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CAS SciFinder 2026

劉全哲 博士　Customer Success Manager

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You can think of a database as an electronic filing system.

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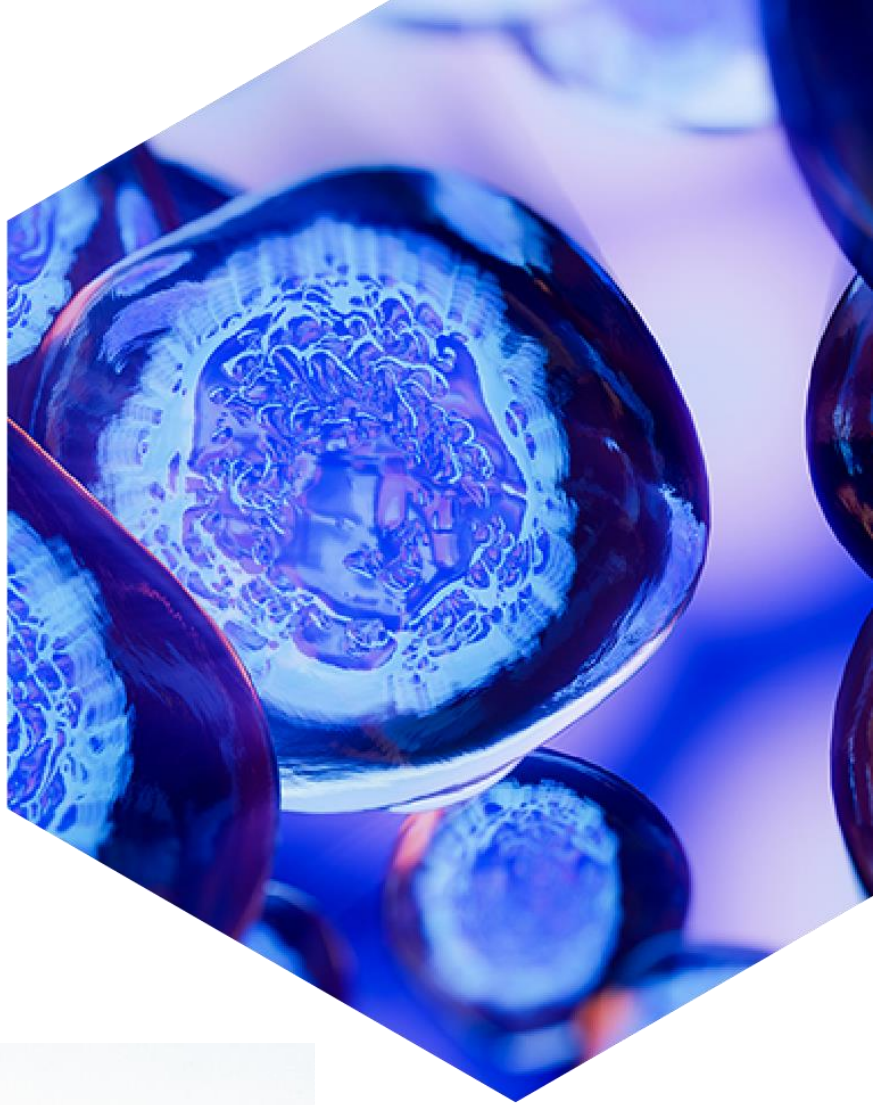
What do we need database?

- Data is easier to manager
  - Too much data in one reference
  - Too many references
  - Too many language for reference
- Databases can better enforce data quality
- Leads to better data integration
- Databases are used to store, organize and retrieve data, quickly!!

About CAS



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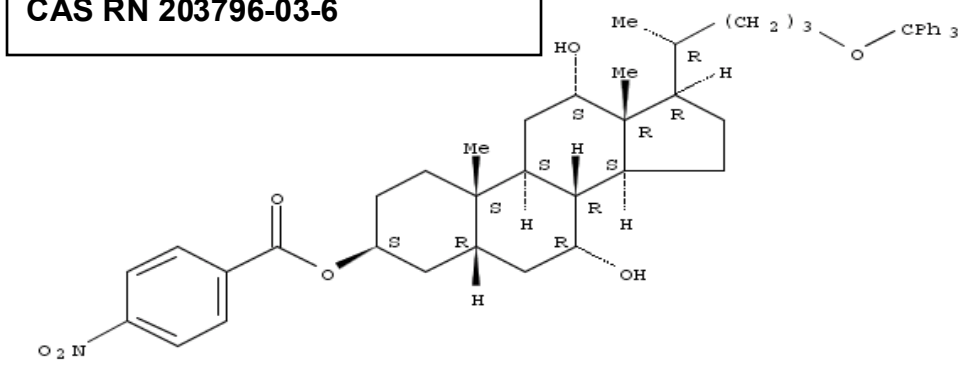
CAS scientists find the chemistry, and save you time!

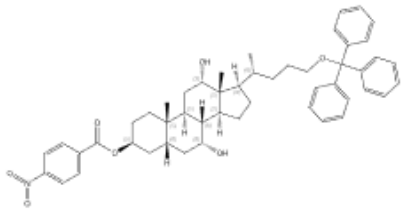
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 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

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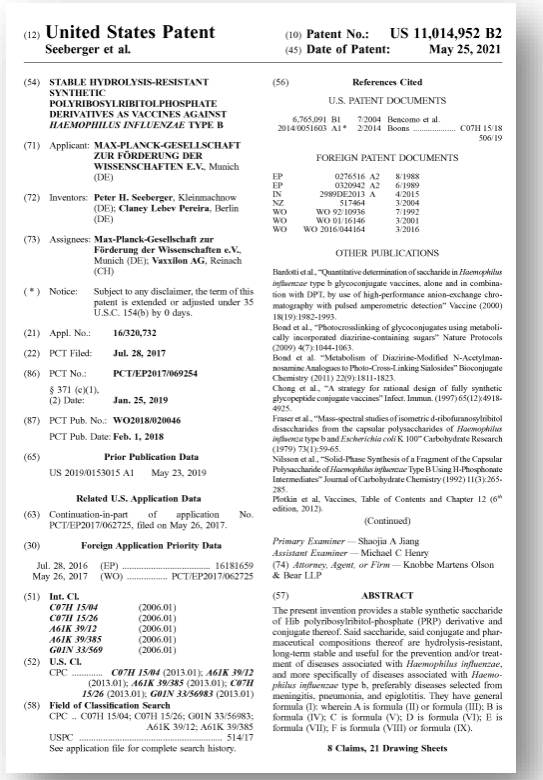
CAS curation extracts knowledge

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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(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

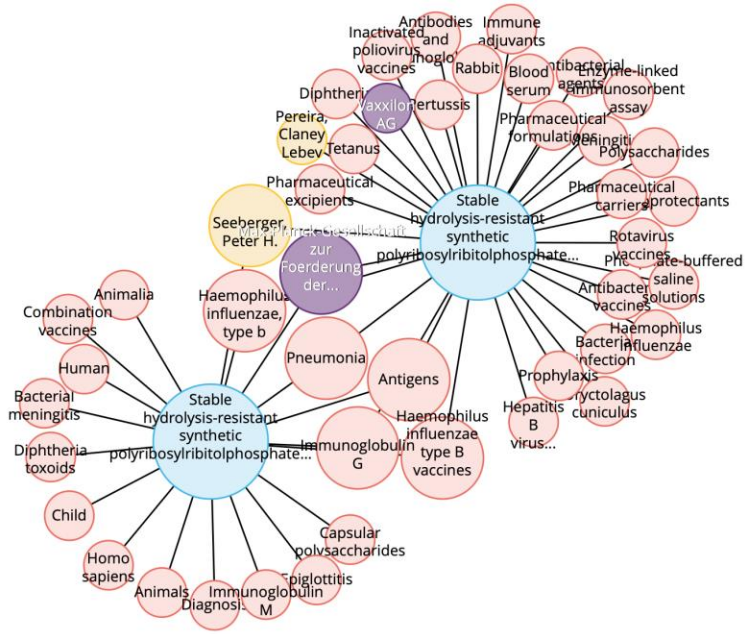
136 substances

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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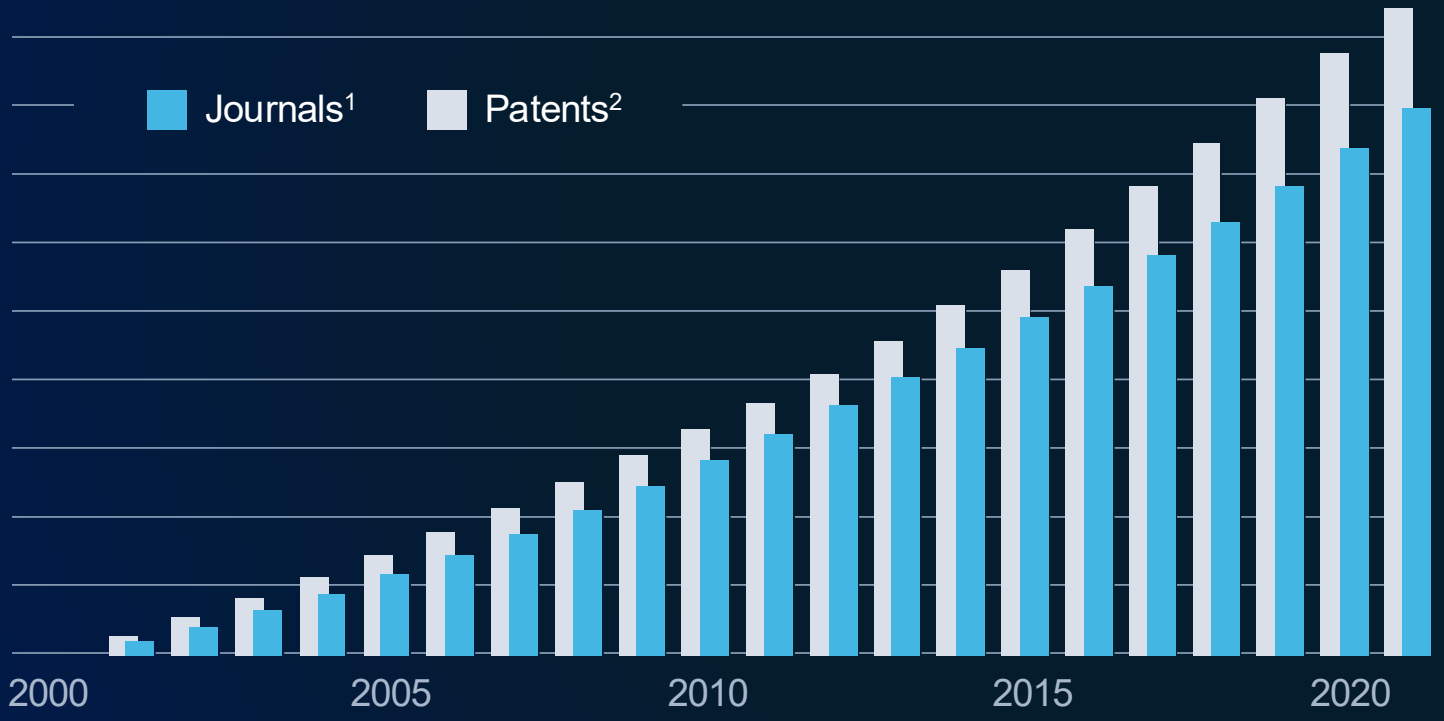
The volume and complexity of scientific information is escalating exponentially

Growth of published science last 20 years



HIGH VOLUME
Limits holistic perspective

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Hinders effective analysis

POOR COMPATIBILITY
Reduces digitalization ROI

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2. WIPO statistics database. Last updated: November 2023

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- Data confirmation
- Published research analysis

