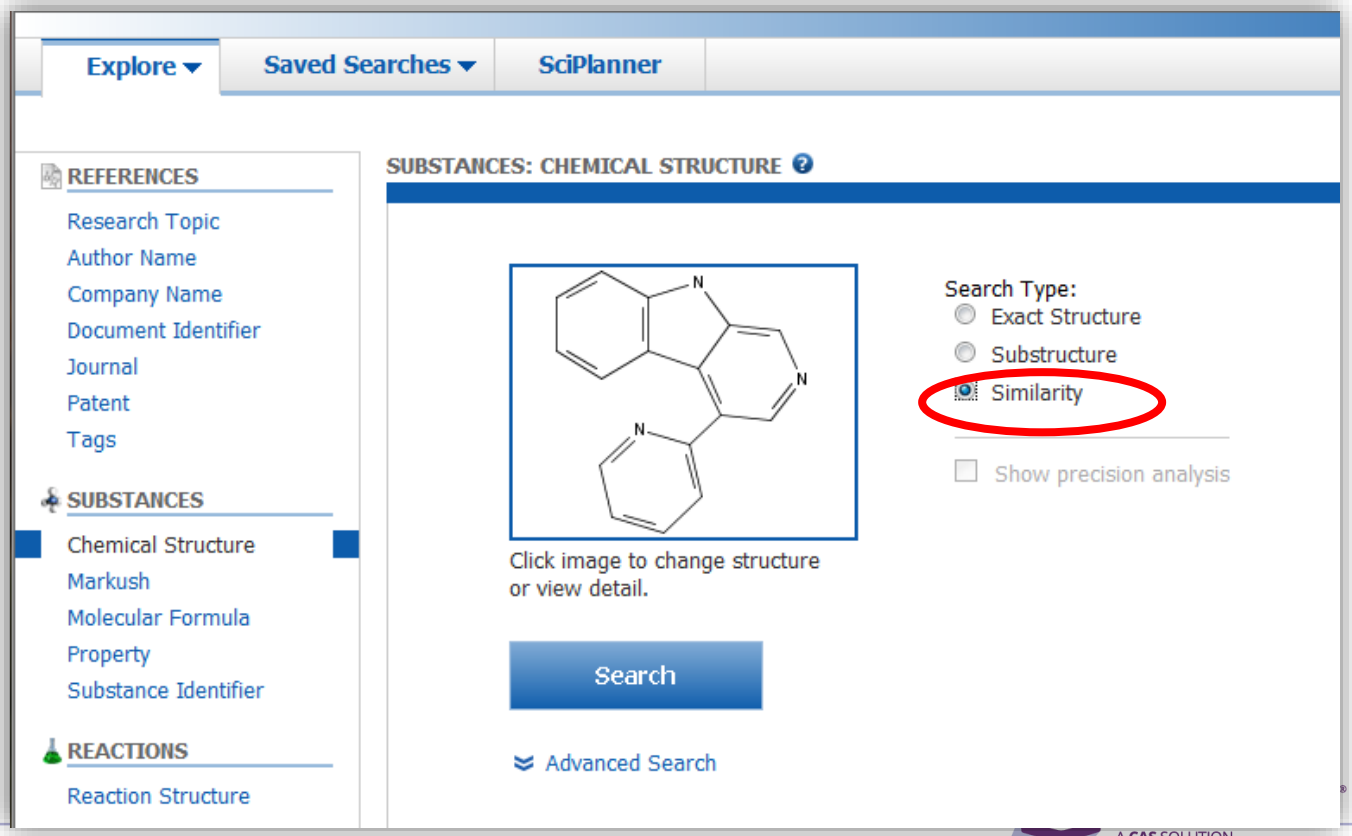
Substructure gives 2 substances.

No reactions available

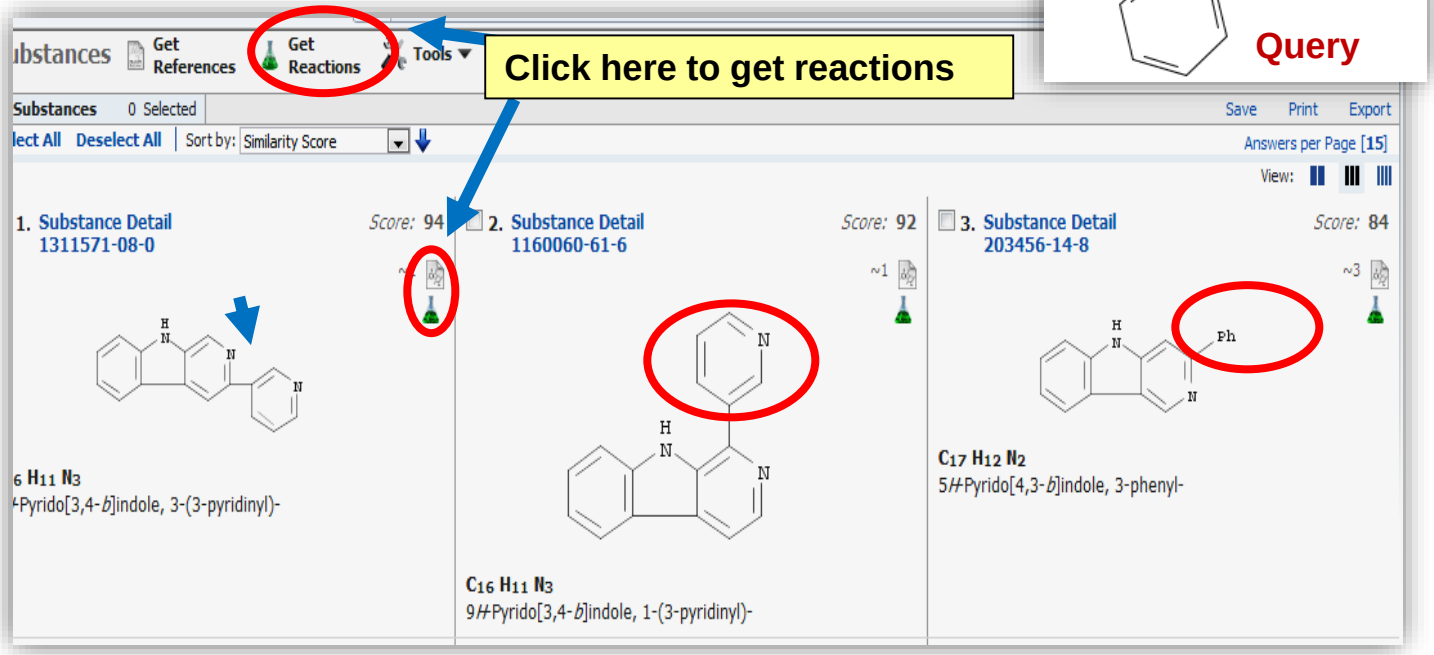
reactions available but too complex structure

Since, there are no processes leading to the final compound –

Let’s locate processes discussing preparation of similar molecules.



A CAS SOLUTION

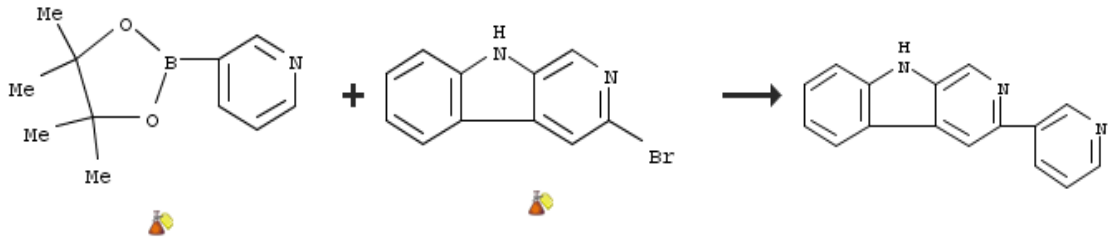


SciFinder®
A CAS SOLUTION

Lets study reactions of similar substance

1. View Reaction Detail Link Similar Re

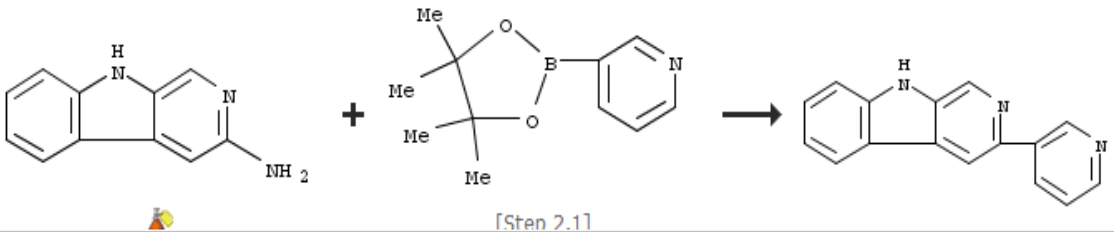
Single Step *Hover over any structure for more options.*



Overview

2. View Reaction Detail Link

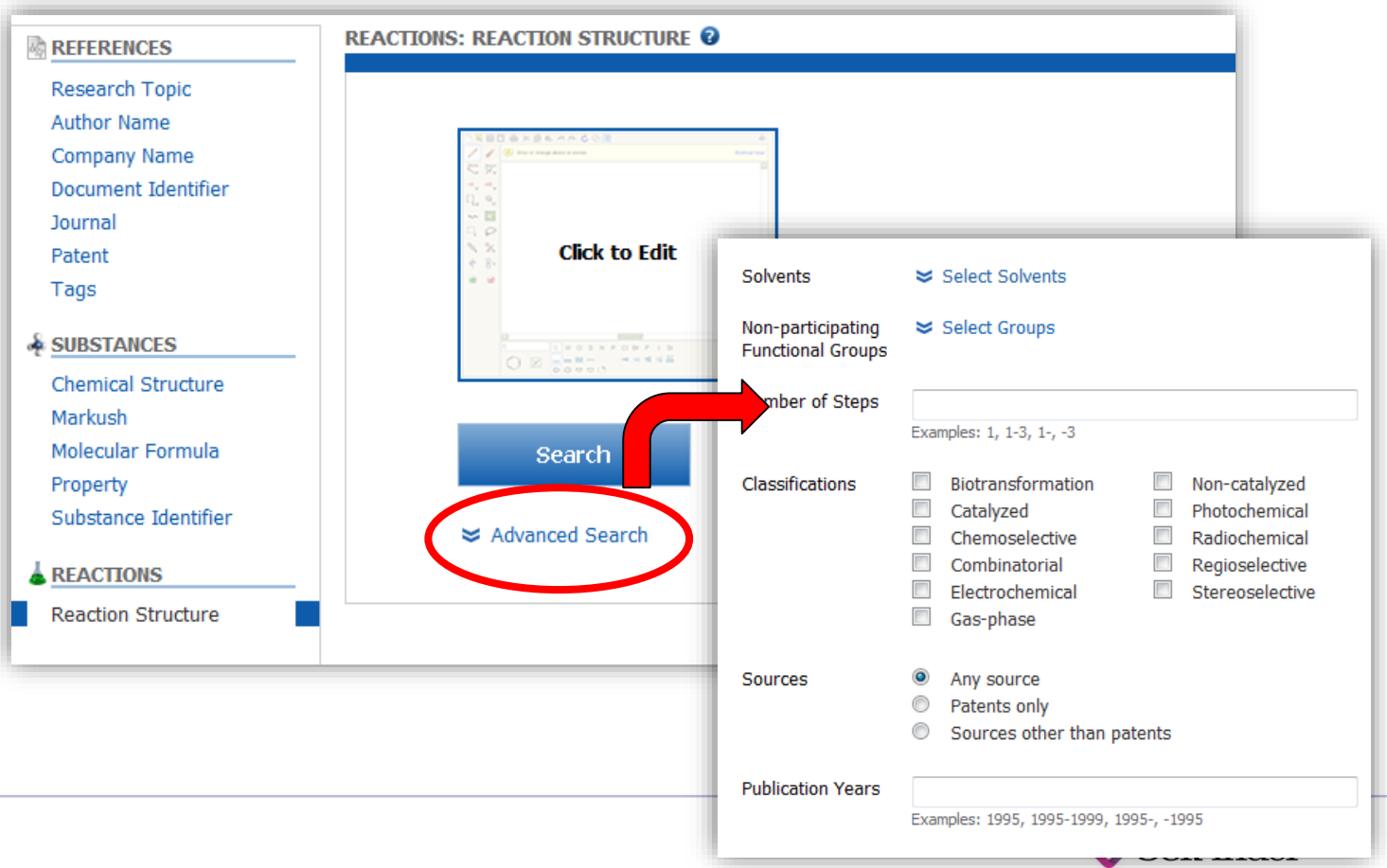
2 Steps *Hover over any structure for more options.*



[Step 2.1]

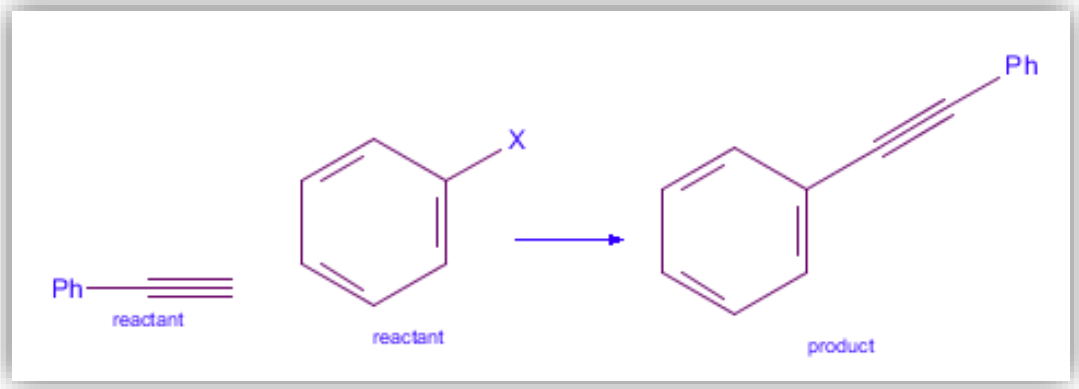
A CAS SOLUTION

Reaction searching



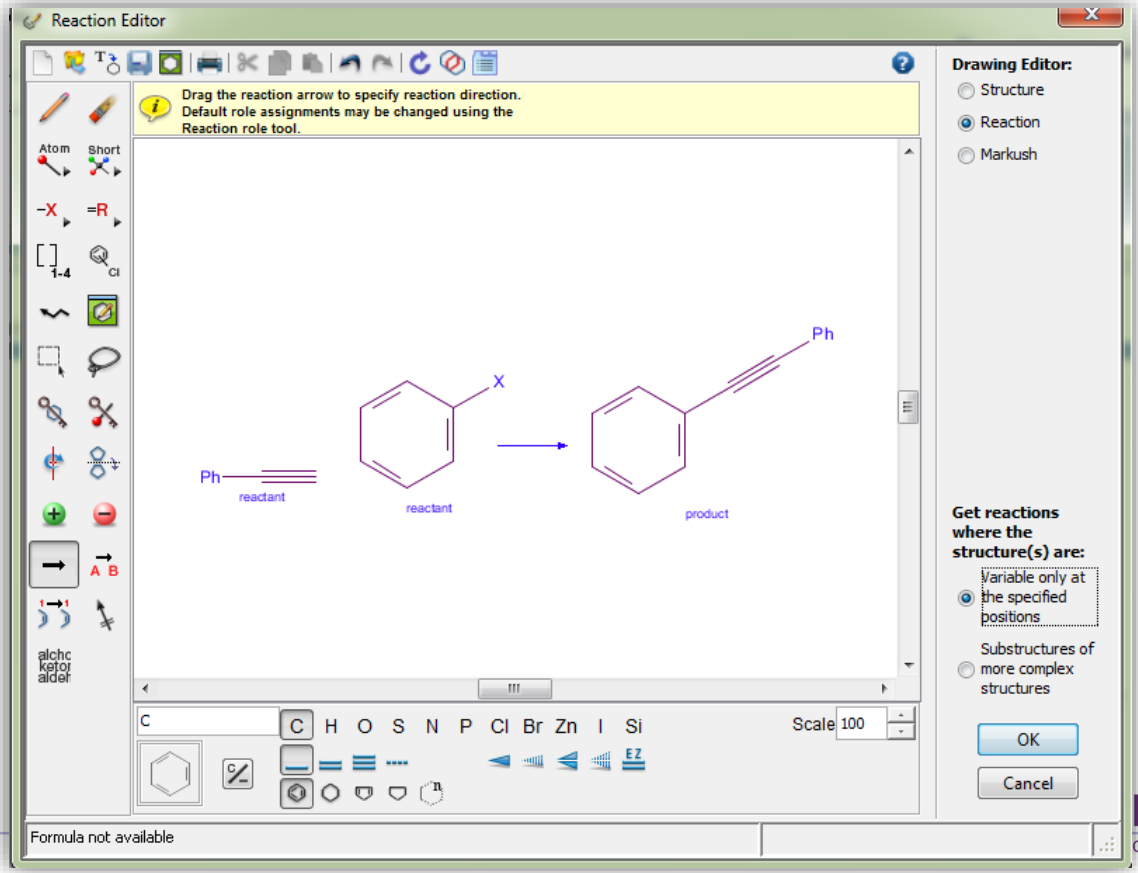
Case Study

Locate reactions with experimental procedures for the following reaction



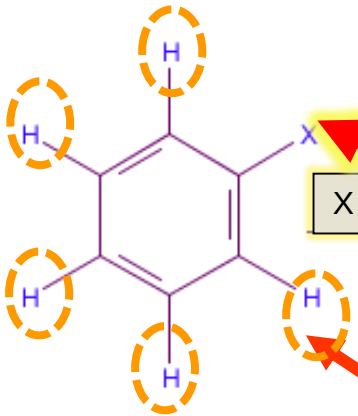
SciFinder®
A CAS SOLUTION

Draw the reaction



Variable at Specified Position

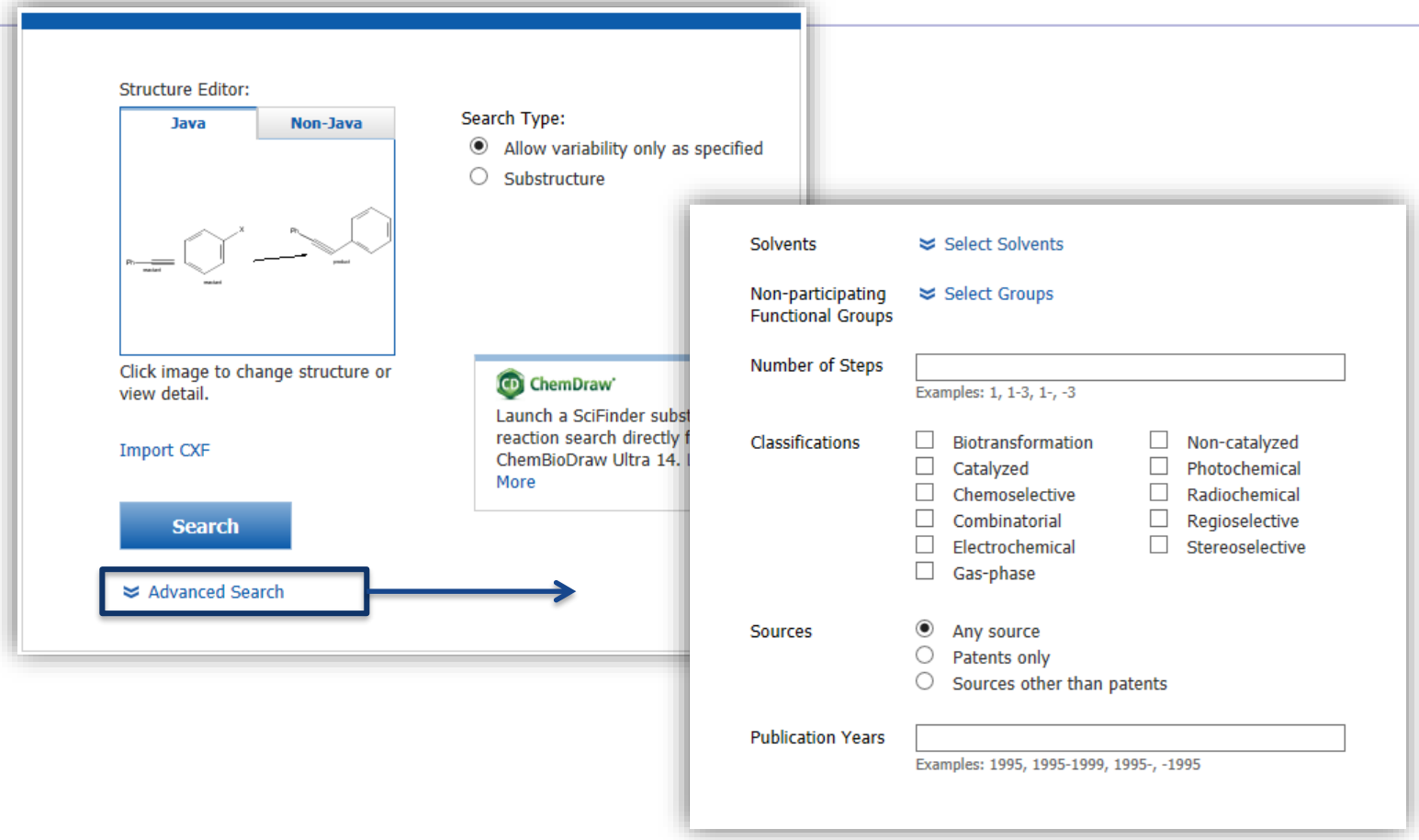
"Variable at specified positions" as the name indicates would consider on the specified positions as variable, rest of the positions would be satisfied by hydrogen



X can be any halogen like Cl, F , Br etc..

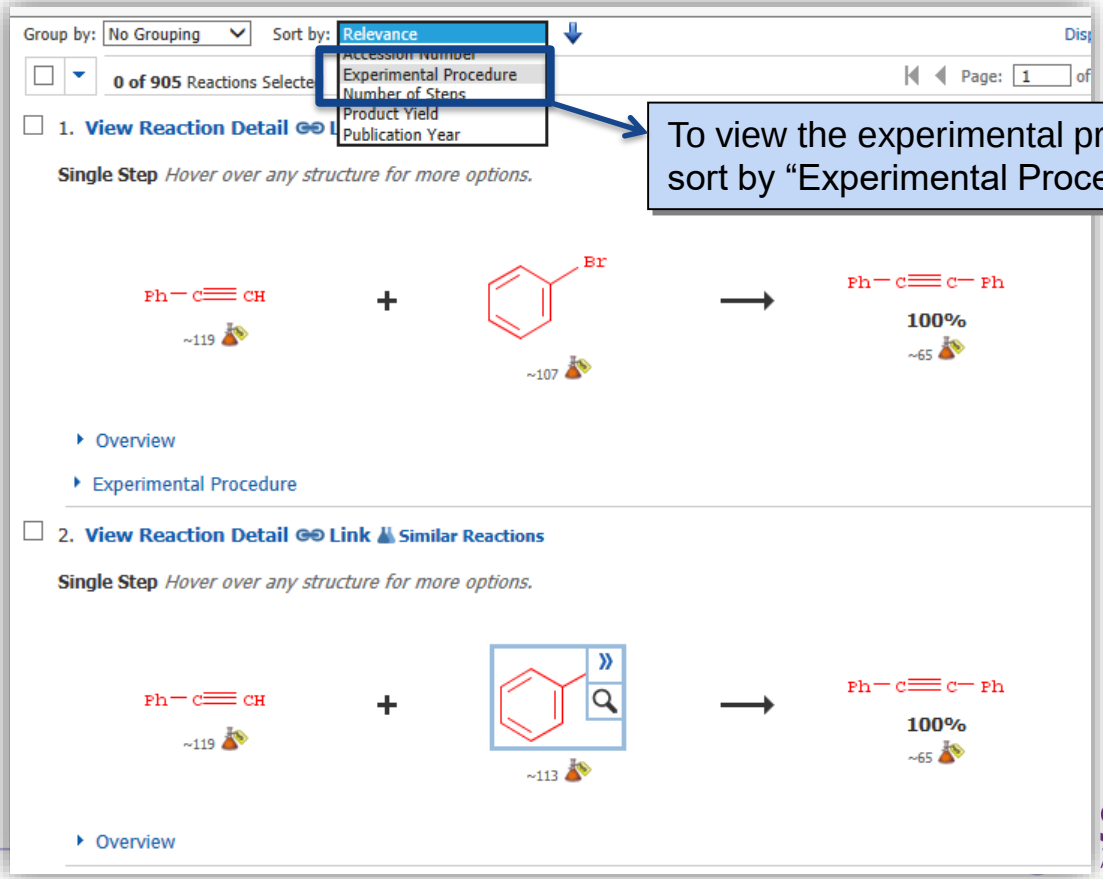
Open position here is considered to have hydrogen

SciFinder®
A CAS SOLUTION



SciFinder®
A CAS SOLUTION

Reaction Searching



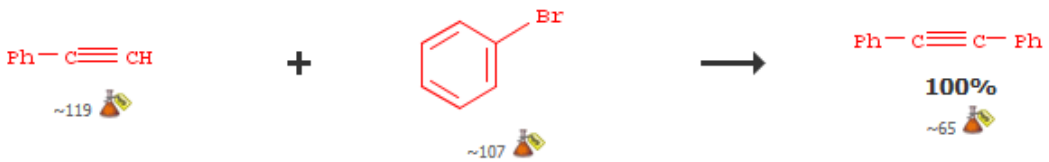
To view the experimental procedures, sort by “Experimental Procedures”

SCIFINDER®
A CAS SOLUTION
SciFinder®

Reactions with experimental procedures

1. View Reaction Detail Link Similar Reactions

Single Step *Hover over any structure for more options.*



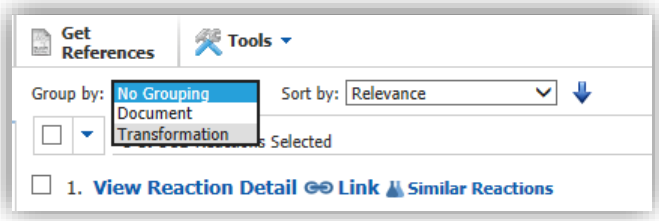
▸ Overview

▾ Experimental Procedure

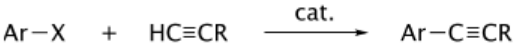
ORGANOMETALLICS

Procedure for Monitoring Cross-Coupling Reactions. In a typical procedure, catalyst precursor (0.01 or 0.05 mmol) and PPh_3 or $PBut_3$ in the desired ratio were dissolved in 3 mL of THF (for reactions carried out at 50°C) or DMF (for reactions carried out at 100°C), and the mixture was stirred at 50°C under argon as outlined previously.4b,d (Heating of a solution of I and two equivalents of PPh3 in DMF at 100°C resulted in the precipitation of palladium metal and hence reduced cross-coupling yields.) Triethylamine (0.4 mL, 2.8 mmol), bromobenzene (0.11 mL, 1.1 mmol), phenylacetylene (0.10 mL, 1 mmol), CuI (where appropriate, 19 mg, 0.1 mmol), and nhexadecane (0.1 mL, 0.34 mmol) were added to the mixture, which was stirred at 50 or 100°C for up to 24 h under argon. Aliquots (0.2 mL) were removed at specified intervals, diluted to 10 mL in a volumetric flask with THF or toluene, and then run through the GC.

