如何運用CAS SciFinderN優化研究

劉全哲
Tliu2@acs-i.org

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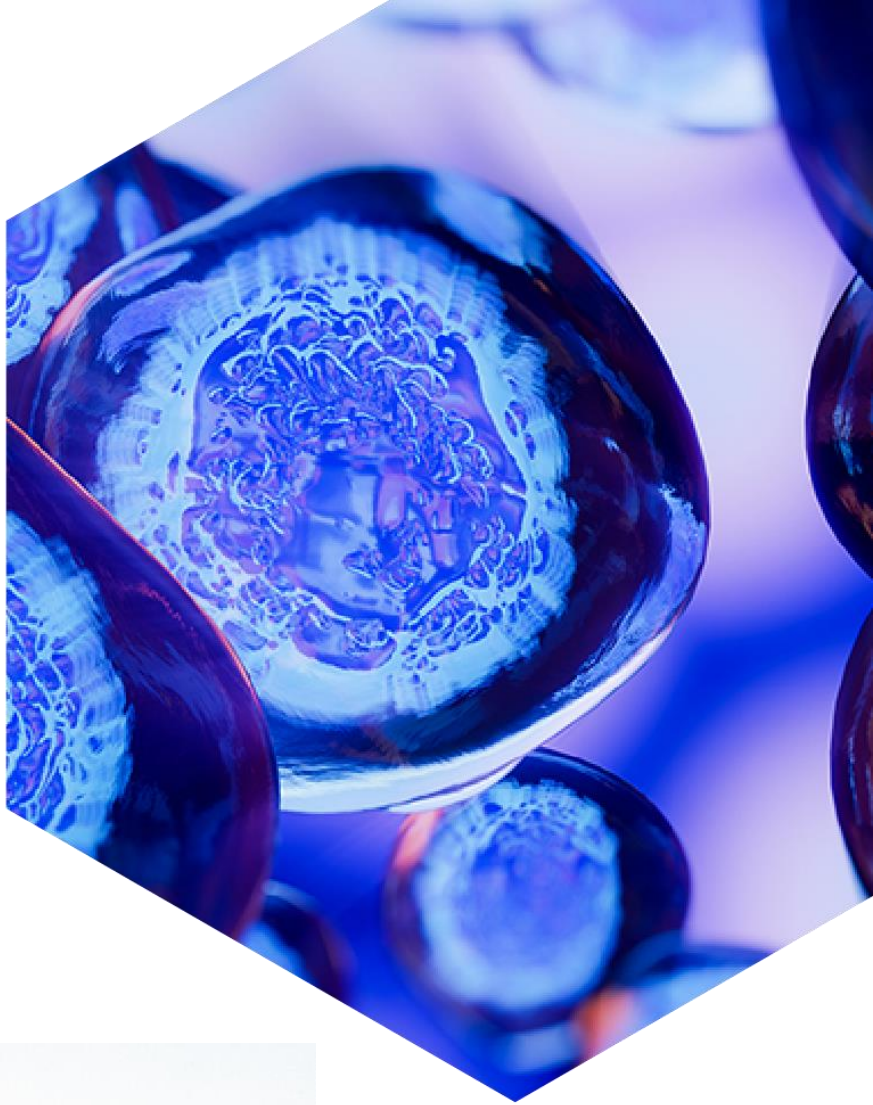
About CAS



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PHARMA

48 of the **TOP 50** pharma companies[1]

ACADEMIC

100 of the **TOP 100** universities[2]

GOVERNMENT

10 of the **TOP 10** global patent offices[3]

BIOTECH

25 of the **TOP 25** biotech companies[4]

CHEMICAL

44 of the **TOP 50** chemical companies[5]

1. https://cdn.sanity.io/files/0vv8moc6/pharmexec/339f103f01e043f652e39f8c0e72f3795fb71f60.pdf/PharmaceuticalExecutive_June2022_watermark.pdf
2. https://www.shanghairanking.com/rankings/gras/2022/RS0103
3. https://www.wipo.int/edocs/pubdocs/en/wipo-pub-943-2021-en-wipo-ip-facts-and-figures-2021.pdf
4. https://www.genengnews.com/a-lists/top-25-biotech-companies-of-2022/
5. https://cen.acs.org/business/finance/CENs-Global-Top-50-2022/100/i26

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CAS connects you to the world's published science for better insights

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50K
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million substances

Over
50
languages translated

109
patent offices worldwide

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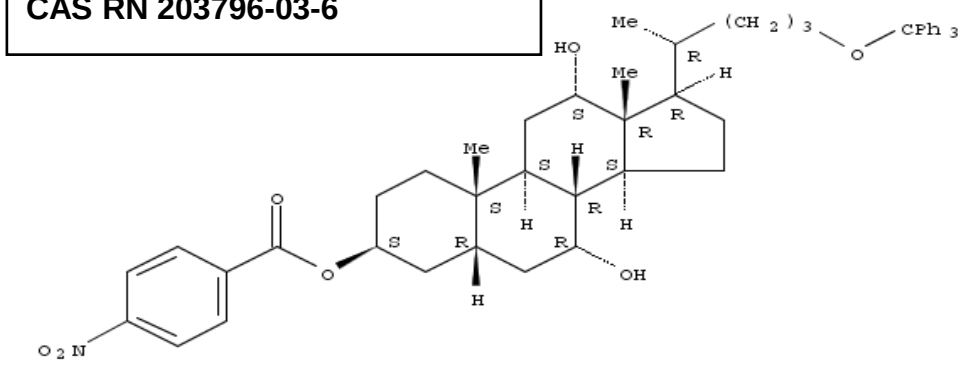
CAS scientists find the chemistry, and save you time!

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 (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding $NaHCO_3$ solution followed by extraction with EtOAc (3x50 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 ($CDCl_3$, 300 MHz) δ 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, 9 H)5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 128.88, 127.86, 126.98, 123.70, 86.47, 73.24, 73.00, 68.70, 64.22, 47.79, 46.79, 42.15, 39.76, 37.47, 35.52, 35.34, 34.23, 33.79, 32.46, 31.12, 28.74, 27.

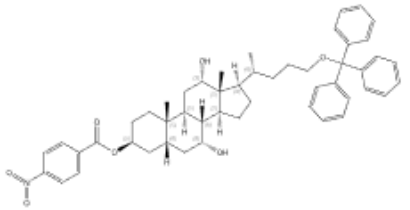
(thioglyce

CAS RN 203796-03-6



Absolute stereochemistry.

203796-03-6



Absolute stereochemistry shown

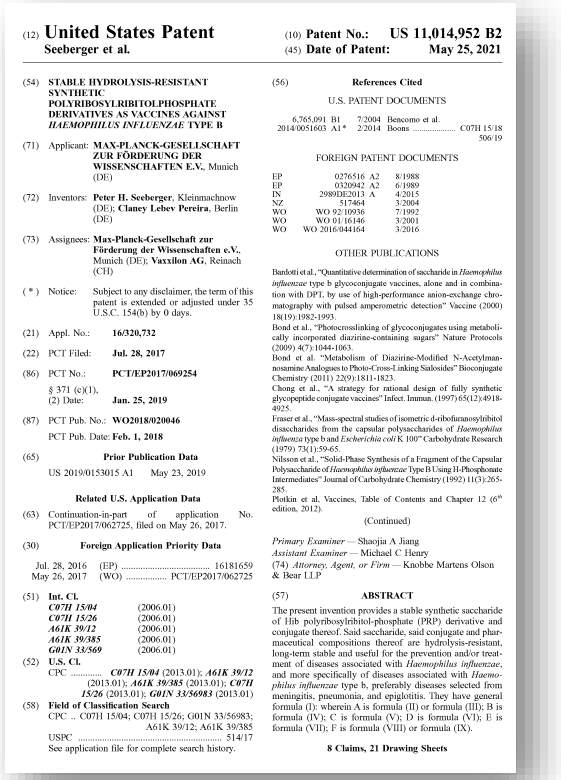
$C_{50}H_{59}NO_7$

Cholane-3,7,12-triol, 24-(tripheny lmethoxy)-, 3-(4-nitrobenzoate), (3β, 5β,7α,12α)-

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

CAS curation extracts knowledge

Current patent example



(12) **United States Patent**
Seeberger et al.

(10) **Patent No.: US 11,014,952 B2**
(45) **Date of Patent: May 25, 2021**

(54) **STABLE HYDROLYSIS-RESISTANT SYNTHETIC POLYRIBOSYLRIBITOLPHOSPHATE DERIVATIVES AS VACCINES AGAINST *HAEMOPHILUS INFLUENZAE* TYPE B**

(71) Applicant: **MAX-PLANCK-GESELLSCHAFT ZUR FÖRDERUNG DER WISSENSCHAFTEN E.V.**, Munich (DE)

(72) Inventors: **Peter H. Seeberger**, Kleinmachnow (DE); **Claney Lebev Pereira**, Berlin (DE)

(73) Assignees: **Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V.**, Munich (DE); **Vaxxilon AG**, Reinach (CH)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: **16/320,732**

(22) PCT Filed: **Jul. 28, 2017**

(86) PCT No.: **PCT/EP2017/069254**
§ 371 (c)(1),
(2) Date: **Jan. 25, 2019**

(87) PCT Pub. No.: **WO2018/020046**
PCT Pub. Date: **Feb. 1, 2018**

(65) **Prior Publication Data**
US 2019/0153015 A1 May 23, 2019

Related U.S. Application Data
(63) Continuation-in-part of application No. PCT/EP2017/062725, filed on May 26, 2017.

(30) **Foreign Application Priority Data**
Jul. 28, 2016 (EP) 16181659
May 26, 2017 (WO) PCT/EP2017/062725

(51) **Int. Cl.**
C07H 15/04 (2006.01)
C07H 15/26 (2006.01)
A61K 39/12 (2006.01)
A61K 39/385 (2006.01)
G01N 33/569 (2006.01)

(52) **U.S. Cl.**
CPC ***C07H 15/04*** (2013.01); ***A61K 39/12*** (2013.01); ***A61K 39/385*** (2013.01); ***C07H 15/26*** (2013.01); ***G01N 33/56983*** (2013.01)

(58) **Field of Classification Search**
CPC .. C07H 15/04; C07H 15/26; G01N 33/56983; A61K 39/12; A61K 39/385
USPC 514/17
See application file for complete search history.

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Nilsson et al., "Solid-Phase Synthesis of a Fragment of the Capsular Polysaccharide of *Haemophilus influenzae* Type B Using H-Phosphonate Intermediates" Journal of Carbohydrate Chemistry (1992) 11(3):265-285.
Plotkin et al, Vaccines, Table of Contents and Chapter 12 (6th edition, 2012).
(Continued)

Primary Examiner — Shaojia A Jiang
Assistant Examiner — Michael C Henry
(74) *Attorney, Agent, or Firm* — Knobbe Martens Olson & Bear LLP

(57) **ABSTRACT**

The present invention provides a stable synthetic saccharide of Hib polyribosylribitol-phosphate (PRP) derivative and conjugate thereof. Said saccharide, said conjugate and pharmaceutical compositions thereof are hydrolysis-resistant, long-term stable and useful for the prevention and/or treatment of diseases associated with *Haemophilus influenzae*, and more specifically of diseases associated with *Haemophilus influenzae* type b, preferably diseases selected from meningitis, pneumonia, and epiglottitis. They have general formula (I): wherein A is formula (II) or formula (III); B is formula (IV); C is formula (V); D is formula (VI); E is formula (VII); F is formula (VIII) or formula (IX).