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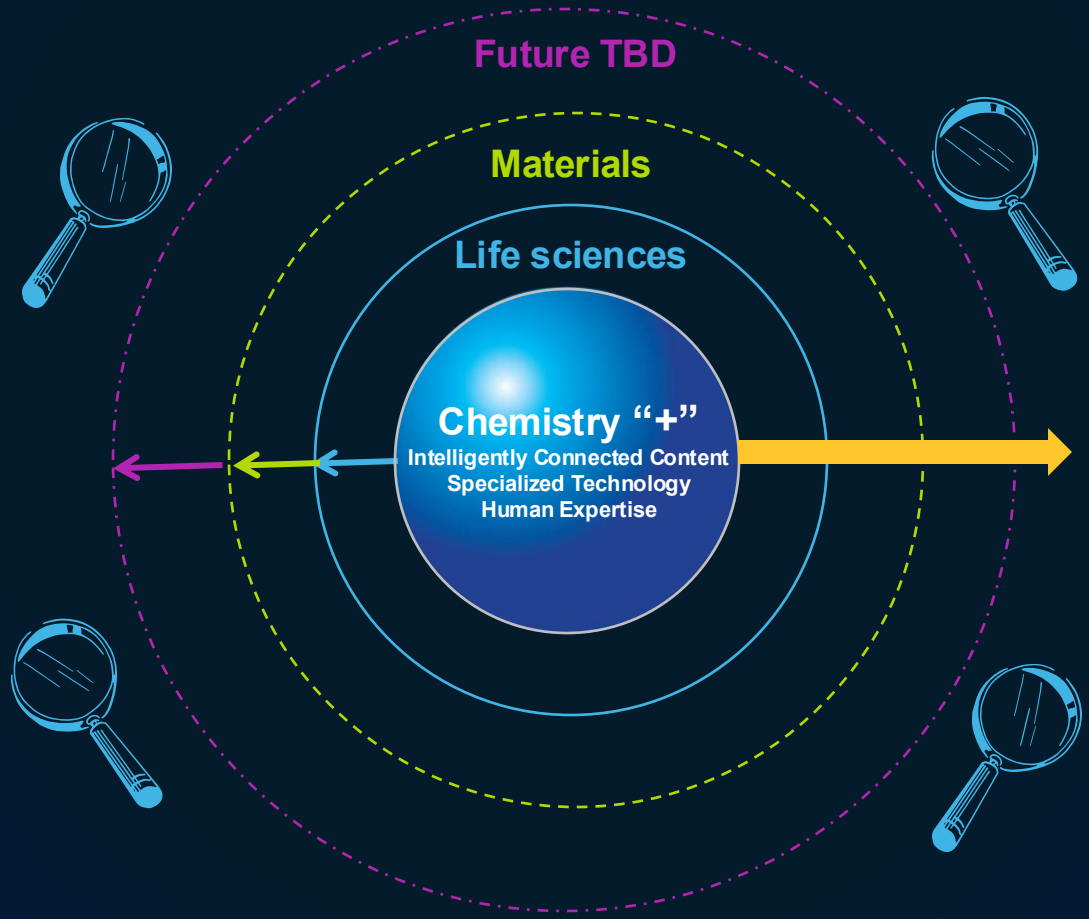

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Materials science solution (future)

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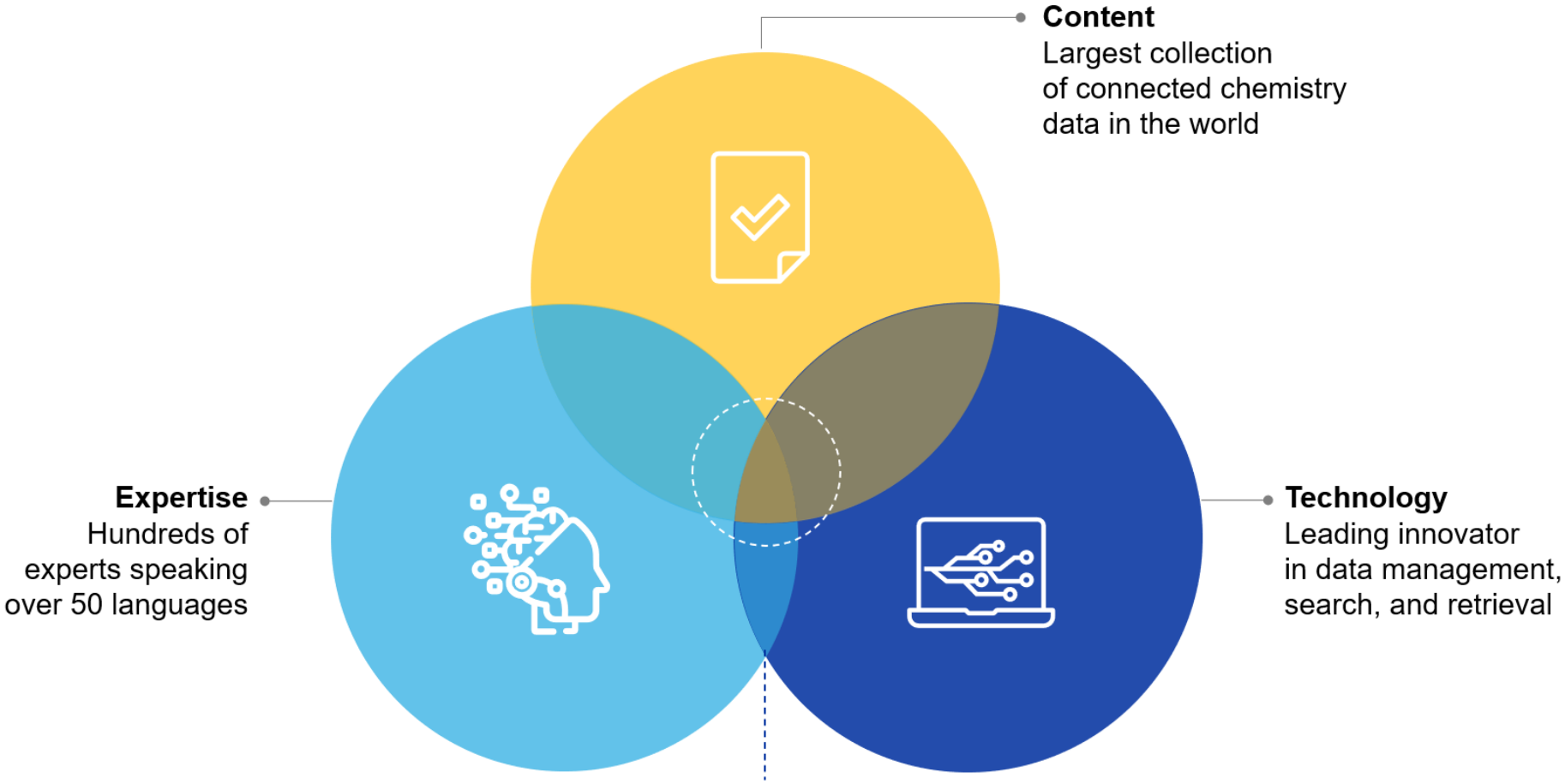

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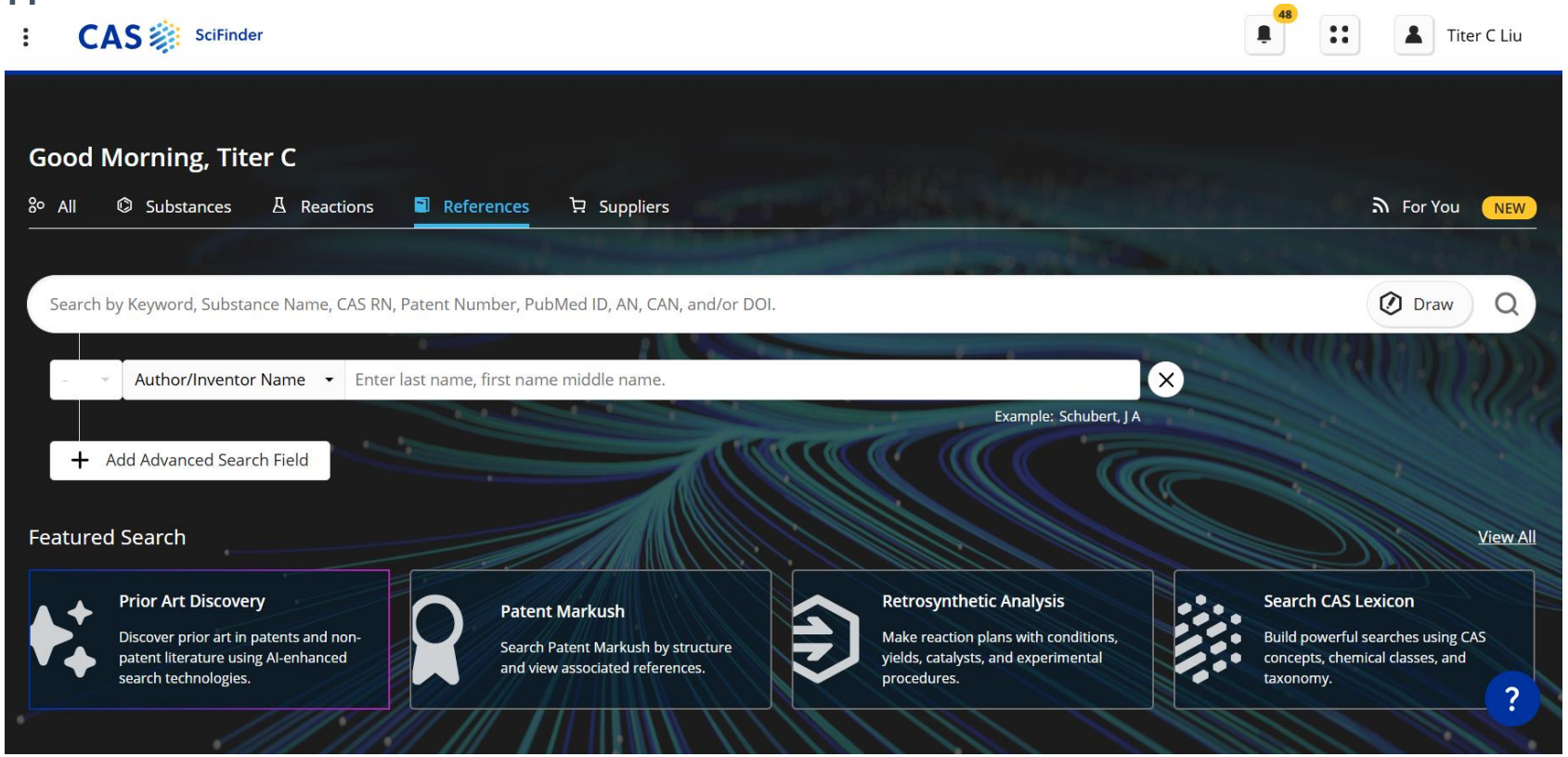
CAS SciFinder Discovery platform

*SciFinder

Top 5 key searching function

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



*CAS Formulation

*CAS Analytical Methods

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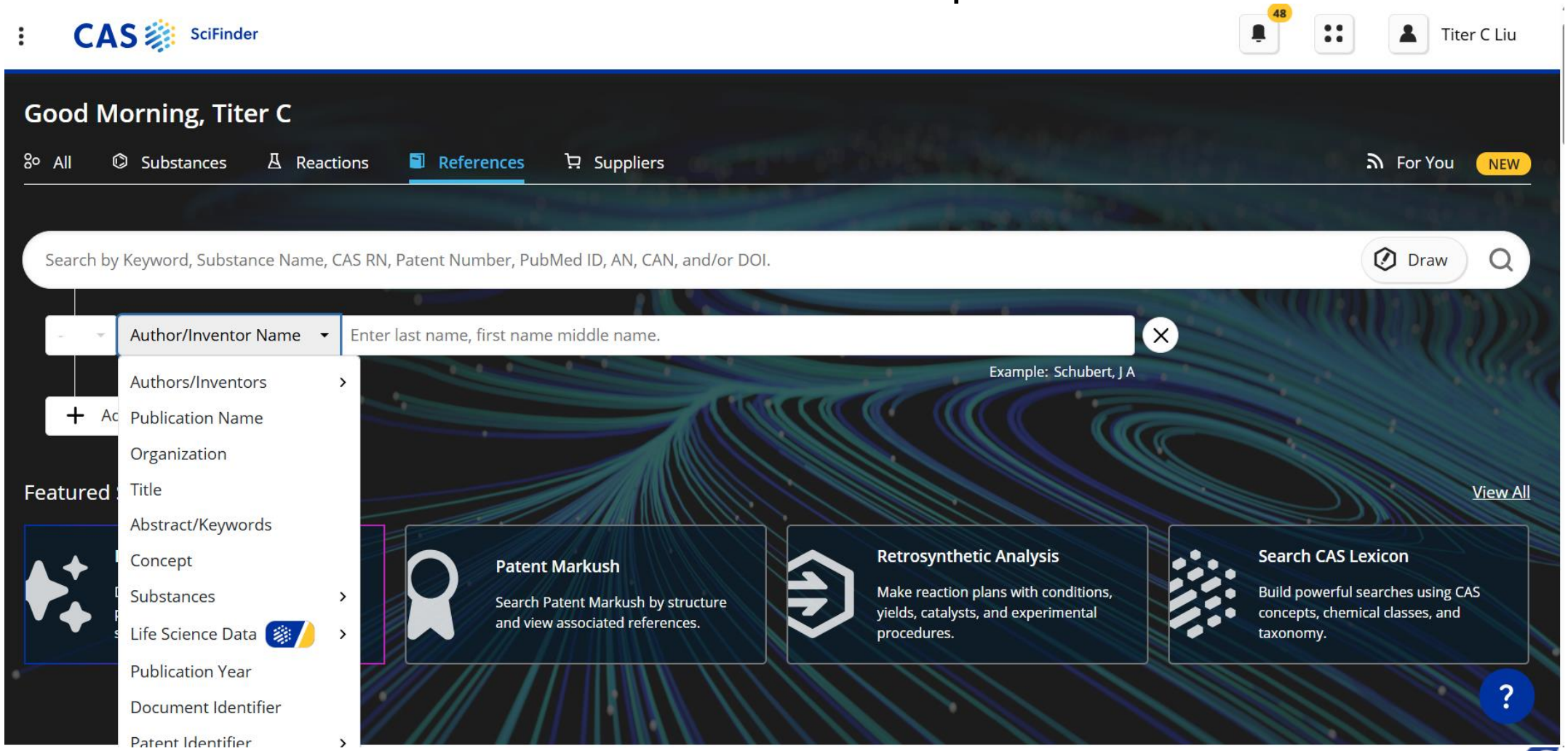
Reference searching