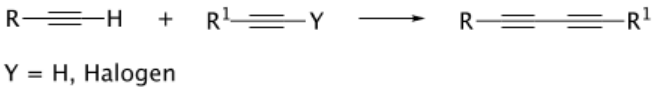
Group by Document



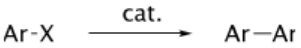
1. **Aryl-Alkyne Coupling/ Stephens-Castro Coupling/ Sonogashira Coupling**
869 Reactions



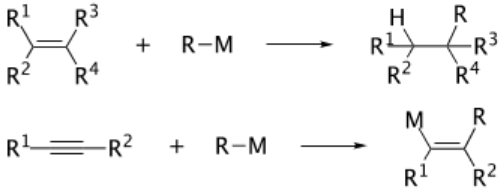
2. **Cadiot-Chodkiewicz Alkyne Coupling/ Eglinton, Glaser or Hay Reactions**
18 Reactions



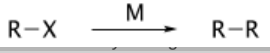
3. **Coupling of Aryl Halides/ Ullmann Reaction**
4 Reactions



4. **Addition of Organometallics to Unactivated Double or Triple Bonds**
3 Reactions

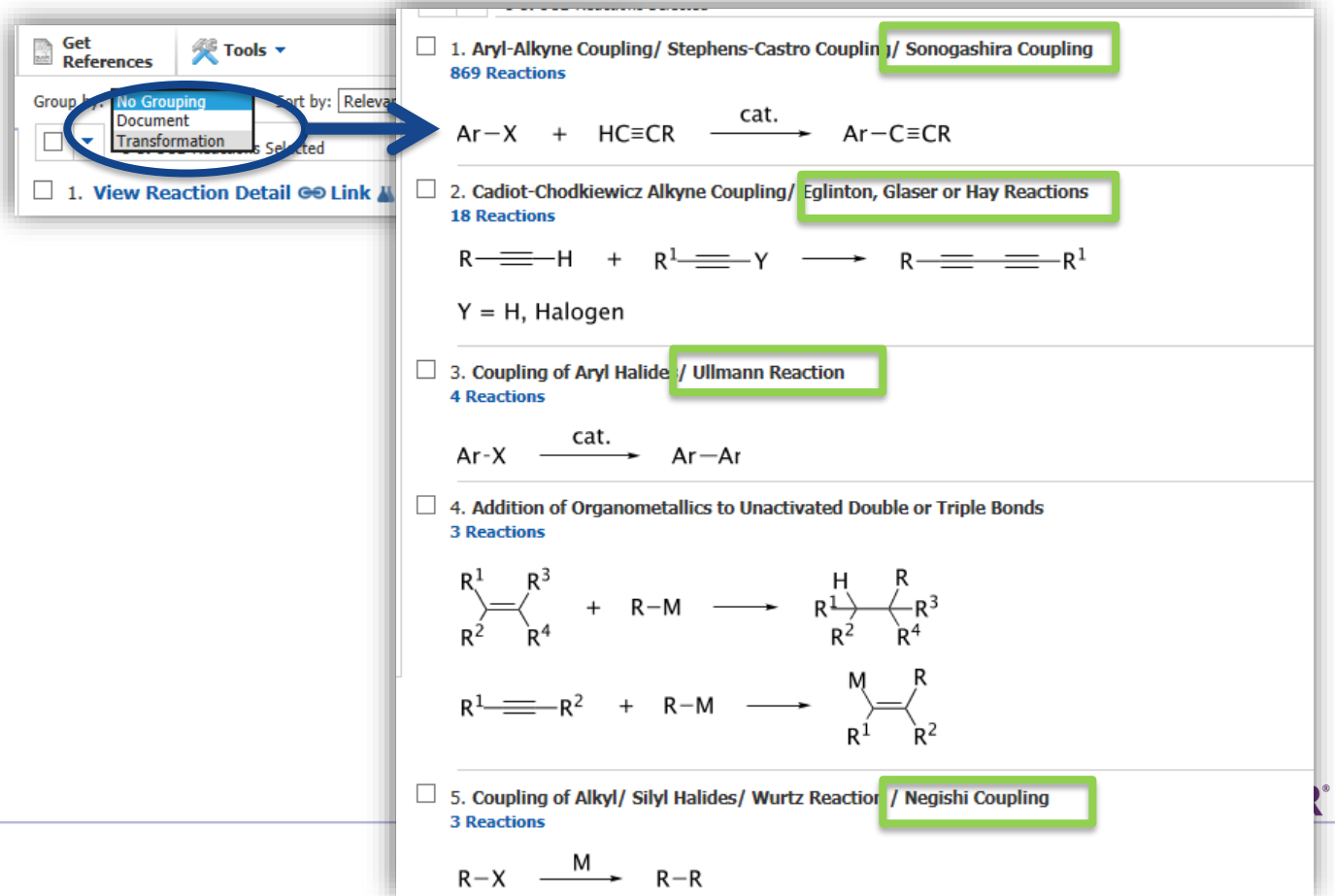


5. **Coupling of Alkyl/ Silyl Halides/ Wurtz Reaction / Negishi Coupling**
3 Reactions



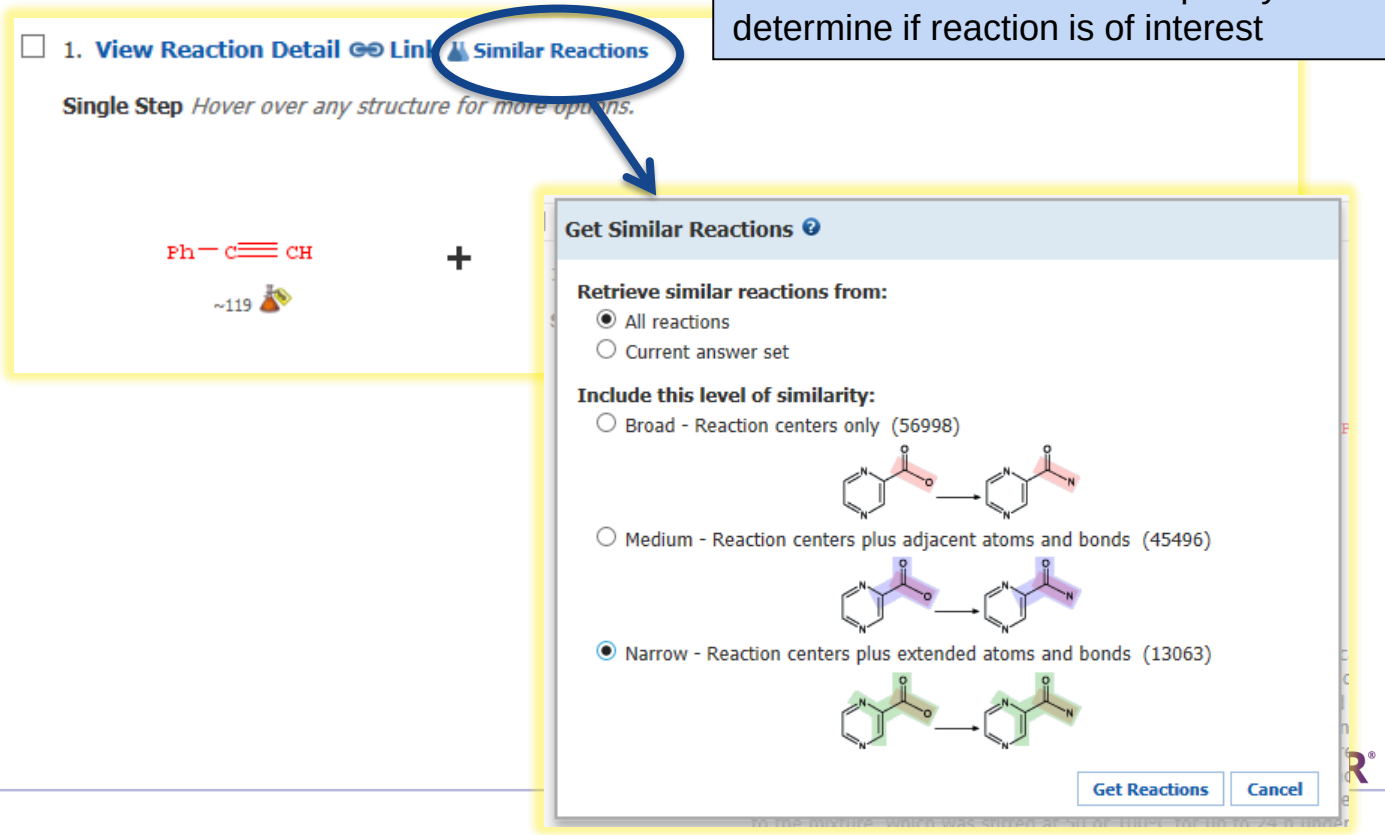
CAS is a division
Copyright 2016 Ameri

Group by Transformation



Similar Reactions

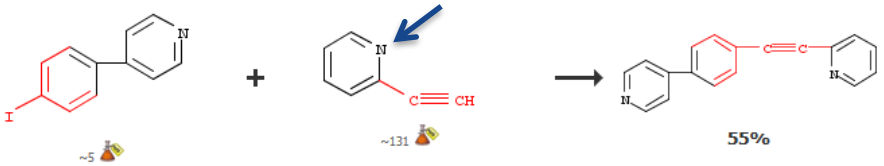
Benefit: Provides details to quickly determine if reaction is of interest



Similar Reactions

11685. **View Reaction Detail** **Link** **Similar Reactions**

Single Step *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 R:Et_3N, C:$Pd(PPh_3)_4$, C:$PdCl_2(PPh_3)_2$, C:CuBr, S:Et_3N, 20°C → reflux; 40 h, reflux

Notes

Heck reaction, Reactants: 2, Reagents: 1, Catalysts: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Stereoselective Association of Binuclear Metallacycles in Coordination Polymers

Quick View Full Text

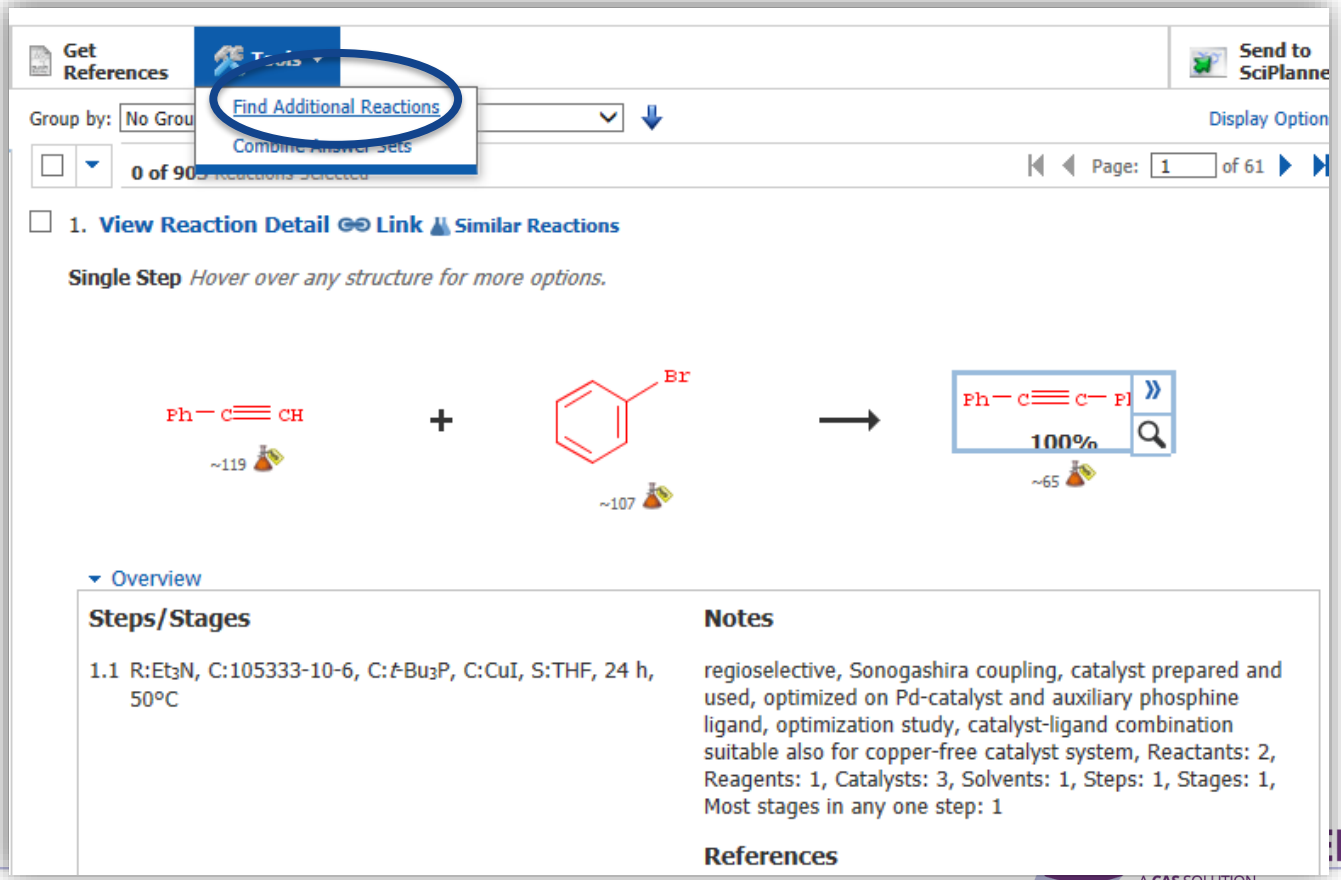
By Khlobystov, Andrei N. et al

From Journal of the American Chemical Society, 125(22), 6753-6761; 2003

Experimental Procedure

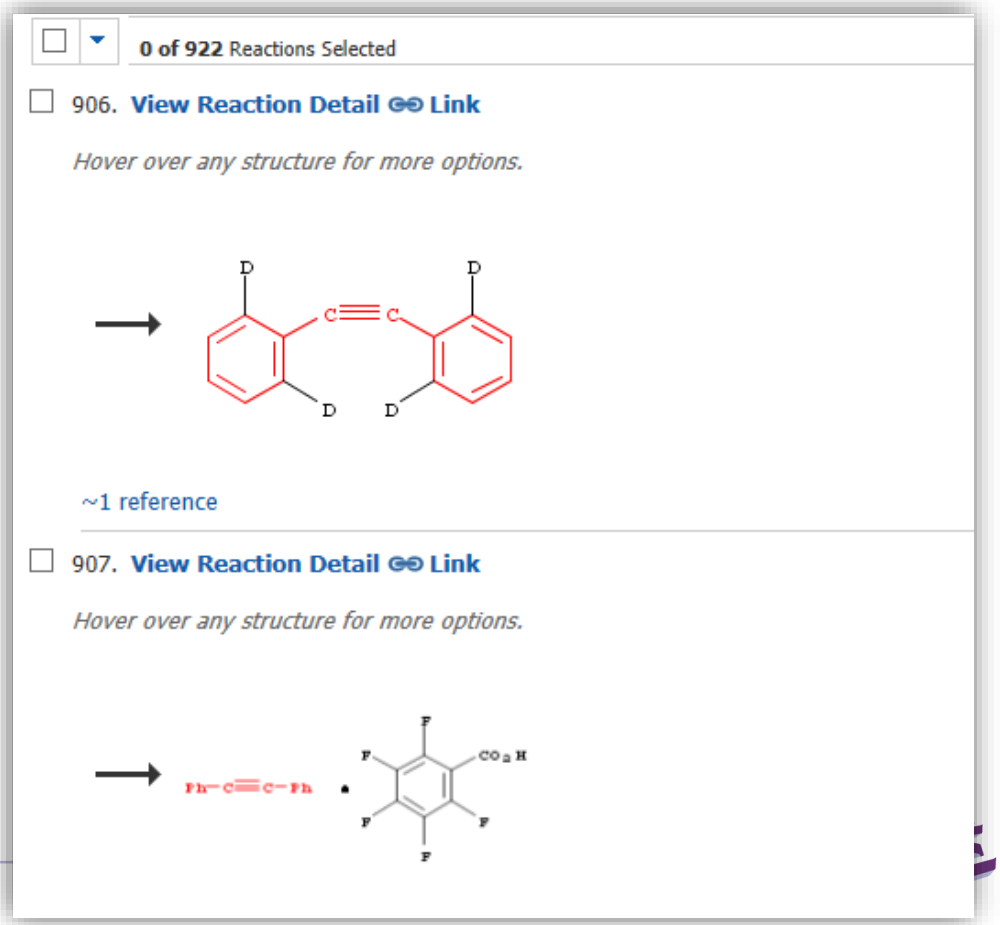
SciFinder® A CAS SOLUTION

Additional Reactions



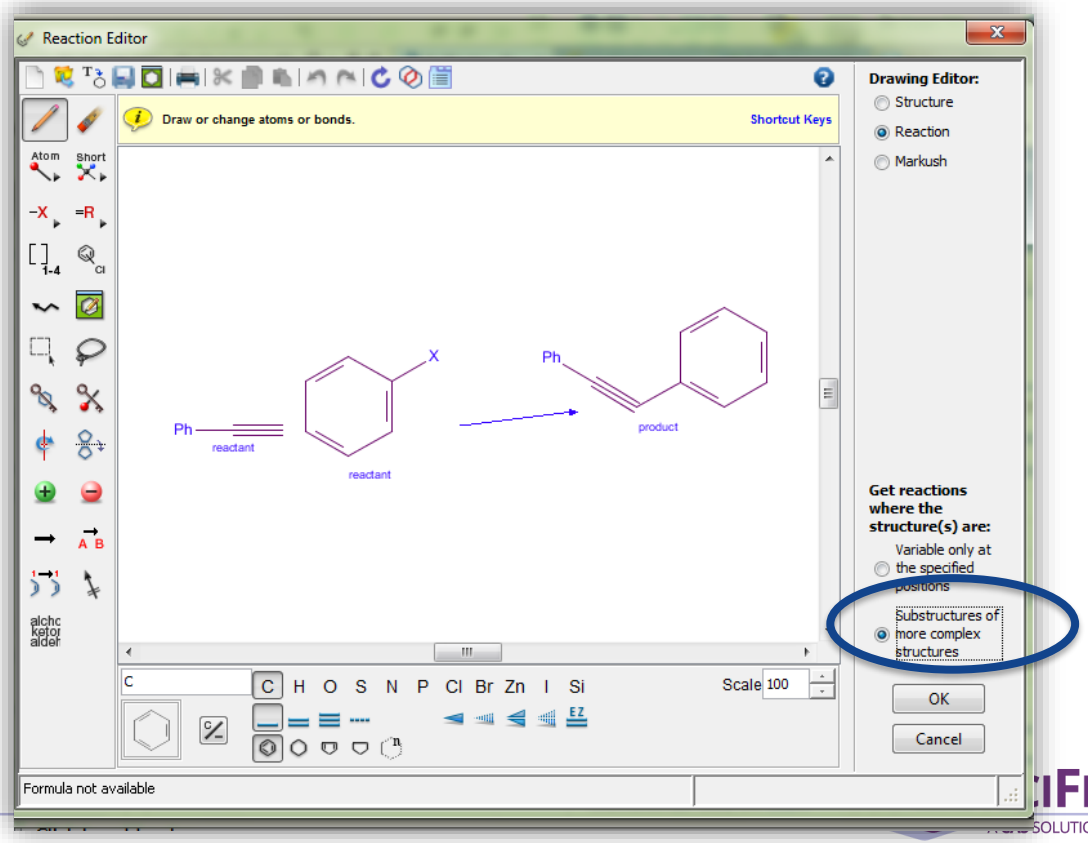
A CAS SOLUTION
SciFinder®

Additional Reactions



SciFinder®
A CAS SOLUTION

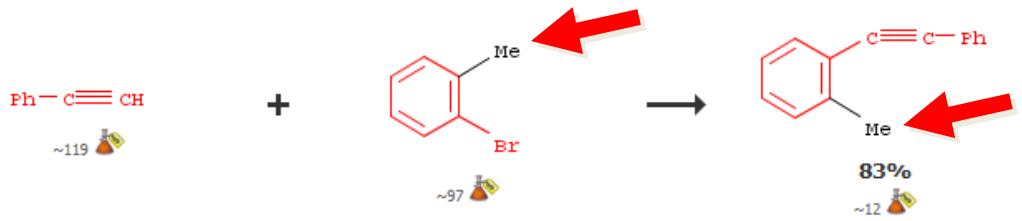
Search Type- Substructure of more complex structure



Substructure reaction results

1486. **View Reaction Detail** **Link** **Similar Reactions**

Single Step *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 C:937378-01-3, C:$PdCl_4$ •2Na, C:CuI, S:i-Pr_2NH, 16 h, 80°C

Notes

Sonogashira coupling, catalyst mixture in diisopropylammonium bromide, Reactants: 2, Catalysts: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

9-Fluorenylphosphines for the Pd-catalyzed Sonogashira, Suzuki, and Buchwald-Hartwig coupling reactions in organic solvents and water

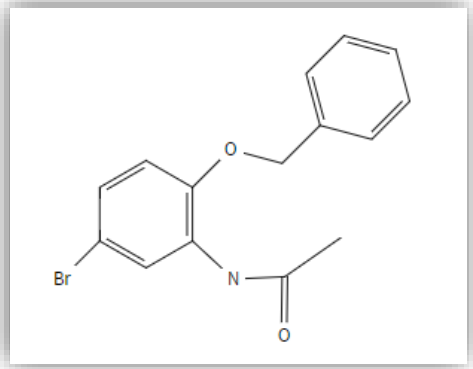
Quick View Full Text

By Fleckenstein, Christoph A. and Plenio, Herbert

From Chemistry - A European Journal, 13(9), 2701-2716; 2007

How can I find?

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

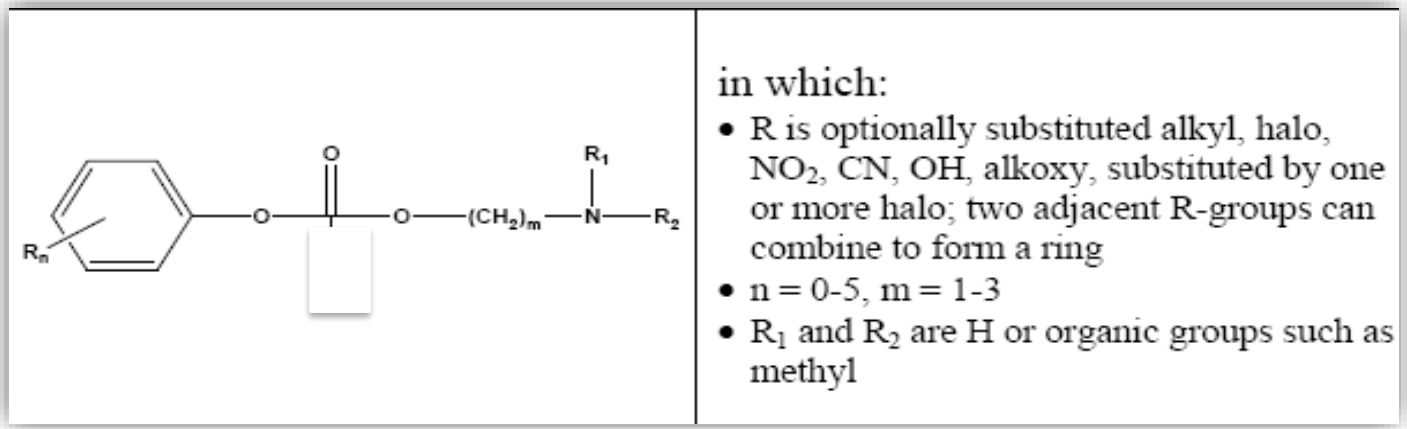


Answer is : Markush Searching !!

SciFinder®
A CAS SOLUTION

What is Markush Structure?

- A generalized formula or description for a related set of chemical compounds, used in patent applications.
- Markush structures are used in patents to cover a range of structures in a single structure drawing.



* Named after dye chemist Eugene Markush, the first inventor to successfully defend the right to use these types of claims in a patent.

A CAS SOLUTION
SciFinder®

Indexing of Substances

A patent may contain two kinds of substance representations:

- Specific substances, represented by specific chemical structures/names and is assigned a specific CAS Registry Number
- Generic substances, represented by generic Markush Structures. Each Markush structure may represent hundreds , or even thousands of chemical substances.