8 Claims, 21 Drawing Sheets

CAS curation yields:

29 concepts

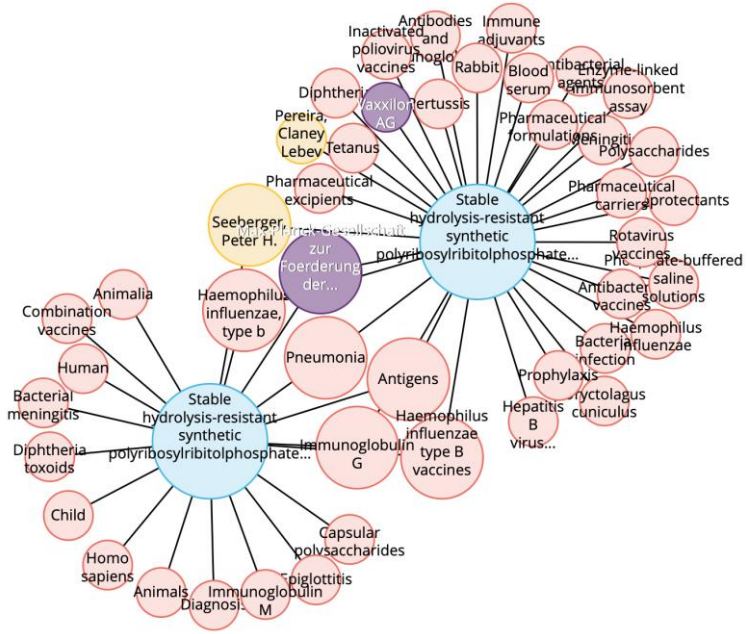
136 substances

1,405 reactions

16 patent family members

25 cited documents

Patent knowledge graph reveals connections



US11014952B2

Stable hydrolysis-resistant synthetic polyribosylribitolphosphate derivatives as vaccines against Haemophilus influenzae type B

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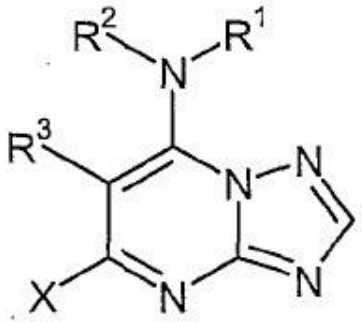
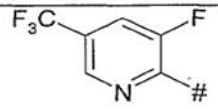
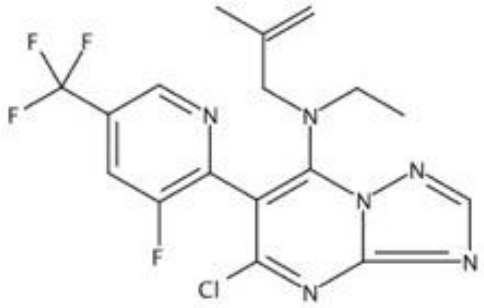
CAS curated chemistry content and technology improve similarity hit rates

Target Patent



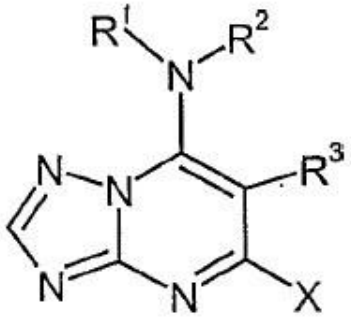
(I)

Bsp. Nr.	R^1	R^2	R^3	X	logP	Fp.(°C):
4	$-CH_2-C(CH_3)=CH_2$	$-C_2H_5$		-Cl	3,51	Paste



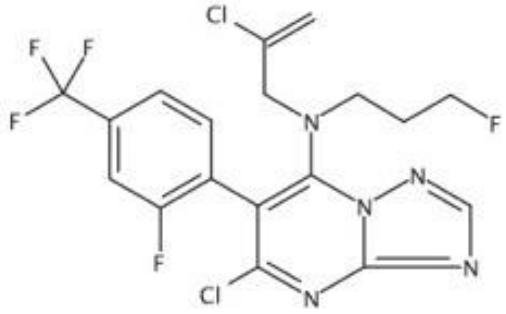
Substance Similarity Match

Prior Art



(I)

Bsp. Nr.	R^1	R^2	R^3	X	logP
52	2-Chlorallyl	3-Fluorpropyl	2-Fluor-4-trifluor-methylphenyl	-Cl	3,77



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- Data harmonization
- API applications

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- Trend analysis
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- Landscaping & whitespace analysis
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•Develop mitigation strategies to minimize delays and respond to emerging threats quickly

•Optimize your inventory and avoid resource waste by predicting market demands and supply needs

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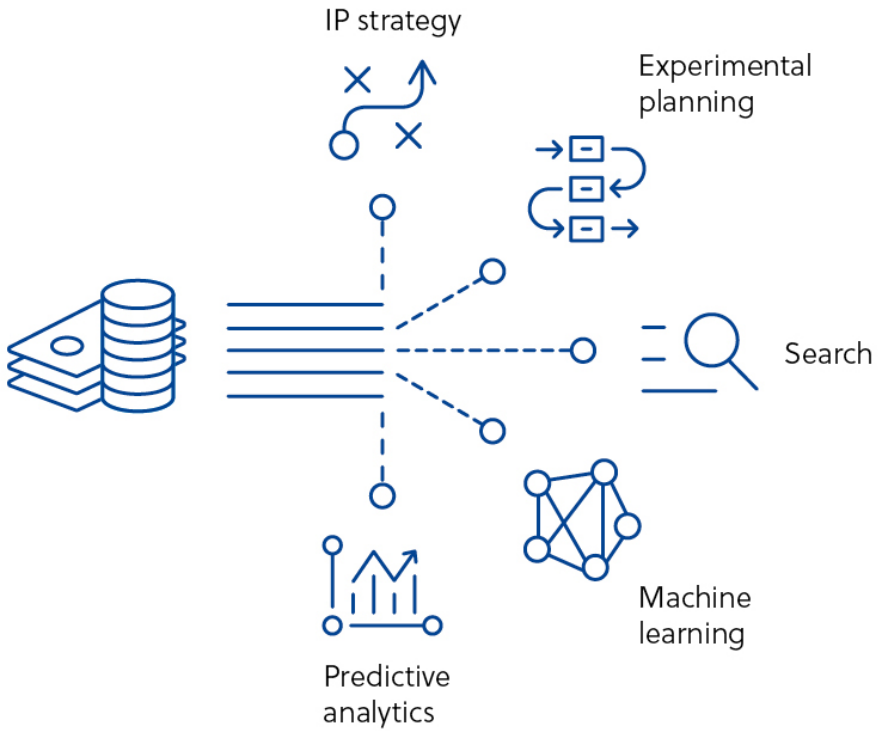
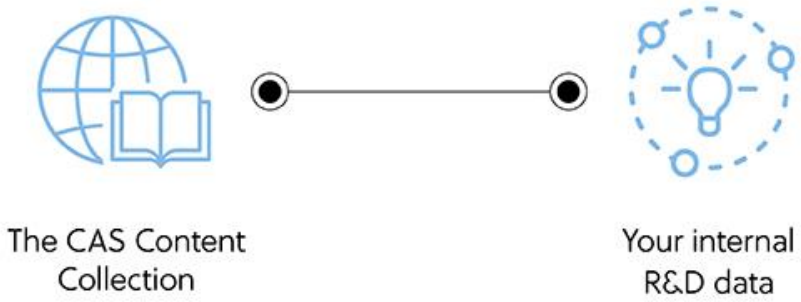
Dark Data Analytics and knowledge management



Unstructured, inaccessible data cannot be leveraged to drive future discoveries.



Associated data

- CAS Registry Number
- Molecular properties
- Chemical structure
- Chemical names
- Regulatory information
- Reaction schemes
- Experimental procedures
- Additional data fields...

Connecting an organization's data with the world's published science.

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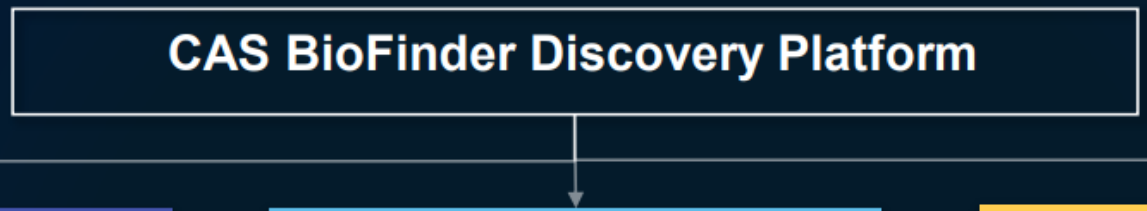
CAS BioFinder Discovery Platform

Elements of a Life Sciences relationship



CAS SciFinder

Primary Research…

- Bioactivity view by Document
- Bioactivity view by Structure
- Advanced search by target, structure, document
- Enhanced Target Search
- Reference Knowledge Graph

CAS BioFinder

Analytics…

- Ligand search (text and structure)
- Scaffold search (text and structure)
- Target Search (text, ID…)
- Pharmacology tables and analysis plots
- Substance, Scaffold, Target, Disease detail view
- Project missing target interactions for existing ligands
- Predict interactions for novel ligands with all targets in the data base
- Predict Common metabolites
- Interactive IP Landscape (based on target coverage)
- Drug Repurposing workflow in KG
- …

Customer Integration

Informatics (workflow)…

- Bioactivity API Endpoints
  - Search by Substance (Structure, Name, Identifiers)
  - Search by Scaffold
  - Search by Target (Name, Acronym, Identifiers)
  - Search by Disease (Name, Identifiers)
  - Search by Document (Patent and Journal identifiers)
- Biomarker API Endpoints
  - Search by Biomarker Molecule (Names, Identifiers)
  - Search by Disease (Names, Identifiers)
  - Search by Document (Patent and Journal identifiers)

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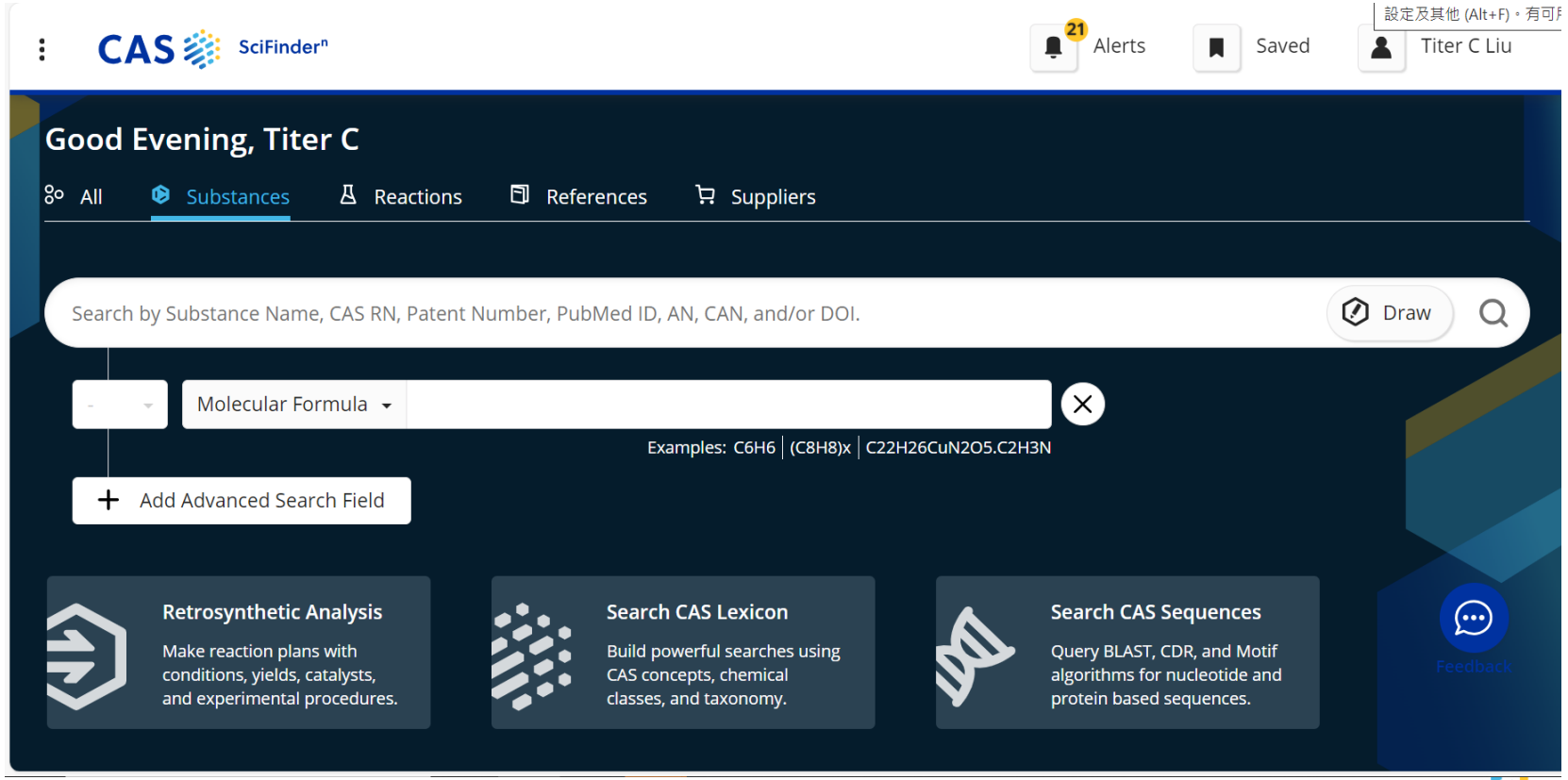
Scifinder^{n} Discovery platform

*SciFinder

Top 6 key searching function

- Reference searching
- Reaction searching
- Substance searching
- Supplier searching
- Sequence searching
- Retrosynthesis