CAS SciFinder halves the time needed to perform literature reviews*



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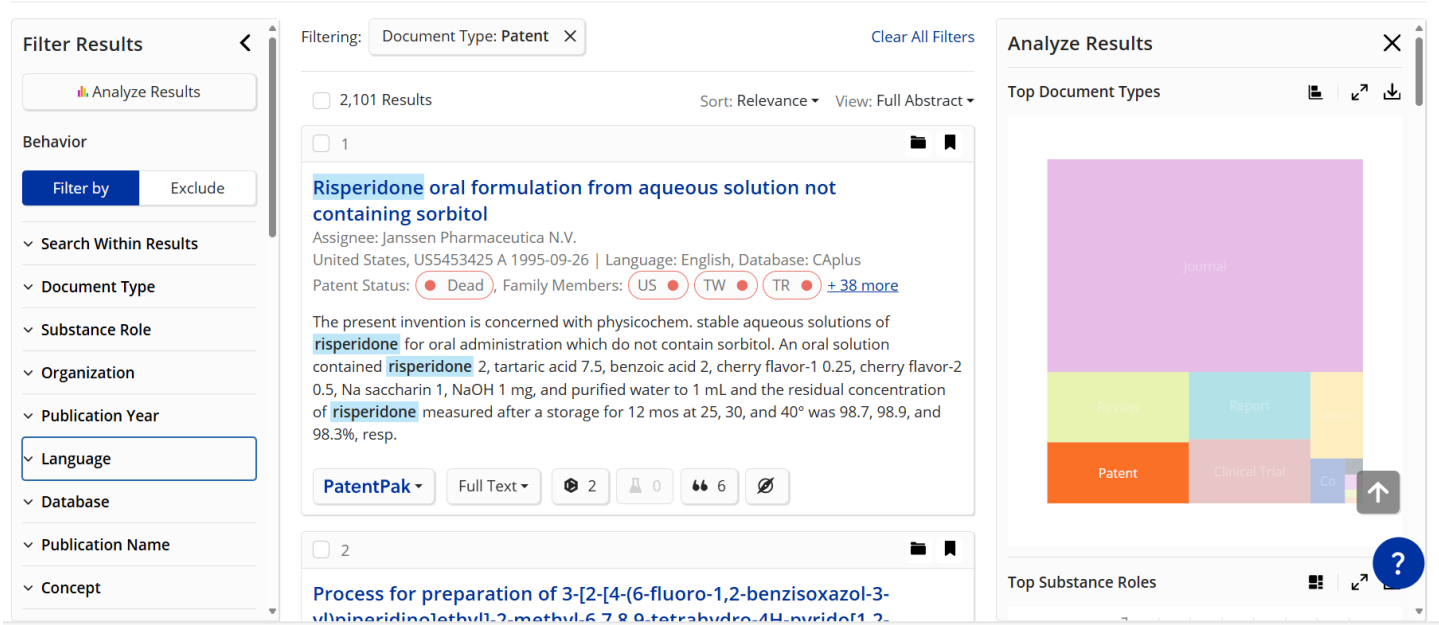

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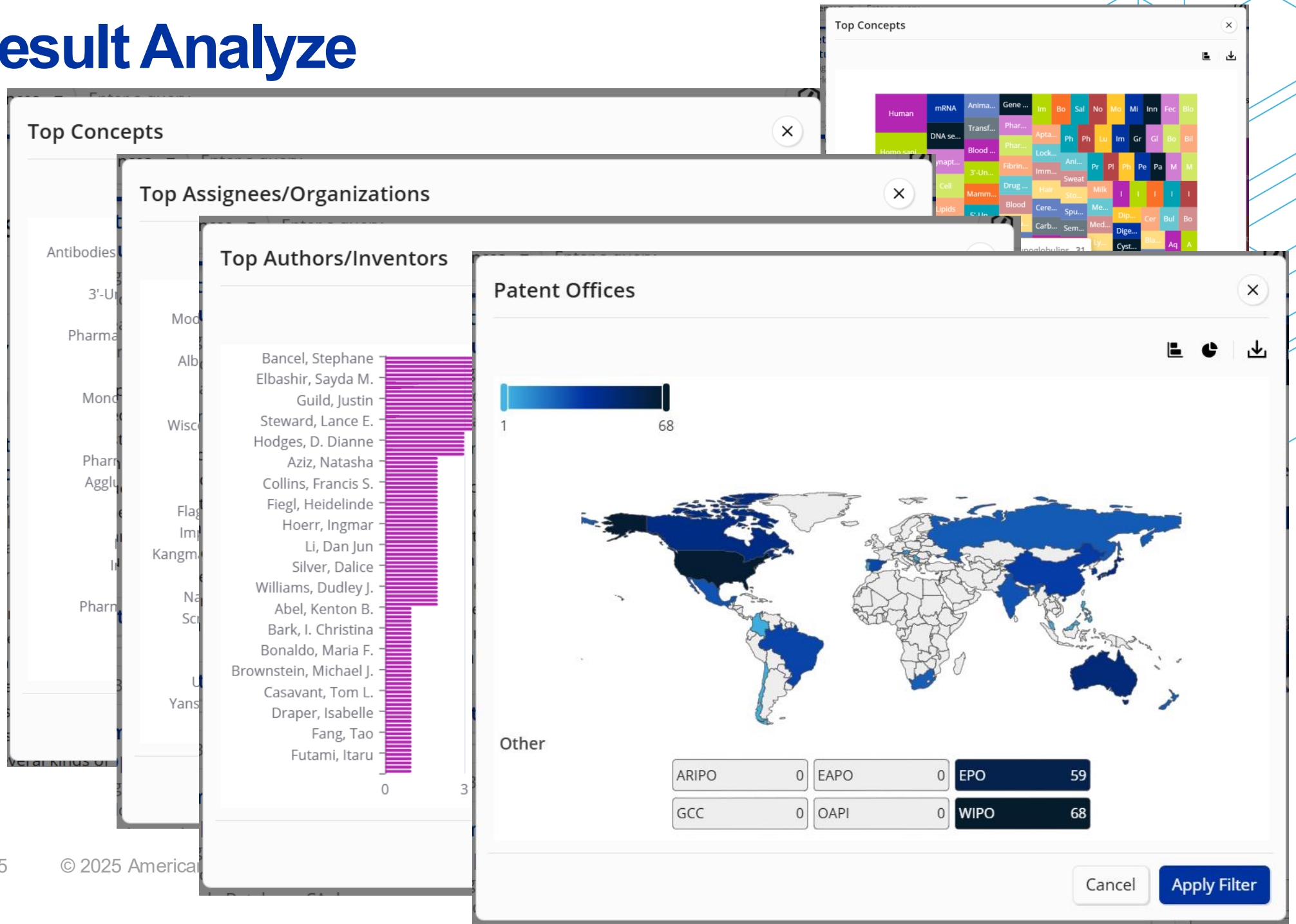
Result Analyze



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Process for preparation of risperidone

3 | 1 | 1 | Citation Map

In this Patent

Inventors: Zhang, Guiling; Zhu, Yidong; Fan, Chuanwen; Zhang, Minghui; Wang, Jingyi

Patent Family

Patent

WO200

CN1013

CN1013

GB2464

GB2464

US2010

Priority

Priority

CN2007

WO200

Claims

Claims tex

1 What

A risp

Chara

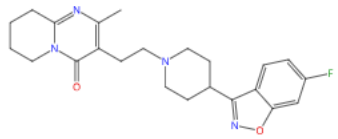
Classifications

Patent	Classification	Codes
WO2009012721 A1	IPCI	C07D 471/04
CN101353347 A	IPCI	C07D 471/04
	CPCI	C07D 471/04
CN101353347 B	IPCI	C07D 471/04
	CPCI	C07D 471/04
GB2464854 A	IPCI	C07D 471/04
	CPCI	C07D 471/04; C07D 471/04
GB2464854 B	IPCI	C07D 471/04
	CPCI	C07D 471/04; C07D 471/04
US20100130740 A1	IPCI	C07D 471/04

Substances

3

106266-06-2

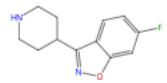


$C_{23}H_{27}FN_4O_2$

Risperidone

Role: Industrial Manufacture, Synthetic Preparation, Preparation

84163-13-3



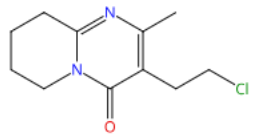
• HCl

$C_{12}H_{13}FN_2O.ClH$

1,2-Benzisoxazole, 6-fluoro-3-(4-piperidinyl)-, hydrochloride (1:1)

Role: Reactant, Reactant or Reagent

63234-80-0



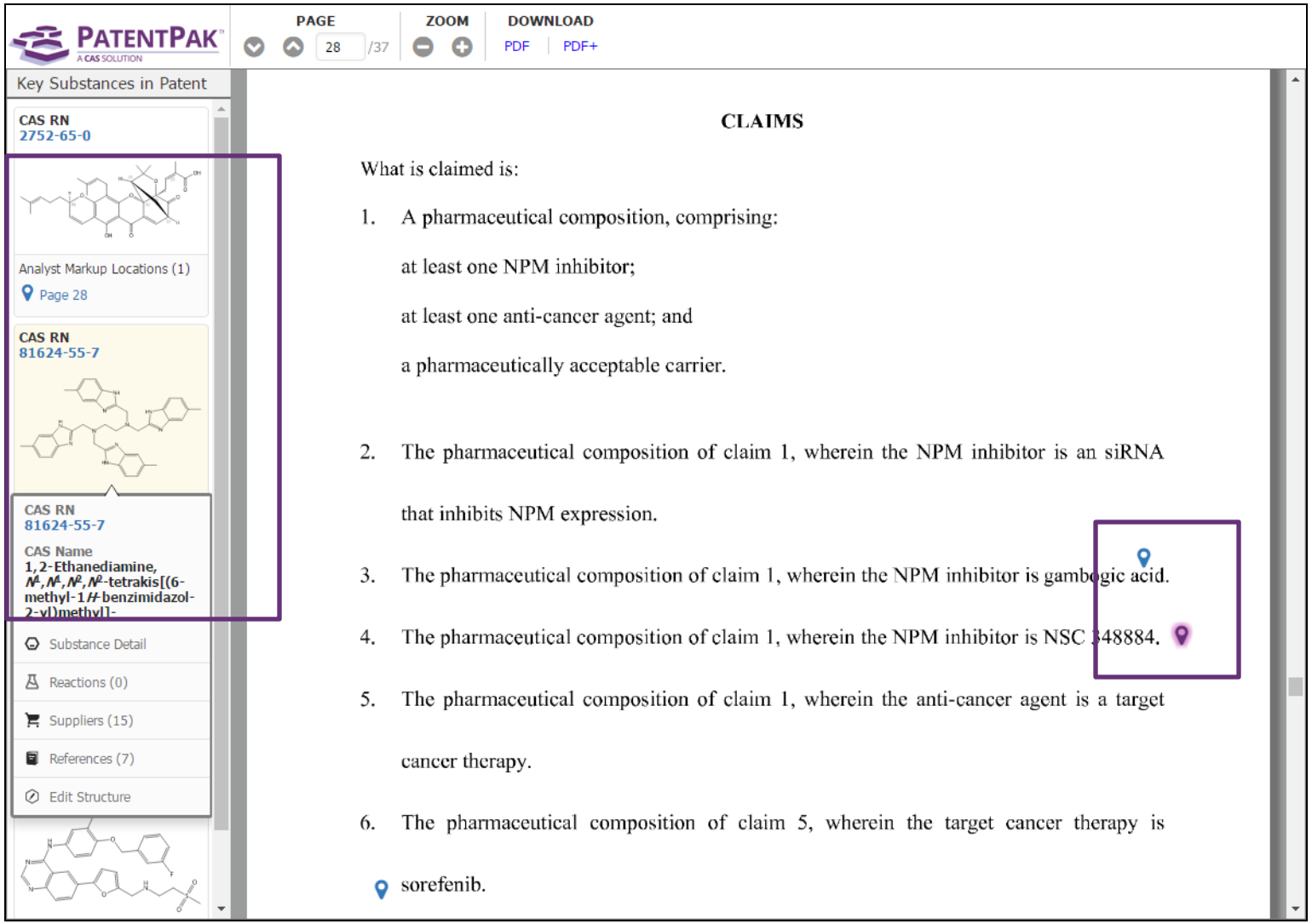
$C_{11}H_{15}ClN_2O$

4*H*-Pyrido[1,2-*a*]pyrimidin-4-one, 3-(2-chloroethyl)-6,7,8,9-tetrahydro-2-methyl-