Indexing of substances in Patents

Illustration: Specific substance

US 6,482,985

Example 1

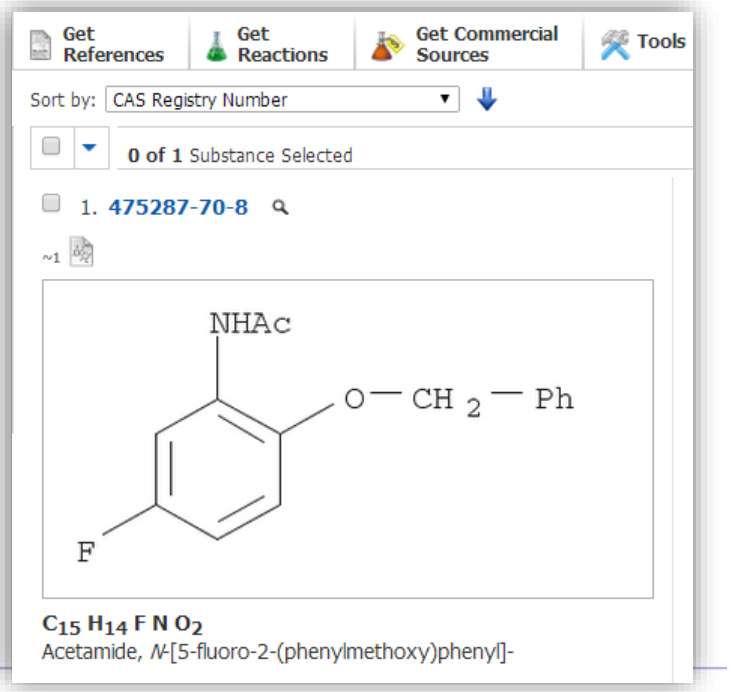
2-Benzyloxy-5-fluoroacetanilide (Formula I; R=CH_3 and X=F)

In a 500-ml flask, place 44.8 g (0.4 m) of 4-fluorophenol (1a; X=F) and 132 ml of acetic acid and stir to a solution. Add 0.6 g of sodium nitrite and cool the solution to 15° C. Add 36.0 g (0.4 m) of 70% nitric acid in drop wise keeping the temperature at 22–27° C. over 10–15 min. Stir the resulting yellow slurry at room temperature for 3 hrs. Warm the mixture to 65° C. to make a clear solution and add 132 ml of warm (65° C.) water slowly. Stir the resulting slurry

SCIFINDER®
A CAS SOLUTION

Indexing of substances in Patents

This specific substance received a CAS RN 475287-70-8 and was indexed in SciFinder



This substance is **searchable** by Name, CAS Registry Number , Molecular formula and Structure Search

SciFinder®
A CAS SOLUTION

Indexing of substances in Patents

Generic Substances

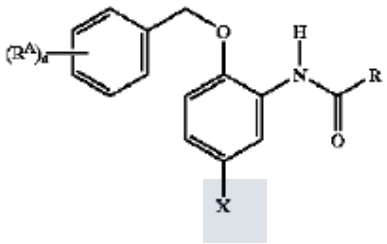
US 6,482,985

Illustration:Generic substances reported in a patent

(57) **ABSTRACT**

Disclosed is a compound comprising a 2-benzyloxy-5-haloacylanilide having the structural formula I:

Formula I



wherein

R is hydrogen or an alkyl group,

R^A is a substituent and n is 0–5; and

X is a halogen.

Also disclosed is a method for preparing a coupler using the compound. The compound and method simplify the preparation of photographic couplers.

5 Claims, No Drawings

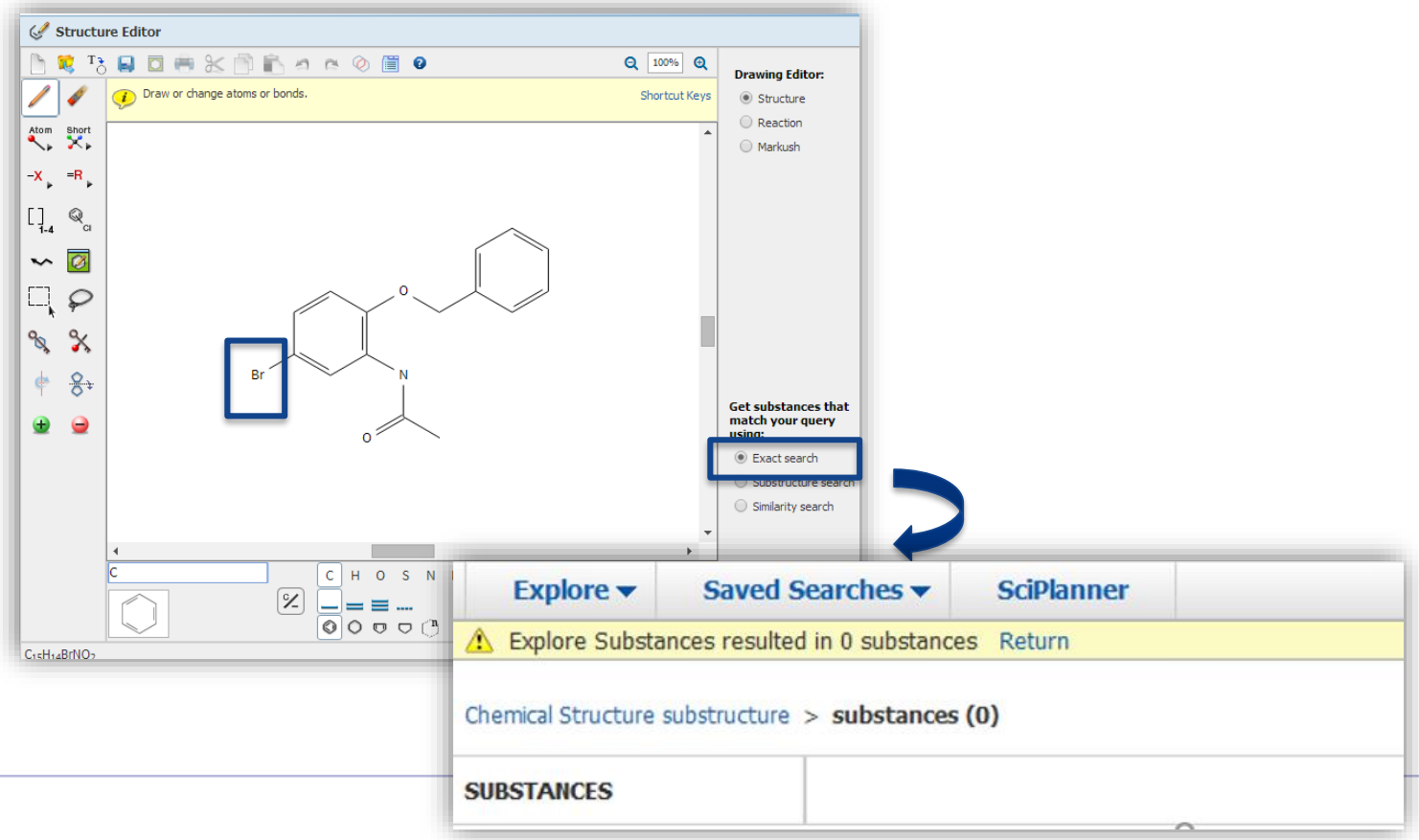
Example discusses substances as 2-Benzoxyl-5 **fluoro**acetanilide .

But claims mentions it as 2-Benzyloxy-5-**Halo**acetanilide

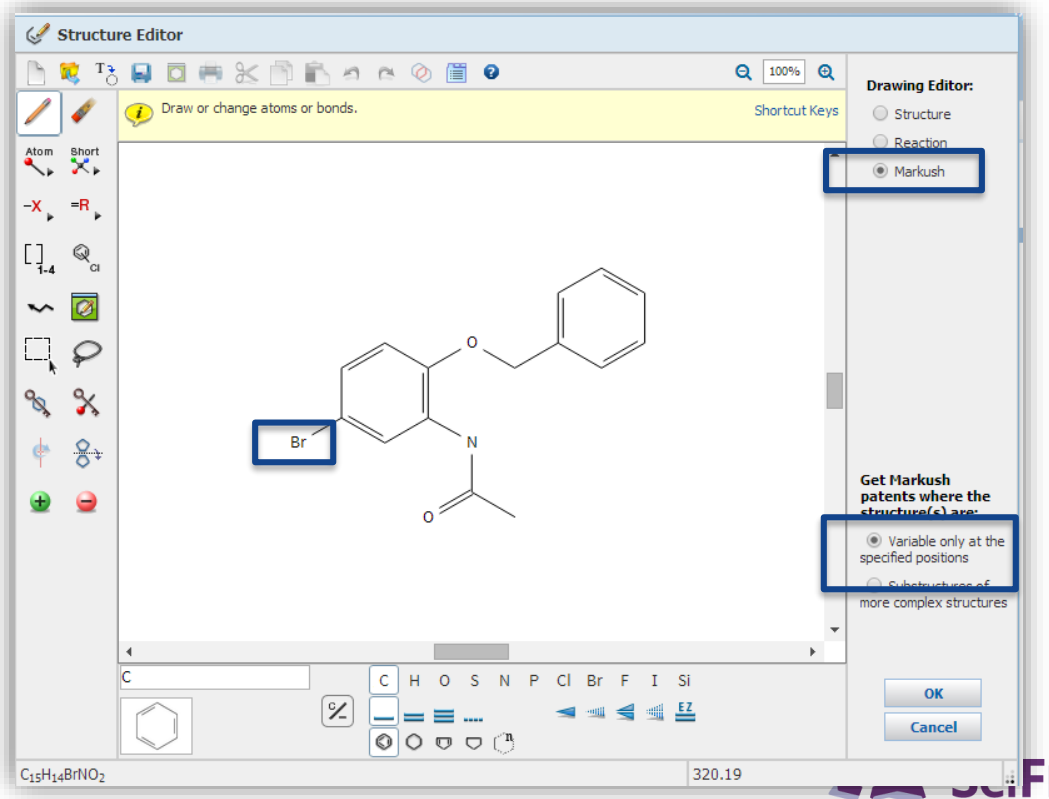
Since, its not specific – It will not be assigned a new RN

SciFinder® A CAS SOLUTION

Lets conduct Structure Search now with Halo as Br !!



Change the search type as Markush



SciFINDER®
A CAS SOLUTION

50 references retrieved!!

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Sort by: Accession Number ▼ Display Options

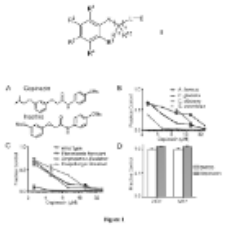
0 of 50 References Selected Page: 1 of 4

1. **Compounds for treating infectious diseases**

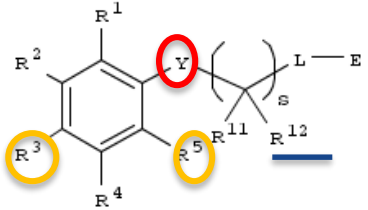
Quick View Full Text

By McLellan, Catherine; Mazitschek, Ralph; Whitesell, Luke; Lindquist, Susan L.

From PCT Int. Appl. (2013), WO 2013192517 A2 20131227. | Language: English, Database: CAPLUS



The invention provides compds. [R^1, R^3, R^4, R^5= H, halo, CN, NO_2, etc.; R^2= H, halogen, OR^x; R^x= (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, etc.; Y= O, S; L= bond, $NR^{13}C(O)$, $C(O)NR^{13}$; R^{11}= H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted carbocyclyl, etc.; R^{12}= H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted carbocyclyl, etc.; R^{13}= H, C_{1-6}alkyl; E= (un)substituted aryl, (un)substituted heteroaryl; s= 1-6], eg. gepinacin, and pharmaceutically acceptable salts compns. Compds. of the invention are useful for inhibiting fungal or parasitic growth. The compds. are useful as inhibitors of glycosylphosphatidylinositol (GPI)-anchor biosynthesis, in particular, as inhibitors of fungal Gwt1 activity. The invention further provides methods of using the compds. described for treating fungal or parasitic infections. The compds. can also be used as biol. probes to study the effects of inhibiting Gwt1 activity. Also disclosed is the prepn. of some compds. of invention.



Indexing of substances in SciFinder

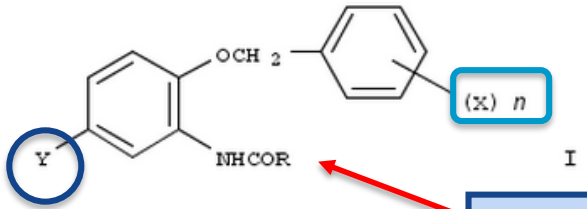
1. **2-(Benzyloxy)-5-halo-N-acylanilines**

Quick View | Full Text | PDF

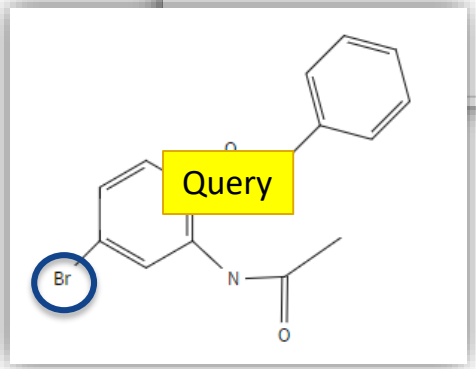
By Kim, Chang-Kyu

From U.S. (2002), US 6482985 B1 20021119. | Language: English, Database: CAPLUS

Disclosed are 2-(optionally substituted benzyloxy)-5-halo-N-acylanilines (I; R = H, alkyl; X = substituent; n = 0-5; Y = halogen). I can be used to prep. phenolic cyan dye-forming couplers with improved efficiency. In an example, I (R = Me; Y = F; n = 0) was prepd. starting with 4-fluorophenol followed by steps of nitration, redn., acetylation, and benzylation.



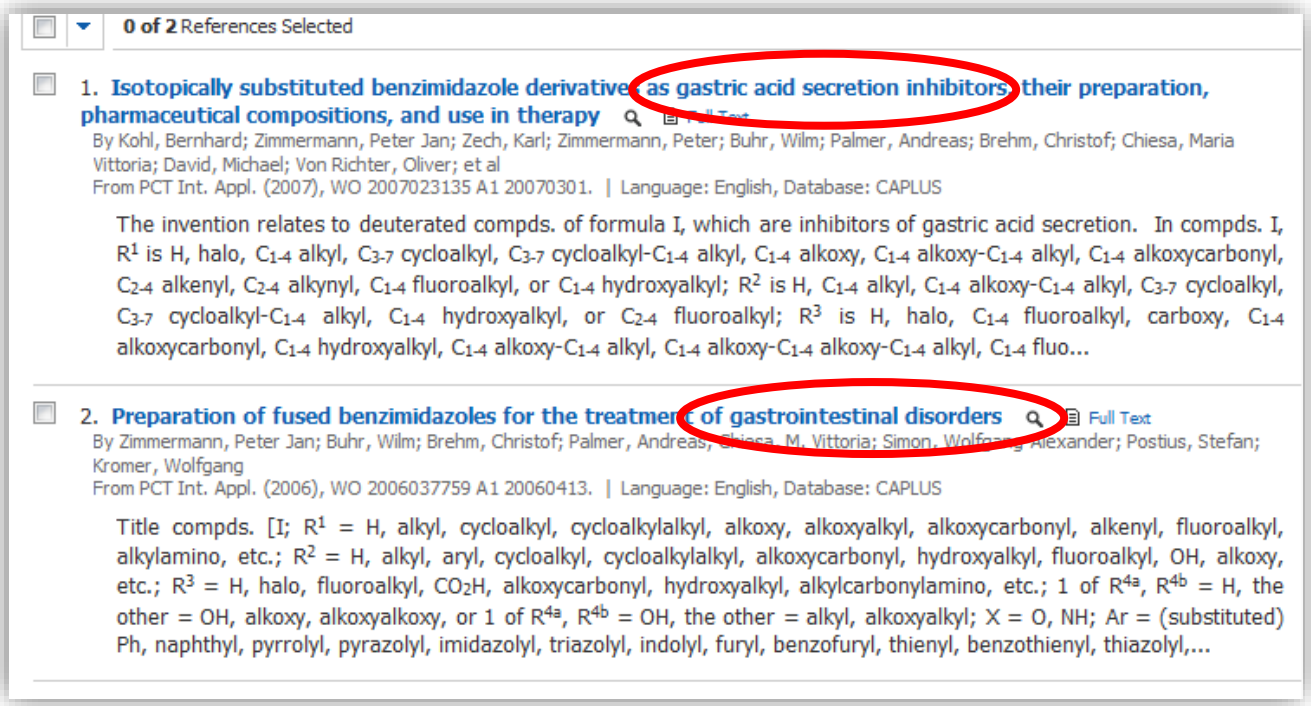
I



- Represented by Markush Structures
- Does not receive CAS RNs.

Searchable only by Markush

Two references found



0 of 2 References Selected

1. **Isotopically substituted benzimidazole derivatives as gastric acid secretion inhibitors, their preparation, pharmaceutical compositions, and use in therapy**

By Kohl, Bernhard; Zimmermann, Peter Jan; Zech, Karl; Zimmermann, Peter; Buhr, Wilm; Palmer, Andreas; Brehm, Christof; Chiesa, Maria Vittoria; David, Michael; Von Richter, Oliver; et al

From PCT Int. Appl. (2007), WO 2007023135 A1 20070301. | Language: English, Database: CAPLUS

The invention relates to deuterated compds. of formula I, which are inhibitors of gastric acid secretion. In compds. I, R^1 is H, halo, C_{1-4} alkyl, C_{3-7} cycloalkyl, C_{3-7} cycloalkyl-C_{1-4} alkyl, C_{1-4} alkoxy, C_{1-4} alkoxy-C_{1-4} alkyl, C_{1-4} alkoxycarbonyl, C_{2-4} alkenyl, C_{2-4} alkynyl, C_{1-4} fluoroalkyl, or C_{1-4} hydroxyalkyl; R^2 is H, C_{1-4} alkyl, C_{1-4} alkoxy-C_{1-4} alkyl, C_{3-7} cycloalkyl, C_{3-7} cycloalkyl-C_{1-4} alkyl, C_{1-4} hydroxyalkyl, or C_{2-4} fluoroalkyl; R^3 is H, halo, C_{1-4} fluoroalkyl, carboxy, C_{1-4} alkoxycarbonyl, C_{1-4} hydroxyalkyl, C_{1-4} alkoxy-C_{1-4} alkyl, C_{1-4} alkoxy-C_{1-4} alkoxy-C_{1-4} alkyl, C_{1-4} fluo...

2. **Preparation of fused benzimidazoles for the treatment of gastrointestinal disorders** Full Text

By Zimmermann, Peter Jan; Buhr, Wilm; Brehm, Christof; Palmer, Andreas; Chiesa, M. Vittoria; Simon, Wolfgang Alexander; Postius, Stefan; Kromer, Wolfgang

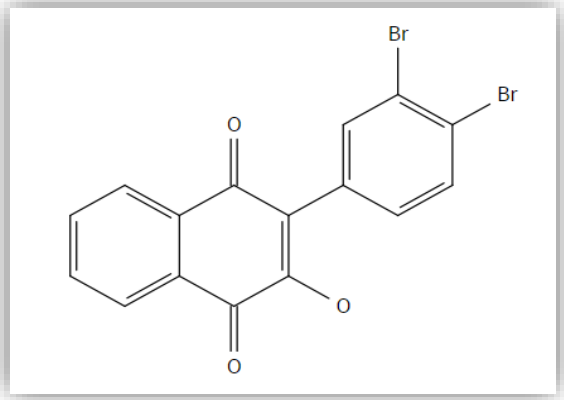
From PCT Int. Appl. (2006), WO 2006037759 A1 20060413. | Language: English, Database: CAPLUS

Title compds. [I; R^1 = H, alkyl, cycloalkyl, cycloalkylalkyl, alkoxy, alkoxyalkyl, alkoxycarbonyl, alkenyl, fluoroalkyl, alkylamino, etc.; R^2 = H, alkyl, aryl, cycloalkyl, cycloalkylalkyl, alkoxycarbonyl, hydroxyalkyl, fluoroalkyl, OH, alkoxy, etc.; R^3 = H, halo, fluoroalkyl, CO_2H, alkoxycarbonyl, hydroxyalkyl, alkylcarbonylamino, etc.; 1 of R^{4a}, R^{4b} = H, the other = OH, alkoxy, alkoxyalkoxy, or 1 of R^{4a}, R^{4b} = OH, the other = alkyl, alkoxyalkyl; X = O, NH; Ar = (substituted) Ph, naphthyl, pyrrolyl, pyrazolyl, imidazolyl, triazolyl, indolyl, furyl, benzofuryl, thienyl, benzothienyl, thiazolyl,...

SciFinder®
A CAS SOLUTION

Difficult to find some substances?

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



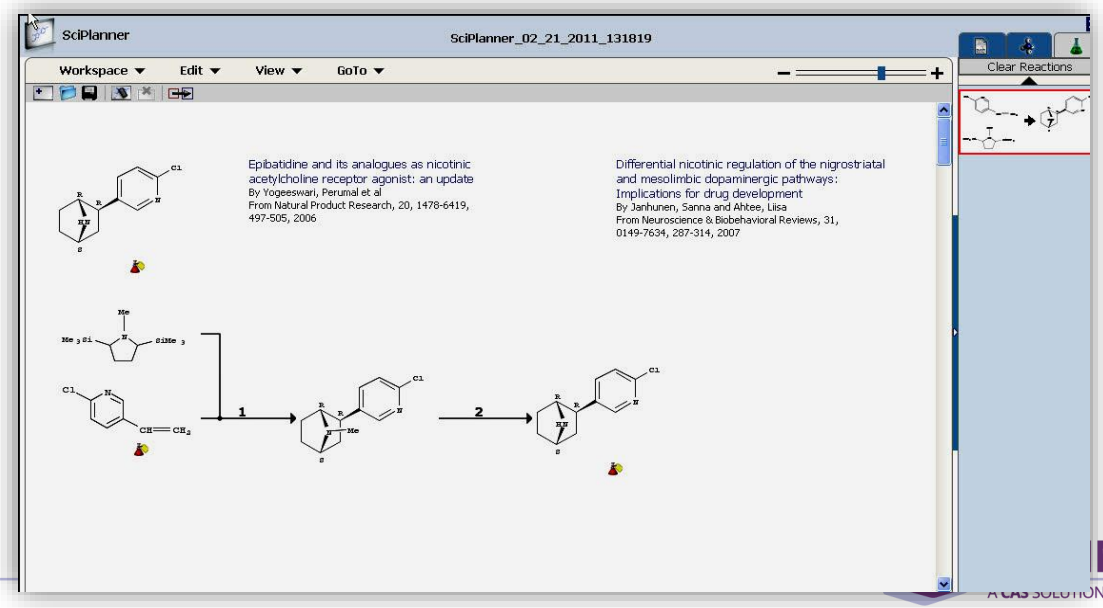
Find it with Markush search

CAS is a division of the American Chemical Society.
Copyright 2018 American Chemical Society. All rights reserved.

SciFinder® A CAS SOLUTION

SciPlanner

SciPlannerTM is an interactive workspace to organize substance, reaction and reference search results, and plan syntheses projects all in one place before heading to the lab or sharing with colleagues.



NDER®
A CAS SOLUTION

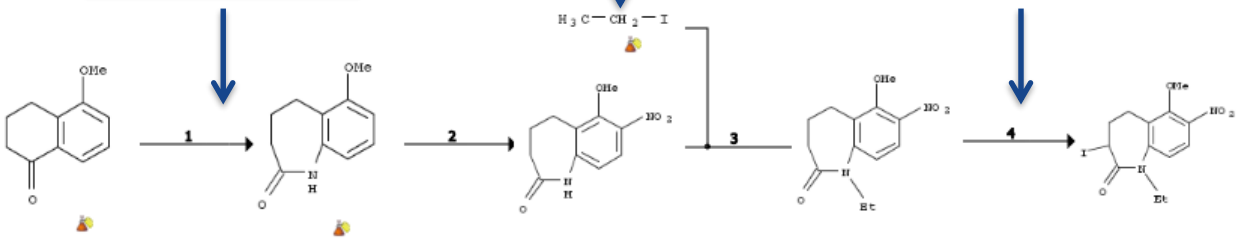
For compiling Multiple Reactions Together From Several Documents

Design the synthetic routes

Reference A (Journal 1999)

Patent B 2010

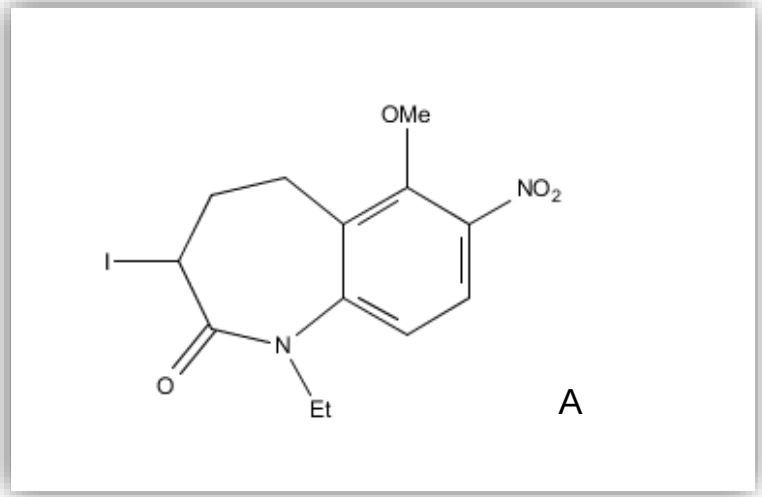
Reference A (Journal 2013)



SciFinder® A CAS SOLUTION

Case Study

Synthesize of following compound

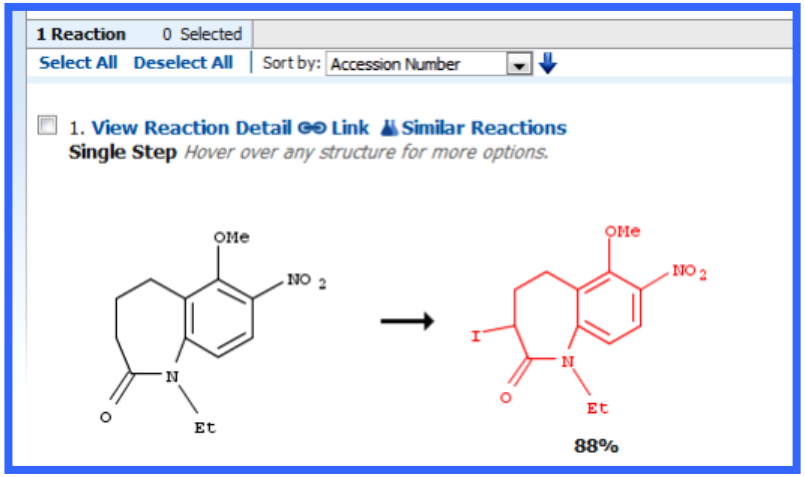


A

SciFinder®
A CAS SOLUTION

Retro-synthesis

- There is only one reaction where desired substance is a product.