*CAS Formulation

*CAS Analytical Methods

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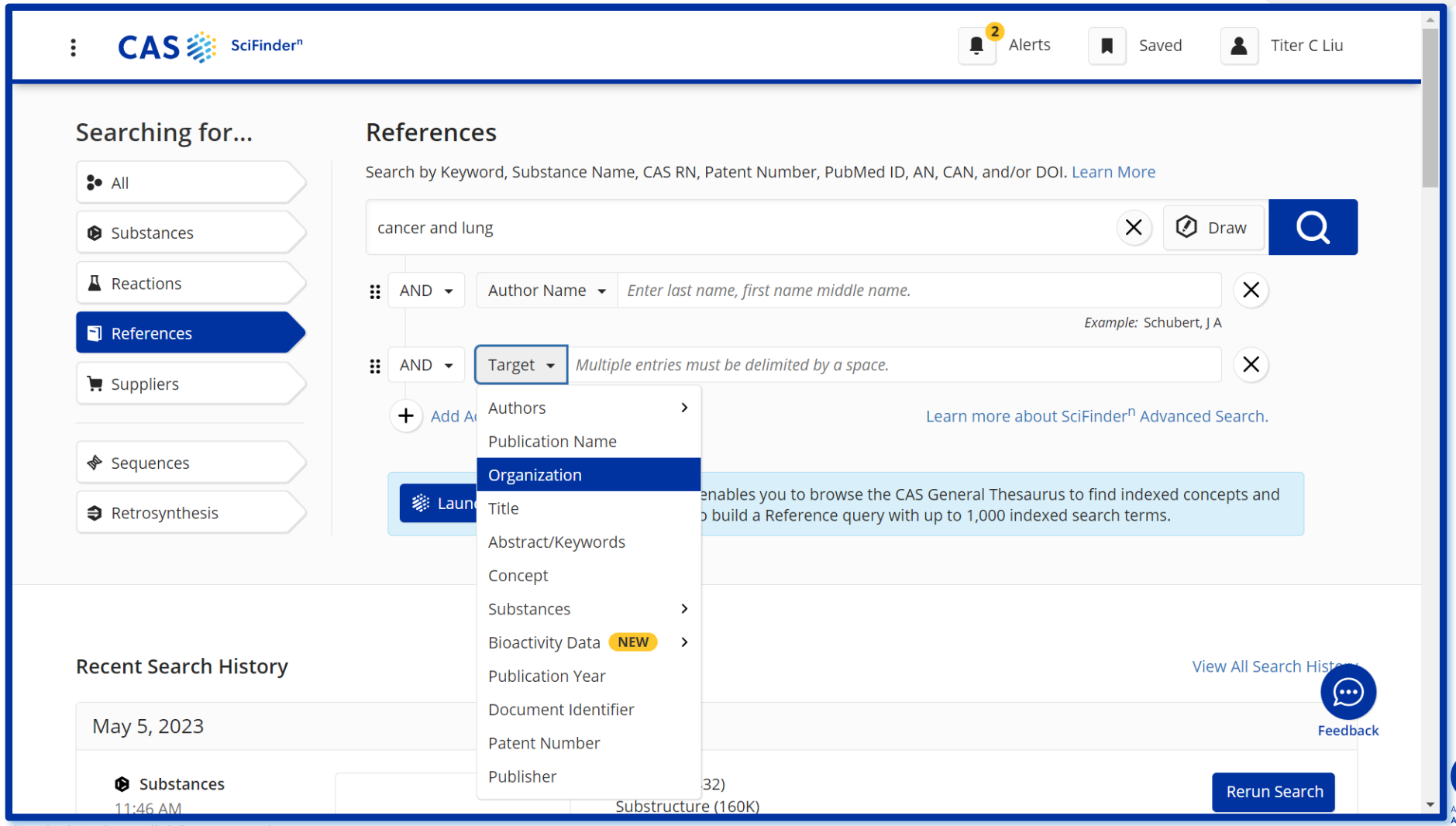
Perform Reference searching

CAS SciFinder^n halves the time needed to perform literature reviews*



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Perform literature reviews

CAS SciFinder^{n} halves the time needed to perform literature reviews*

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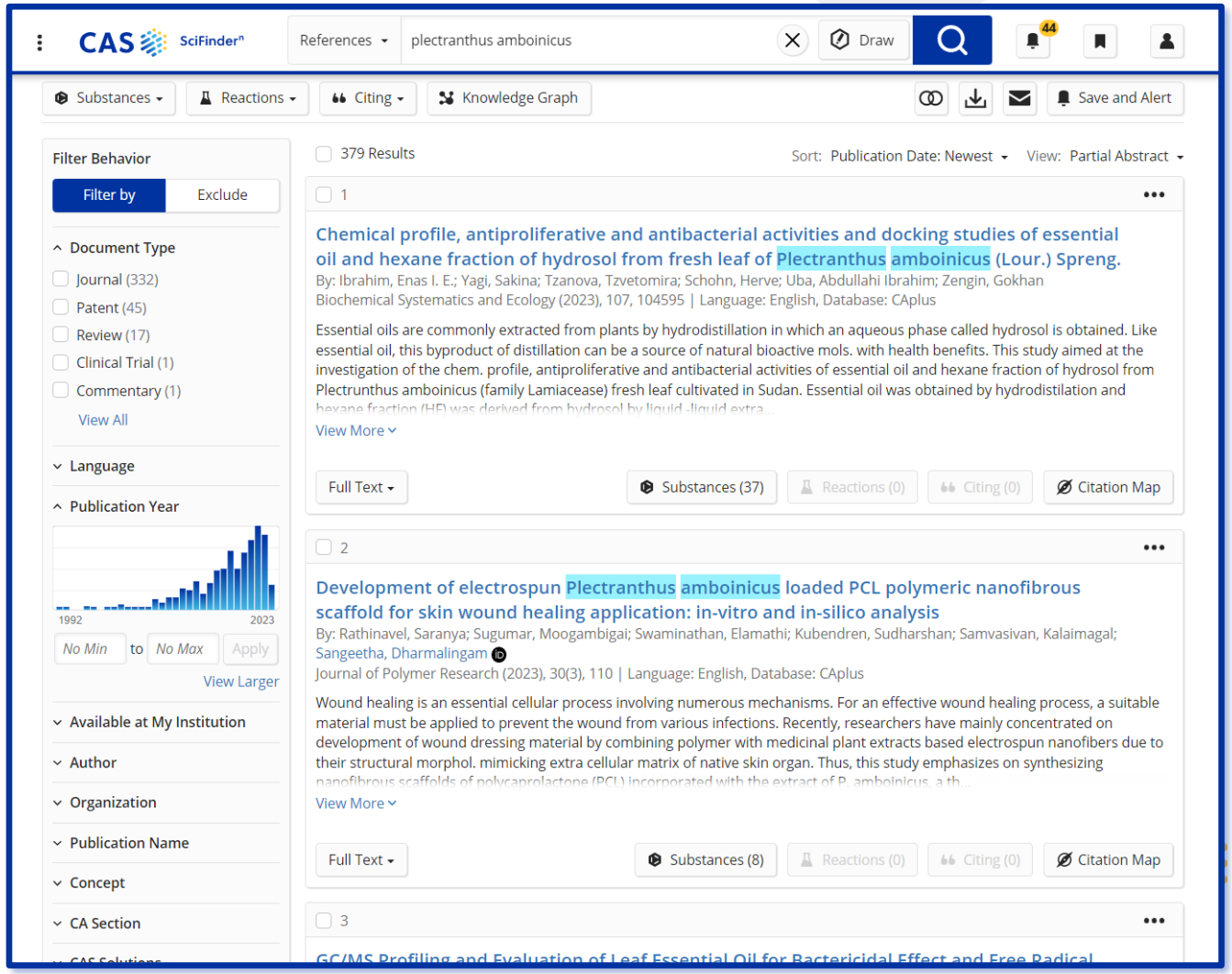


Reference Detail

Substances (6)

Patent

Patent Information

Patent Number
WO2007076701

Publication Date
2007-07-12

Application Number
WO2006-CN3694

Application Date
2006-12-29

Kind Code
A1

Assignee
Zensun (Shanghai) Science & Technology Limited, China

Source
World Intellectual Property Organization

Database Information
AN: 2007:762994
CAN: 147:134439
CAplus

Language
English

Concepts

Alzheimer disease

Animal gene
Modifier: NRG1, NR

Role: Biological Stu
Activity; Therapeuti

Anti-Alzheimer age

Antidiabetic agents

Antitumor agents

Cardiac hypertroph

Cardiomyocyte
Modifier: growth ar

Cardioprotective a

Cardiovascular dis

Cell differentiation
Modifier: cardiomy

Cell proliferation
Modifier: cardiomy

Controlled-release

Diabetes mellitus

Substances

135729-61-2

Absolute stereoch

$C_{19}H_{24}N_2O$
Palonosetron

Role: Pharmacolog
Use, Biological Stu

50-18-0

$C_7H_{15}Cl_2N_2O_2P$
Cyclophospha

Role: Adverse Effec
Pharmacological A
Biological Study, U

Formulations

Collagen Formulation: Anticancer Agents

View **Formulus®** Detail

Location: Article Page 3, 6
Purpose: Antitumor agents
Target: cancer

Component	Function	Amount Reported
Group: cyclic dinucleotides stock solution	-	-
cyclic dinucleotides	-	6.67 µg
endotoxin-free water	solvent	-
Phosphate-buffered saline solutions	buffer	-
collagen stock solution	carrier	3.5-5 mg/mL

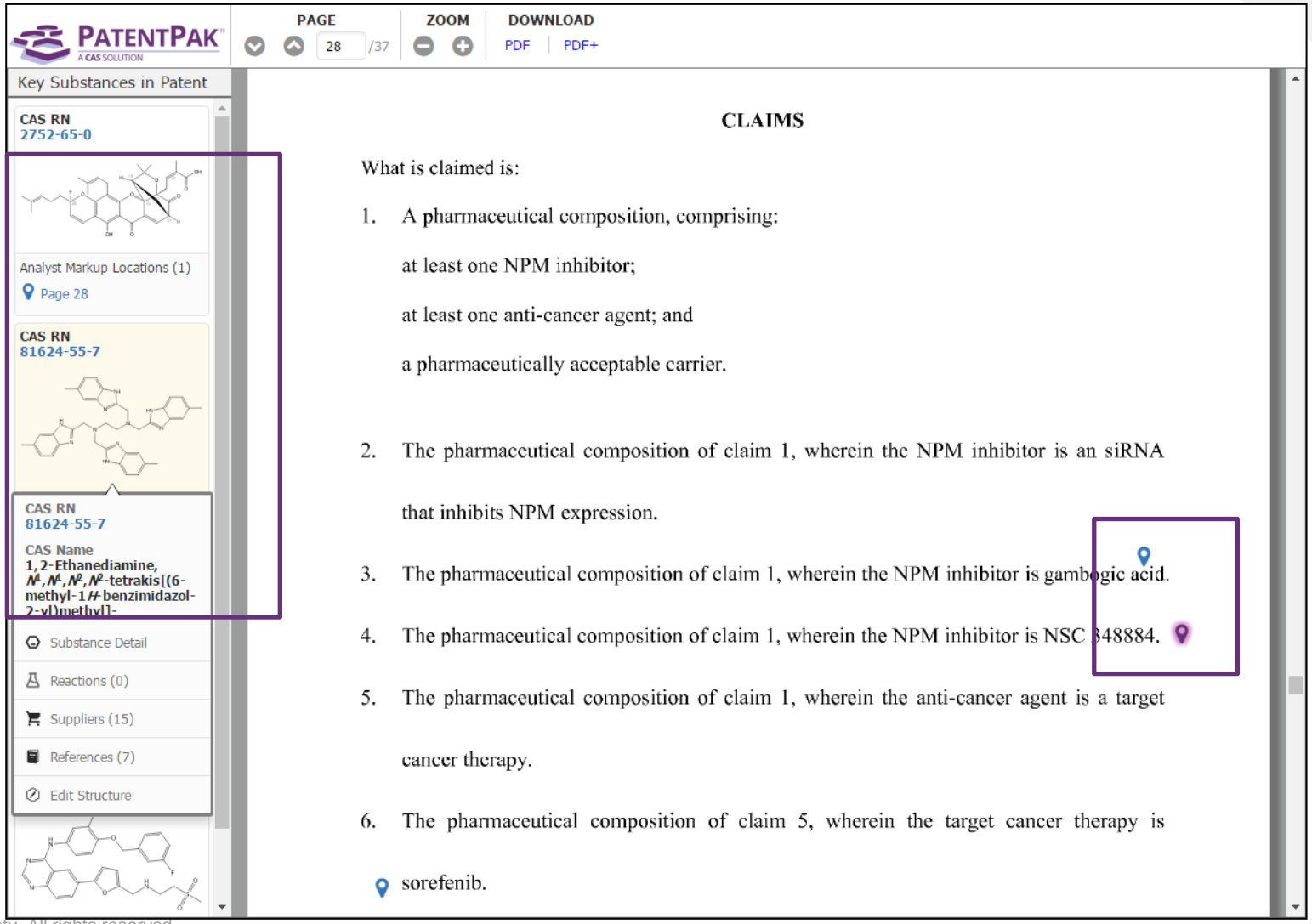
Stingel Formulation: Anticancer Agents

View **Formulus®** Detail

Location: Article Page 3, 6

PatentPak:
Why waste time slogging through dense patent material with direct access to and understanding of the chemistry within the document

Patent chemistry is fully annotated with structures, nomenclature and more!