Role: Reactant, Reactant or Reagent

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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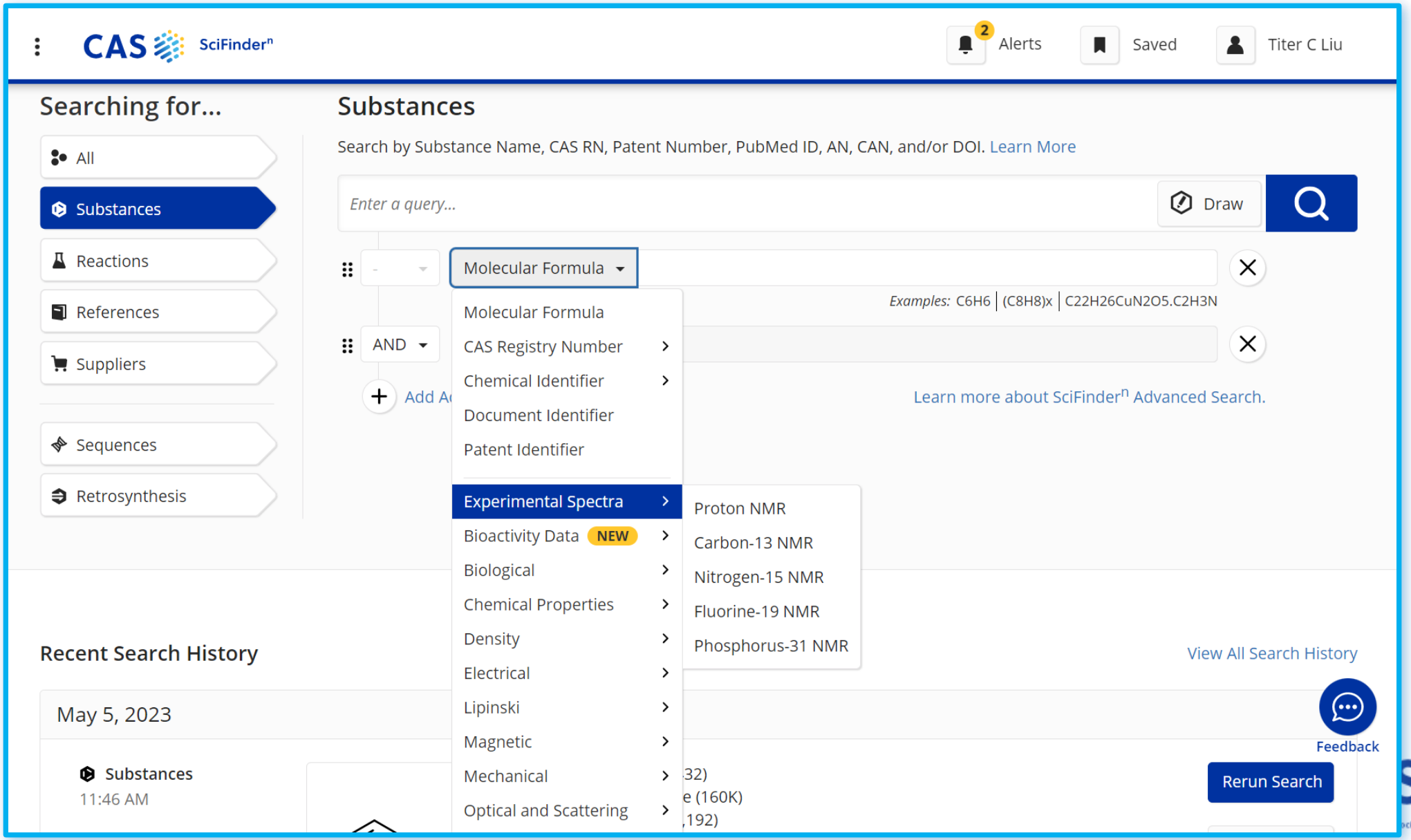
Substance searching



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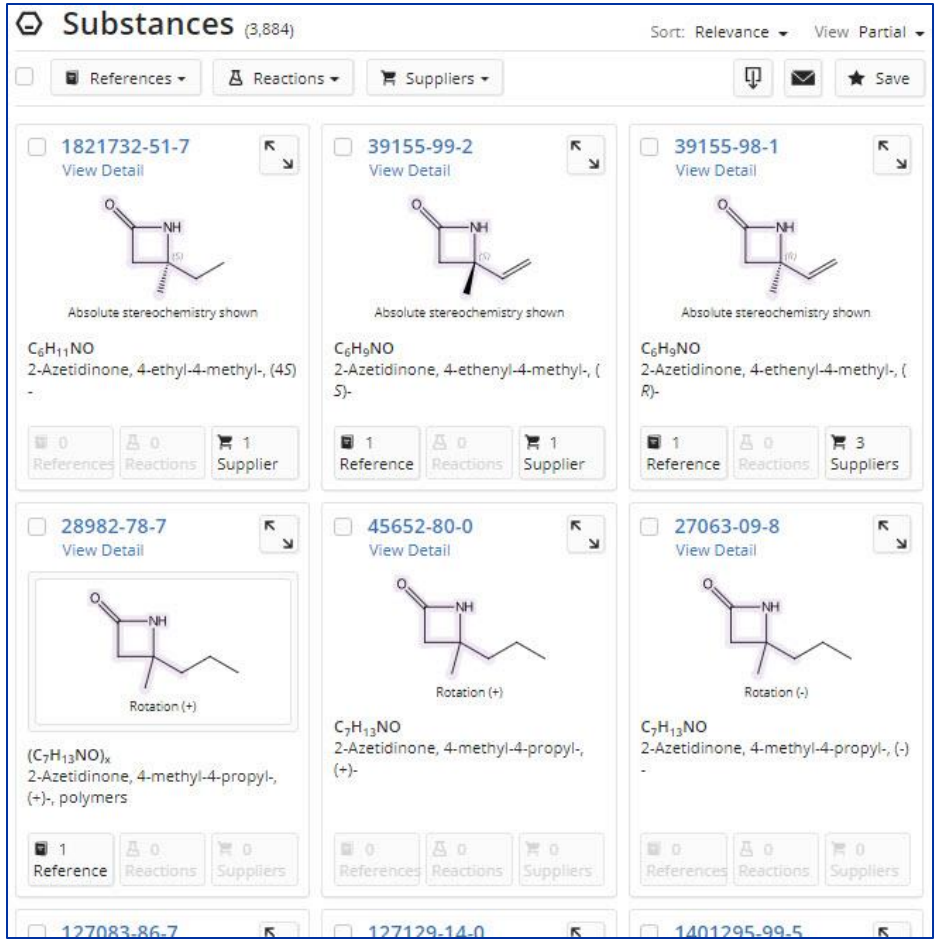

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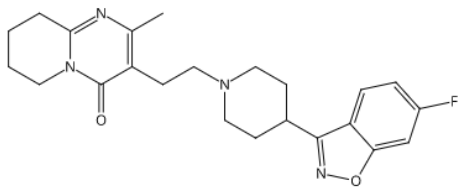
Substances information

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) (2000), 1280 pages, CAplus

Structure Activity Relationships — CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data — CAS LIFE SCIENCES

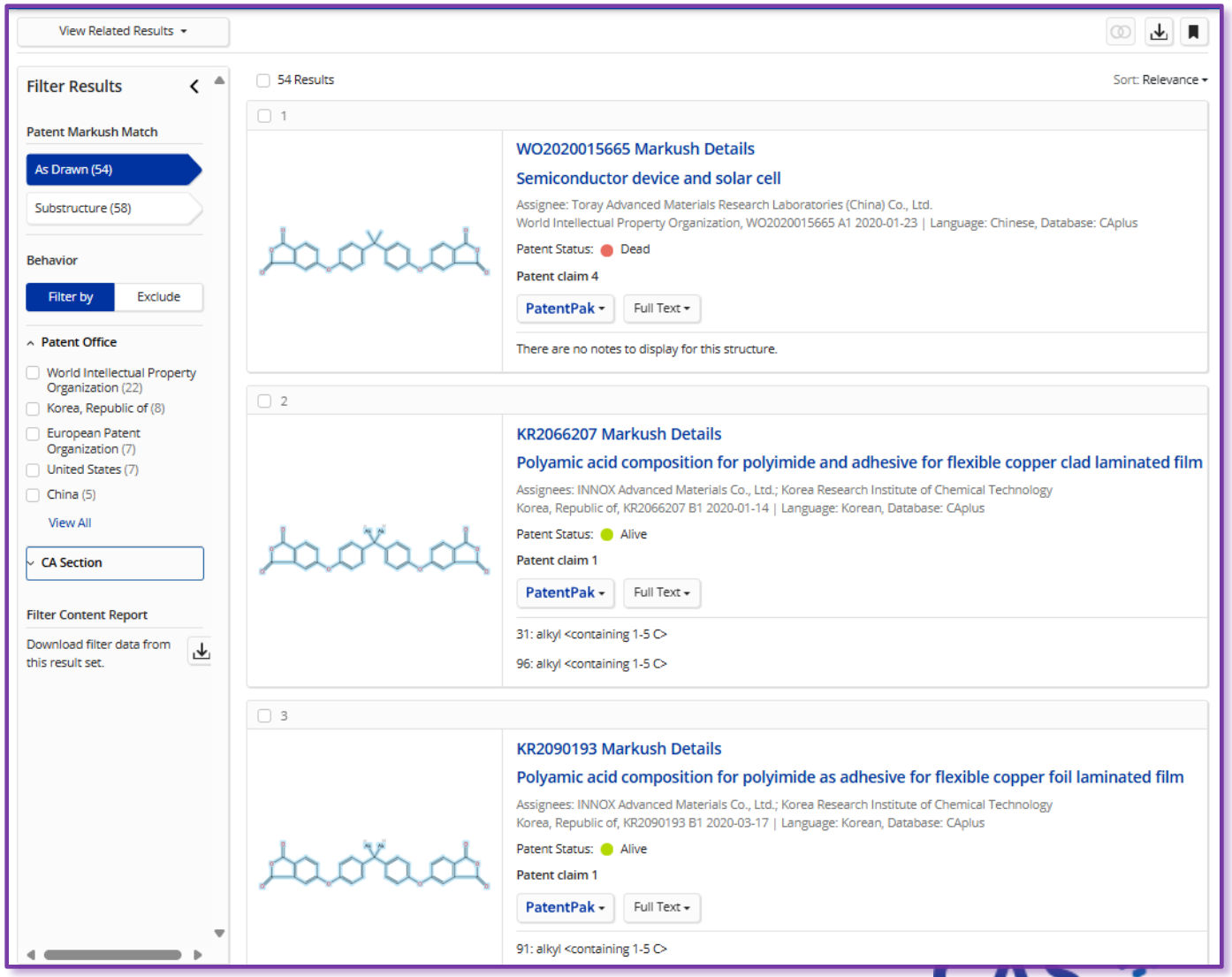
Toxicity — CAS LIFE SCIENCES

Target | Function | Parameter | Disease | Organism

Target	Function	Parameter	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

CAS SciFinder 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.