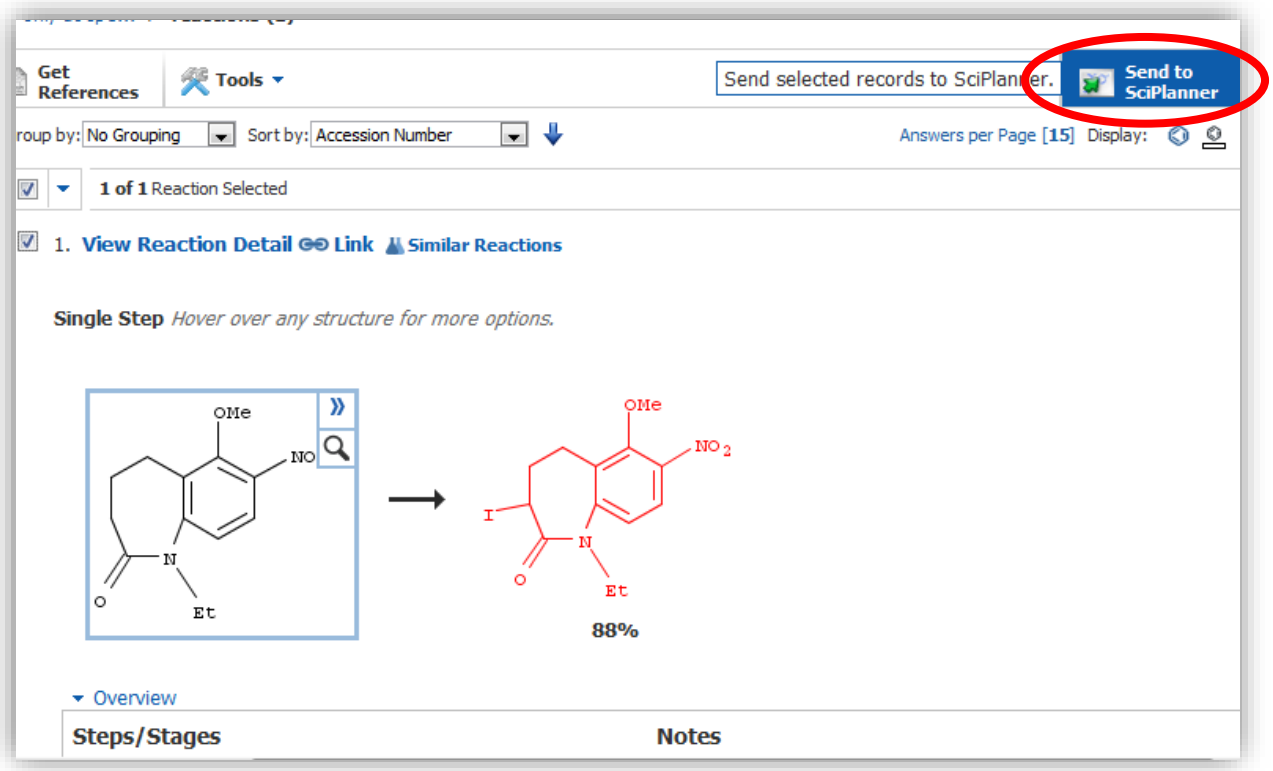


- The reactant is not commercially available

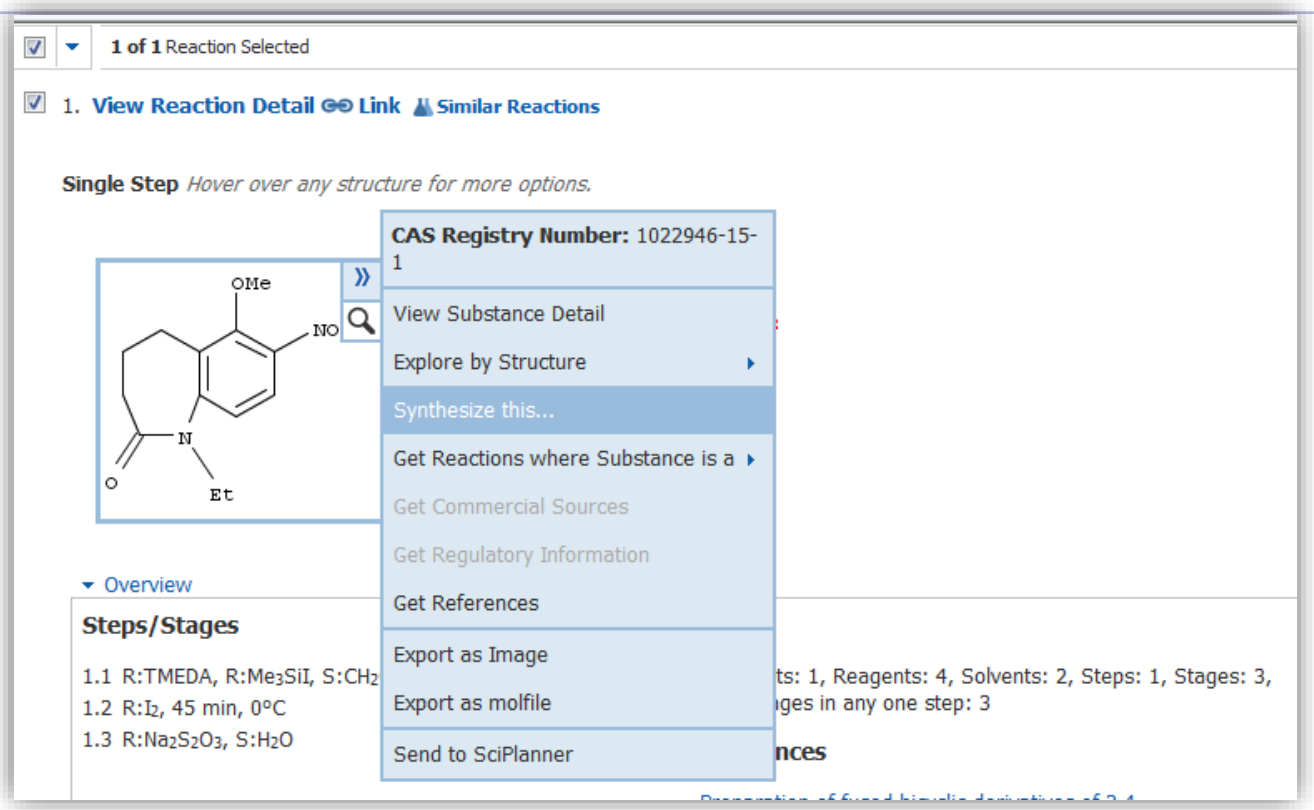
Let's see how to synthesize this reactant using new SciPlanner

SciFinder® A CAS SOLUTION

SciPlanner



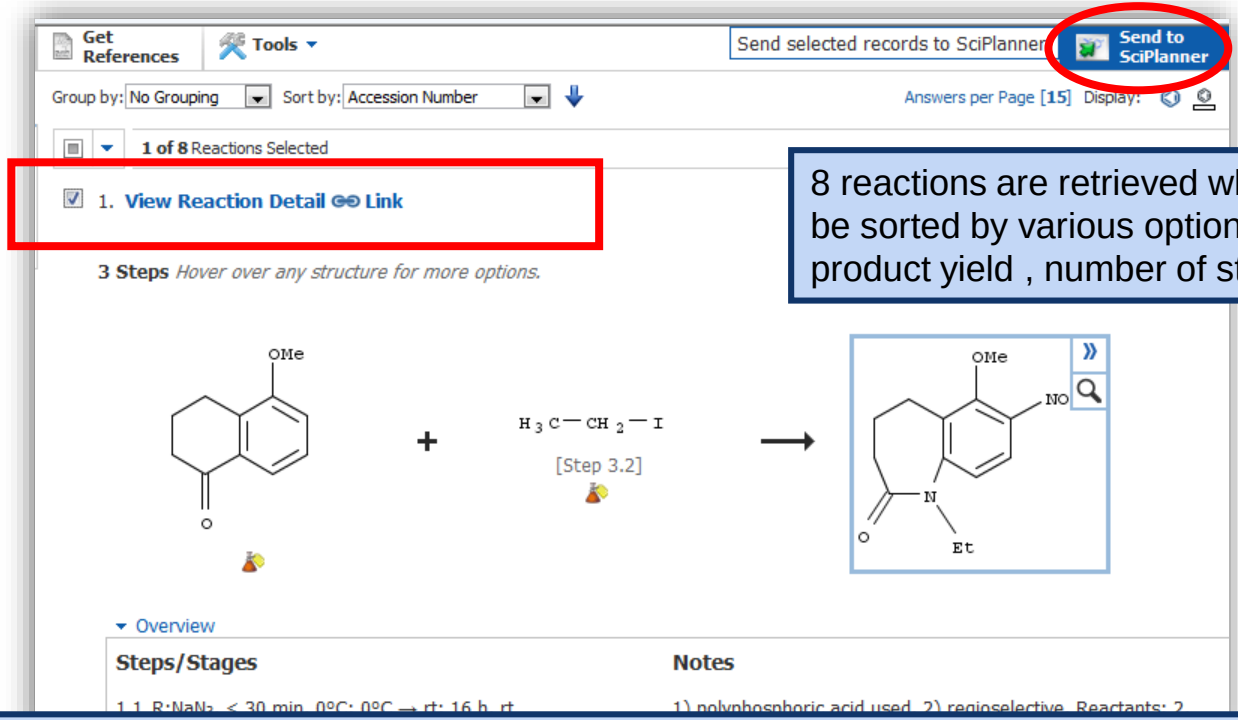
Select the reaction and click on “Send to SciPlanner



Right click on the button of the reactant and select synthesize this…

SciFinder®
A CAS SOLUTION

Select reaction



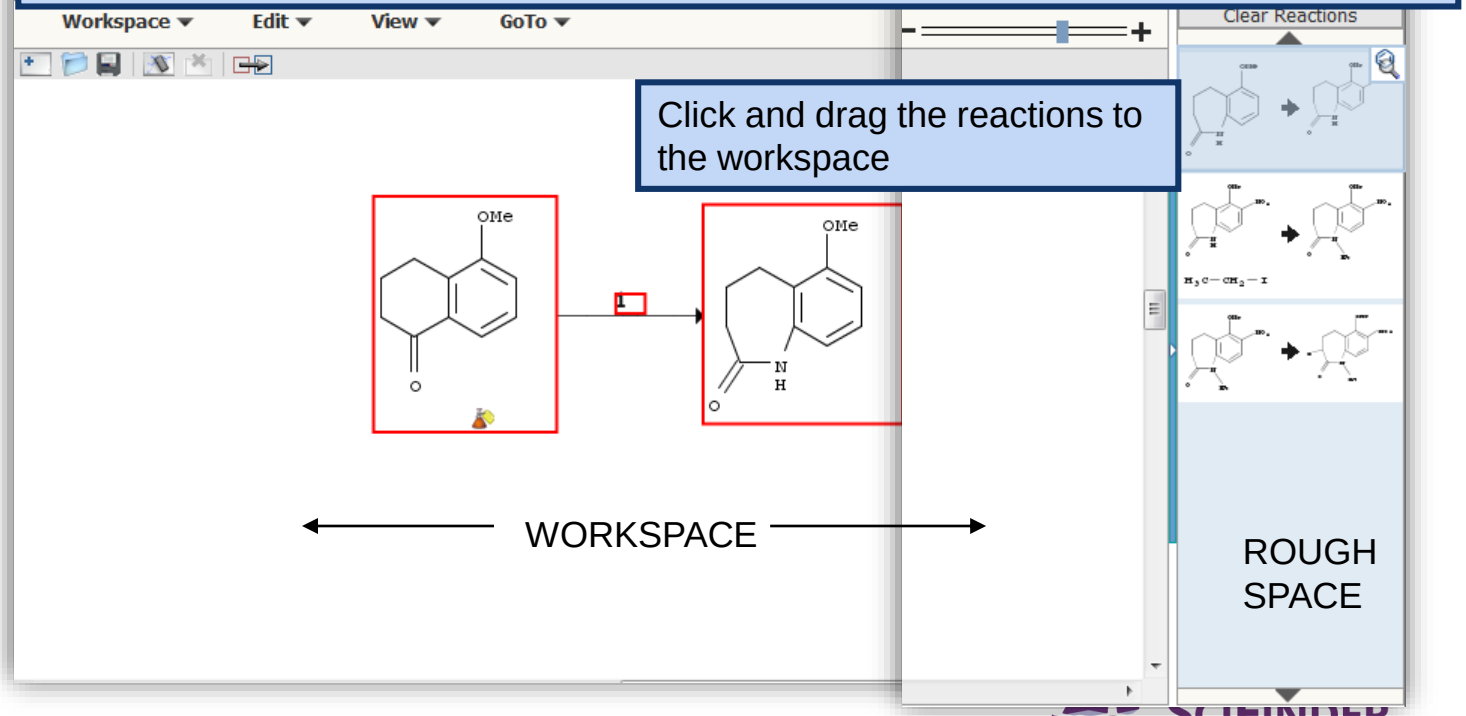
8 reactions are retrieved which can be sorted by various options like product yield , number of steps etc

Select the reaction of interest and click on “Send to SciPlanner” and repeat the steps 2 and 3

SCIFINDER
A CAS SOLUTION

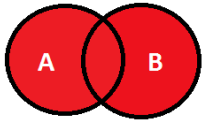
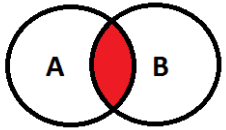
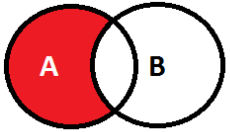
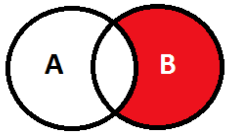
SciPlanner

Once all the reactions are sent to SciPlanner, Organize the reaction in a systematic way in SciPlanner



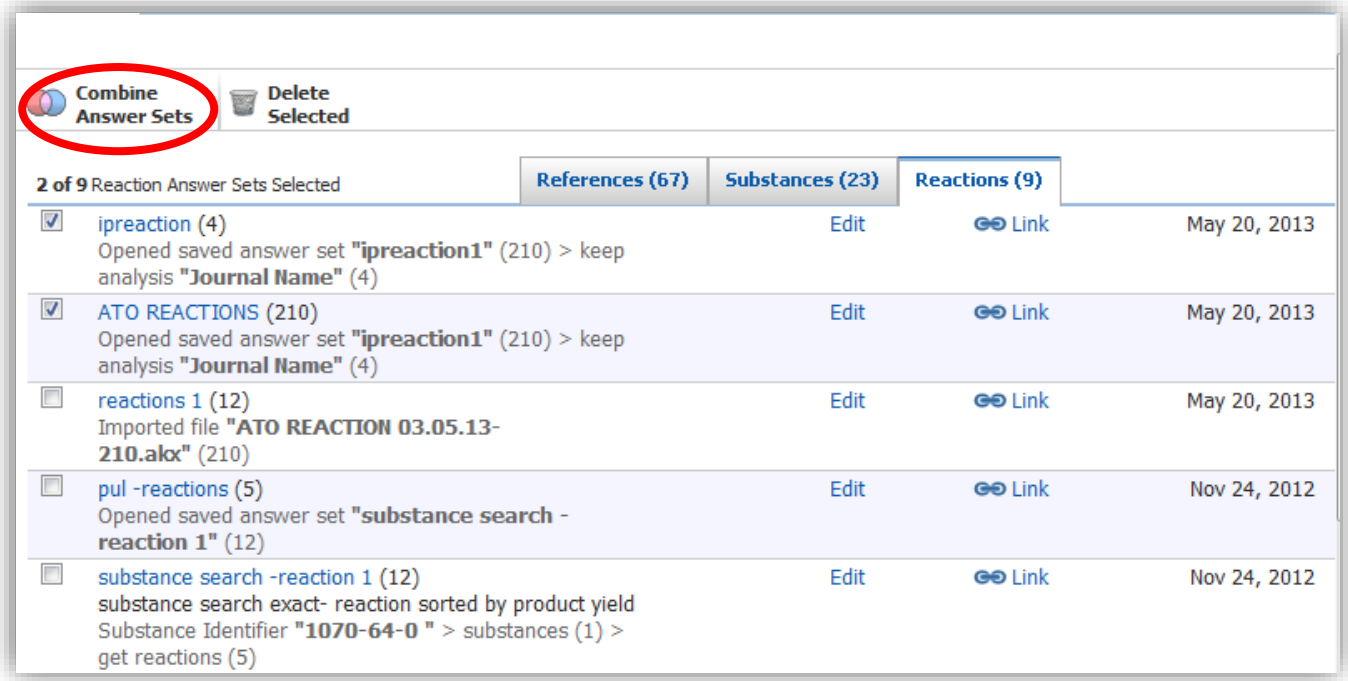
SCIFINDER
A CAS SOLUTION

Combine Answers

For two or more saved answer sets , you can :	Performs a Logical…
 Combine	**OR** combination: The combined answer set includes all answers from both original sets.
 Intersect	**AND** combination: The combined answer set includes only answers that are present in both original sets.i.e common records
 Exclude	**NOT** combination: Contains answers from A which are not in B. The common record gets eliminated.
 Exclude	**NOT** combination: Contains answers from B which are not in A. The common record gets eliminated

SciFinder® A CAS SOLUTION

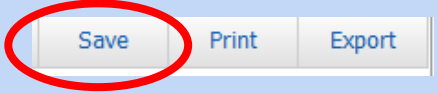
Combine answer sets

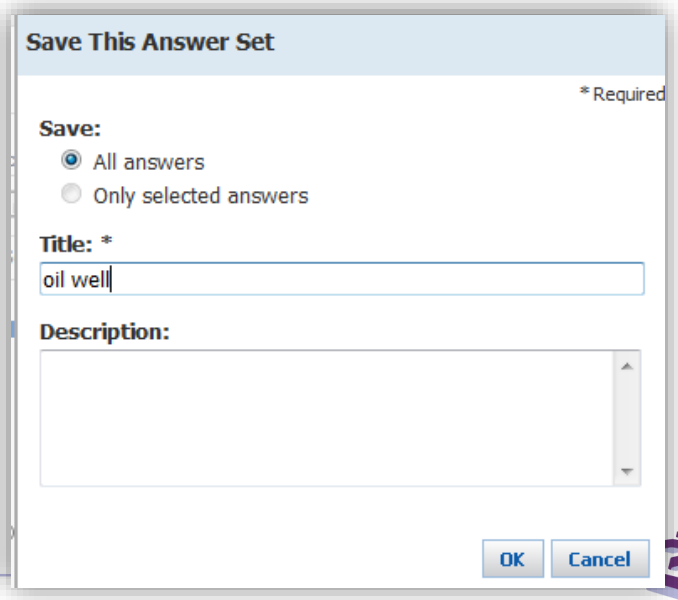


SciFinder®
A CAS SOLUTION

Save Answers

To Save some or all references in an answer set to SciFinder Server, select the references of interest and click “Save”, located in the upper right corner

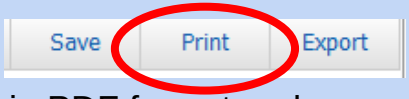




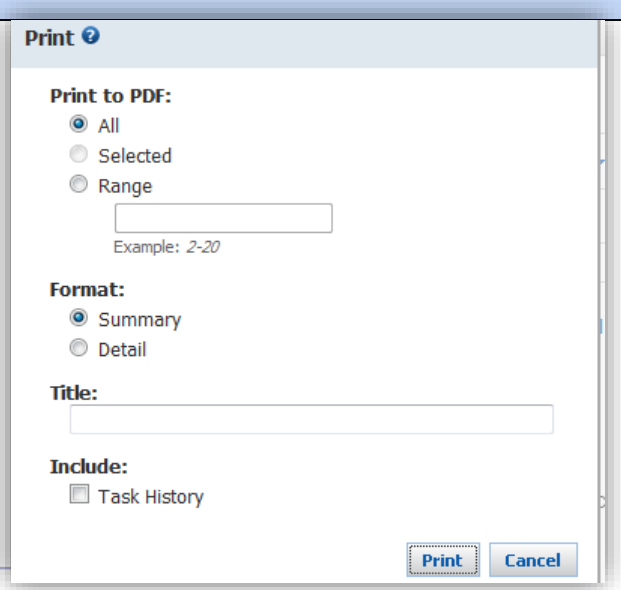
SciFinder®
A CAS SOLUTION

Print Answers

To print some or all references in an answer set, select the references of interest and click “Print”, located in the upper right corner



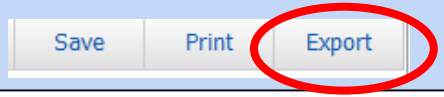
Answer set are printed in PDF format and appear in the new browser tab or window

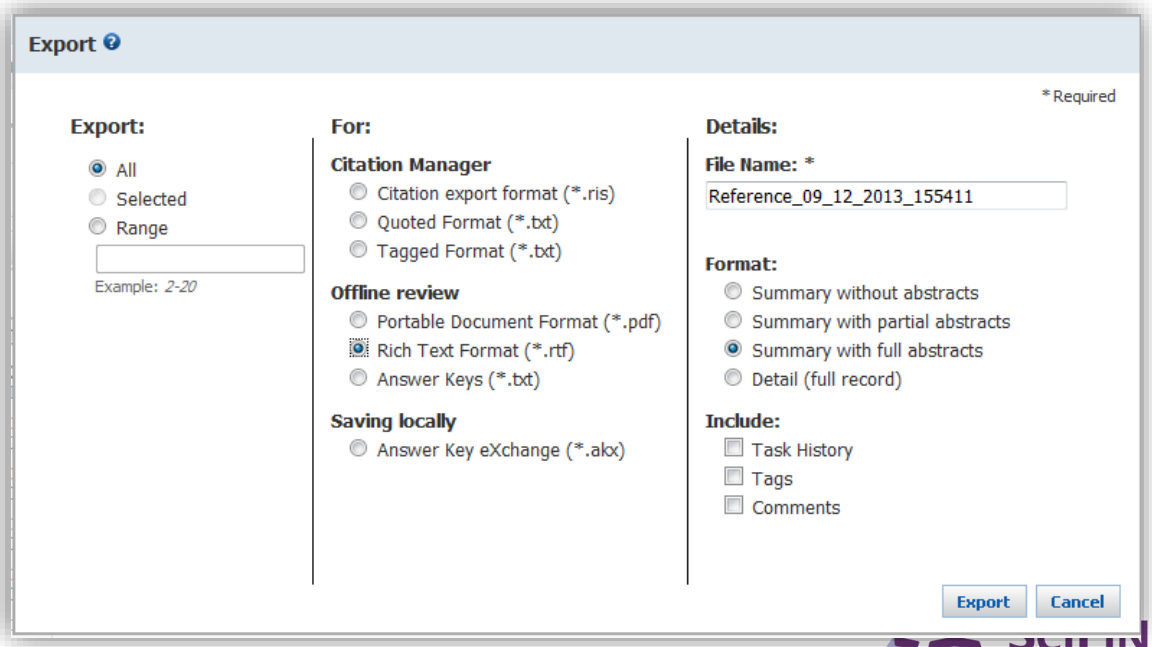


SciFinder®
A CAS SOLUTION

Export Answers

To export some or all references in an answer set to a local or shared file location, select the references of interest and click “Export”, located in the upper right corner





SciFINDER®
A CAS SOLUTION

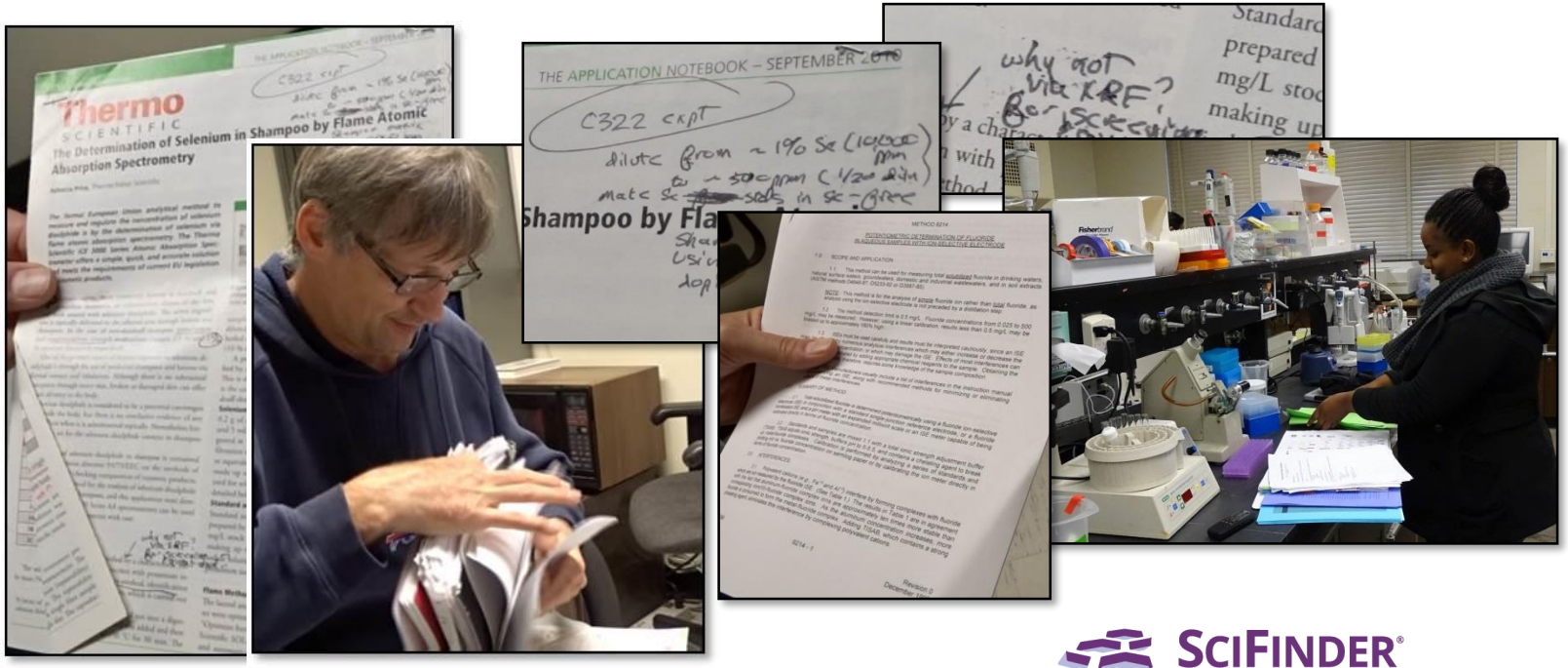
A few enhancements

- New www.cas.org
- SciFinder-n
- PatentPak
- MethodsNow (Analytical)

SciFinder®
A CAS SOLUTION

CAS is making it easier for researchers to find methods for their work

So that stacks of paper will become a thing of the past



MethodsNow™ is a complete CAS solution

- Largest single collection of methods information
  - Addresses core chemistry markets
- CAS-quality indexing and new, value-add templating of key methods from important full-text sources
- Covers both ***synthetic and analytical researcher needs***

SCIFINDER®
A CAS SOLUTION

So what exactly is MethodsNow?