Important chemistry locations are identified by CAS expert scientists

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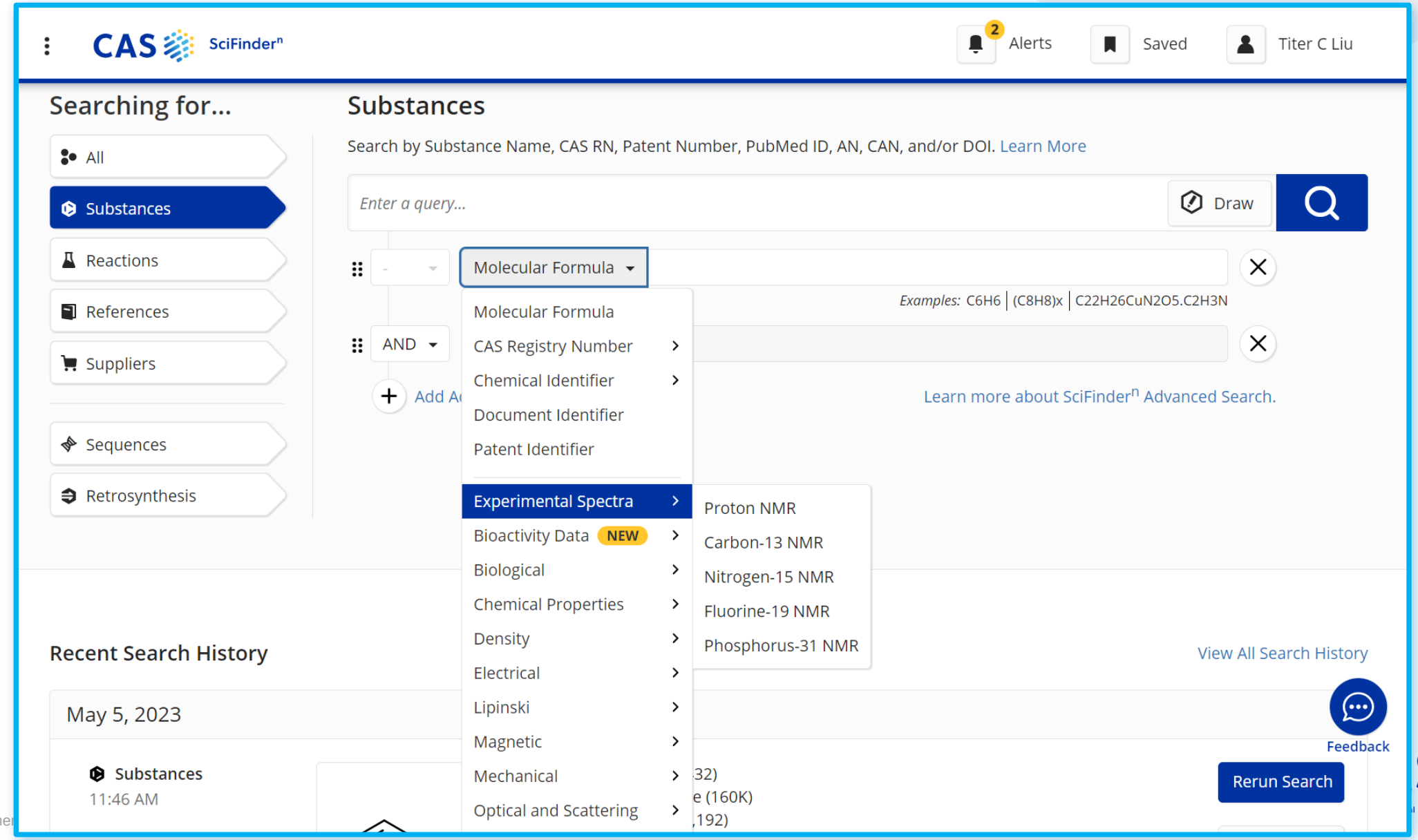
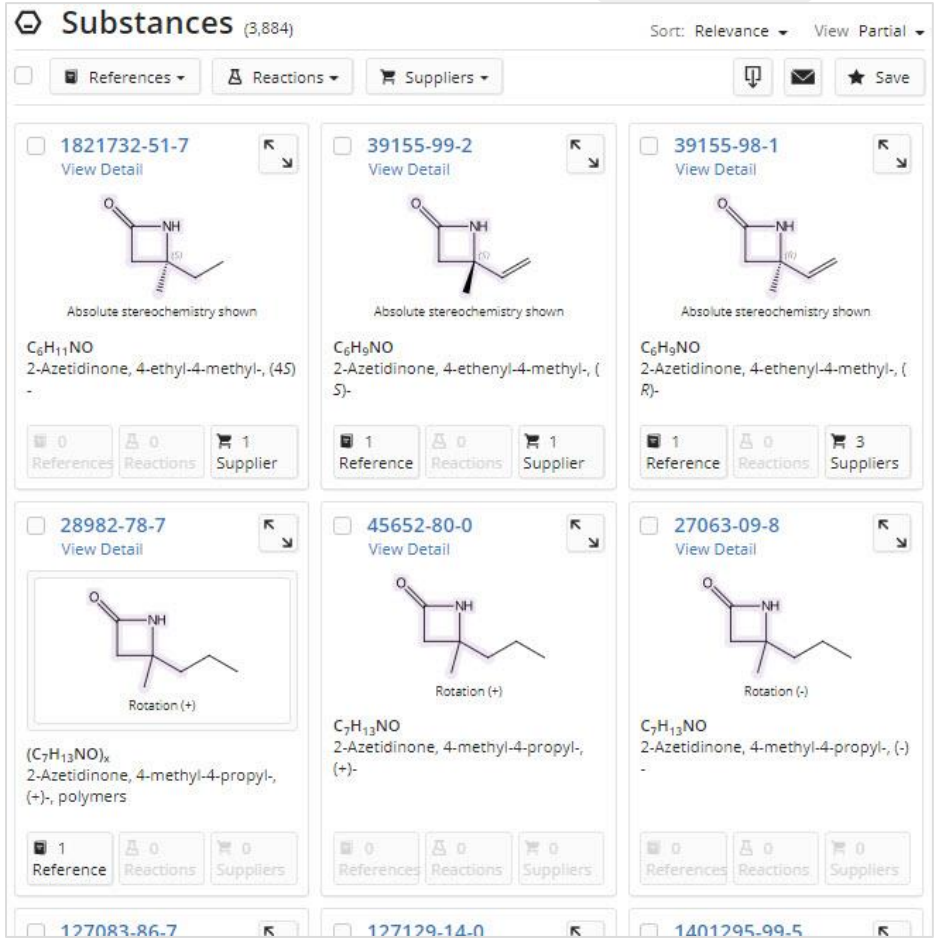
Substance searching



Mine substances and reactions

CAS SciFinder^{n} provides access to the world's most trusted substance resource, CAS REGISTRY®

Inform your research with the one true source for authoritatively identifying a chemical substance and its related chemical structures, chemical names, regulatory information, and properties, including the CAS Registry Number®, as well as reaction schemes, product yields and more.



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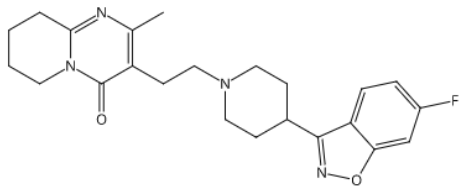
Substances information

CAS Registry Number: 106266-06-2

References (13K) | Reactions (218) | Suppliers (122) | Save



$C_{23}H_{27}FN_4O_2$

4*H*-Pyrido[1,2-*a*]pyrimidin-4-one, 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-2-methyl- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	410.49	-
Melting Point (Experimental)	170 °C	-
Boiling Point (Predicted)	572.4±60.0 °C	Press: 760 Torr
Density (Predicted)	1.38±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	8.07±0.10	Most Basic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names and Identifiers

Experimental Properties

Biological | Chemical | Lipinski | Structure Related | Thermal

Property	Value	Condition	Source
Median Lethal Dose	29.7 mg/kg	Organism: rat; Route: intravenous	(1) APC
Median Lethal Dose	18.3 mg/kg	Organism: dog; Route: oral	(1) APC
Median Lethal Dose	14.1 mg/kg	Organism: dog; Route: intravenous	(1) APC
ADME (Absorption, Distribution, Metabolism, Excretion) - 16 Sources	See Full Text		(2-17) CAS
Half-Life (Biological) - 7 Sources	See Full Text		(18-24) CAS
LC50 - 1 Source	See Full Text		(25) CAS

Sources

(1) (2009), 1280 pages, CAplus

Structure Activity Relationships

CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data

CAS LIFE SCIENCES

Toxicity

CAS LIFE SCIENCES

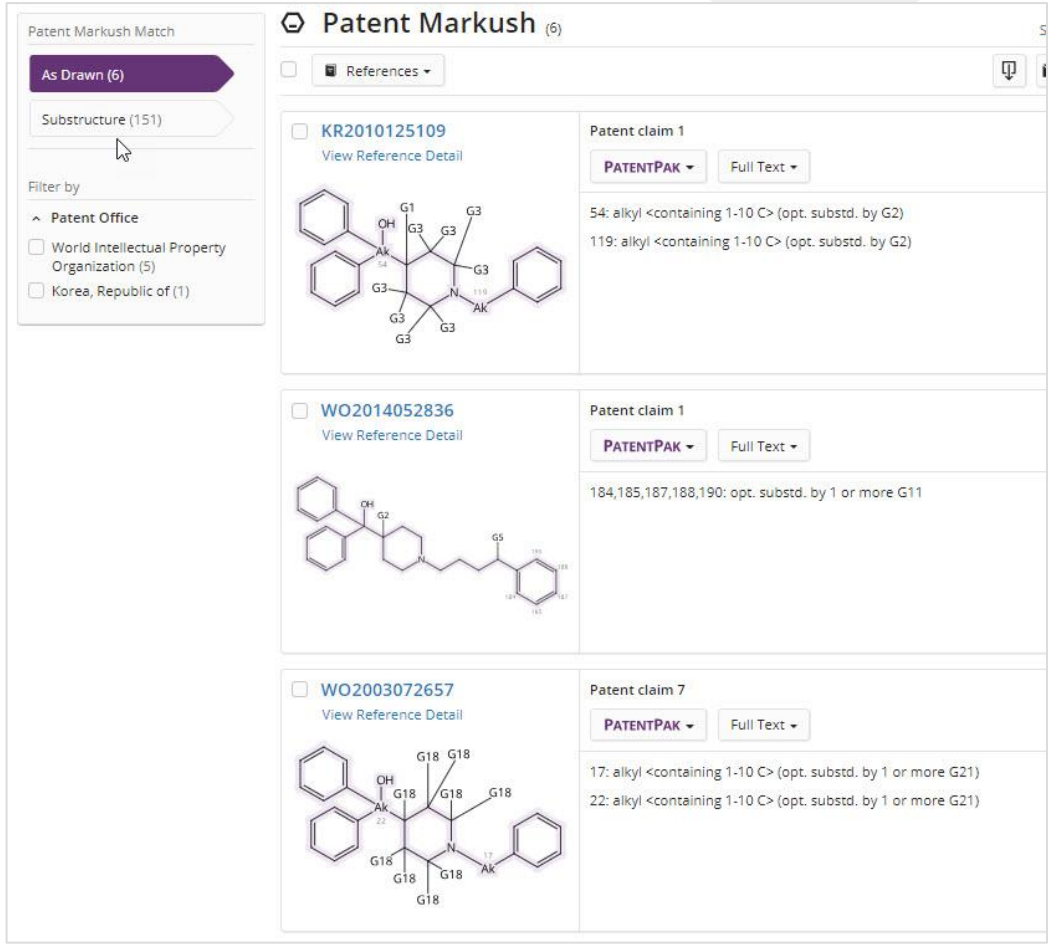
Target | Function | Parameter | Disease | Organism

Target (1)	Function	Parameter (2)	Value	Disease	Organism	Assay	Source
5-HT2A receptors	-	5-HT2C receptor activity	19.7 nM	Schizophrenia	-	View Detail	(1) CAS
Adrenoceptor A1	-	α1 receptor activity	2.8 nM	Schizophrenia	-	View Detail	(1) CAS
Dopamine D_3 receptors	-	D3 receptor activity	10.9 nM	Schizophrenia	-	View Detail	(1) CAS
HEK293 cells and Chang liver cells	Antagonist	IC50	>600 ug/ml	Depression	Mouse	View Detail	(2) CAS
HEK293 cells and Chang liver cells	Antagonist	IC50	238.8 ug/ml	Depression	Mouse	View Detail	(2) CAS
Histamine H1 receptors	-	H1 receptor activity	26.1 nM	Schizophrenia	-	View Detail	(1) CAS
-	-	Adiposity index	Ligand didn't show any significant difference in adiposity index	-	-	View Detail	(3) CAS
-	-	APO level	17.92 mg/kg	Schizophrenia	-	View Detail	(1) CAS
-	-	AUC	Ligand significantly increased AUC values	-	-	View Detail	(3) CAS
-	-	Behavior	1628.3 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1573.7 cm	-	-	View Detail	(3) CAS
-	-	Behavior	0.21	-	-	View Detail	(3) CAS
-	-	Behavior	0.34	-	-	View Detail	(3) CAS
-	-	Behavior	0.38	-	-	View Detail	(3) CAS
-	-	Behavior	0.28	-	-	View Detail	(3) CAS
-	-	Behavior	0.40	-	-	View Detail	(3) CAS
-	-	Behavior	0.43	-	-	View Detail	(3) CAS
-	-	Behavior	47.3	-	-	View Detail	(3) CAS
-	-	Behavior	58.8	-	-	View Detail	(3) CAS
-	-	Behavior	2119.17 cm	-	-	View Detail	(3) CAS
-	-	Behavior	56.1	-	-	View Detail	(3) CAS
-	-	Behavior	62	-	-	View Detail	(3) CAS
-	-	Behavior	73.2	-	-	View Detail	(3) CAS
-	-	Behavior	65.8	-	-	View Detail	(3) CAS
-	-	Behavior	1778 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1768.33 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1937.2 cm	-	-	View Detail	(3) CAS

Inform IP strategy

CAS SciFinder^{n} reduces the time needed to analyze the IP landscape*

Access industry-leading capabilities like patent Markush searching, and content such as patents that have been chemically annotated by our scientists, so you can stay on top of the technology landscape.