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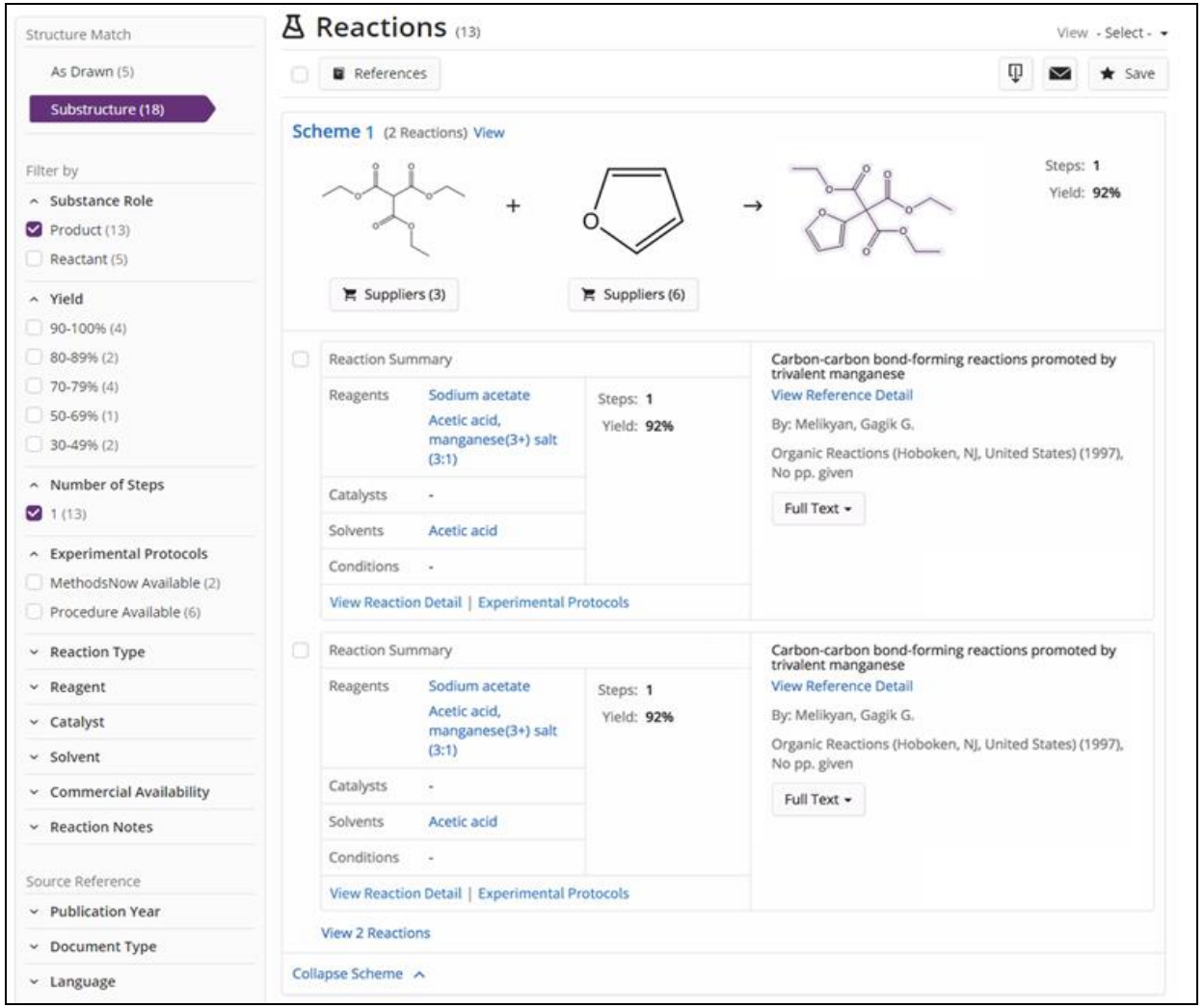
Reaction: Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus



Intuitive information layouts fosters quick comprehension

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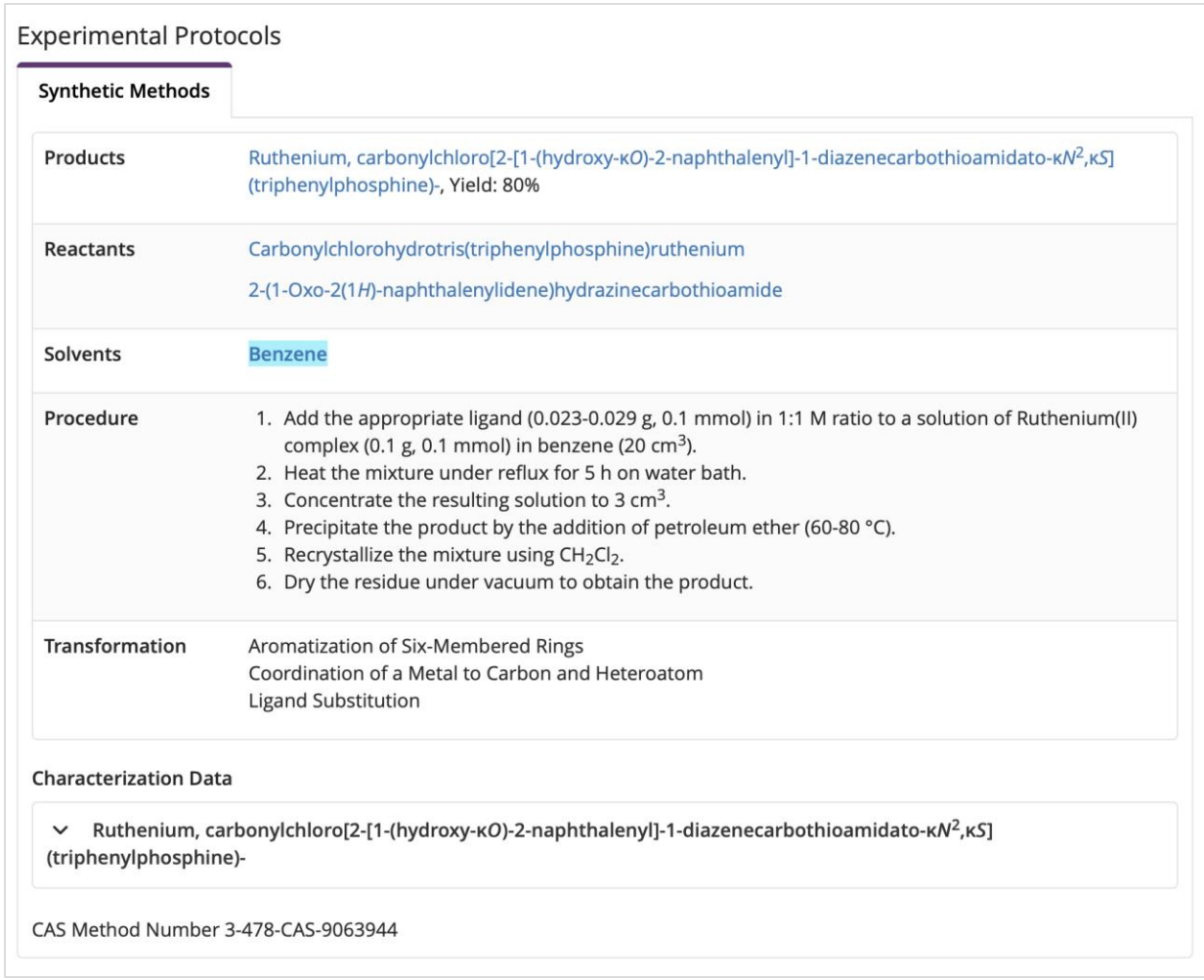
Design efficient bench strategies and work plans

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

Identify opportunities for new breakthroughs in synthetic methods.



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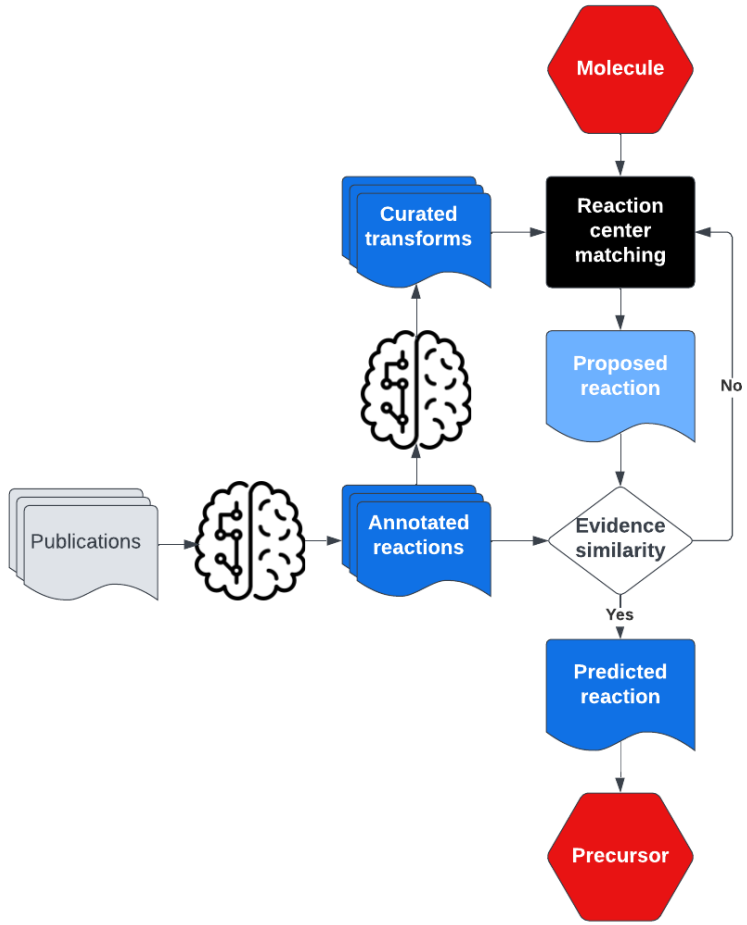
Retrosynthesis – How it works

Evidence based validation of predictive chemistry

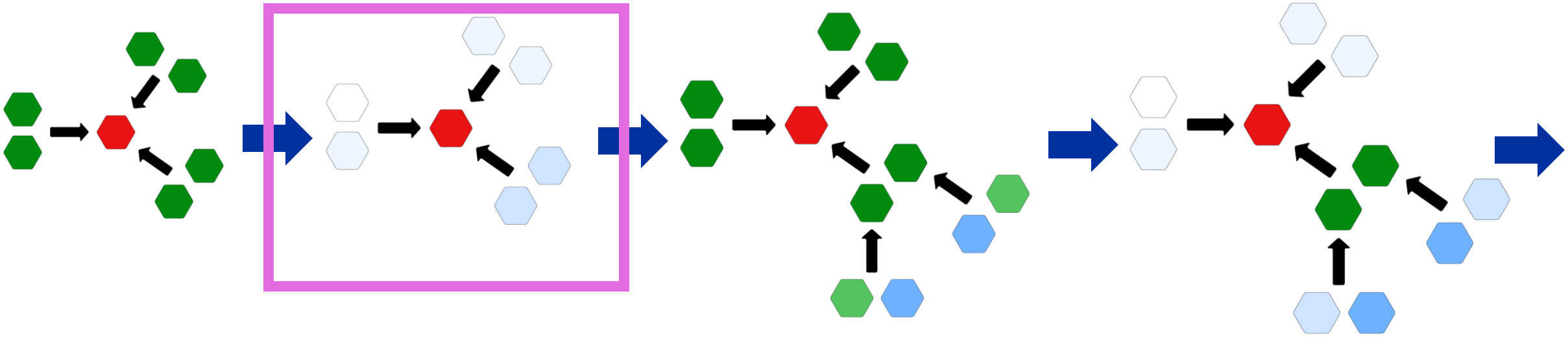
- CAS Reactions are used to generate all potential predicted reactions, then used again to provide specific evidence to evaluate each proposed reaction.
- Similarity to published chemistry is the criteria for accepting predicted reactions.
- Displayed evidence is ordered by relevance to that specific predicted reaction.



Retrosynthesis – How it works

Route guidance by substance-trained AI model

At each step, the top alternatives are selected by synthetic accessibility inference scores.



Explore the best directions for finding starting materials

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Innovate with retrosynthesis plans in real time

Retrosynthesis plans are generated in real-time for both experimental and predictive targets.

Review and evaluate plan steps and alternatives collaboratively, accelerating innovation.

View evidence directly within your plan, enabling precise comparison of alternative predictive synthetic pathways.

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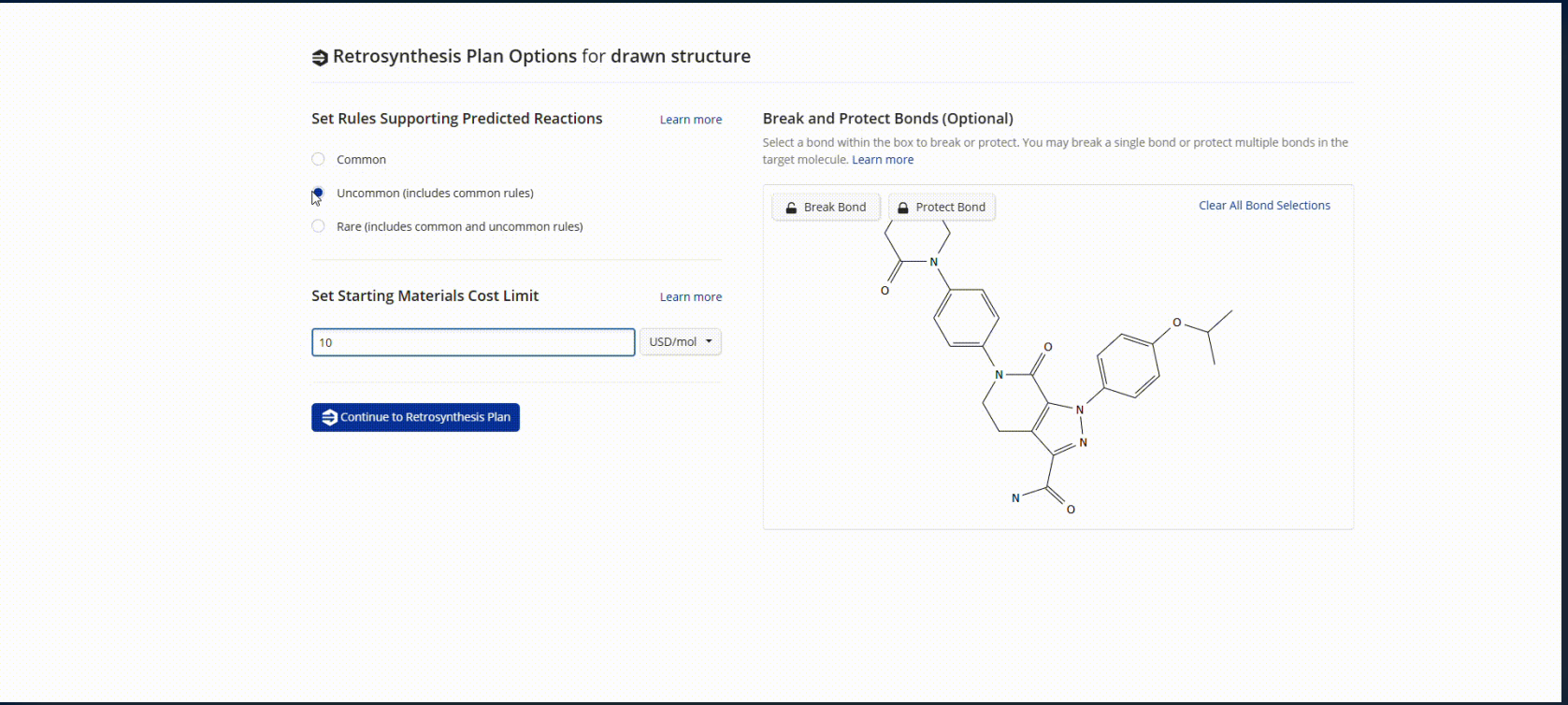
Retrosynthesis – Interactive Search

Real time results



First in the world real-time retrosynthesis planning!