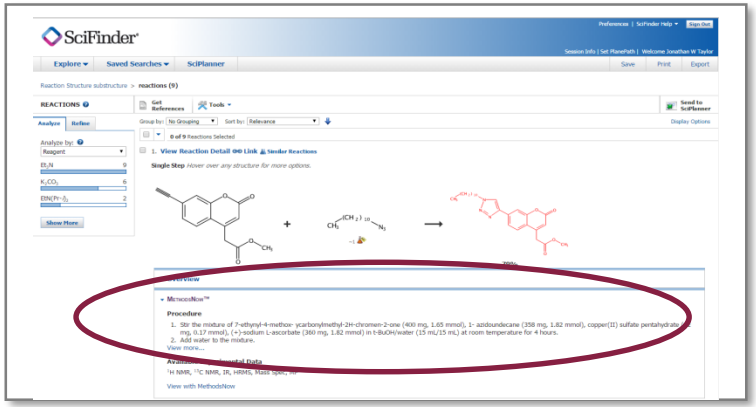
- A collection of over a million ***synthetic and analytic methods*** – with more to come!
  - Focused indexing, step-by-step instruction
  - Details for analytical researchers such as matrix, analyte, instrumentation and comparison capabilities

- Interface options right where the user needs them!
  - Synthetic researchers will find relevant content right inside SciFinder
  - Analytical researchers will find relevant content in a newly-designed interface tailored for their search needs

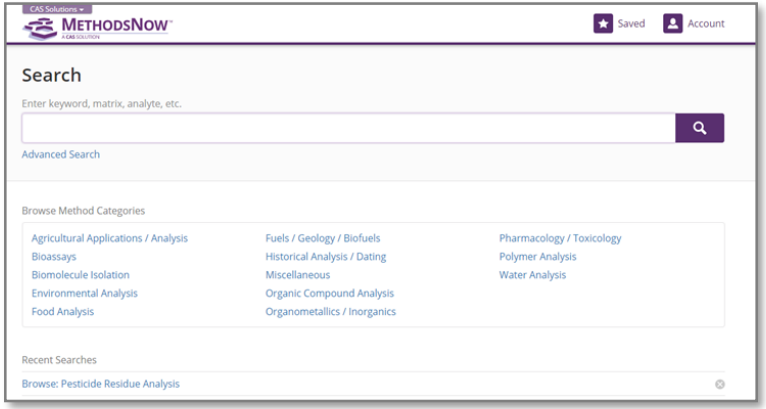
One product, two interfaces

- Research showed that users interested in synthetic methods were often already in SciFinder, but analytical scientists often weren't (though they might be familiar with it)

***Synthetic chemist** looking for great methods?*
They are in SciFinder.

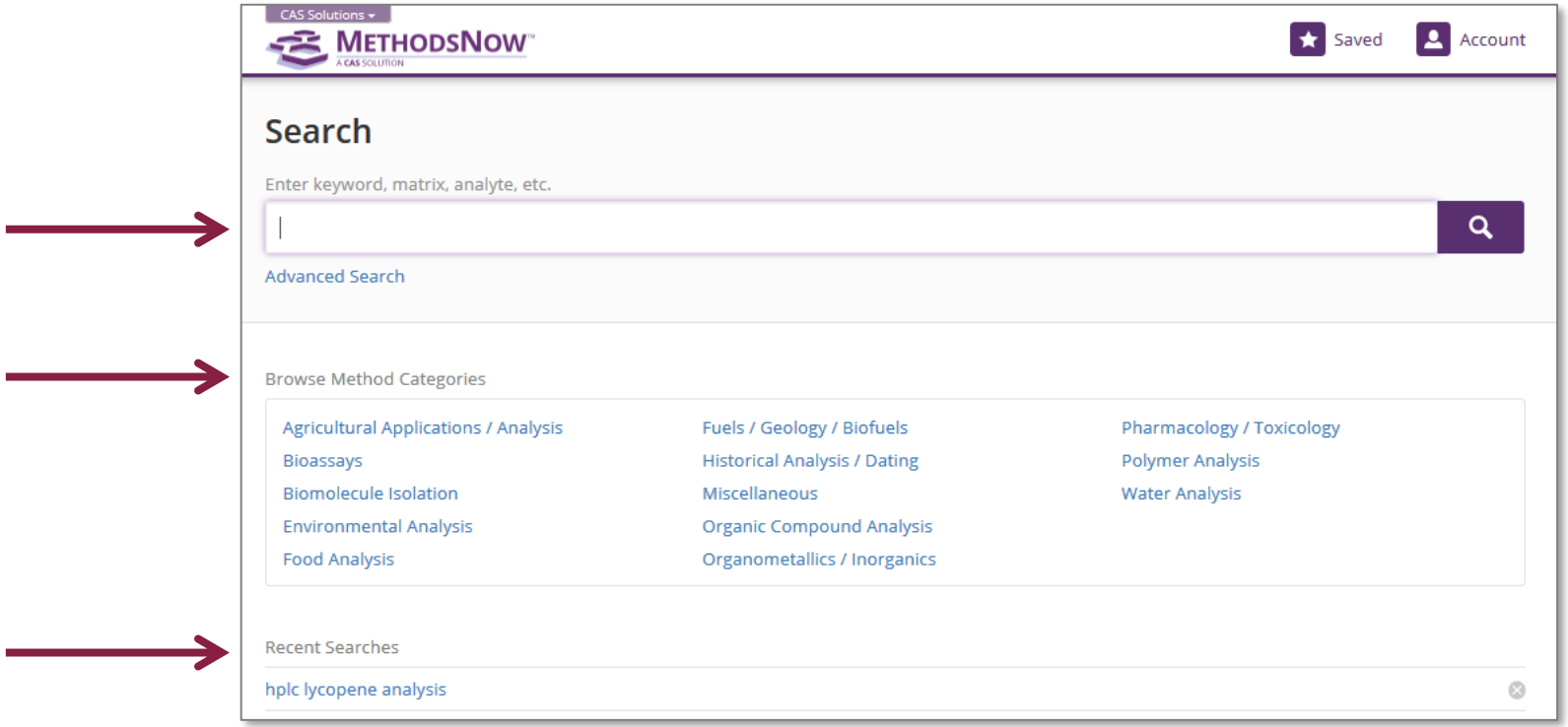


***Analytical scientist** just looking for great methods?*
A new, easy to use interface just for you.

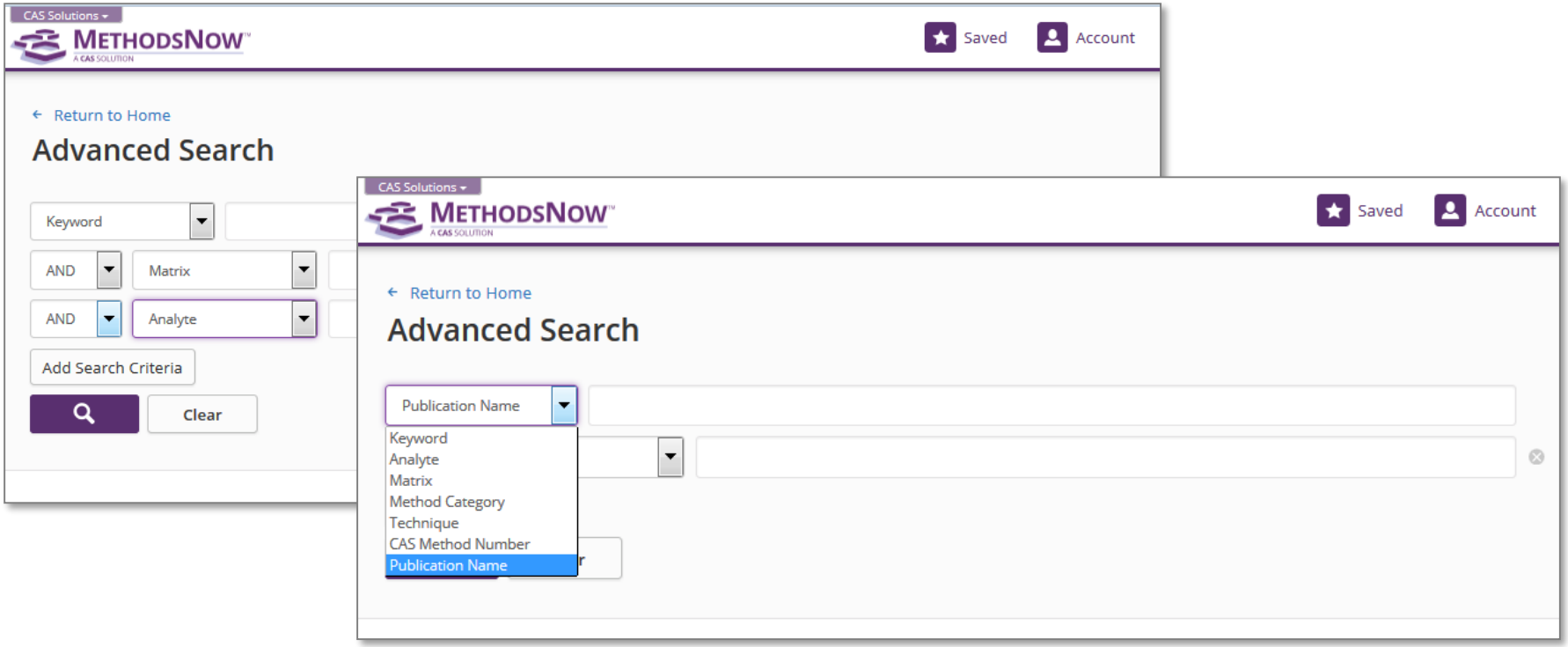


SCIFINDER®
A CAS SOLUTION

MethodsNow – Analytical Scientist Interface

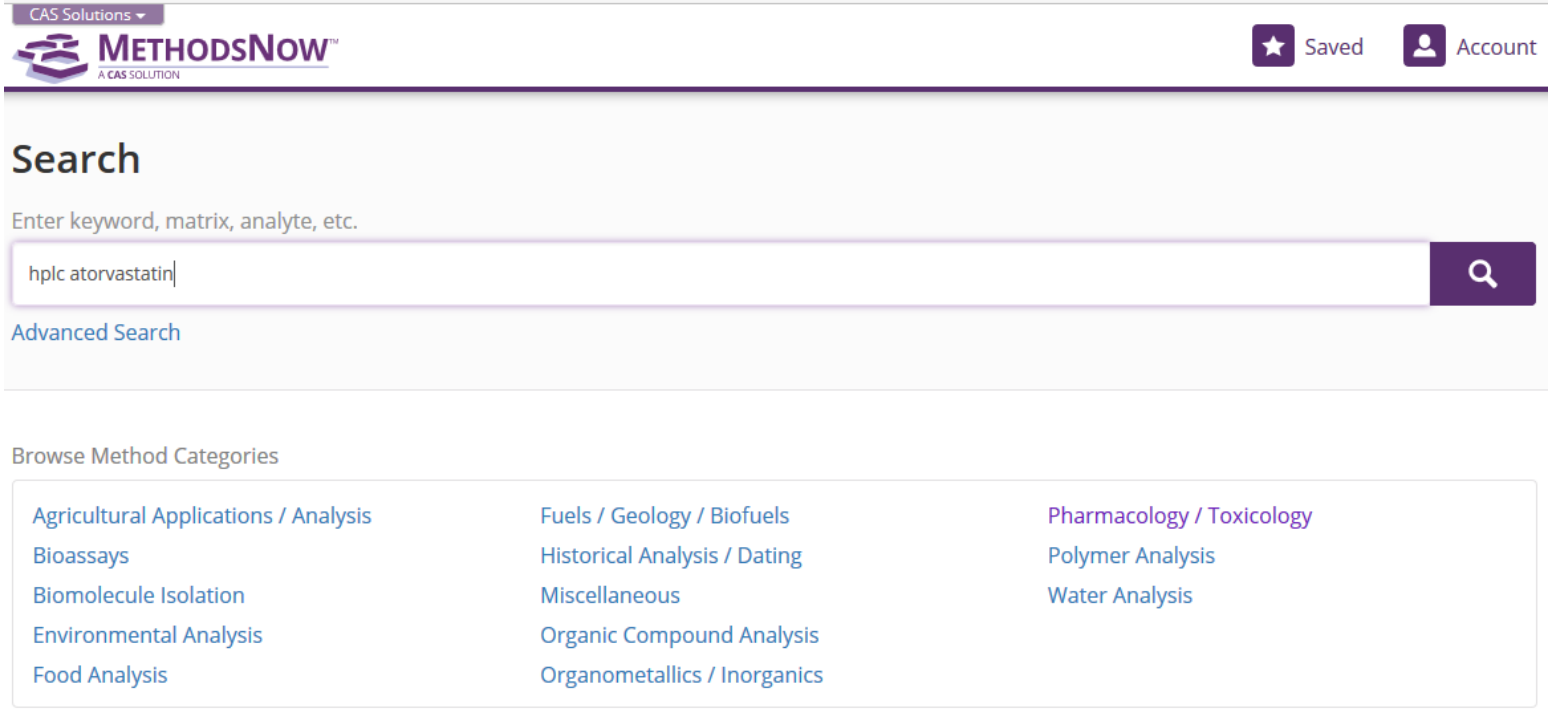


Specify one or many advanced search fields

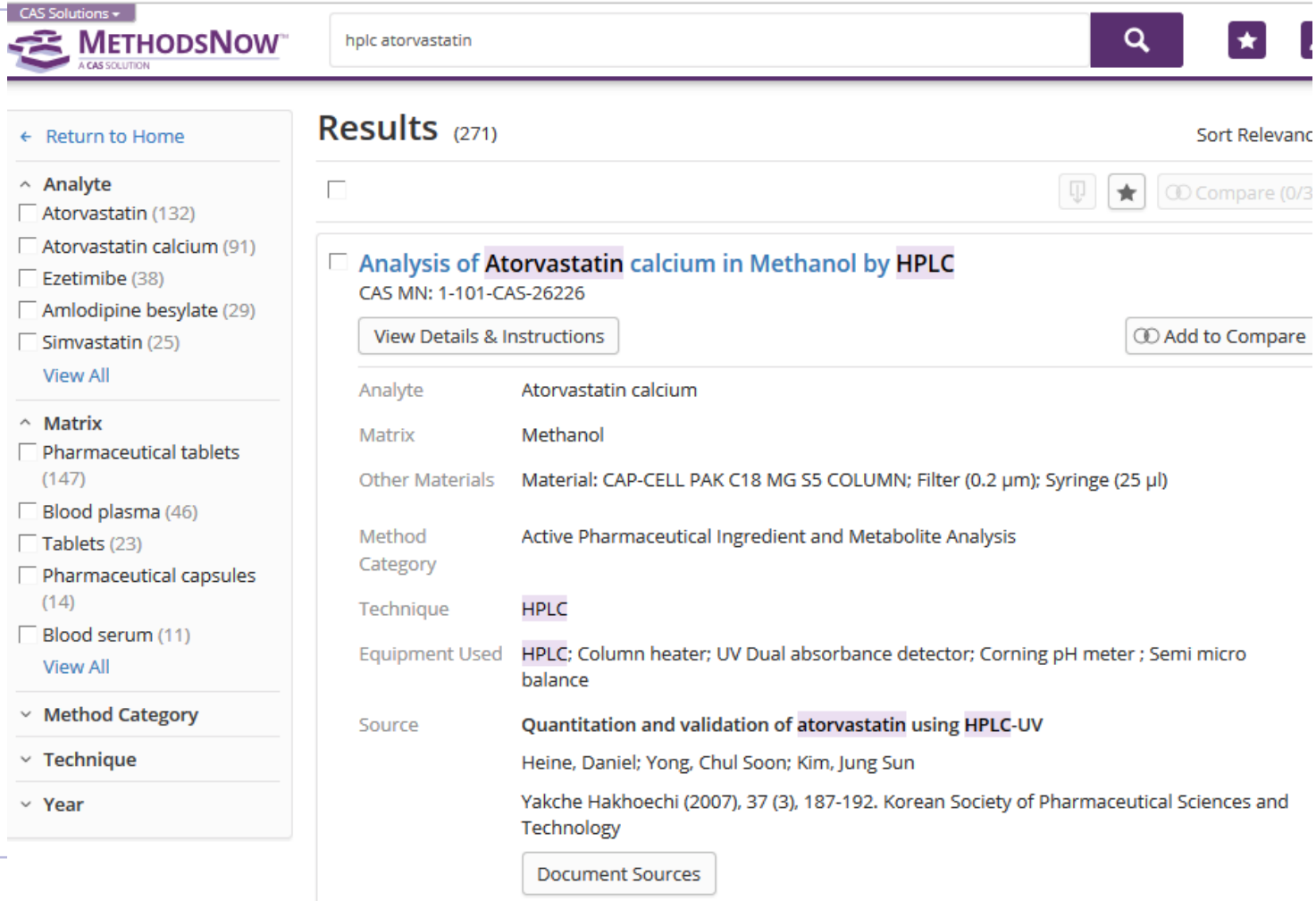


SCIFINDER®
A CAS SOLUTION

Search for HPLC methods for Atorvastatin



Filters allow you to quickly hone in on the most interesting results



Sample record

Analysis of Atorvastatin in Capsule (microbial) by Reversed-phase HPLC

CAS MN: 1-101-CAS-6621

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Reversed-phase HPLC

Materials	Role	Image	CAS RN
Atorvastatin	analyte	View Structure	134523-00-5
Capsule (microbial)	matrix		
C18 column, 250 x 4.6 mm	material		

Source

HPLC method development of atorvastatin by RP-HPLC in its bulk dosage forms

Navaneetha Krishnan, S.; Suresh Kumar, P.; Naveen Kumar, V.; Sunil; Surendernath, Y.

International Journal of Research in Ayurveda & Pharmacy (2011), 2 (5), 1604 - 1606. International Journal of Research in Ayurveda and Pharmacy

CODEN: IJRAC2 | ISSN: 22293566

Document Sources

Abstract ^

A fast, simple, sensitive, precise, accurate, and reproducible reversed phase high performance chromatog. method was developed and validated for the anal. of atorvastatin in bulk dosage forms. The separation was conducted by using C_{18} RP-HPLC column, which was maintained at ambient temperature The mobile phase consisting of potassium di-hydrogen ortho phosphate, methanol and acetonitrile in the ratio 30:20:50 was delivered at a rate of 1 mL/min. The anal. was detected by using UV detector at the wave length of 240 nm. The method is validated for its precision, limit of quantitation (LOQ),

Sample record

Equipment Used

Quaternary isocratic HPLC system, HPLC YL9000 series, Young Lin

Instructions

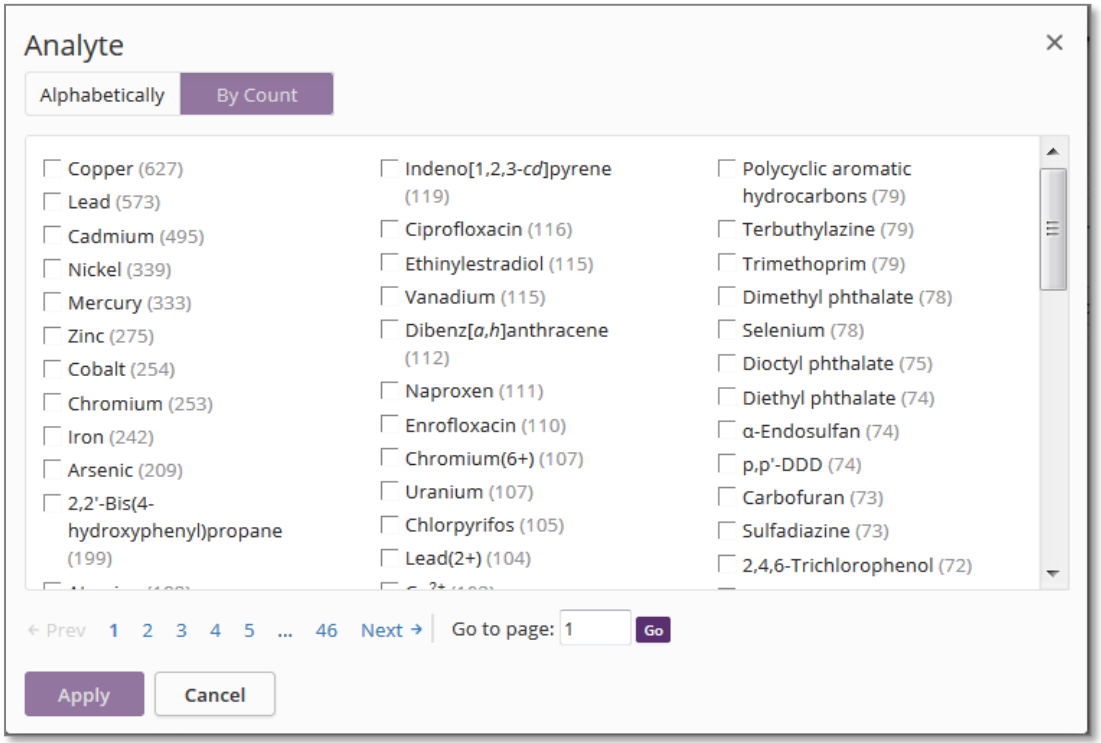
Reversed phase high performance liquid chromatography (RP-HPLC)

1. Inject the capsule sample into the HPLC system.
2. Perform analysis using Quaternary isocratic HPLC (Young Lin HPLC YL9000 series) with YL 9110 Pump and with "autochrom 3000" software and UV-Vis detector YL9120.
3. Carry out separation in inertsil C18 column (250 x 4.6 mm).
4. Mobile phase comprises of potassium di-hydrogen ortho phosphate (adjust to pH 3.5 ± 0.05 with ortho phosphoric acid), methanol and acetonitrile (30:20:50); use water as diluent (pH 7).
5. Filter the mobile phase through a 0.45 µm membrane filter, degas with a helium spurge for 20 min and pump from the respective solvent reservoir to the column (flow rate, 1.0 ml/min), which yield a column back pressure of 653 - 720 psi.
6. Set the run time at 10 min and maintain the column at room temperature.
7. Prior to injecting the drug solution in to the column, equilibrate the column for at least 1 hour with the mobile phase flowing through the system.
8. Monitor the eluent at 240 nm.
9. Store and analyze the data with the software "autochrom-3000" (Young Lin).

Validation

Linearity Range	10 - 100 µg/ml
Limit of Detection	0.086 µg/ml
Limit of Quantitation	0.189 µg/ml
Precision	0.12% (RSD) (intra-day); 0.14% (RSD) (inter-day)
Retention Time	8.32 min

View all on analyte



Compare Methods

Expand All | Collapse All

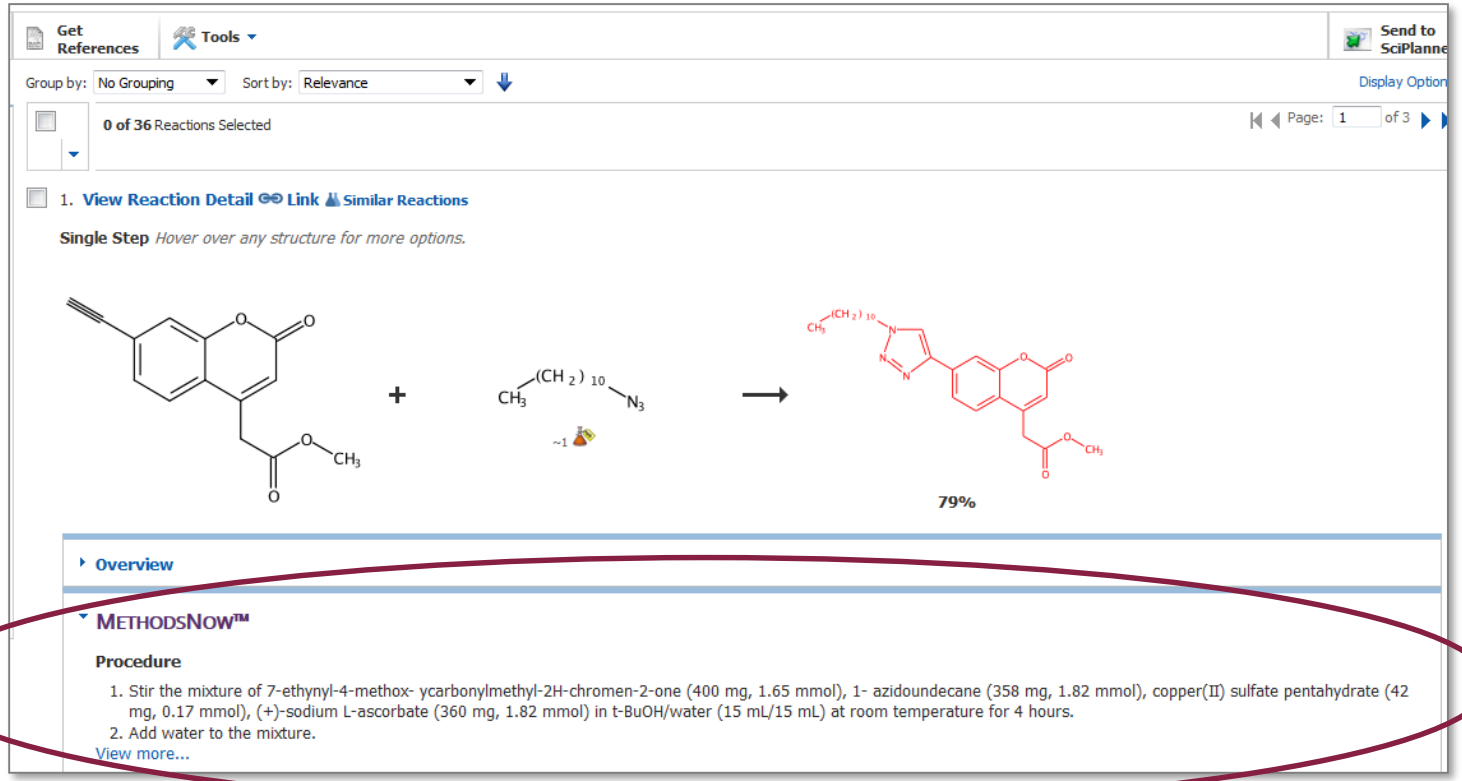
	1	2	3
Title	Analysis of Atorvastatin calcium in Methanol by HPLC	Analysis of Atorvastatin in Capsule (microbial) by Reversed-phase HPLC	Analysis of Atorvastatin in Pharmaceutical tablets by HPLC
CAS Method Number	1-101-CAS-26226	1-101-CAS-6621	1-101-CAS-39815
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	HPLC	Reversed-phase HPLC	UV-visible spectroscopy; HPLC
Analyte	Atorvastatin calcium	Atorvastatin	Atorvastatin
Matrix	Methanol	Capsule (microbial)	Pharmaceutical tablets
Other Materials	CAP-CELL PAK C18 MG S5 COLUMN; Filter (0.2 µm); Syringe (25 µl)	C18 column, 250 x 4.6 mm	C-18 column; 100 µL loop; 0.45 mm membrane filter
Equipment Used	HPLC, 2690, Waters, MA, USA; Column heater, Waters; UV Dual absorbance detector; Corning pH meter , 440; View All	Quaternary isocratic HPLC system, HPLC YL9000 series, Young Lin	High performance liquid chromatographic system; UV-VIS detector, SPO-6A V, Shimadzu
Conditions			**Instrument:** Detection wavelength, 245 nm. **Chromatographic:** Injection volume, 100 µL; mobile phase, water - View All