*CAS SciFinder^{n} Productivity Survey 2020

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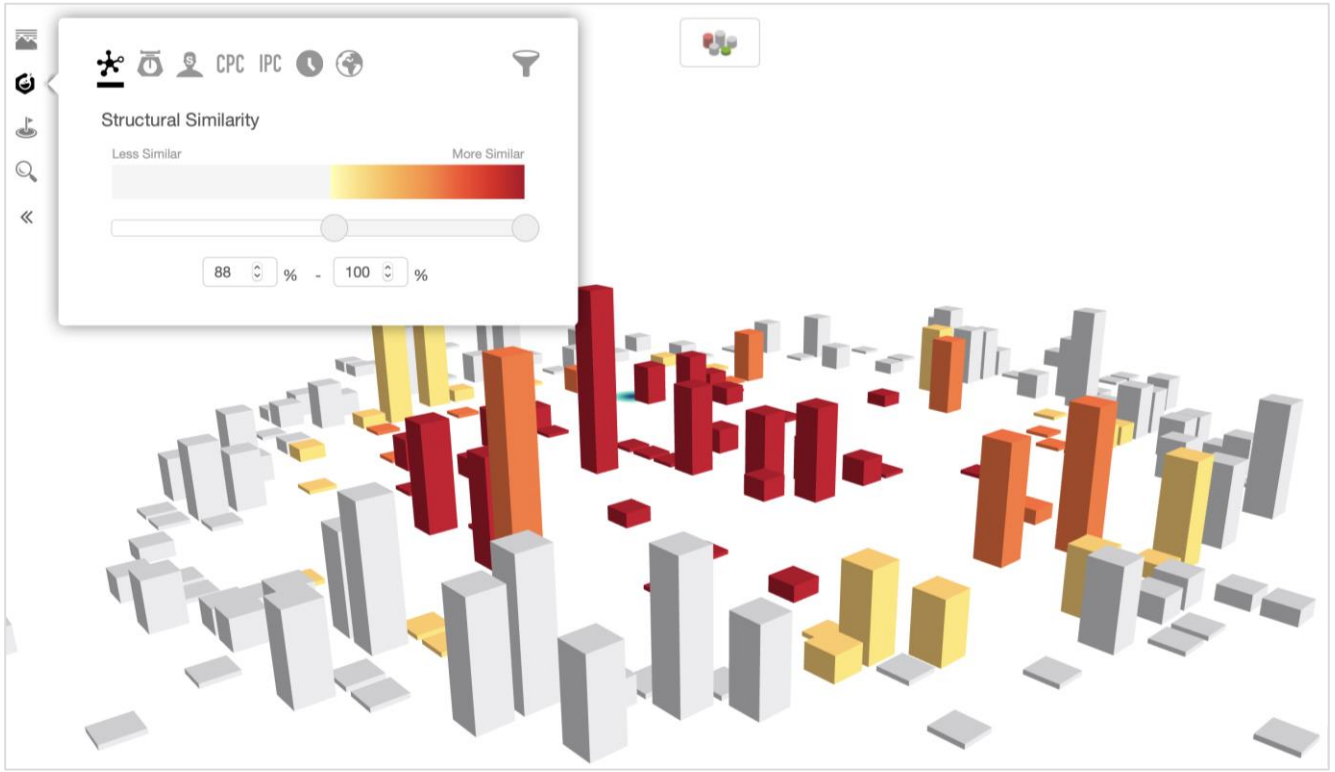
Visualize search results

CAS SciFinder^{n} offers visual context for substance and biosequence result sets

Graphically explore the structural similarity of chemicals compared to one another and the patents associated with them.

Review visualized biosequence search results and evaluate sequence space from an IP perspective.



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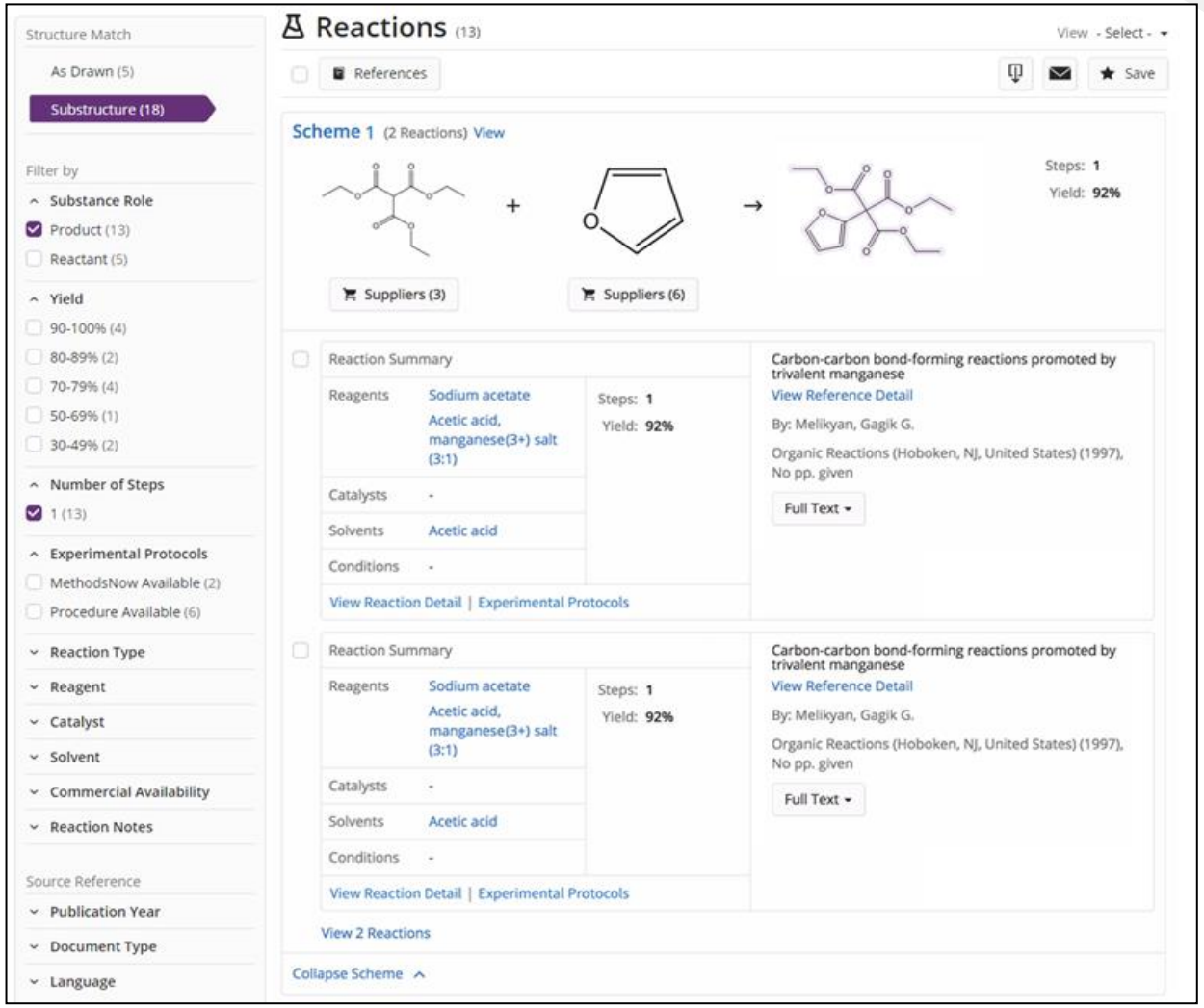
Reaction: Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus



Intuitive information layouts fosters quick comprehension

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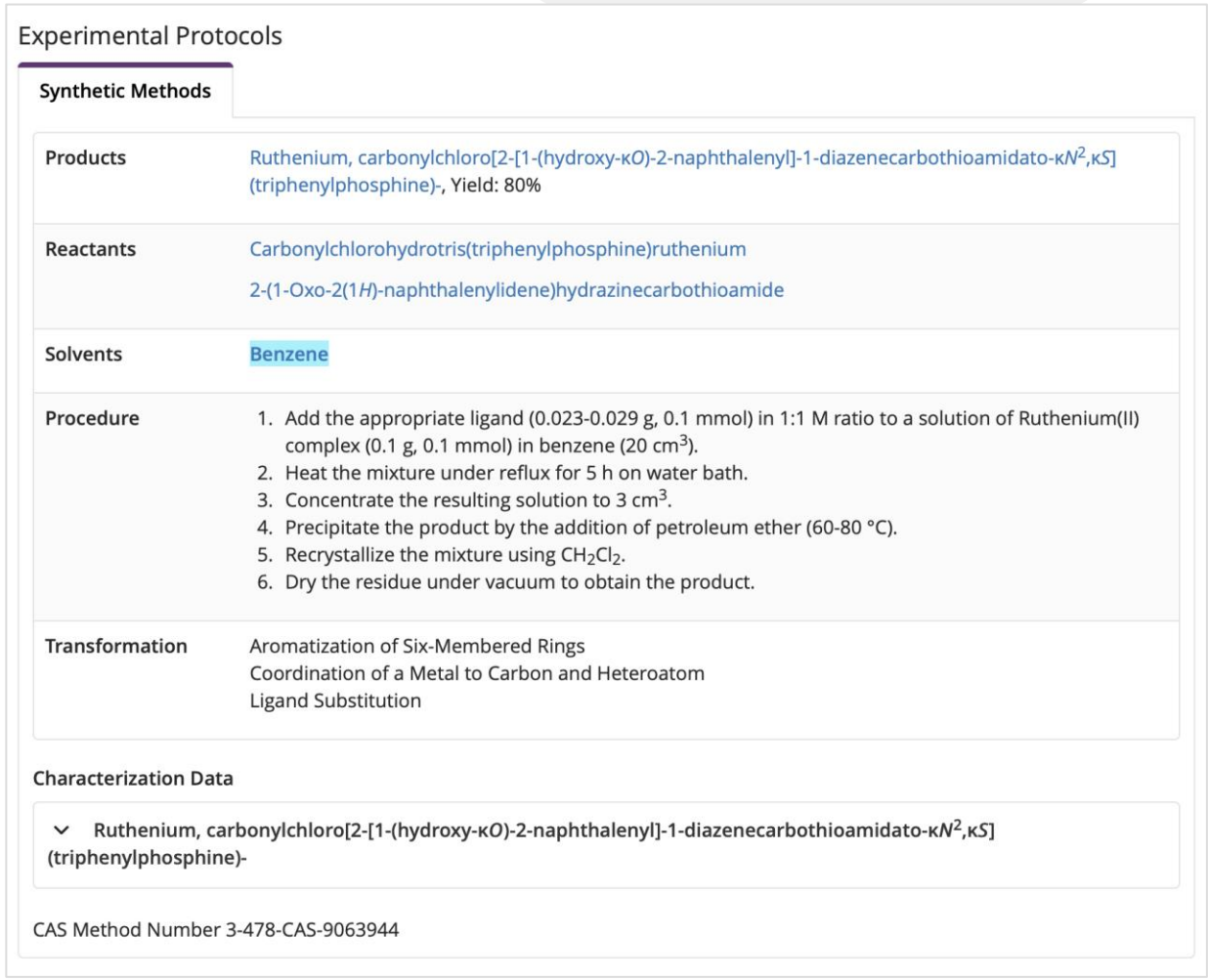
Design efficient bench strategies and work plans

Find practical methods and pathways for production synthesis, extracted directly from the literature.

Identify opportunities for new breakthroughs in synthetic methods.



Experimental Protocols

Synthetic Methods

Products	Ruthenium, carbonylchloro[2-[1-(hydroxy-κ*O*)-2-naphthalenyl]-1-diazenecarbothioamidato-κN^2,κ*S*](triphenylphosphine)-, Yield: 80%
Reactants	Carbonylchlorohydrotris(triphenylphosphine)ruthenium 2-(1-Oxo-2(1*H*)-naphthalenylidene)hydrazinecarbothioamide
Solvents	Benzene
Procedure	1. Add the appropriate ligand (0.023-0.029 g, 0.1 mmol) in 1:1 M ratio to a solution of Ruthenium(II) complex (0.1 g, 0.1 mmol) in benzene (20 cm^3). 2. Heat the mixture under reflux for 5 h on water bath. 3. Concentrate the resulting solution to 3 cm^3. 4. Precipitate the product by the addition of petroleum ether (60-80 °C). 5. Recrystallize the mixture using CH_2Cl_2. 6. Dry the residue under vacuum to obtain the product.
Transformation	Aromatization of Six-Membered Rings Coordination of a Metal to Carbon and Heteroatom Ligand Substitution

Characterization Data

Ruthenium, carbonylchloro[2-[1-(hydroxy-κ*O*)-2-naphthalenyl]-1-diazenecarbothioamidato-κN^2,κ*S*](triphenylphosphine)-

CAS Method Number 3-478-CAS-9063944

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Retro-Synthetic Planning

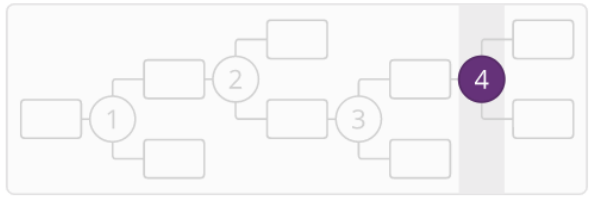
CAS SciFinder^n | Reactions | Enter a query... | Draw | 2

Retrosynthesis Plan Options for 106266-06-2

Powered by ChemPlanner®

Select Synthetic Depth Learn more.