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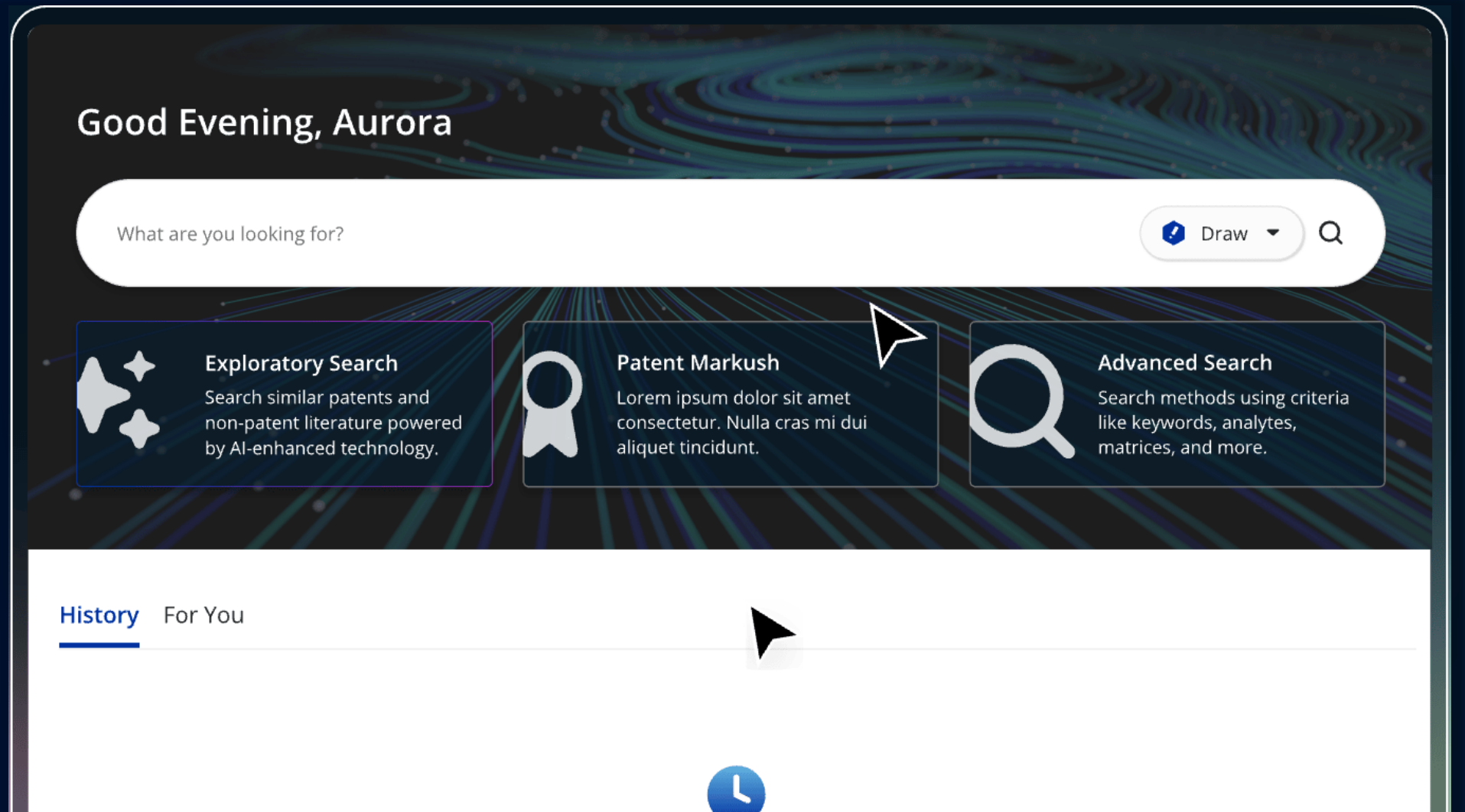
Our solutions are continuously evolving

CAS SciFinder powered by AI



Prior Art Discovery ensures researchers can find relevant prior art leveraging proprietary AI trained by CAS experts

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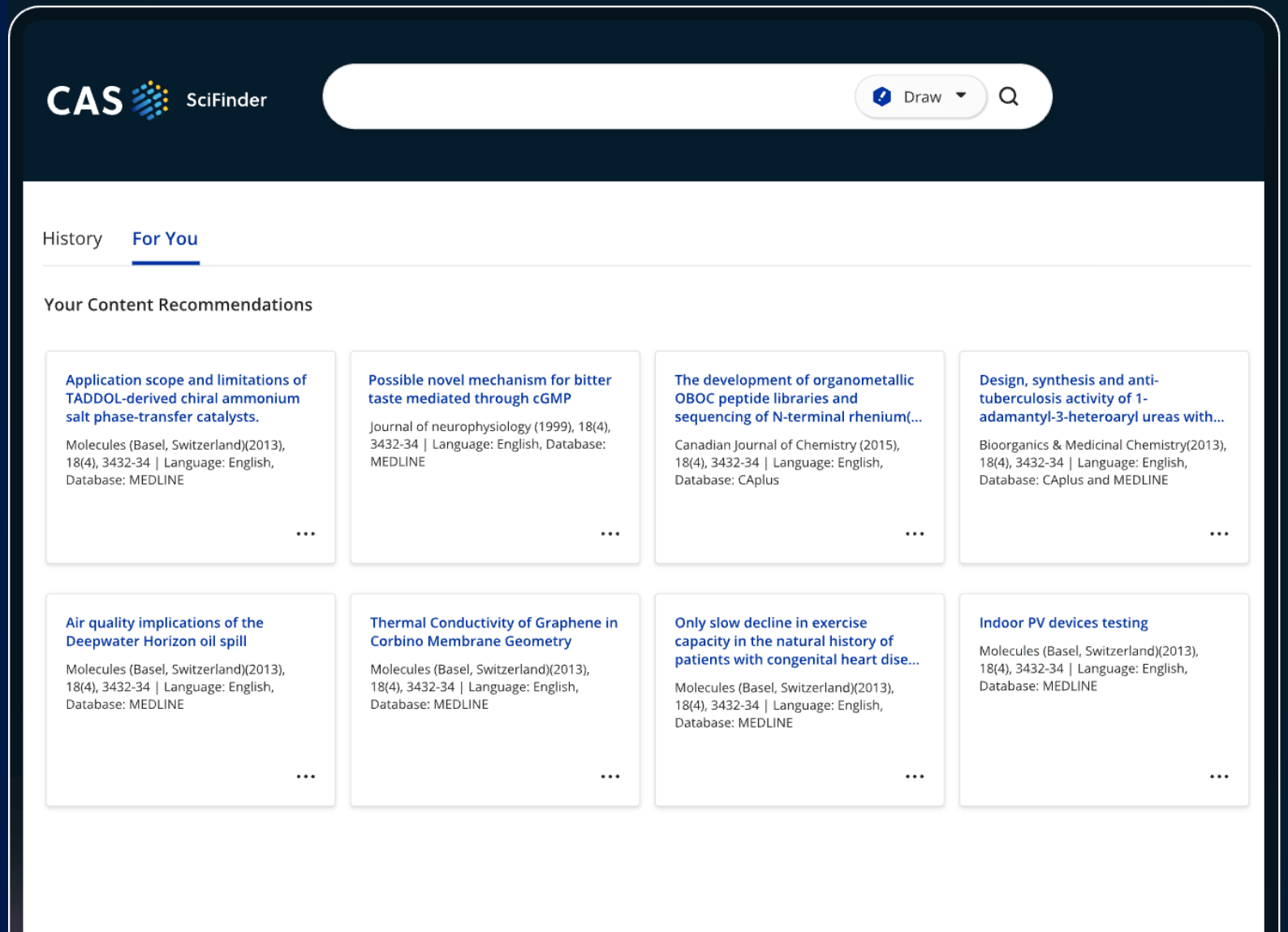
Our solutions are continuously evolving

CAS SciFinder powered by AI



- Natural language search
- Personalized recommendations
- Scientifically accurate summaries

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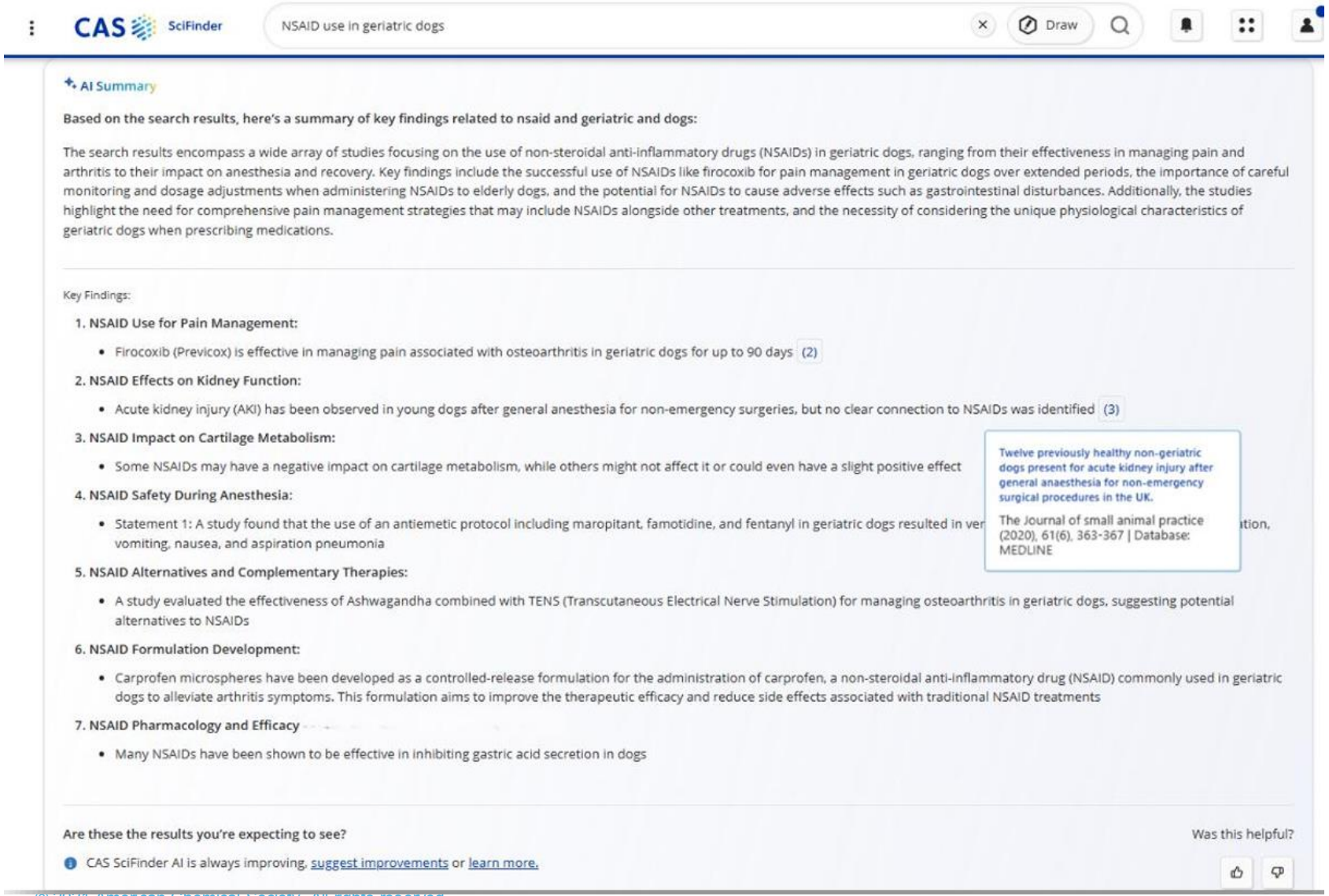
AI-powered Result Summaries!