Source	Quantitation and validation of atorvastatin using HPLC-UV View All	HPLC method development of atorvastatin by RP-HPLC in its bulk dosage forms View All	Validation of HPLC method for determination of atorvastatin in tablets and for monitoring stability View All
Preparation	**Preparation of atrovastatin (AS)** 1. Dilute the AS stock to samples View All		**Preparation of sample solution** 1. Weigh ten tablets of atorvastatin View All
Method	1. Perform sample injections manually with a 25 µL syringe View All	**Reversed phase high performance liquid chromatography (RP-HPLC)** View All	**High performance liquid chromatography with UV detection** View All
Linearity Range	0.2 – 50 µg/ml	10 - 100 µg/ml	0.04 mg/mL - 0.4 mg/mL
Limit of Detection	≅0.1 µg/ml	0.086 µg/ml	0.035 mg/mL
Accuracy	81.19 – 111.09 (intra day); 92.92 –114.04 (inter day)		100.91 ± 0.73%, 99.95 ± 0.37% and 100.22 ± 0.63% (Recovery) for 0.1000, 0.2000 and 0.4000 mg/mL spiked View All
Limit of Quantitation		0.189 µg/ml	0.015 mg/mL
Precision		0.12% (RSD) (intra-day); 0.14% (RSD) (inter-day)	0.983%, 0.668% and 0.742% for 0.1000, 0.2000 and 0.4000 mg/mL spiked (RSD, Intra-day); 0.881% View All
Retention Time		8.32 min	6.5 minutes

MethodsNow for analytical scientists: Great content sources

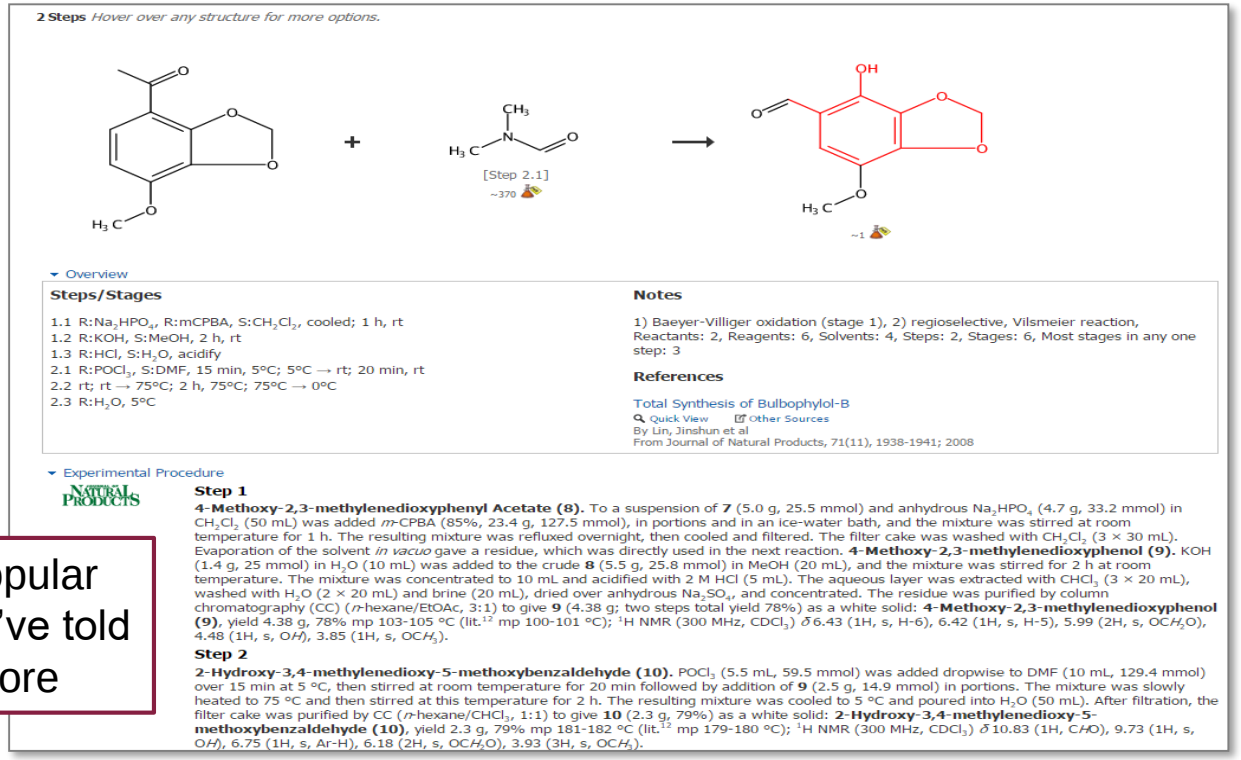
Content from years	2000 - present
Number of methods	~150,000 at launch – more than any other single source
Content Coverage	Broad range: Key focus in Pharma, Ag, and chemical as well as others
Source Focus	Full CAplus℠ database. Future investment may include regulatory agencies and instrumentation
Example journal titles	Food Chemistry, Journal of Chromatography A and B, Journal of Agricultural and Food Chemistry, Talanta, Analytica Chimica Acta
Language	English only

MethodsNow – Synthetic Chemist Interface

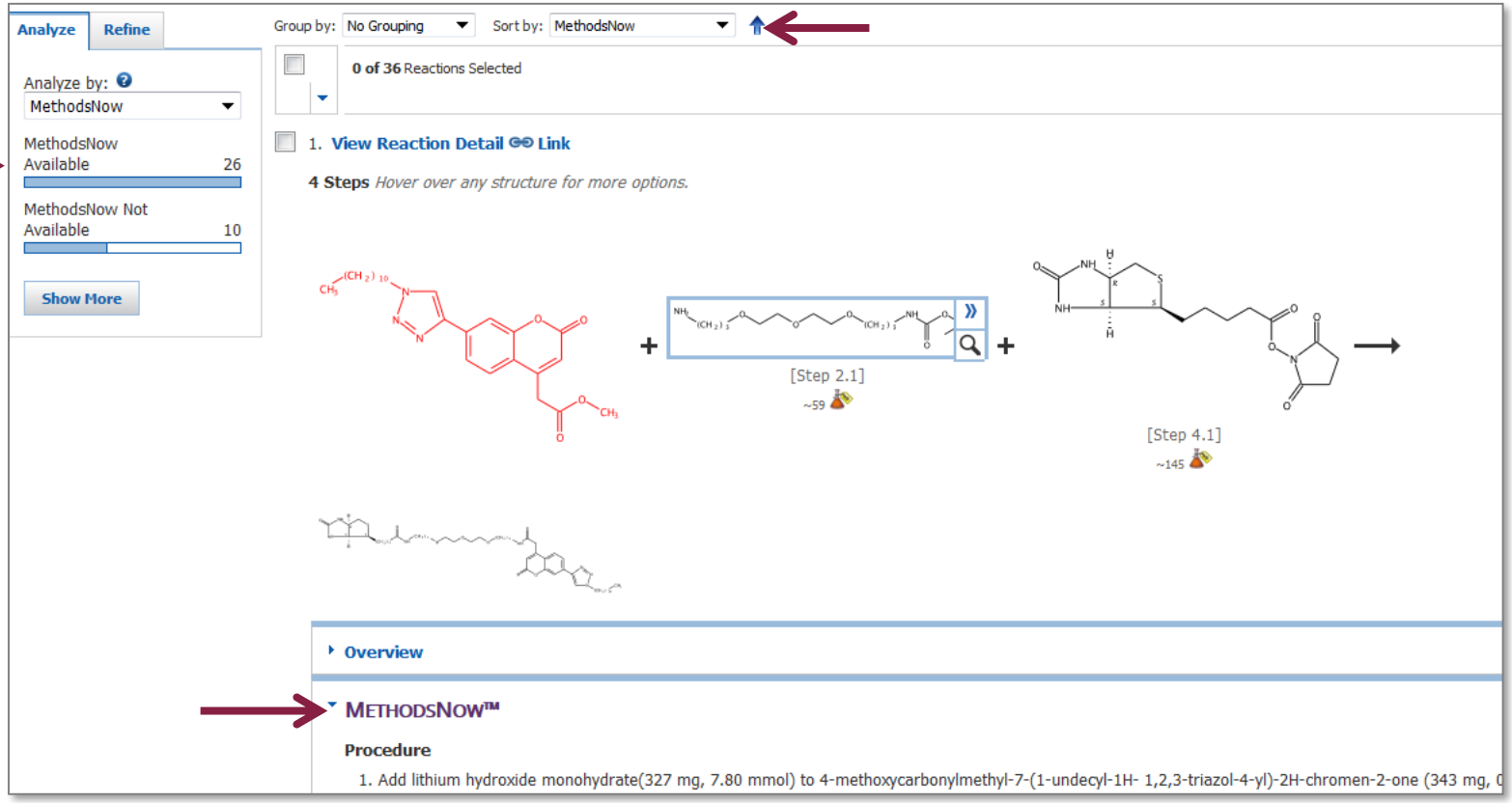


SciFinder® A CAS SOLUTION

SciFinder has the largest collection of experimental procedures for reactions



It is our most popular feature, but you've told us we can do more

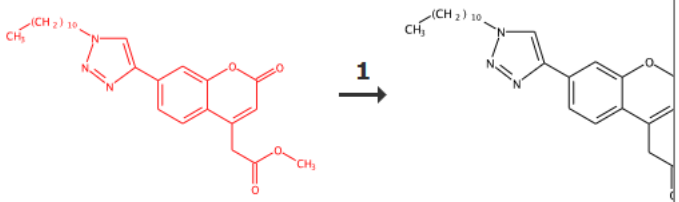

Analyze
Refine
Group by: No Grouping
Sort by: MethodsNow
Analyze by:
MethodsNow
MethodsNow Available 26
MethodsNow Not Available 10
Show More
0 of 36 Reactions Selected
1. View Reaction Detail Link
4 Steps Hover over any structure for more options.
[Step 2.1]
~59
[Step 4.1]
~145
Overview
METHODSNOW™
Procedure
1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H- 1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg,

MethodsNow

7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule microarrays

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha
From Tetrahedron, 68(30), 6038-6053; 2012
Published by Elsevier Ltd.

Reaction Steps 1 2 3 4



Products	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-tria 1384966-77-1
Reactants	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-tria 1384966-75-9
Reagents	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
Solvents	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

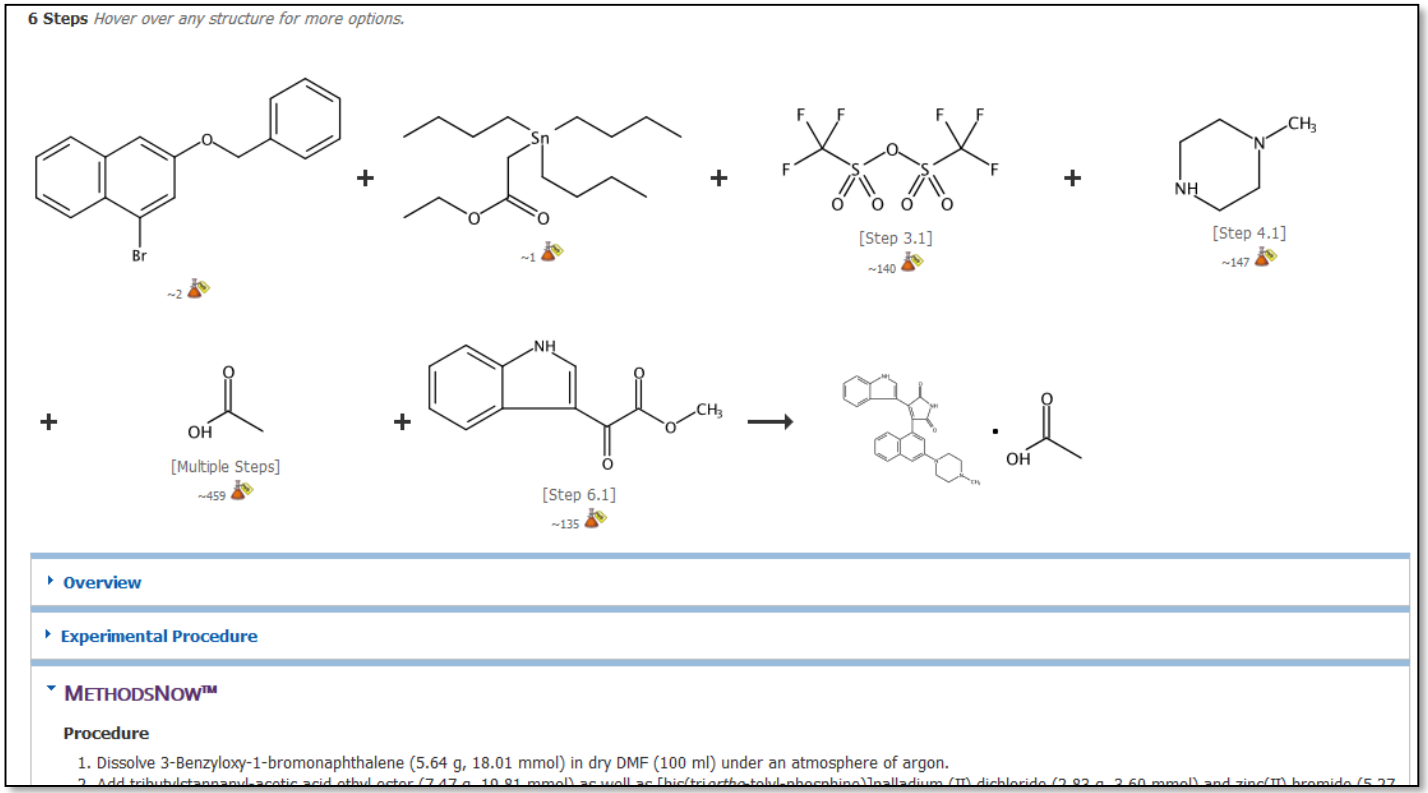
MethodsNow

Procedure	1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H- 1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature. 2. Stir the reaction mixture for 3 hours at room temperature. 3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid. 4. Partition the reaction mixture between ethyl acetate and water. 5. Extract the aqueous layer with ethyl acetate. 6. Dry the combined organic layer over magnesium sulfate.
Scale	milligram
^{1}H NMR	^{1}H NMR (300 MHz, acetone- d_6): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, *J* = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, *J* = 6.8 Hz, 3H).
^{13}C NMR	^{13}C NMR (125 MHz, DMF-d_7, 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).
IR	IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm^{-1}.
HRMS	HRMS (EI): m/z calculated for $C_{24}H_{31}N_3O_4$: 425.2315 [M$^+$]; found: 425.2315.
Mass Spec	MS (ESI): m/z: 426 [M+H$^+$].
MP	235.5±0.8 °C.
CAS Method Number	3-352-CAS-78415

Print/Export Close

SciFinder® A CAS SOLUTION

A reaction with experimental procedure and MethodsNow



MethodsNow synthetic chemistry content sources

Content from years	2000 - present
Number of protocols	>1 million at launch; 2 million within months; 3 million later this year
Content Coverage	Small molecule synthesis
Source Focus	180+ journals titles including new coverage from Wiley, RSC and Elsevier in addition to ACS, Springer, Taylor&Francis, WO patents (2010-present)
Example journal titles	Organic Letters, Catalysis Letters, Journal of Coordination Chemistry, Journal of Medicinal Chemistry, Journal of the American Chemical Society, Angewandte Chemie, Tetrahedron, Chemical Science
Language	English only

MethodsNow Benefits

- Readily integrates into your workflow
- Lets you quickly compare analytical methods side by side
- Saves time with easy searching and direct access to method details – no more searching through full-text documents
- Displays experimental details in easy-to-read table format
- Includes materials, instrumentation, validation data, conditions and more

PatentPak

- 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®
A CAS SOLUTION

Issues faced while searching Patents….

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 (Car 1.356 mmol). The mixture was degassed thoroughly refilling with nitr to 60 °C for 2 hrs. The mixture was filtered through silica and washed The filtrate was passed through SCX-2 resin (30g 0.67 mmol /g) eluti (250 ml) followed by 2M ammonia in MeOH (250 ml). The ammonia/MeOH washings were evaporated to dryness and the resulting crude residue was purified by 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®
A CAS SOLUTION

Issues faced while searching Patents….

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

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid

dissolved in THF (50 mL) and added to the paste. The resu

ambient temperature overnight. Water (100 mL) was adde

slightly basic by adding $NaHCO_3$ solution followed by ext

mL). The combined extracts were washed with brine once and dried over anhydrous Na_2SO_4. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO_2 chromatography (Et_2O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm^{-1} ; ^1H NMR ($CDCl_3$,

8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m,

(bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14

Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01

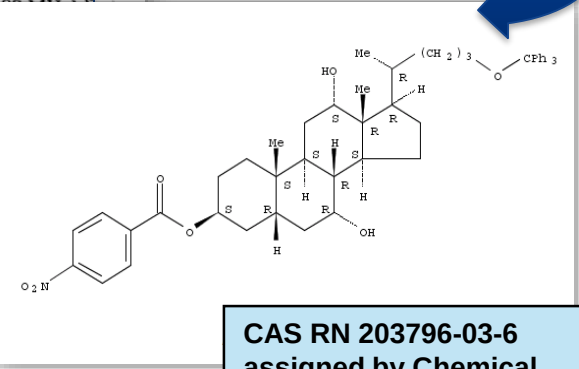
(d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.21, 1

144.70, 136.79, 130.77, 128.88, 127.86, 126.98, 123.70, 86.47, 73.24, 73.

64.22, 47.79, 46.79, 42.15, 39.76, 37.47, 35.52, 35.34, 34.23, 33.79, 32.4

28.74, 27.71, 26.85, 26.30, 25.16, 23.41, 17.98, 12.77; HRFAB-MS (thioglycerol+Na^+ matrix) m/e: ([M+Na]$^+$) 808.4203 (53.8%), calcd. 808.

CAS scientists find details, like structure information in text, that others miss

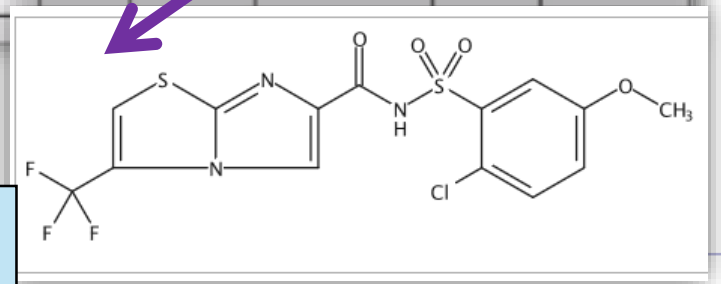


CAS RN 203796-03-6 assigned by Chemical Abstract Service

Issues faced while searching Patents….

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

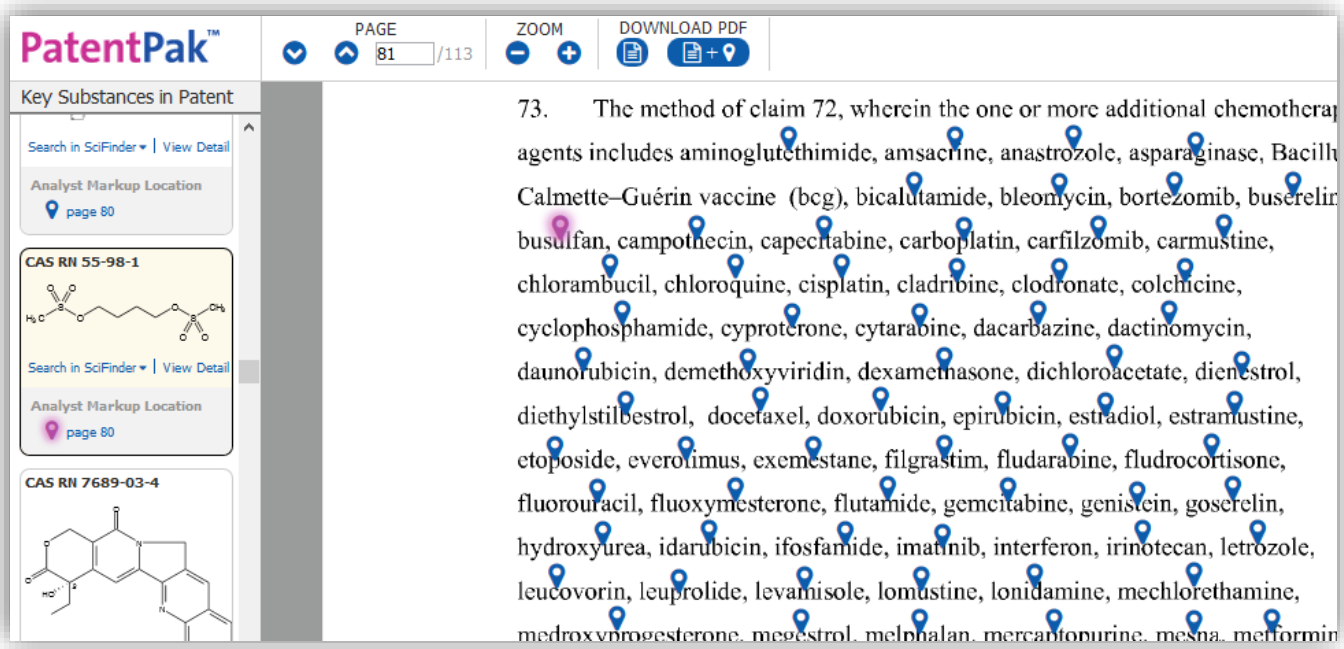
Example	R^1	n	A	R^a	R^b	R^c	R^d	R^e	Remarks
I-1-28	2-CF_3	1	CH	CH_3	H	H	Cl	H	
I-1-29	3-CF_3	1	C-R^1	Cl	H	H	OMe	H	NMR
I-1-30	3-CF_3	1	C-R^1	Cl	H	H	H	Cl	NMR
I-1-31	3-CF_3	1	C-R^1	Cl	H	H	Cl	H	NMR
I-1-32	3-CF_3	1	C-R^1	Cl	H	H	CH_3	H	
I-1-33	3-CF_3	1	C-R^1	Cl	H	H	F	H	
I-1-34	3-CF_3	1	C-R^1	CH_3	H	H	Cl	H	
I-1-35	3-CF_3	1	C-R^1	F					



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

Issues faced while searching Patents….