- 1
- 2
- 3
- 4 (selected)



Set Rules Supporting Predicted Reactions Learn more.

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

Set Starting Materials Cost Limit Learn more.

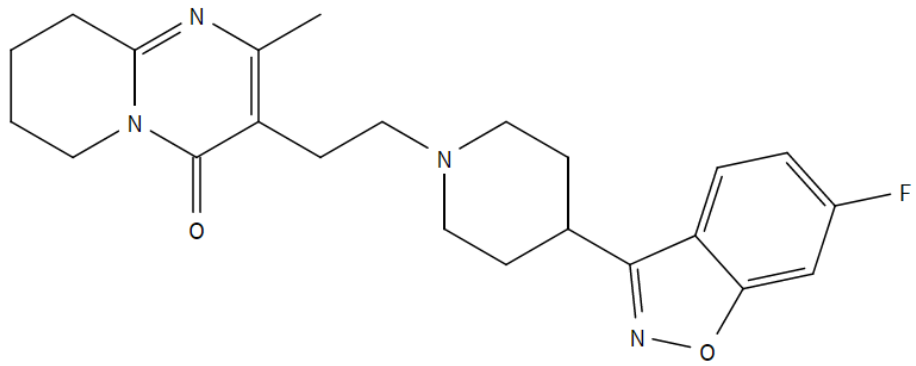
1000 USD/mol

☑ Email me when my plan is complete

Create Retrosynthesis Plan

Break and Protect Bonds Learn more.

Break Bond | Protect Bond | Clear All Bond Selections



Feedback

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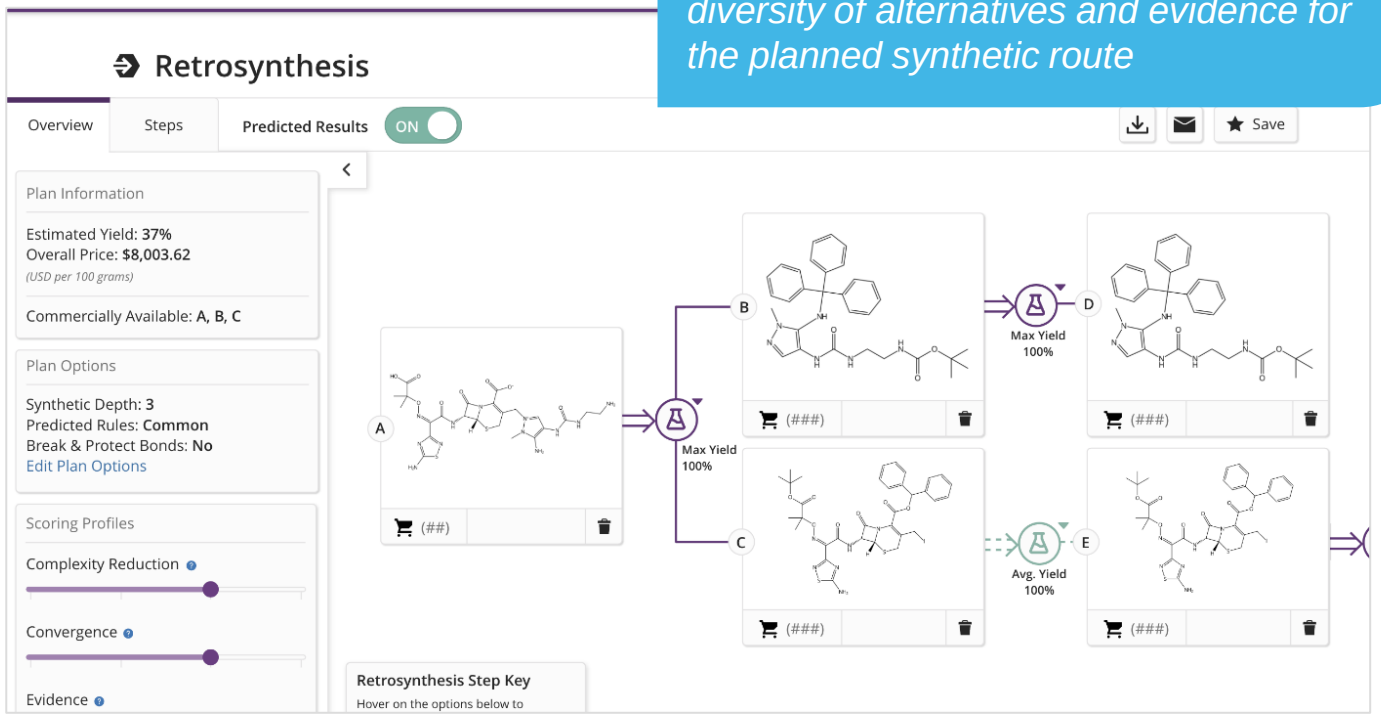
CAS SciFinder Discovery Platform for Synthetic Planning

CAS SciFinder^{n} is a catalyst for unlocking research productivity

- Synthesize new molecular innovations
- Scale up levels of production synthesis
- Identify opportunities for new breakthroughs in methods development

Researchers can clearly understand the diversity of alternatives and evidence for the planned synthetic route



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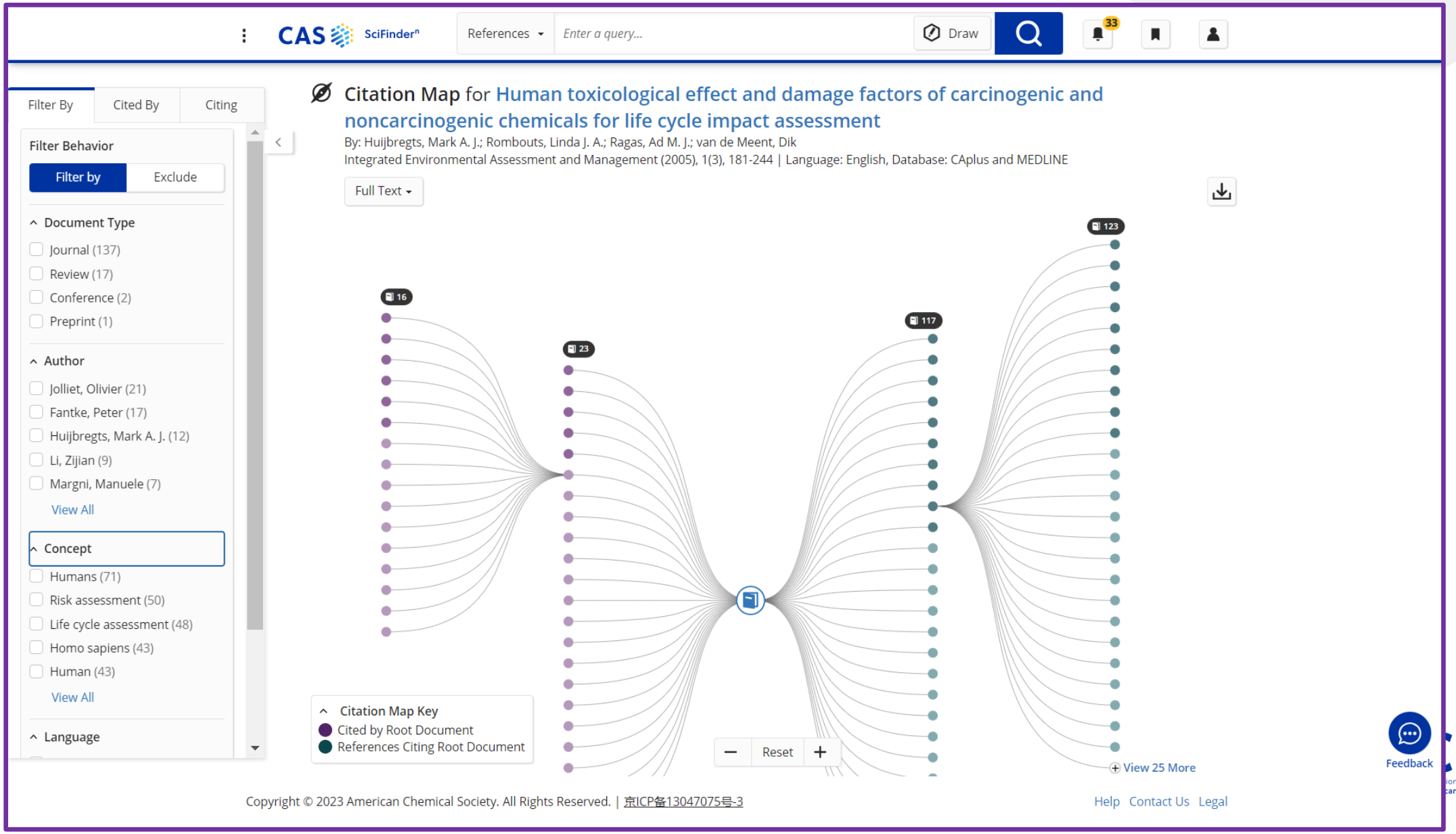
Citation Map



Sequence Search

Why is it important to an Academic Account

Sequences are important for investigators to probe…

- Underlying genomic and proteomic mechanisms.
- Answer questions associated with physiological phenomena, pathological conditions, environmental sciences, agricultural inventions, etiological factors…

CAS provides the world's largest biosequence collection and integrated BLAST/CDR/Motif searching.

- >70M biosequences curated by CAS scientists.
- >700 million additional proteins and nucleotides.

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CAS SciFinder Discovery Platform for Molecular Biologists

Enhancing biological research with biosequence searching in SciFinder^n

UNMATCHED CONTENT

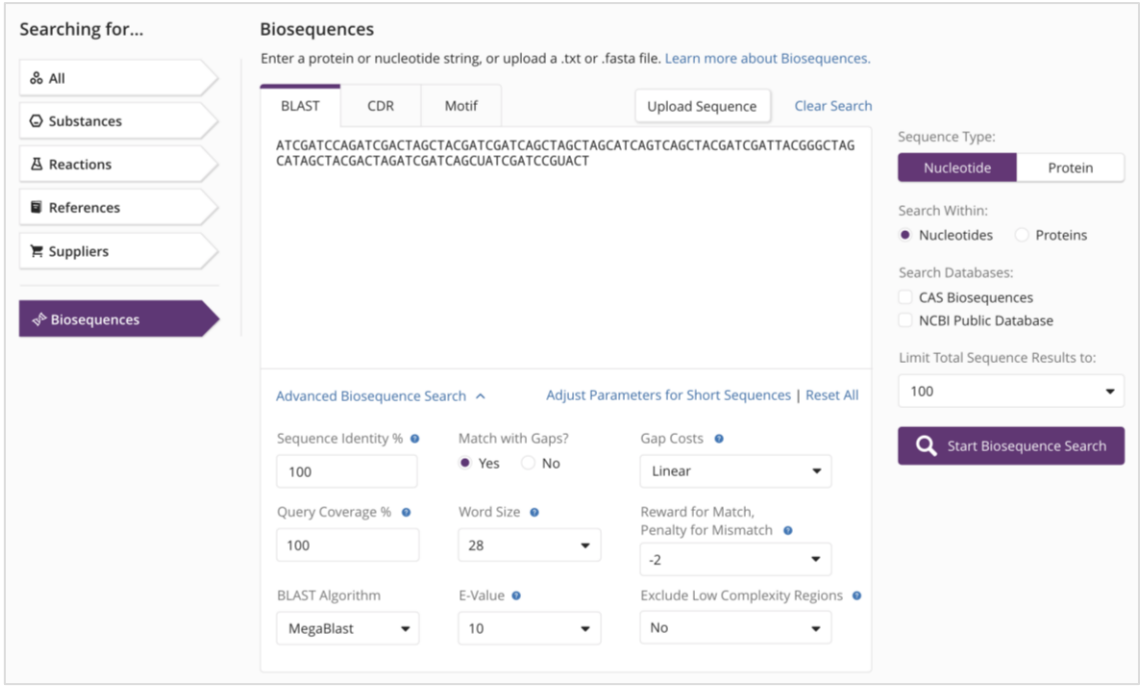
Newly enhanced collection of 700M+ proteins and nucleotides from 60+ patent authorities dating back to 1957

SPECIALIZED TECHNOLOGY

Multiple search options to support your sequence search needs, including BLAST, CDR search for antibody and T-cell receptors, and Motif search

HUMAN EXPERTISE

Human and machine-curated biosequence collection including sequences not found in electronic sequence listings and other databases