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References

- **References by Author**
- *Query Examples:*
- smith, john
- john smith on MEIS1 gene
- **References by Journal**
- *Query Example:* documents published in jacs
- **References by Document Type**
- *Query Example:* patents about waterborne coating

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Substances and Their Properties

Search for a substance by property or a substance's physical, experimental, and predicted properties using simple keywords, with or without Boolean operators, and natural language

- ***Example queries:***
- amines with boiling point <100
- what is the glass transition point of PMMA
- boiling point of 79-09-4
- benoxaprofen median lethal dose
- ketones with H acceptors >2
- acids with pKa <0.5
- substances that self-ignite over 70 F
- compounds with melting point between 114.6-115.5 degrees C

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- ibuprofen carbon nmr
- spectra of benzene
- 51234-28-7 spectra
- Visible Absorption Spectrum of CH2Cl2
- GHS data for toluene
- where can I find the regulation information on sulfur dioxide
- how hazardous is the chemical nitrogen dioxide
- safety regulations for chlorine
- benzene cost
- cost of 51234-28-7
- who sells acetone
- where to buy triostin a
- source for 1,2,4-trimethylbenzene

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Reaction

- *Water as a solvent for synthesis of toluene*
- What can I synthesize with Fmoc-Gly-OH and iron catalyst?
- Chromium dichloride catalyzed Nozaki-Hiyama-Kishi reactions
- how to synthesize benzenamine, 3-methoxy- with copper catalyst
- protocols to make toluene catalyzed by copper
- how to make ibuprofen
- suzuki coupling procedures
- synthesis of ibuprofen with 80-86% yield with pdcl2 catalyst
- Water as a solvent for synthesis of toluene with high yield
- Michael addition yield = 80

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

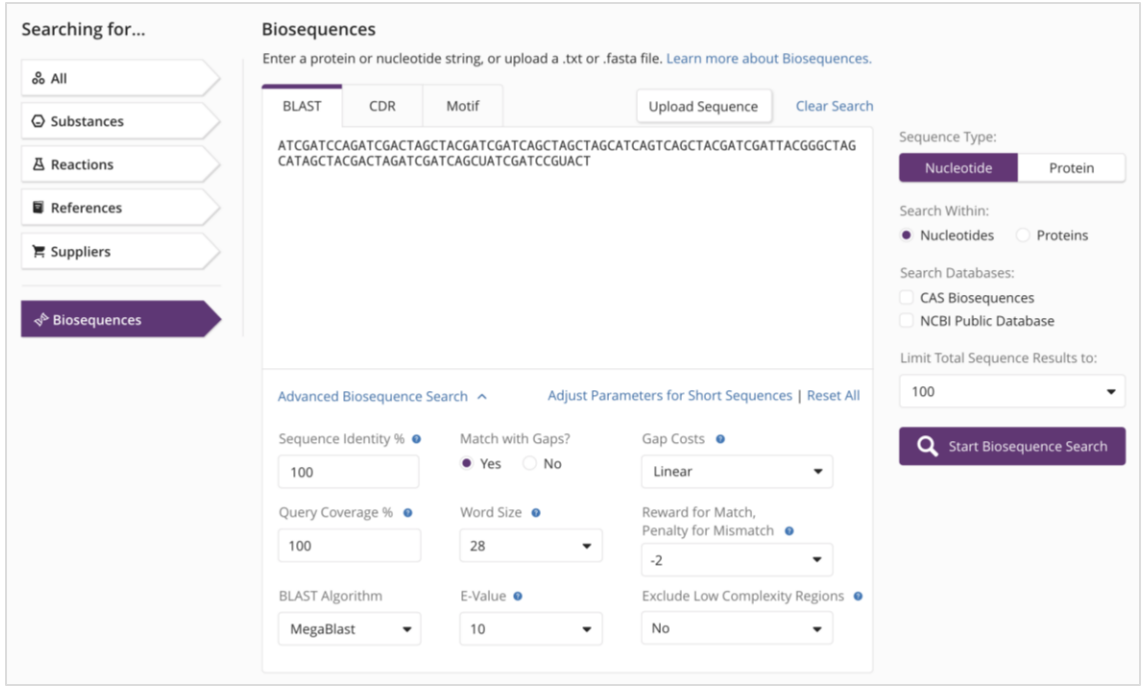
Newly enhanced collection of 700M+ proteins and nucleotides from 60+ patent authorities dating back to 1957

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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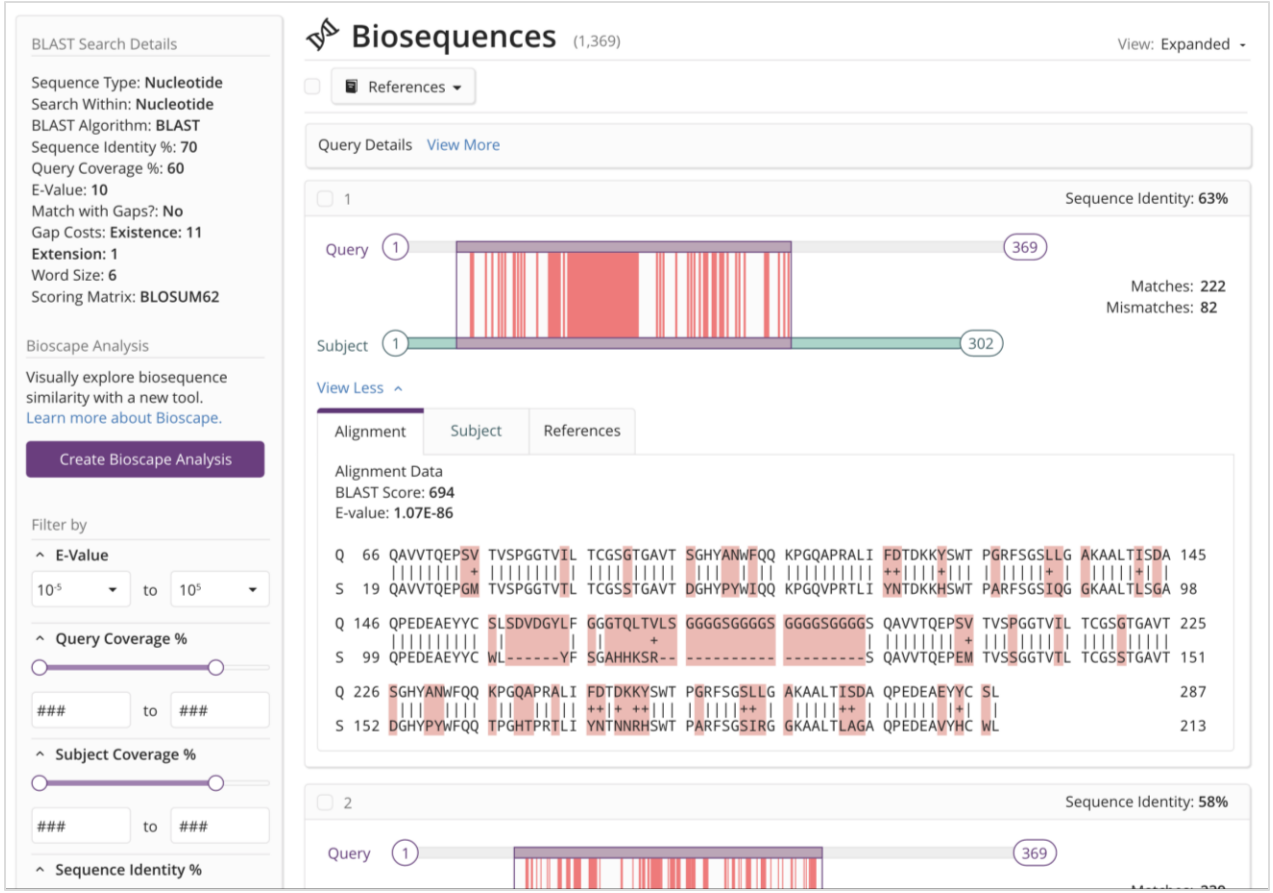
Conduct comprehensive biologics research

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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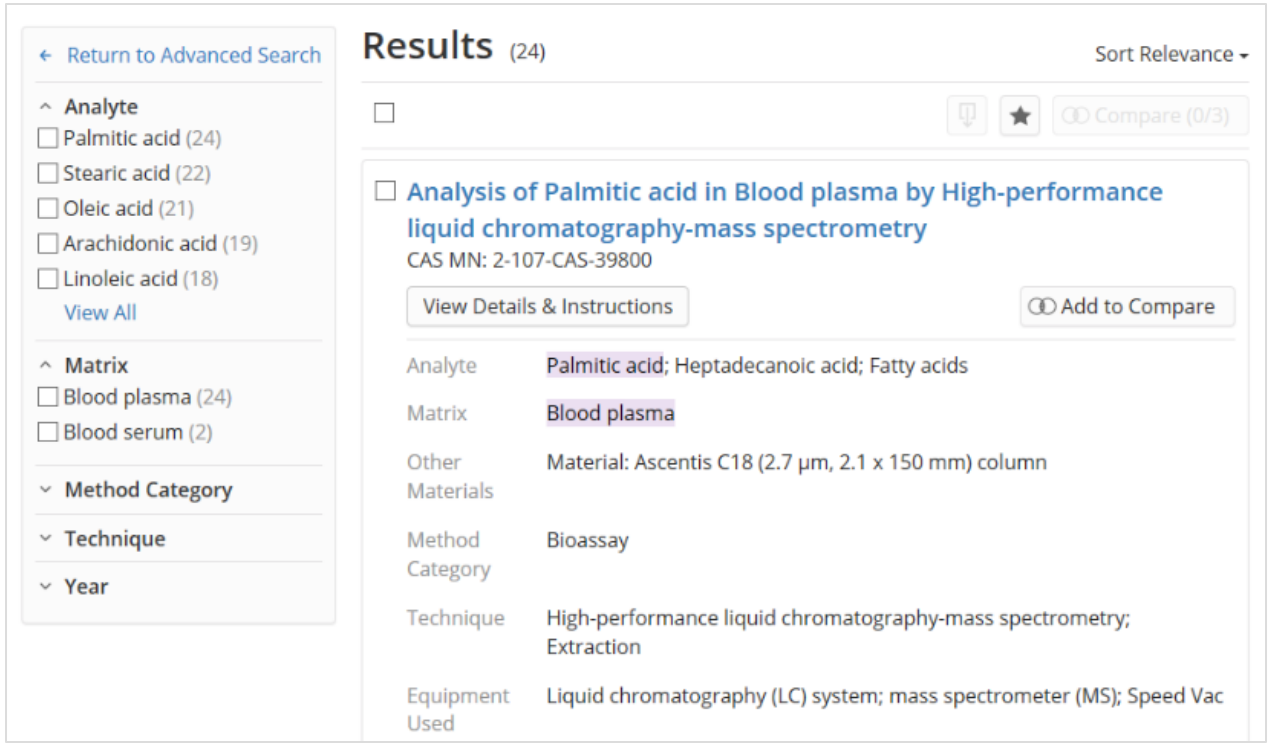
CAS SciFinder Discovery Platform for Analytical Chemists