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

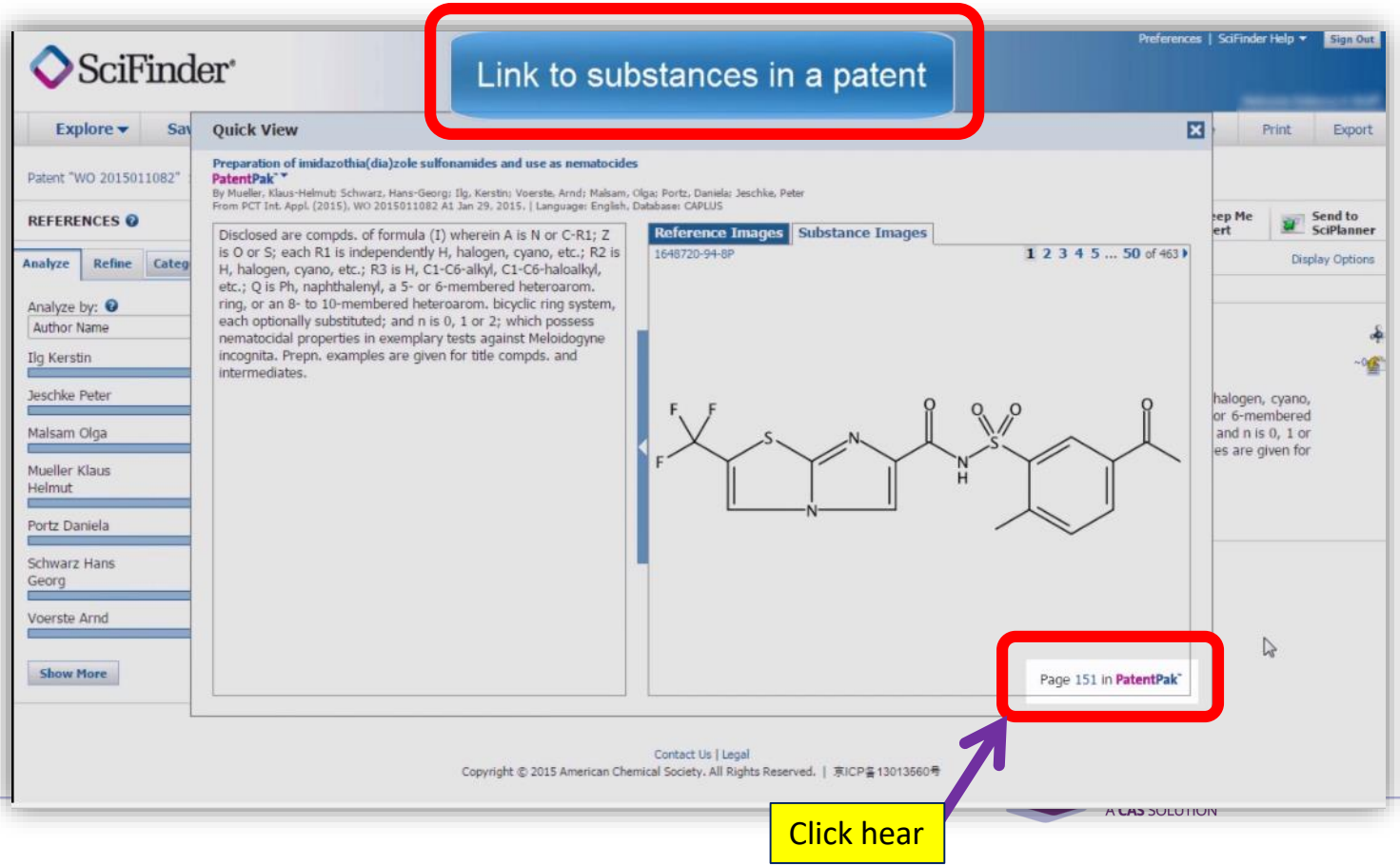


We had searched by "Sulfabutin" and were not aware that it's also called "busulfan"

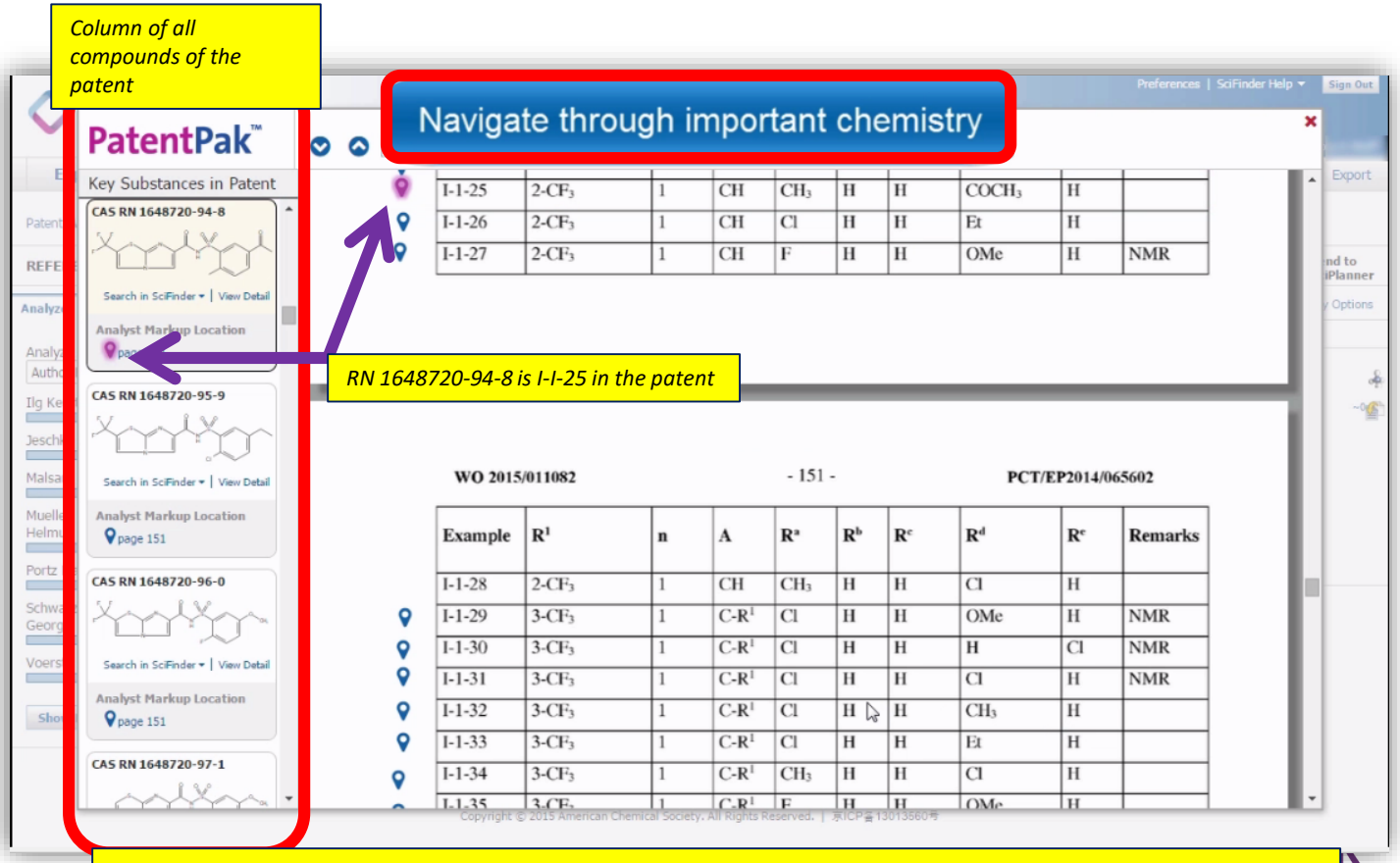
SCIFINDER®
A CAS SOLUTION

What is PatentPak ?…… and How does it work?

When you locate a compound of your interest in a patent in SciFinder

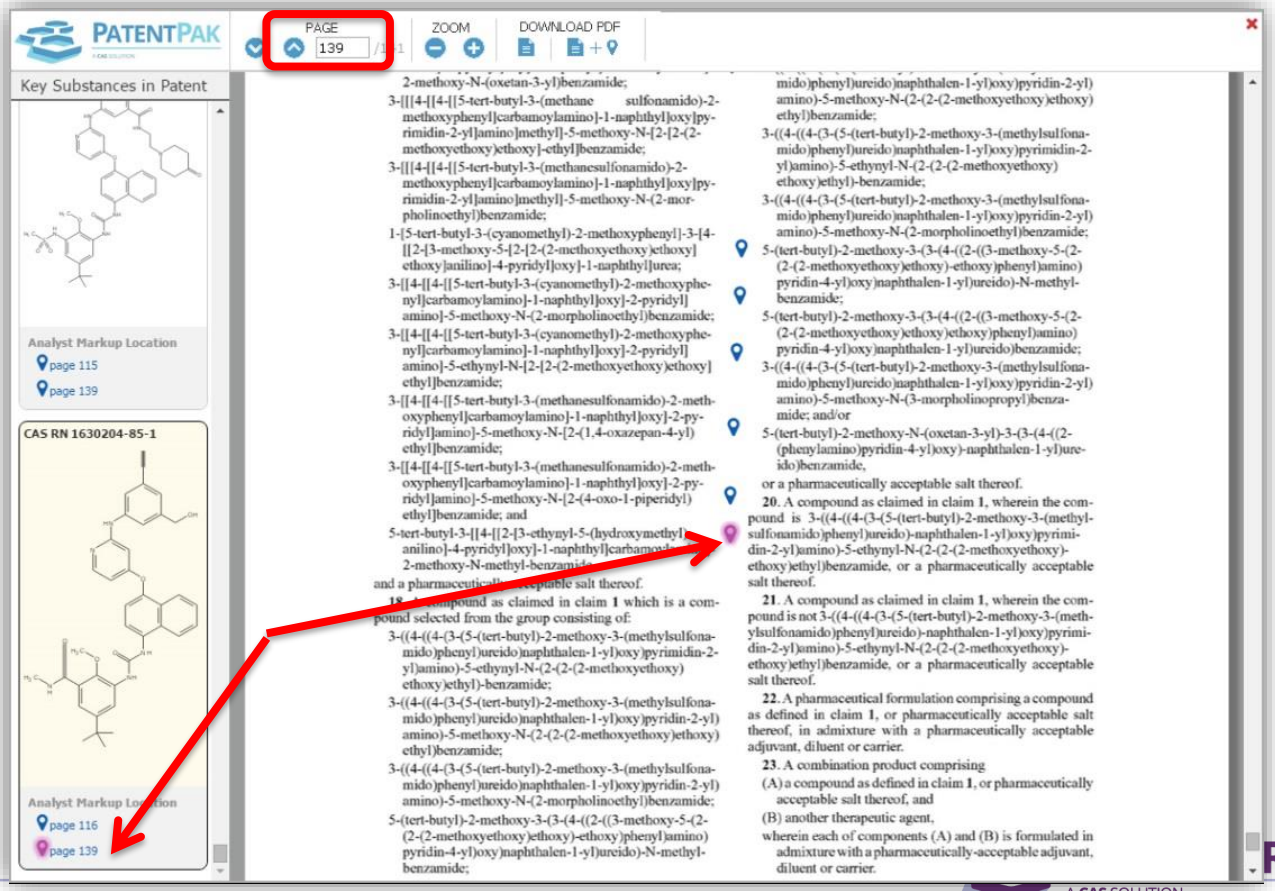


PatentPak viewer would come up



PatentPak viewer is interactive and hence if you click any blue tag – it'll automatically take you to the structure and CAS RN on the left column

PatentPak takes you right to it saving you hours of hunting!



A CAS SOLUTION

Thank You!

For any additional information, please contact us at

info@acs-i.org

CAS is a division of the American Chemical Society.
Copyright 2016 American Chemical Society. All rights reserved.

SciFinder®
A CAS SOLUTION

CAS Coverage includes key areas of Polymer Science

- Block & Graft Polymers
- Composites
- Conductive Polymers
- Elastomer
- Resins
- Fibre reinforced plastics
- Additives
- Photosensitive polymers
- Plastic Manufacturing and processes
- Polyacrylates

And many more....

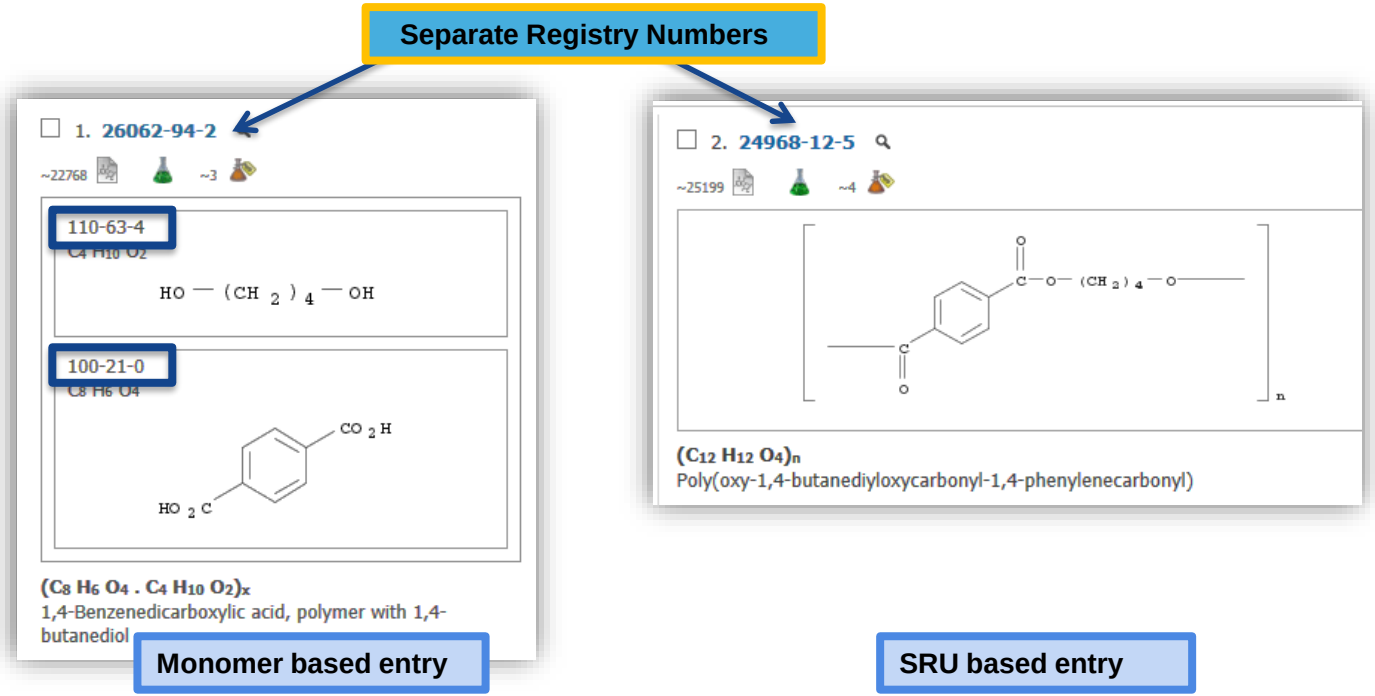
SciFinder®
A CAS SOLUTION

Polymers in SciFinder represent an important group of substances

- CAS REGISTRY℠ contains over 100 million substances
- At present, more than 1.7 million substances are polymers or oligomers
- CAS assigns a specific CAS Registry Number® for each polymer based on:
  - ✓ **Its monomers**
  - ✓ **The structural repeating unit (SRU)**
  - ✓ **Manual registration**

SciFinder®
A CAS SOLUTION

Polymer Registrations in SciFinder



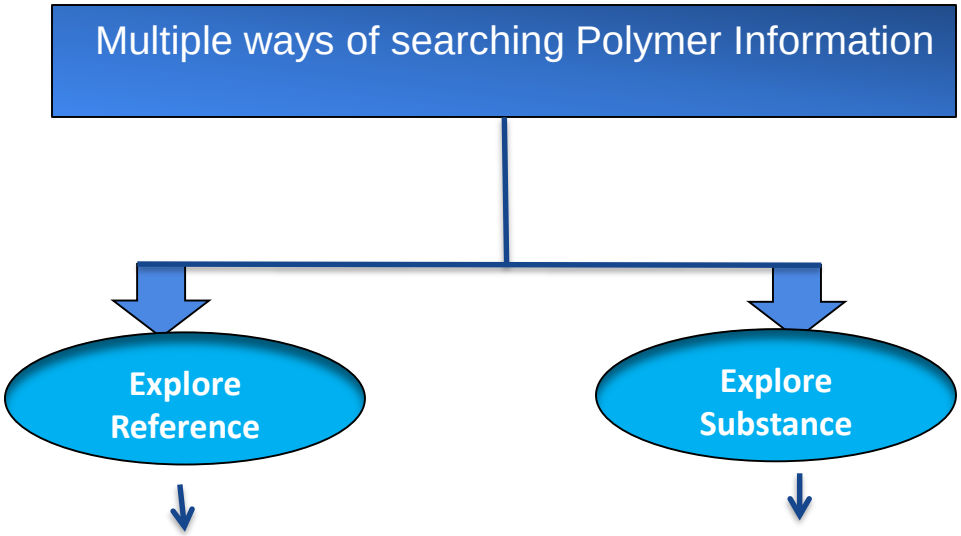
SciFinder®
A CAS SOLUTION

Polymers have unique rules for their records in SciFinder

- The CAS Registry Number for a polymer is specific to the building blocks (monomers) of the polymer
- Polymers with specified stereochemistry (tacticity) are registered separately
- Block, diblock, triblock (etc.), graft or alternating polymers are registered separately
- The molecular weight (distribution), number of repeating units, component ratio, physical characteristics, or initiators or catalysts used do not influence the registration

SciFinder®
A CAS SOLUTION

Locating Polymer Information



- **Keyword Based search**

- **Chemical/Trade Name**
- **CAS Registry Number**
- **Molecular Formula**
- **Chemical Structure**

SciFinder®
A CAS SOLUTION

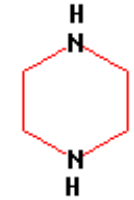
Polymer molecular formulas have a unique format

- For addition polymers and most condensation polymers put the molecular formula of the monomers, separated by dots, within brackets, and close with an “X”
  - (C3H6)x for propene homopolymer
  - (C8H8 . C5H8)x for styrene-isoprene copolymers
  - (C8H8 . C4H6 . C2H4)x for styrene-butadiene-ethene polymers
- For structural repeating units of symmetric condensation polymers put the formula of the repeating unit within brackets and close with a “n”
  - (C14H12O4)n for polybutylene terephthalate
  - (C2H4O)nCH4O for α-methyl-ω-hydroxy PE

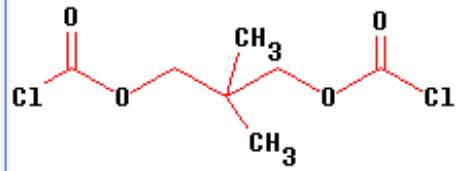
SciFinder® A CAS SOLUTION
SciFinder®

Polymer Search by Molecular Formula

Locate the polymer retrieved by the polymerization of these monomers-



Monomer A

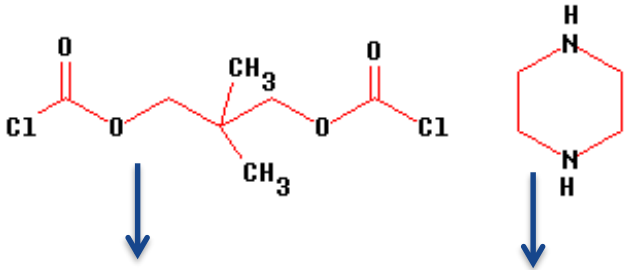


Monomer B

SciFinder®
A CAS SOLUTION

Search Strategy:

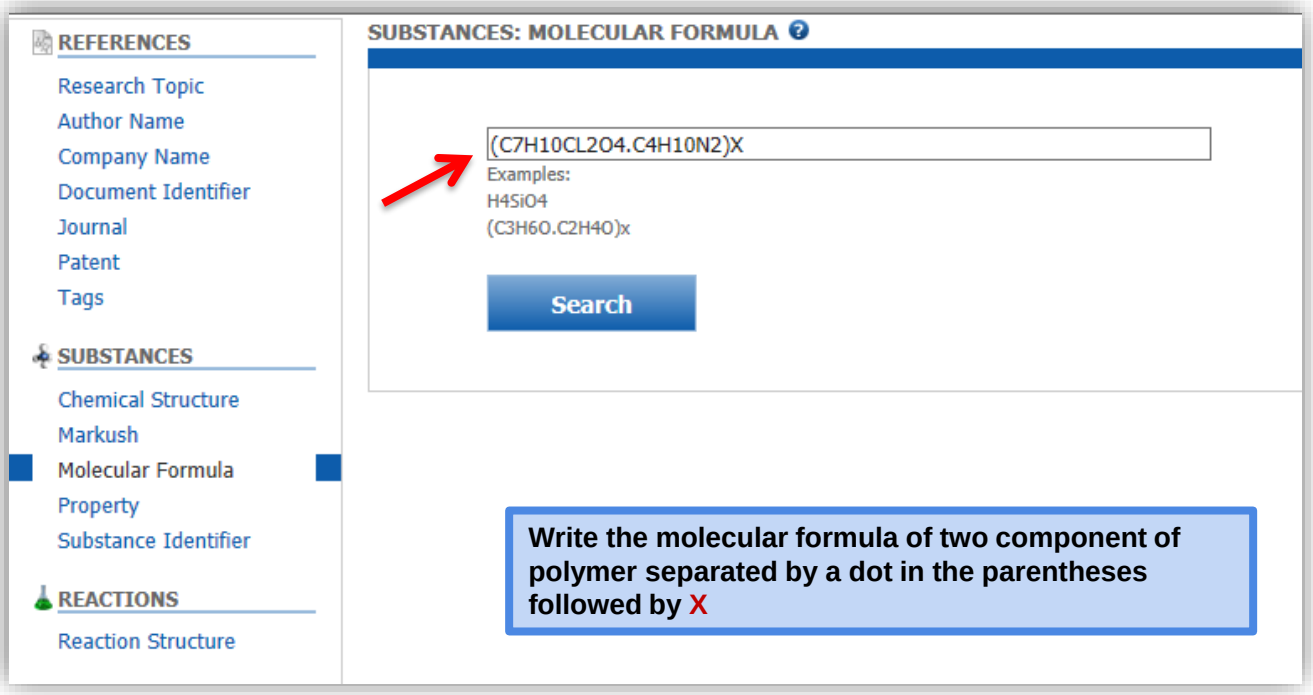
- Identify the molecular formula.
- Explore Substance by Molecular formula.



(C7H10Cl2O4.C4H10N2)X ← Use X for copolymers

SciFinder®
A CAS SOLUTION

Searching by Molecular formula

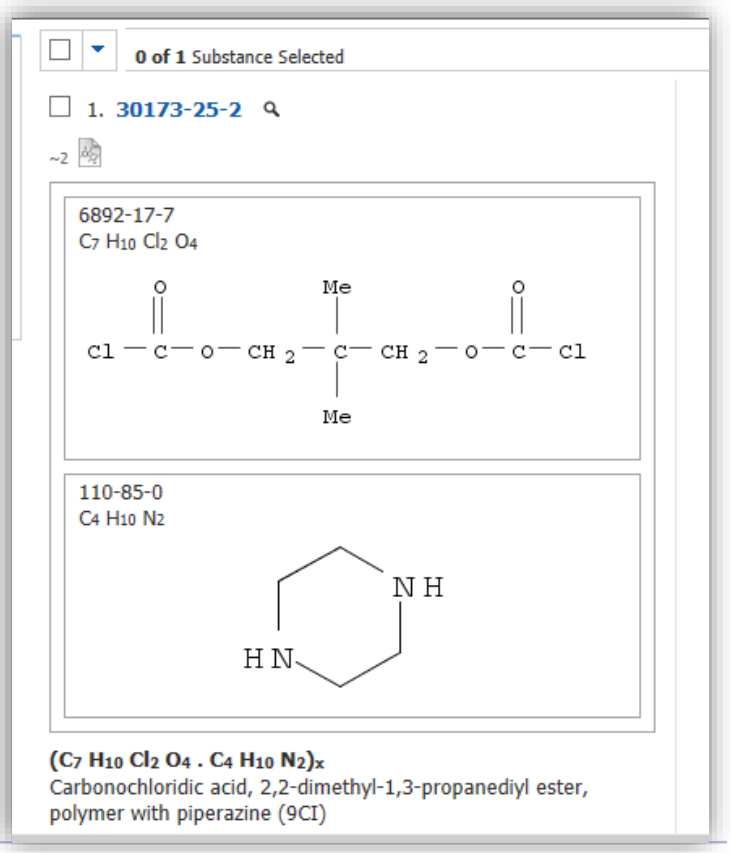


For searching SRU structure search, use N instead of X . For e.g. (C6H10O2)N

SciFinder® A CAS SOLUTION

SciFinder®

Results



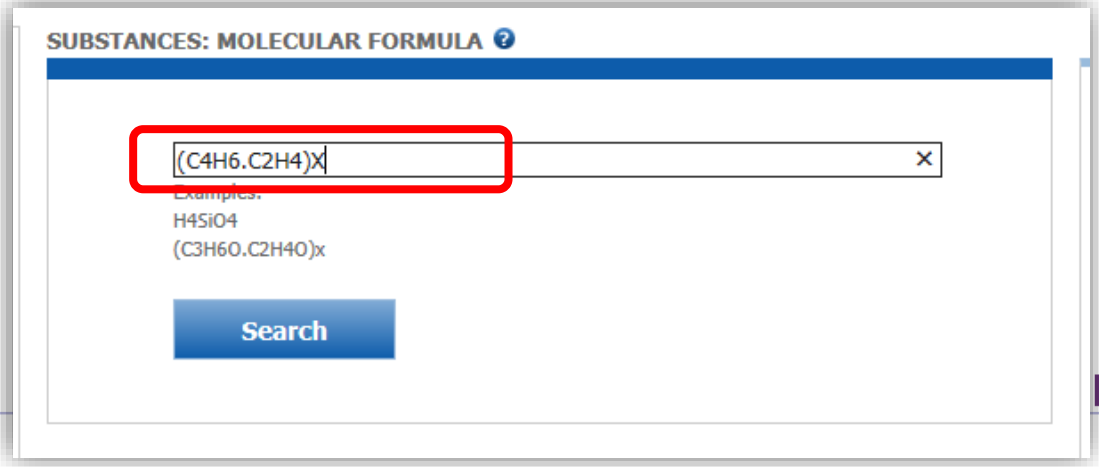
SciFinder®
A CAS SOLUTION

Case Study

Locate Copolymer of 1,3 Butadiene and ethylene

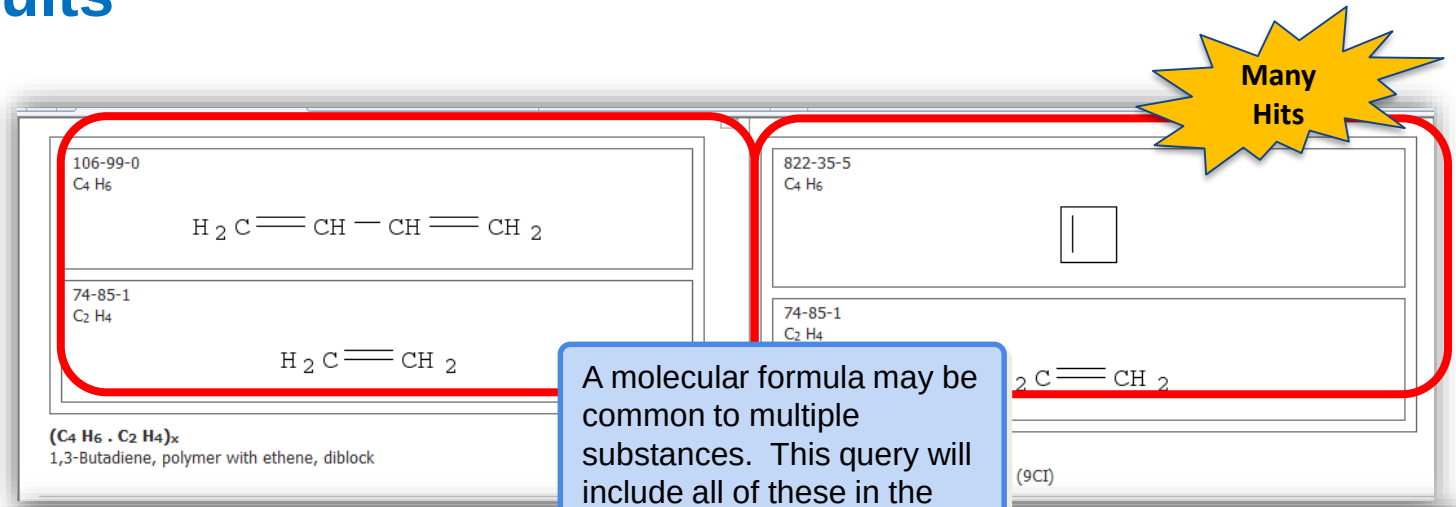
Search Strategy :

- Explore by Molecular formula-(C4H6.C2H4)X
- Refine by chemical structure.