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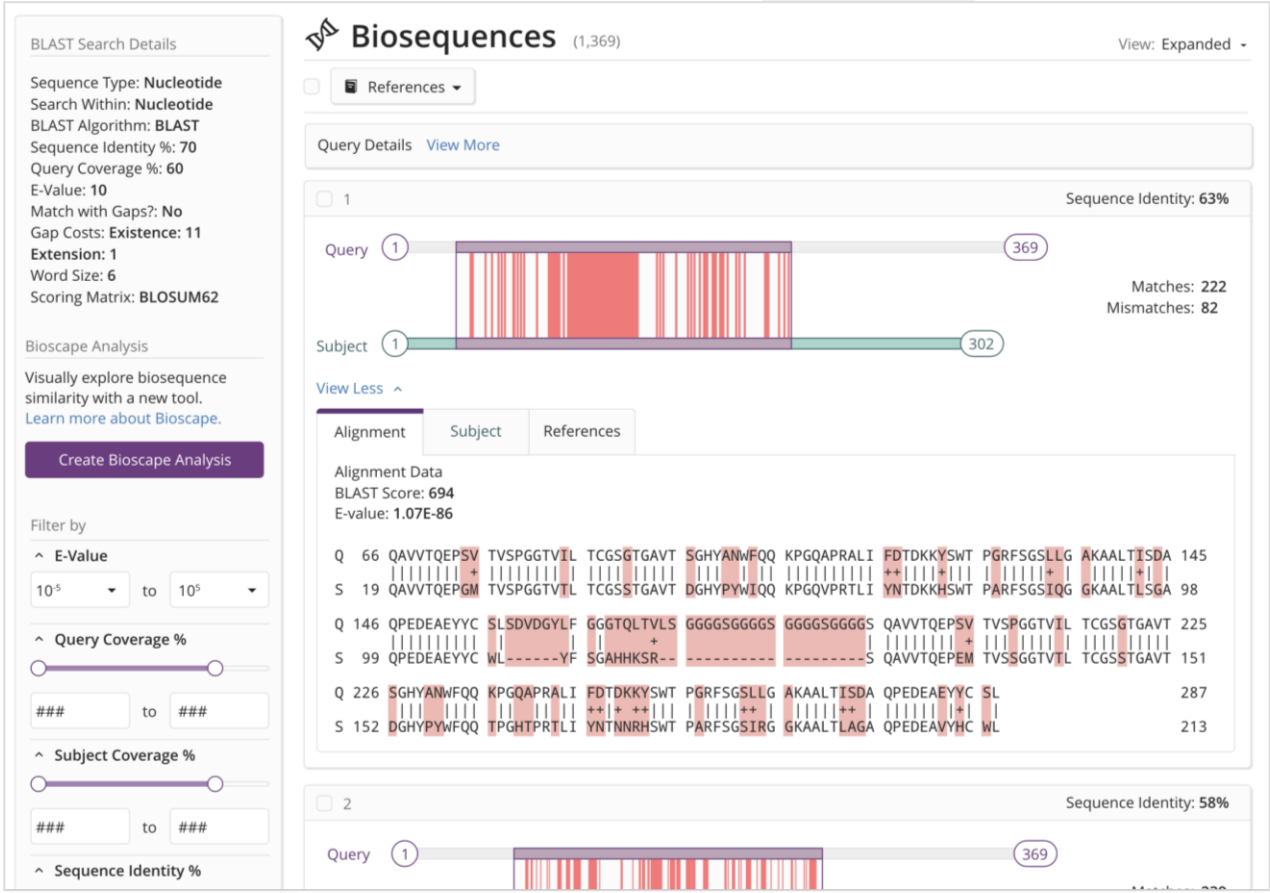
Conduct comprehensive biologics research

CAS SciFinder^{n} powers your biologics R&D to new levels

Uncover connections between biosequences and patent and non-patent* literature that you can't see anywhere else.

Tap into one of the largest collections of scientific journal records, including PubMed's biomedical and life science articles and abstracts.



*Coming soon

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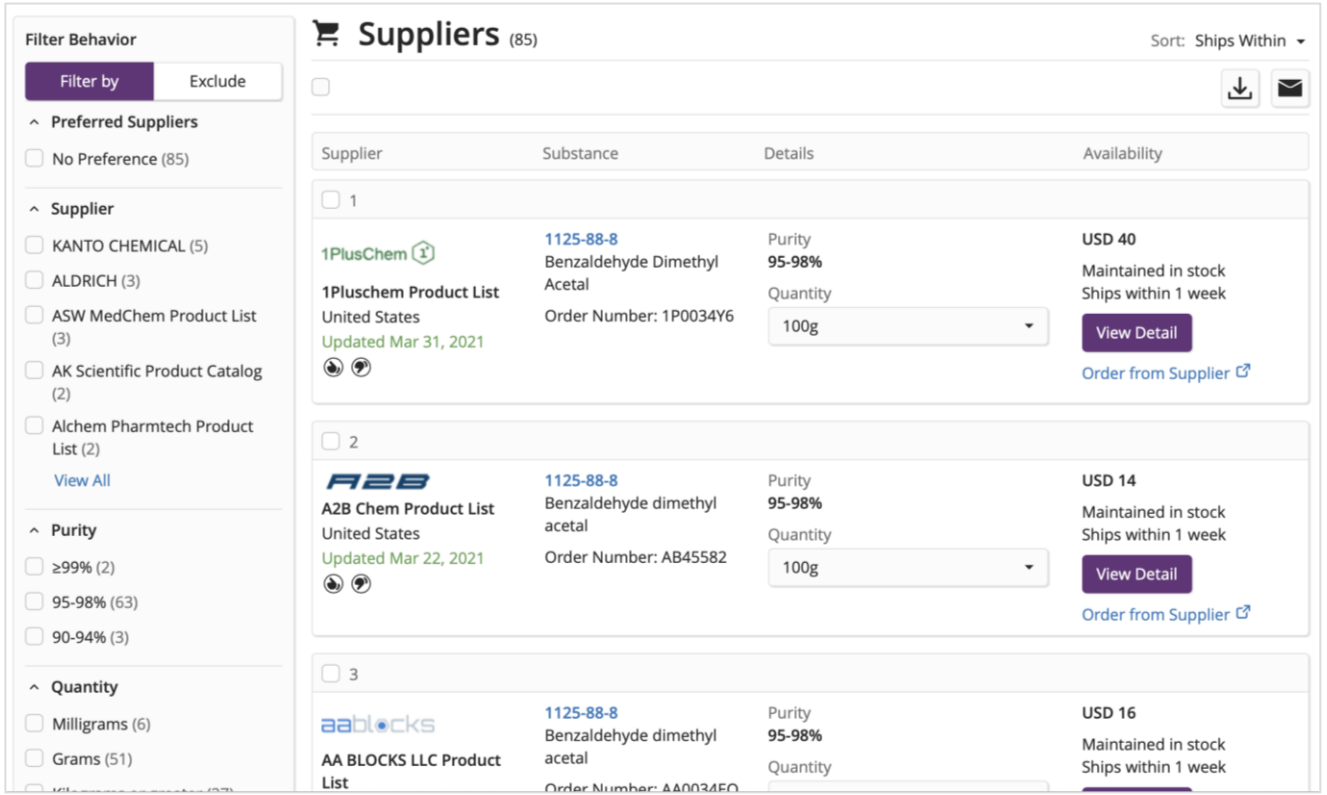
Find commercially available chemicals

CAS SciFinder^{n} contains the market-leading index of chemicals from worldwide suppliers

Learn which suppliers have your needed materials with information on available quantities and prices for millions of chemical products from hundreds of vendors.



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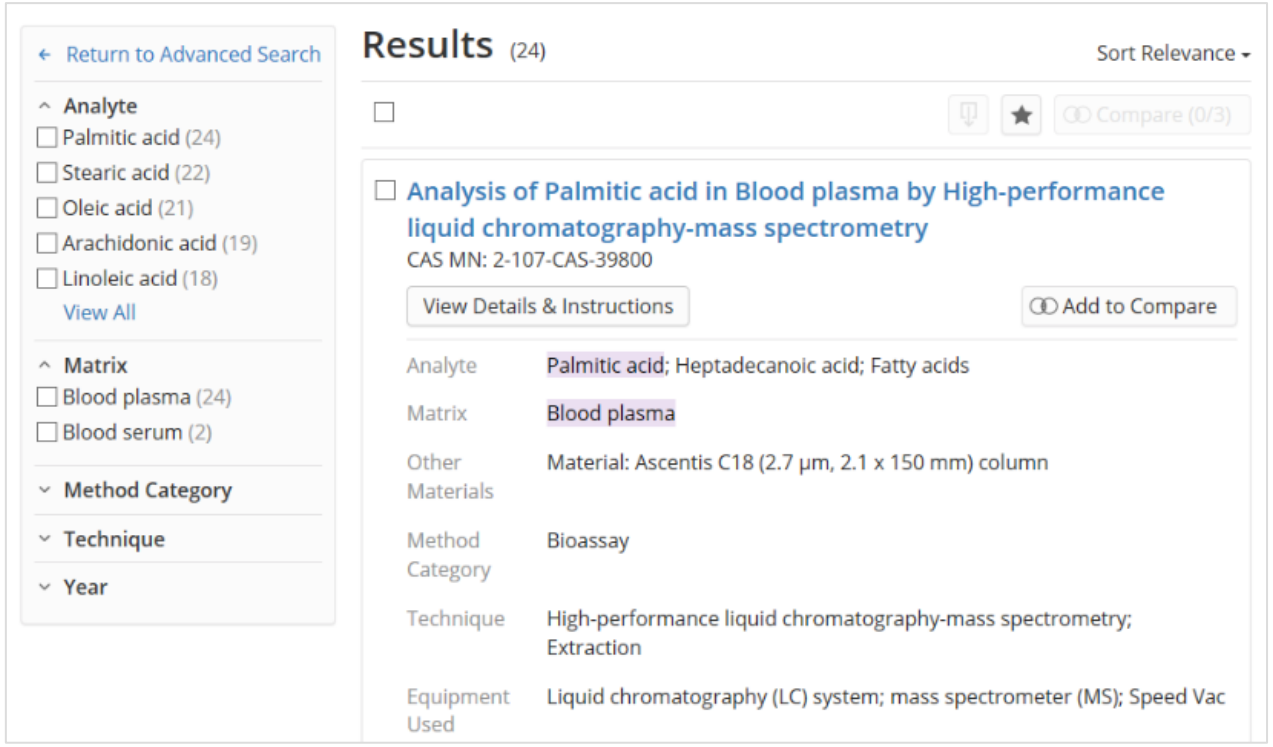
CAS SciFinder Discovery Platform for Analytical Chemists

CAS Analytical Methods is a single source for in-depth scientific methods

- Save time with easy access to method details from millions of disclosed procedures
- Compare analytical methods side-by-side to understand key similarities and differences
- Organize experimental details in an easy-to-read format
- Get materials, instrumentation, and conditions



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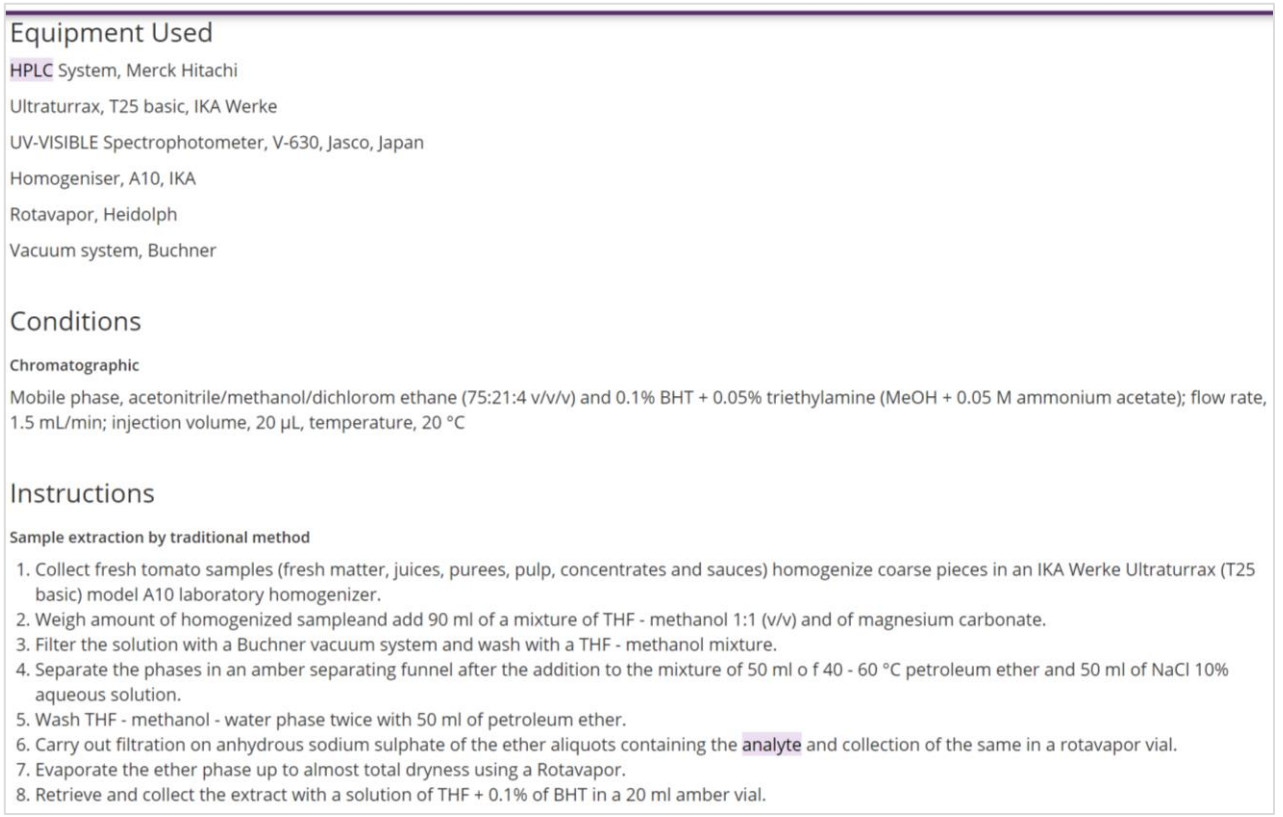
Test and validate innovations

Search and filter hundreds of thousands of analytical methods extracted from published references to find the best option for your work.