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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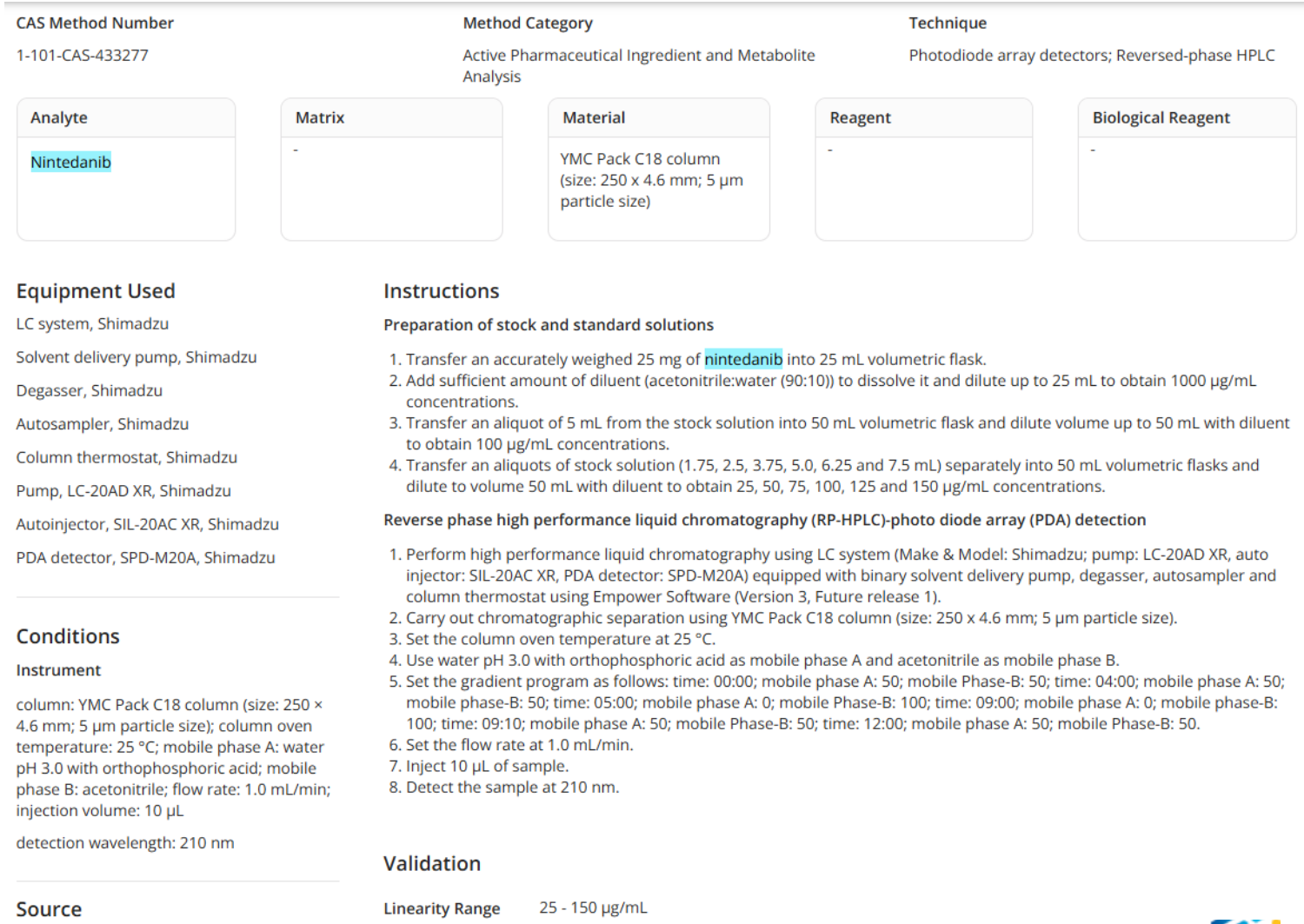
Test and validate innovations

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



CAS Method Number	Method Category	Technique
1-101-CAS-433277	Active Pharmaceutical Ingredient and Metabolite Analysis	Photodiode array detectors; Reversed-phase HPLC

Analyte	Matrix	Material	Reagent	Biological Reagent
Nintedanib	-	YMC Pack C18 column (size: 250 x 4.6 mm; 5 µm particle size)	-	-

Equipment Used

LC system, Shimadzu

Solvent delivery pump, Shimadzu

Degasser, Shimadzu

Autosampler, Shimadzu

Column thermostat, Shimadzu

Pump, LC-20AD XR, Shimadzu

Autoinjector, SIL-20AC XR, Shimadzu

PDA detector, SPD-M20A, Shimadzu

Conditions

Instrument

column: YMC Pack C18 column (size: 250 × 4.6 mm; 5 µm particle size); column oven temperature: 25 °C; mobile phase A: water pH 3.0 with orthophosphoric acid; mobile phase B: acetonitrile; flow rate: 1.0 mL/min; injection volume: 10 µL

detection wavelength: 210 nm

Source

Instructions

Preparation of stock and standard solutions

1. Transfer an accurately weighed 25 mg of nintedanib into 25 mL volumetric flask.
2. Add sufficient amount of diluent (acetonitrile:water (90:10)) to dissolve it and dilute up to 25 mL to obtain 1000 µg/mL concentrations.
3. Transfer an aliquot of 5 mL from the stock solution into 50 mL volumetric flask and dilute volume up to 50 mL with diluent to obtain 100 µg/mL concentrations.
4. Transfer an aliquots of stock solution (1.75, 2.5, 3.75, 5.0, 6.25 and 7.5 mL) separately into 50 mL volumetric flasks and dilute to volume 50 mL with diluent to obtain 25, 50, 75, 100, 125 and 150 µg/mL concentrations.

Reverse phase high performance liquid chromatography (RP-HPLC)-photo diode array (PDA) detection

1. Perform high performance liquid chromatography using LC system (Make & Model: Shimadzu; pump: LC-20AD XR, auto injector: SIL-20AC XR, PDA detector: SPD-M20A) equipped with binary solvent delivery pump, degasser, autosampler and column thermostat using Empower Software (Version 3, Future release 1).
2. Carry out chromatographic separation using YMC Pack C18 column (size: 250 x 4.6 mm; 5 µm particle size).
3. Set the column oven temperature at 25 °C.
4. Use water pH 3.0 with orthophosphoric acid as mobile phase A and acetonitrile as mobile phase B.
5. Set the gradient program as follows: time: 00:00; mobile phase A: 50; mobile Phase-B: 50; time: 04:00; mobile phase A: 50; mobile phase-B: 50; time: 05:00; mobile phase A: 0; mobile Phase-B: 100; time: 09:00; mobile phase A: 0; mobile phase-B: 100; time: 09:10; mobile phase A: 50; mobile Phase-B: 50; time: 12:00; mobile phase A: 50; mobile Phase-B: 50.
6. Set the flow rate at 1.0 mL/min.
7. Inject 10 µL of sample.
8. Detect the sample at 210 nm.

Validation

Linearity Range	25 - 150 µg/mL

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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

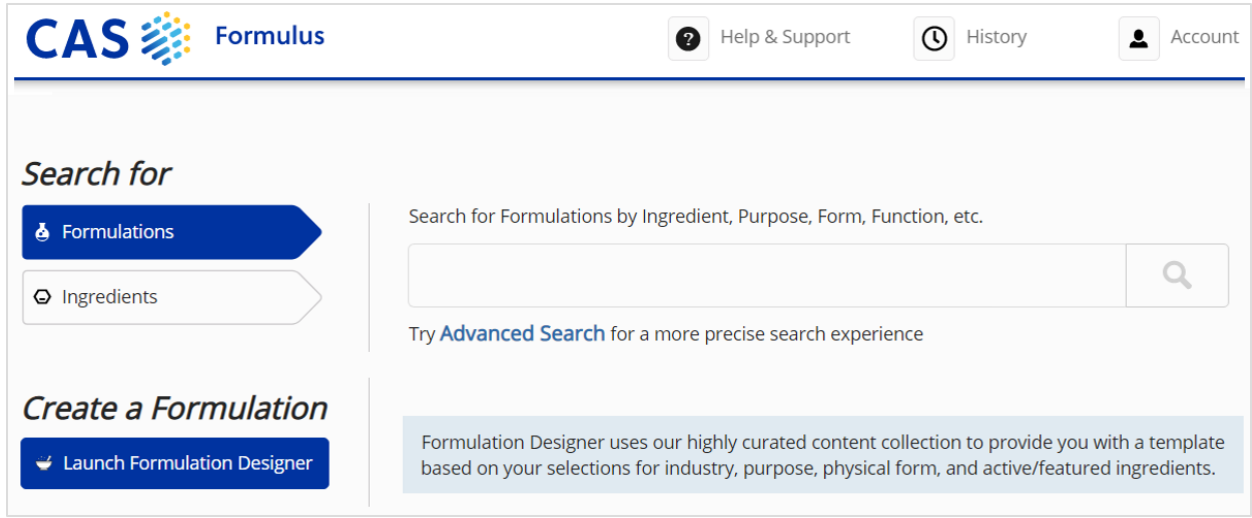
Understand a formulation's effectiveness with quick access to the best information for active ingredients and excipients

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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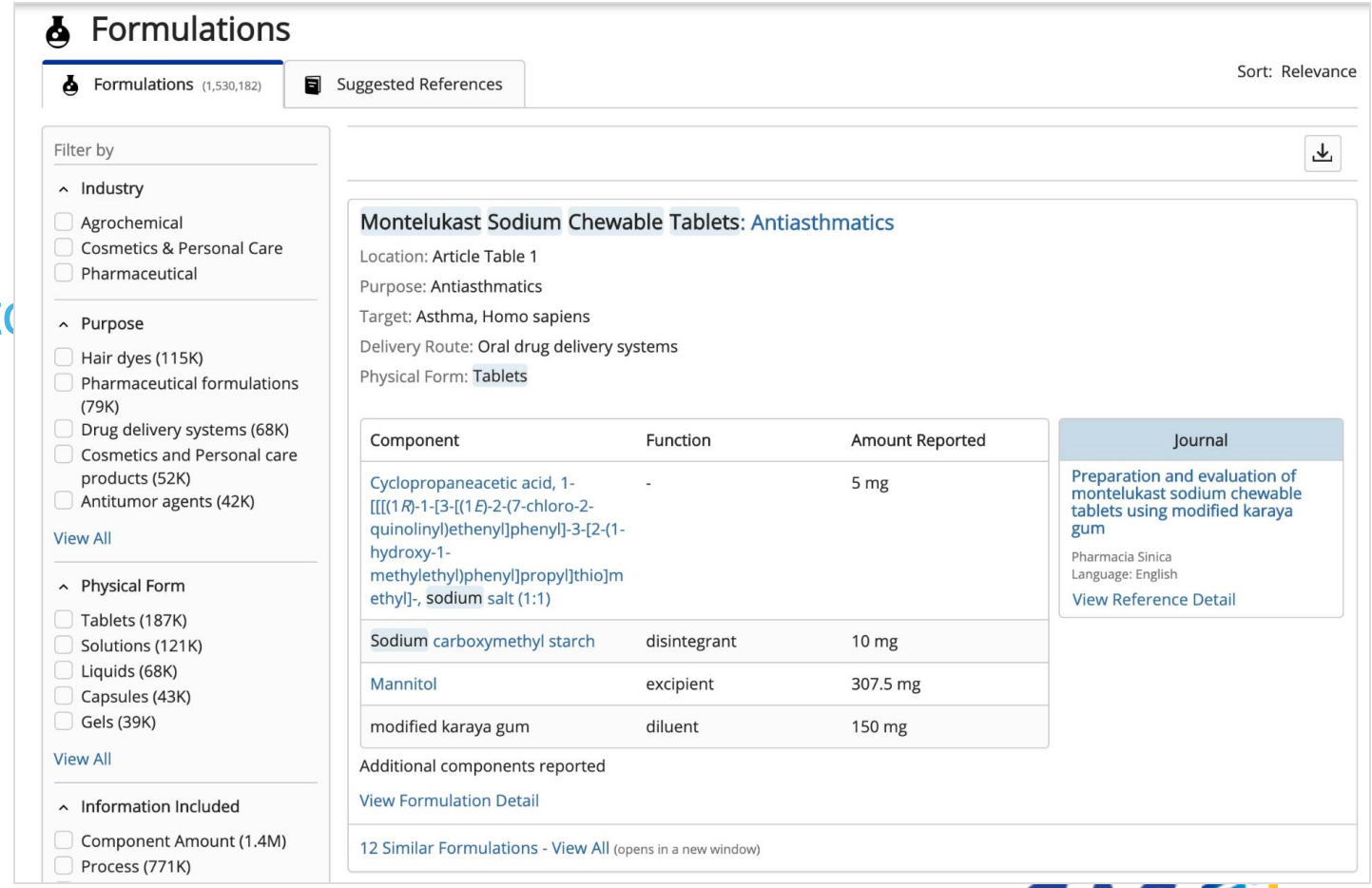
Develop differentiating formulations and manufacture-to-scale

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



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Thank you！

謝謝！

For more information

CAS Representative Office

Tliu2@acs-i.org

+886-975-765358

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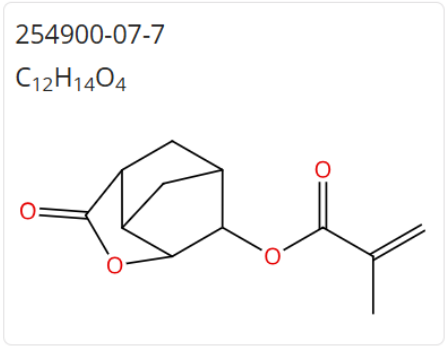
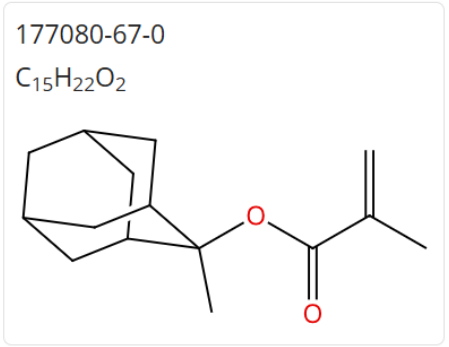
- 請查詢貴單位發表,並限制在2025年以後的文獻.
- 含有Mo金屬的所有物質,特別是有機金屬化合物.
- 高分子搜尋





- 抗凝血藥物 Apixaban的分析方法與逆合成分析
- What is the advantage of Perovskite Solar Cells?