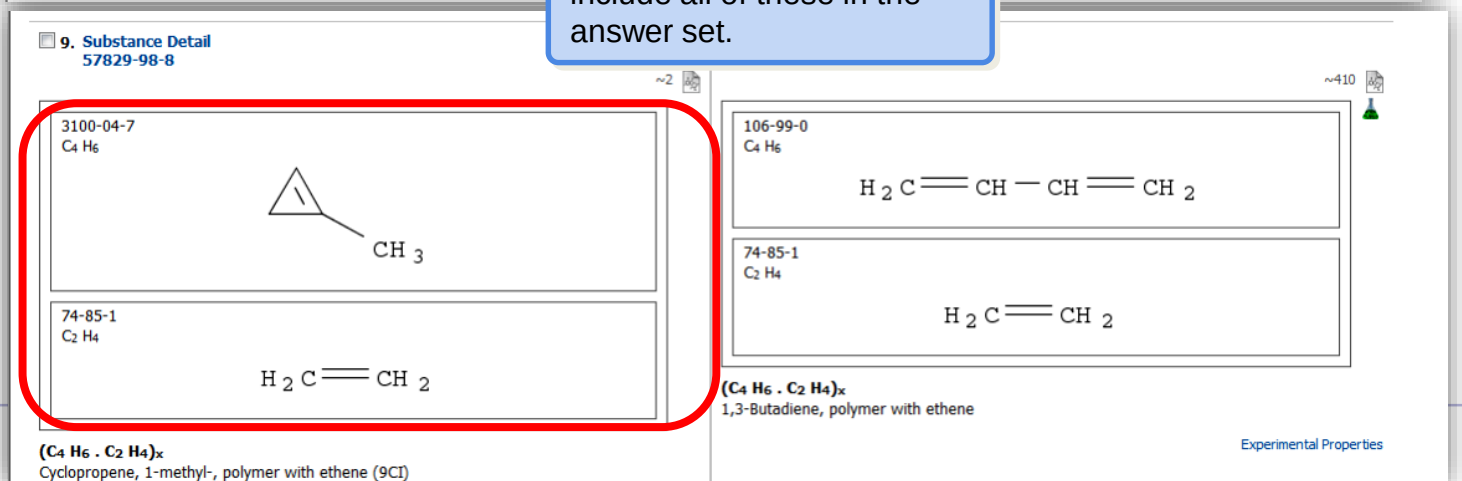


DER®

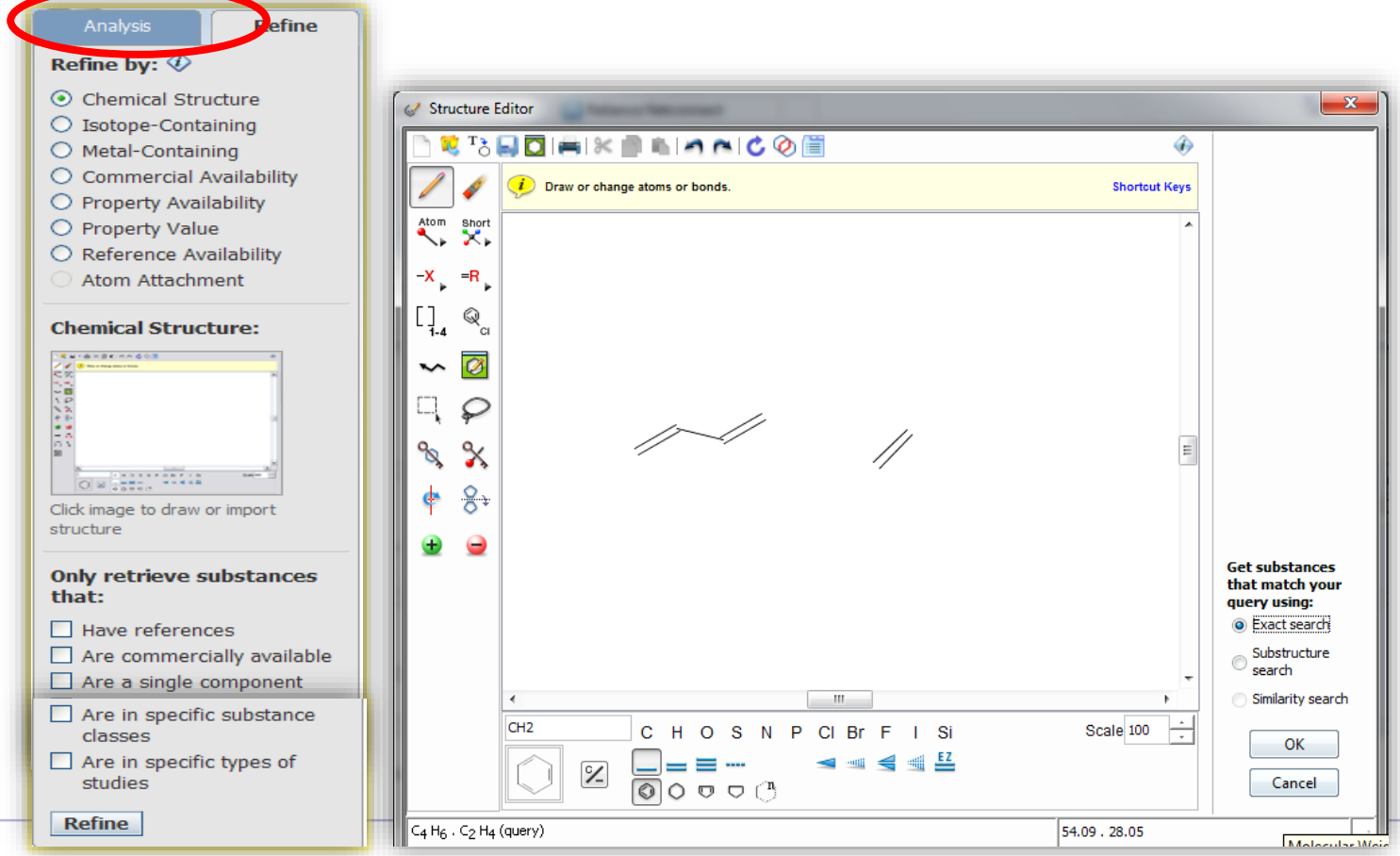
Results



A molecular formula may be common to multiple substances. This query will include all of these in the answer set.



Refine by Structure



Substances | Get References | Get Reactio | Tools | Send to

7 Copolymers of 1,3 Butadiene and ethylene

7 Substances | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Nu | Answers per Page [15]

View:

1. **Substance Detail**
   1356014-87-3
   ~1

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Tetrablock

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, tetrablock

2. **Substance Detail**
   827596-73-6
   ~5

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Triblock

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, triblock

3. **Substance Detail**
   733047-67-1
   ~9

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Diblock

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, diblock

4. **Substance Detail**
   126643-93-4
   ~9

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Alternating

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, alternating (9CI)

5. **Substance Detail**
   117708-05-1
   ~15

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Graft

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, graft (9CI)

6. **Substance Detail**
   117318-45-3
   ~32

   106-99-0
   C_4H_6
   $H_2C{=}CH{-}CH{=}CH_2$

   74-85-1
   C_2H_4
   $H_2C{=}CH_2$

   Block

   $(C_4H_6 . C_2H_4)_x$
   1,3-Butadiene, polymer with ethene, block

A CAS SOLUTION

Case Study

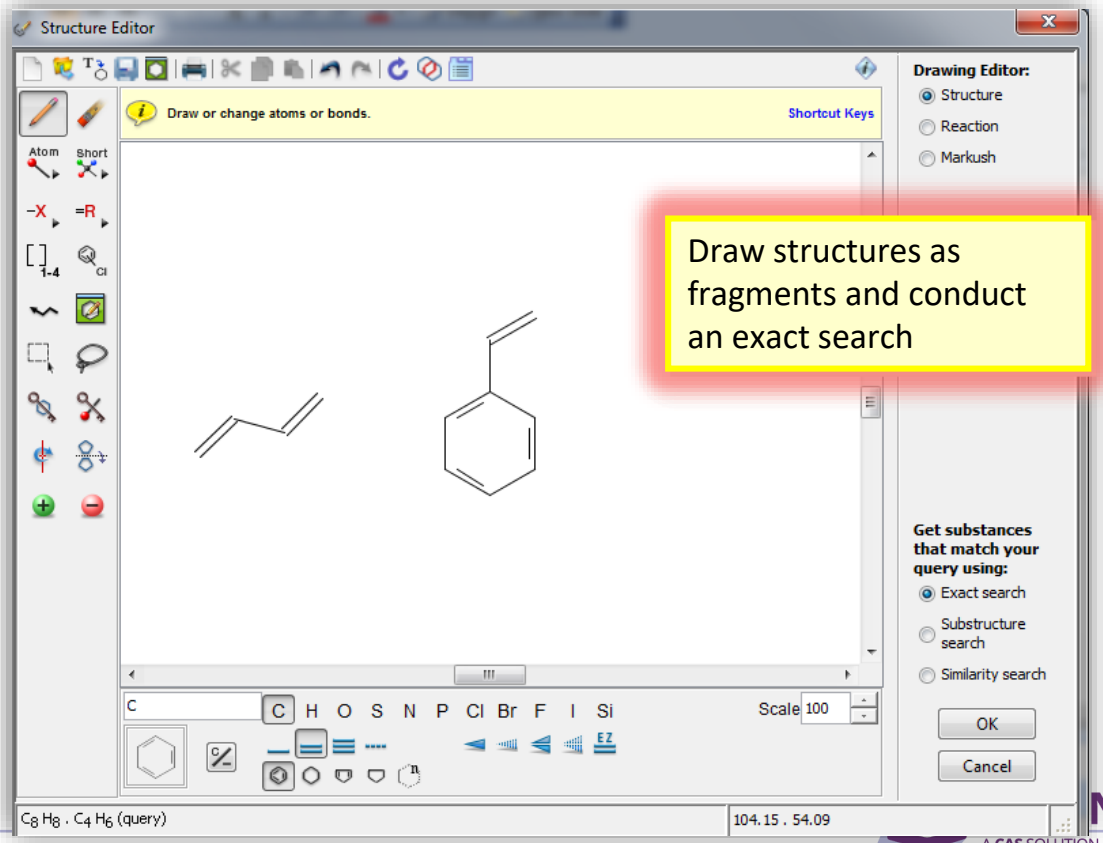
Locate copolymer of Styrene and 1,3- Butadiene

Search Strategy :

- Explore by structure-chemical structure
- Limit by characteristics-single component and type-polymers

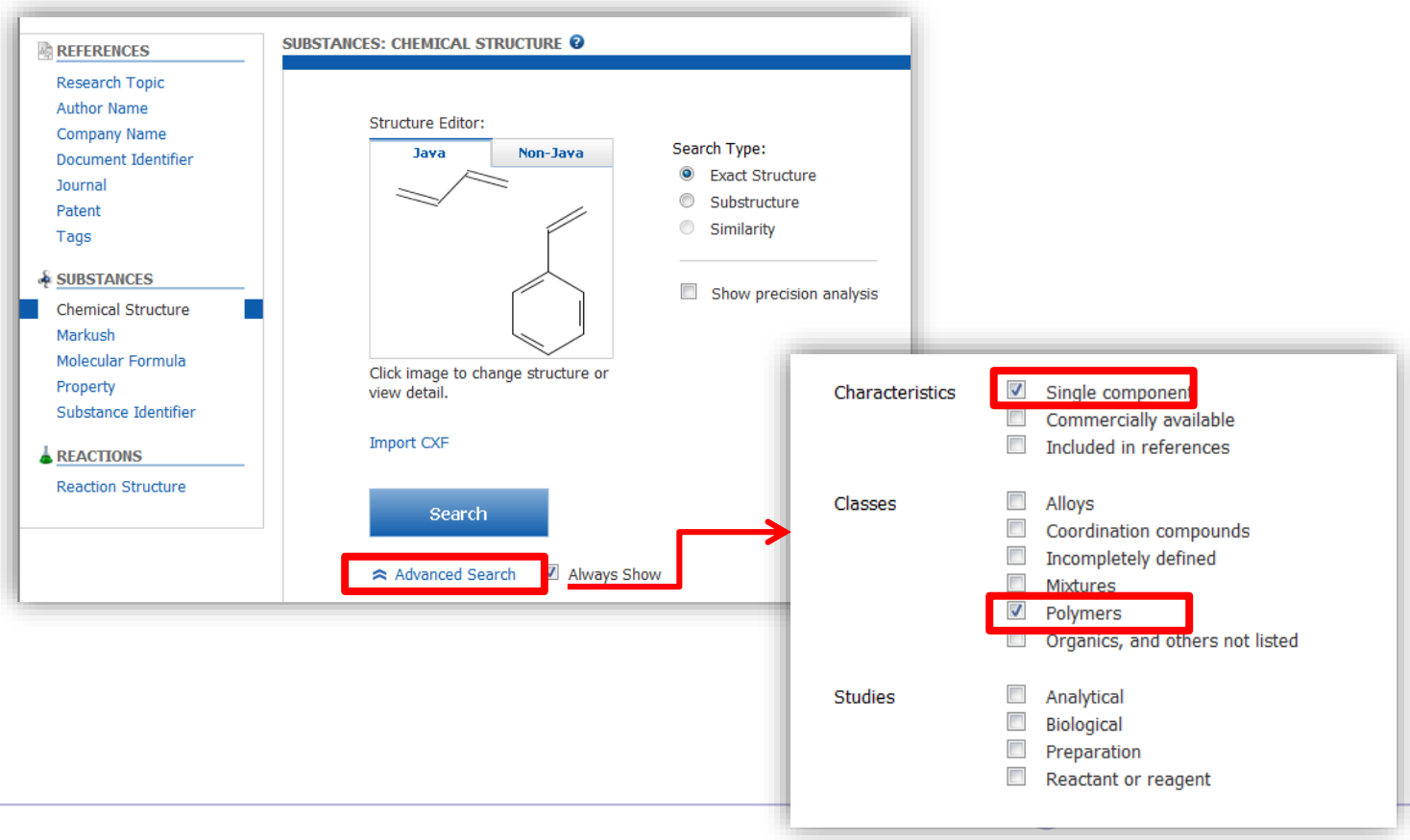
SciFinder®
A CAS SOLUTION

Structure Drawing



NDER®
A CAS SOLUTION

Search by Structure



27 Substances 0 Selected

Save Print Export

Select All Deselect All | Sort by: CAS Registry Number

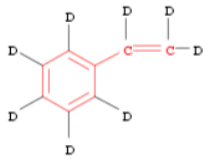
Answers per Page [15] 1 2

View:

1. Substance Detail
1196999-06-0

~1

19361-62-7
$C_8 D_8$



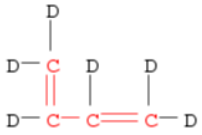
106-99-0
$C_4 H_6$

$(C_8 D_8 . C_4 H_6)_x$
Benzene-*1,2,3,4,5-d5*, 6-(ethenyl-*1,2,2-d3*)-, polymer with 1,3-butadiene, diblock

2. Substance Detail
1012312-98-9

~2

1441-56-1
$C_4 D_6$



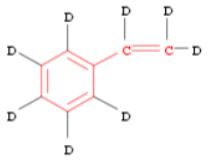
100-42-5
$C_8 H_8$

$(C_8 H_8 . C_4 D_6)_x$
Benzene, ethenyl-, polymer with 1,3-butadiene-*1,1,2,3,4,4-d6*, diblock

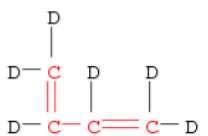
3. Substance Detail
873195-13-2

~2

19361-62-7
$C_8 D_8$



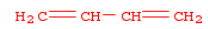
1441-56-1
$C_4 D_6$



4. Substance Detail
869196-18-9

~2

106-99-0
$C_4 H_6$



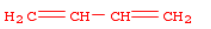
100-42-5
$C_8 H_8$

$(C_8 H_8 . C_4 H_6)_x$
Benzene, ethenyl-, polymer with 1,3-butadiene, graft, triblock

5. Substance Detail
853997-61-2

~1

106-99-0
$C_4 H_6$



100-42-5
$C_8 H_8$

$(C_8 H_8 . C_4 H_6)_x$
Benzene, ethenyl-, polymer with 1,3-butadiene, syndiotactic, pentablock (9CI)

6. Substance Detail
853997-60-1

~1

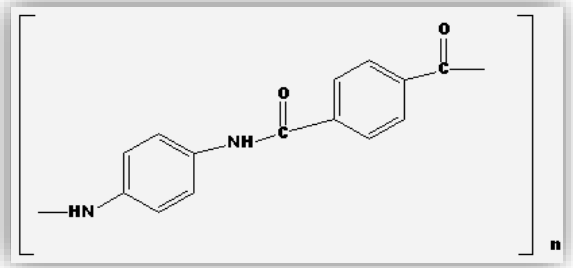
106-99-0
$C_4 H_6$

100-42-5
$C_8 H_8$

$(C_8 H_8 . C_4 H_6)_x$
Benzene, ethenyl-, polymer with 1,3-butadiene, syndiotactic, triblock (9CI)

Case Study

Find any information in SciFinder relating to the polymer below.

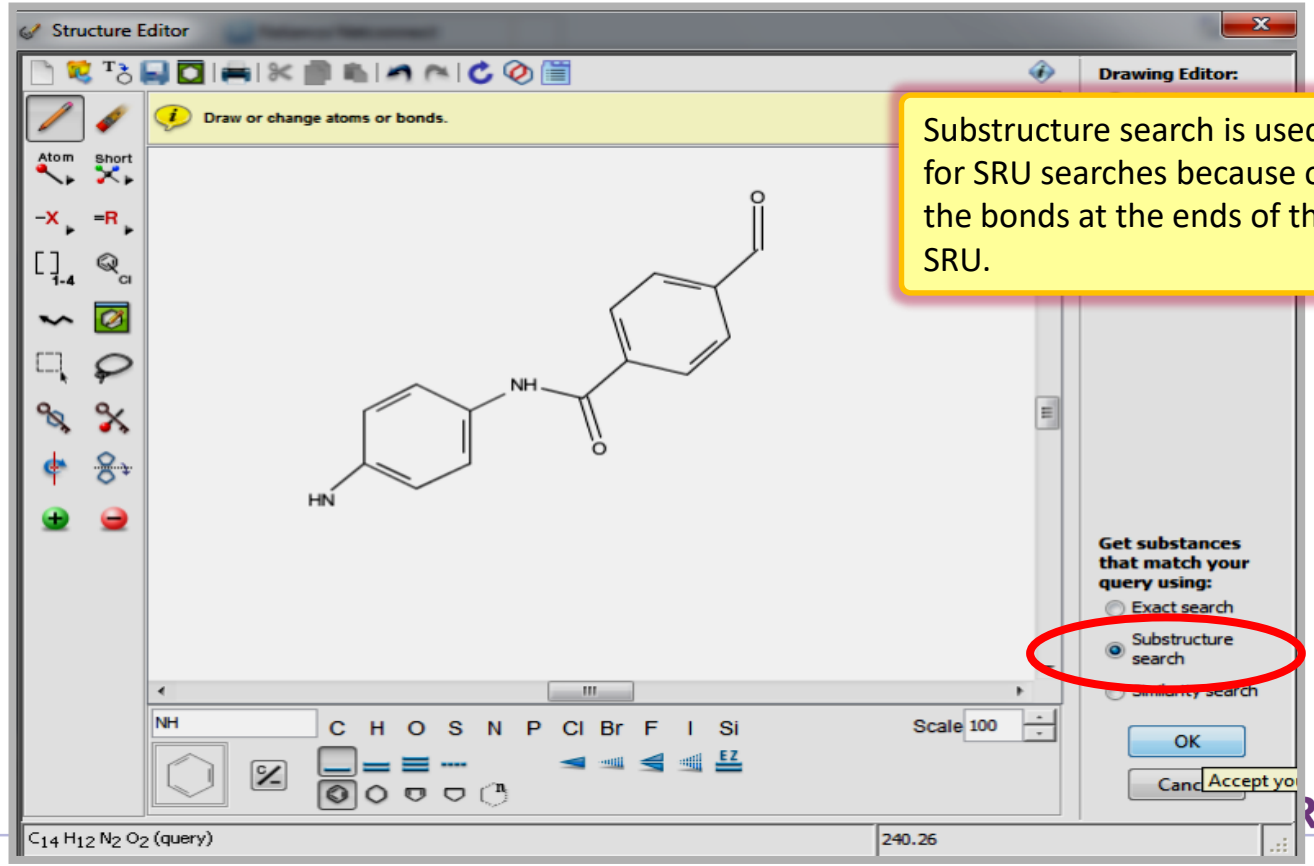


Search Strategy :

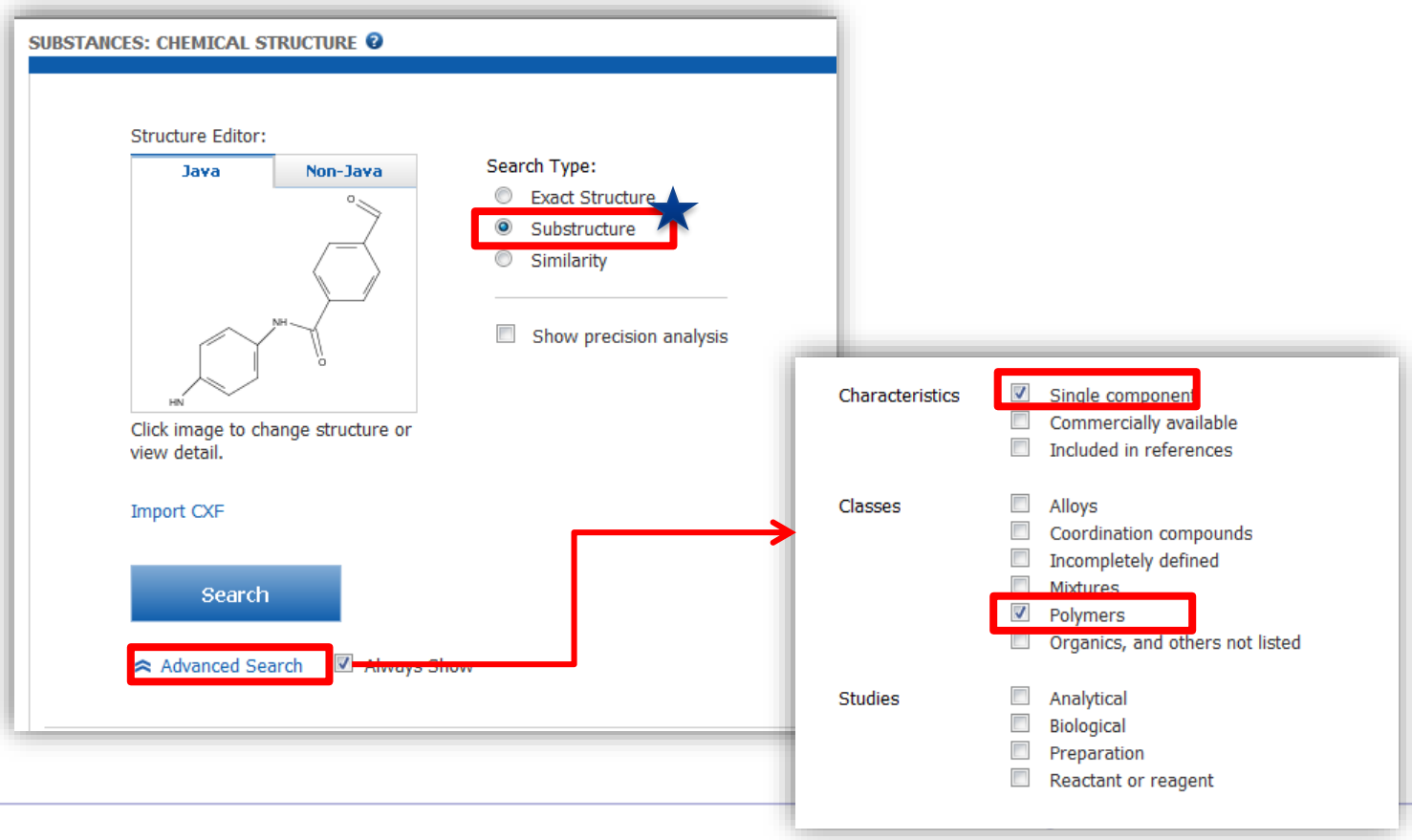
- Explore by structure-chemical structure
- Limit by characteristics-single component and type-polymers

SciFinder®
A CAS SOLUTION

Structure Drawing



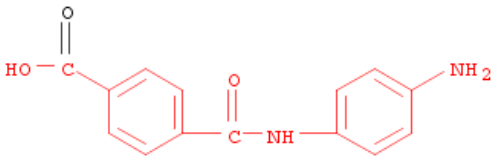
Limiting our search



1. **Substance Detail**
89885-24-5

~4

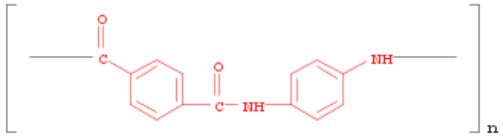
89846-77-5
$C_{14}H_{12}N_2O_3$



$(C_{14}H_{12}N_2O_3)_x$
Benzoic acid, 4-[[(4-aminophenyl)amino]carbonyl]-, homopolymer (9CI)

2. **Substance Detail**
24938-64-5

~4998

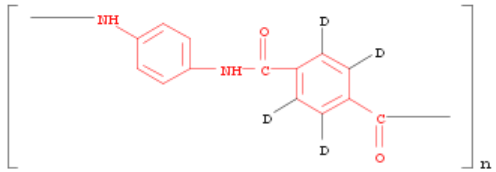


$(C_{14}H_{10}N_2O_2)_n$
Poly(imino-1,4-phenyleneiminocarbonyl-1,4-phenylenecarbonyl)

Experimental Properties

3. **Substance Detail**
143859-85-2

~3

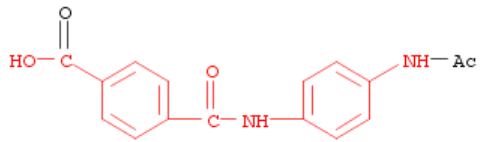


$(C_{14}H_6D_4N_2O_2)_n$
Poly[imino-1,4-phenyleneiminocarbonyl(1,4-phenylene-*2,3,5,6-d*4)carbonyl] (9CI)

4. **Substance Detail**
124239-34-5

~1

124239-33-4
$C_{16}H_{14}N_2O_4$



$(C_{16}H_{14}N_2O_4)_x$
Benzoic acid, 4-[[[4-(acetylamino)phenyl]amino]carbonyl]-, homopolymer