Equipment Used

HPLC System, Merck Hitachi

Ultraturrax, T25 basic, IKA Werke

UV-VISIBLE Spectrophotometer, V-630, Jasco, Japan

Homogeniser, A10, IKA

Rotavapor, Heidolph

Vacuum system, Buchner

Conditions

Chromatographic

Mobile phase, acetonitrile/methanol/dichlorom ethane (75:21:4 v/v/v) and 0.1% BHT + 0.05% triethylamine (MeOH + 0.05 M ammonium acetate); flow rate, 1.5 mL/min; injection volume, 20 µL, temperature, 20 °C

Instructions

Sample extraction by traditional method

1. Collect fresh tomato samples (fresh matter, juices, purees, pulp, concentrates and sauces) homogenize coarse pieces in an IKA Werke Ultraturrax (T25 basic) model A10 laboratory homogenizer.
2. Weigh amount of homogenized sampleand add 90 ml of a mixture of THF - methanol 1:1 (v/v) and of magnesium carbonate.
3. Filter the solution with a Buchner vacuum system and wash with a THF - methanol mixture.
4. Separate the phases in an amber separating funnel after the addition to the mixture of 50 ml o f 40 - 60 °C petroleum ether and 50 ml of NaCl 10% aqueous solution.
5. Wash THF - methanol - water phase twice with 50 ml of petroleum ether.
6. Carry out filtration on anhydrous sodium sulphate of the ether aliquots containing the analyte and collection of the same in a rotavapor vial.
7. Evaporate the ether phase up to almost total dryness using a Rotavapor.
8. Retrieve and collect the extract with a solution of THF + 0.1% of BHT in a 20 ml amber vial.

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CAS Analytical Methods

Why is it important to an Academic Account?

Collection of diverse methods indexed to help solve chemical problems or teach research techniques.

Procedures from +5000 journals & peer reviewed publications.

- Including top journals like: Food Chemistry, Analytical Chemistry, and Analyst.

Coverage spans from wastewater analysis to active pharmaceutical ingredient analysis.

- Step-by-step methods curated by CAS and formatted to take into the lab.
- Easily locate relevant methods.
  - Advanced search, faceting, and compare options.

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CAS SciFinder Discovery Platform for Formulation Scientists

Develop safe and effective products with CAS Formulus®

FASTER ITERATION

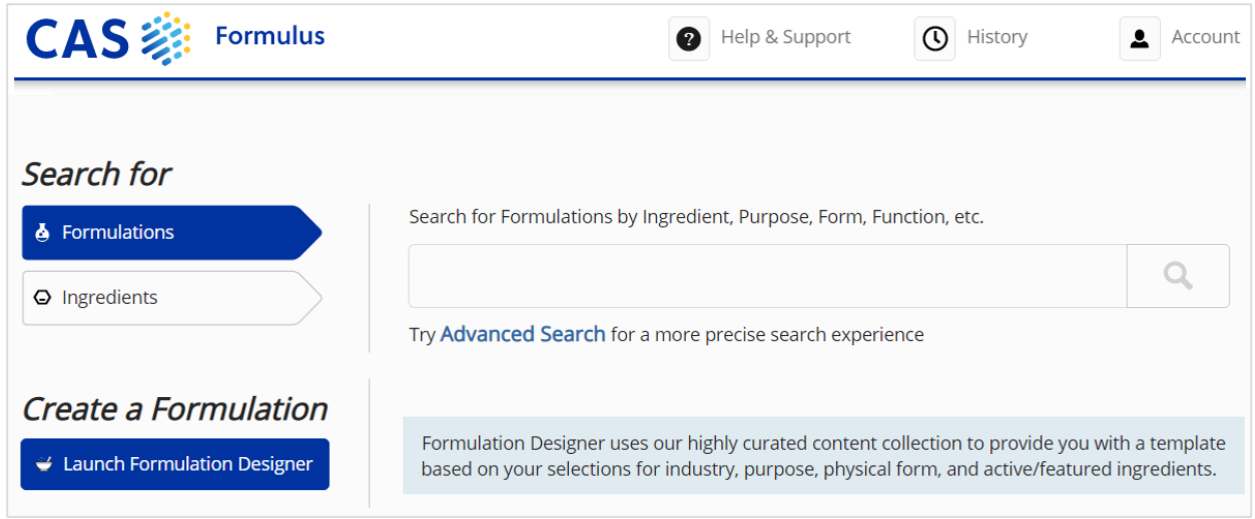
Understand a formulation's effectiveness with quick access to the best information for active ingredients and excipients

MORE EFFICIENCY

Get insights beyond literature and interact with formulations data curated from patents, journals, and product inserts more effectively

COMPREHENSIVENESS

Evaluate ingredients, find alternative suppliers, and explore regulatory requirements in one easy interface



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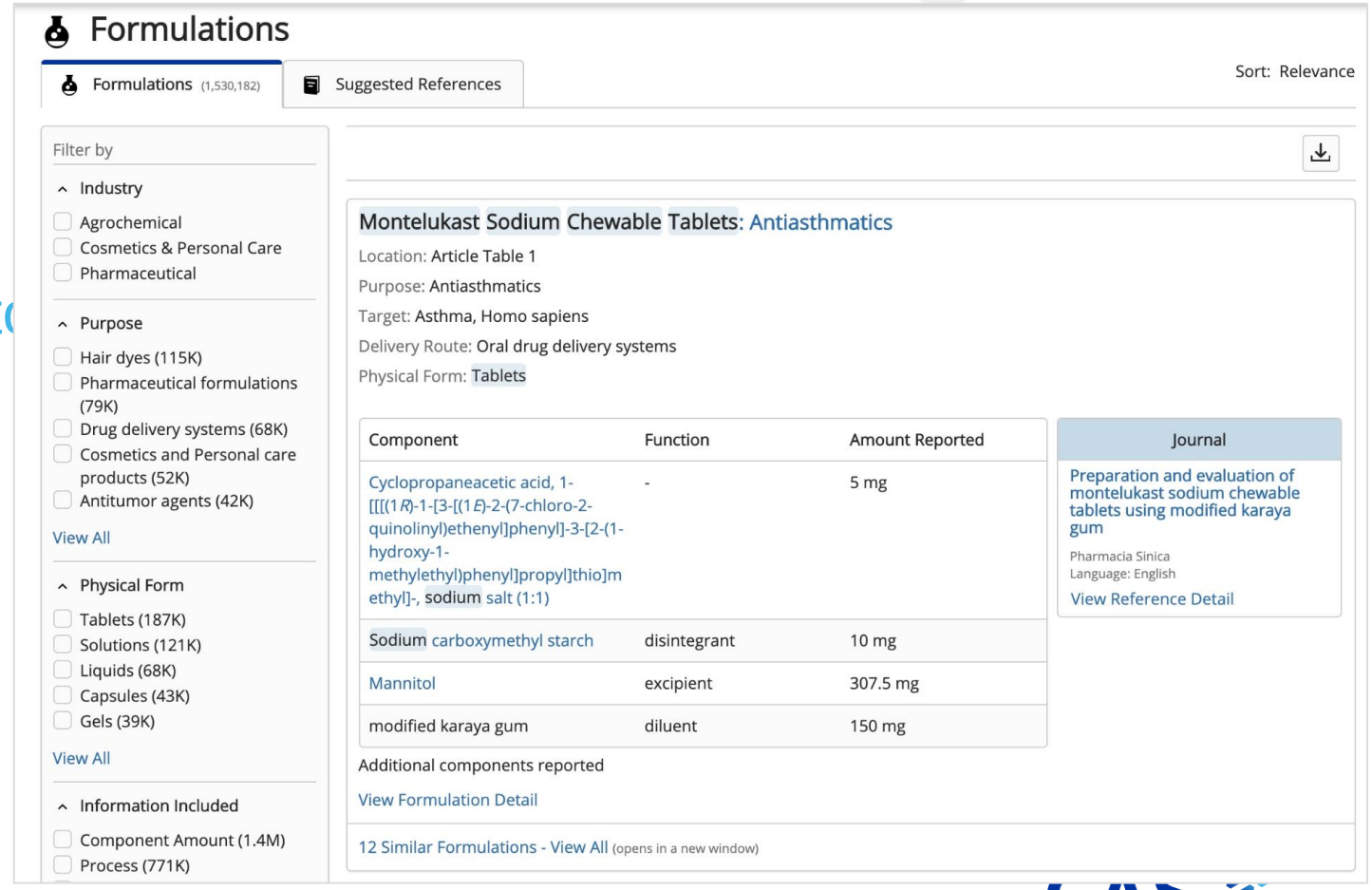
Develop differentiating formulations and manufacture-to-scale

Evaluate a formulation's effectiveness with quick access to the best information for active ingredients and excipients.



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Accelerate breakthroughs and get discoveries to market faster

Titer Liu
Senior Account Consultant
Tliu2@acs-i.org

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CAS SciFinder^{n}

speeds your science

INNOVATION

84%

of researchers agree CAS SciFinder^{n} allows them **to be more innovative** than other research solutions.*

SPEED

77%

of researchers agree CAS SciFinder^{n} allows them **to work more quickly** than other research solutions.*

CONFIDENCE

84%

of researchers agree CAS SciFinder^{n} allows them **to work more confidently** compared to other research solutions.*

*CAS SciFinder^{n} Productivity Survey 2020.

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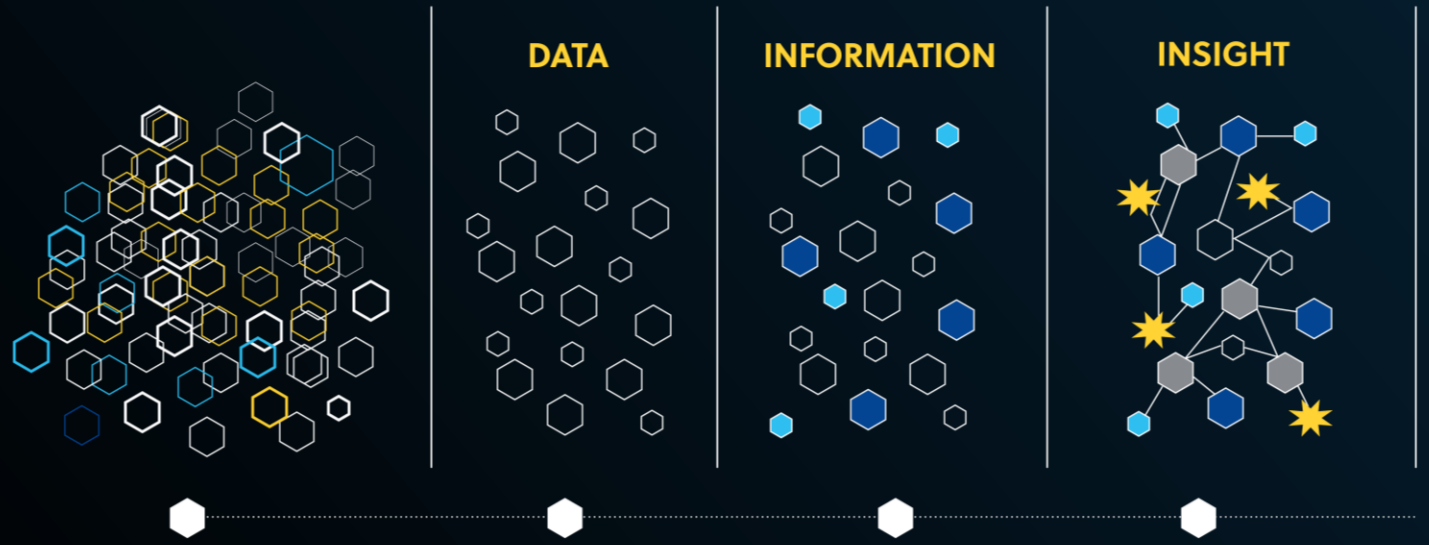
CAS scientists curate, connect, and analyze scientific knowledge



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Our unique solutions and capabilities

streamline success

DISCOVERY

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need

INTELLECTUAL PROPERTY

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets

CUSTOM SOLUTIONS

CAS Custom Services℠

Maximize the value of information assets and fuel digitalization success with customized data, analytics and insights

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