CAS SciFinderN

劉全哲
Tliu2@acs-i.org

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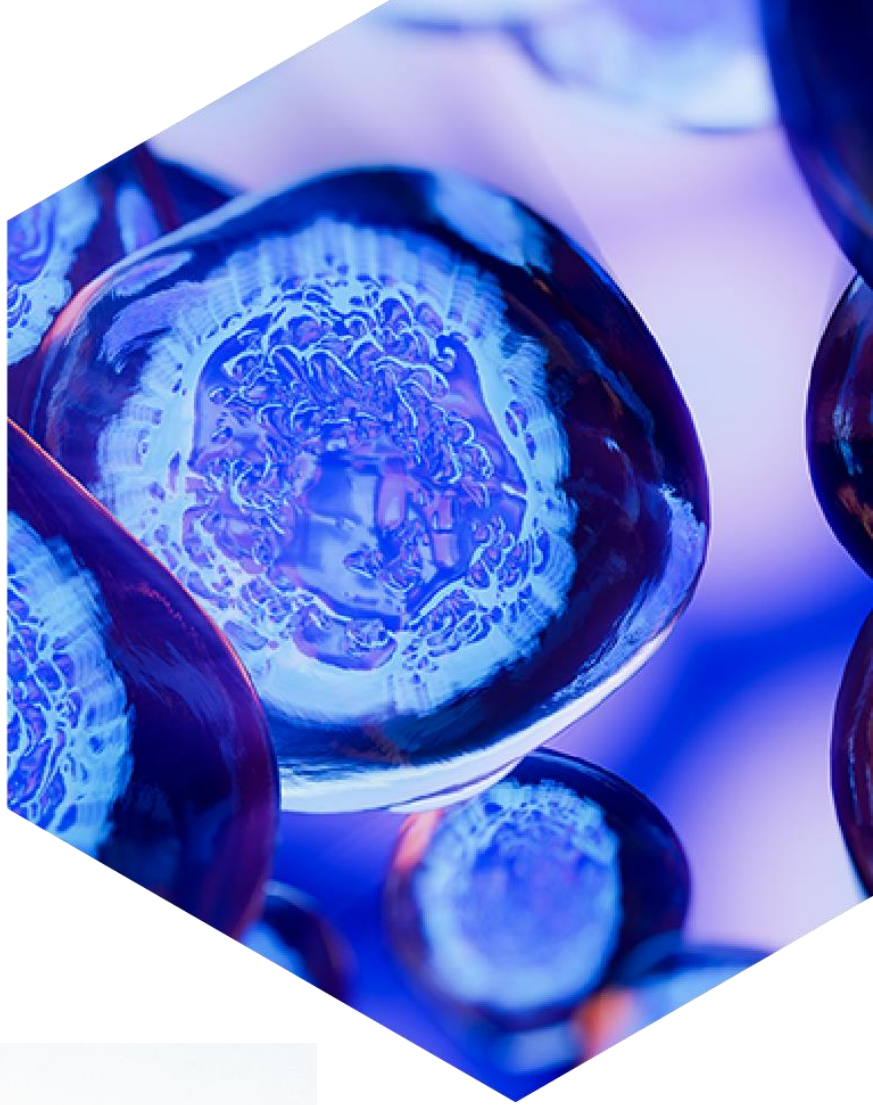
About CAS



Founded in 1907, chemists around the world understood the value to research in aggregating scientific information.

Today we are a global organization of expert scientists, technologists, and business leaders with a long and successful history of harnessing scientific information to support valuable research insights.

Approximately 1,600 staff members – including CAS scientists, speaking 50 languages among them (600+ Ph.D. Scientists)

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CAS is a trusted partner

to innovation leaders across industries

PHARMA

48

of the top 50

ACADEMIC

100

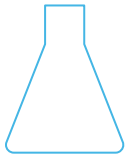
of the top 100

BIOTECH

20

of the top 25

CHEMICAL



48

of the top 50

GOVERNMENT

10

of the top10 global patent offices

1. Pharm Exec's Top 50 Companies 2020. **2.** ShanghaiRanking's Global Ranking of Academic Subjects 2020. **3.** Genetic Engineering & Biotechnology News Top 25 Biotech Companies of 2019. **4.** C&EN's Global Top 50 for 2020. **5.** WIPO IP Facts and Figures 2019.

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CAS has the most comprehensive collection of connected science

Over
50K
scientific journals and documents

Over
250
million substances

Over
50
languages translated

64
patent offices worldwide

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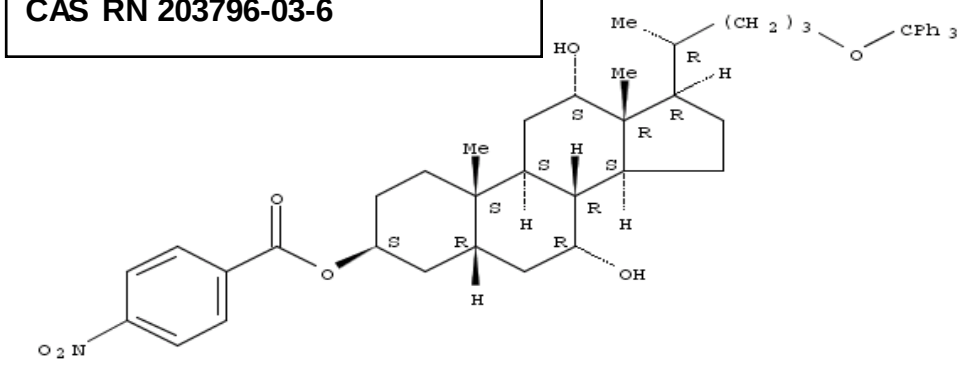
CAS scientists find the chemistry, and save you time!

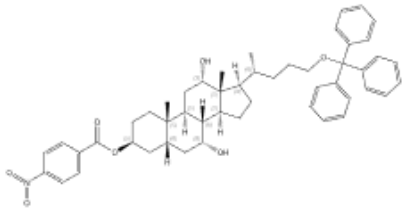
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87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

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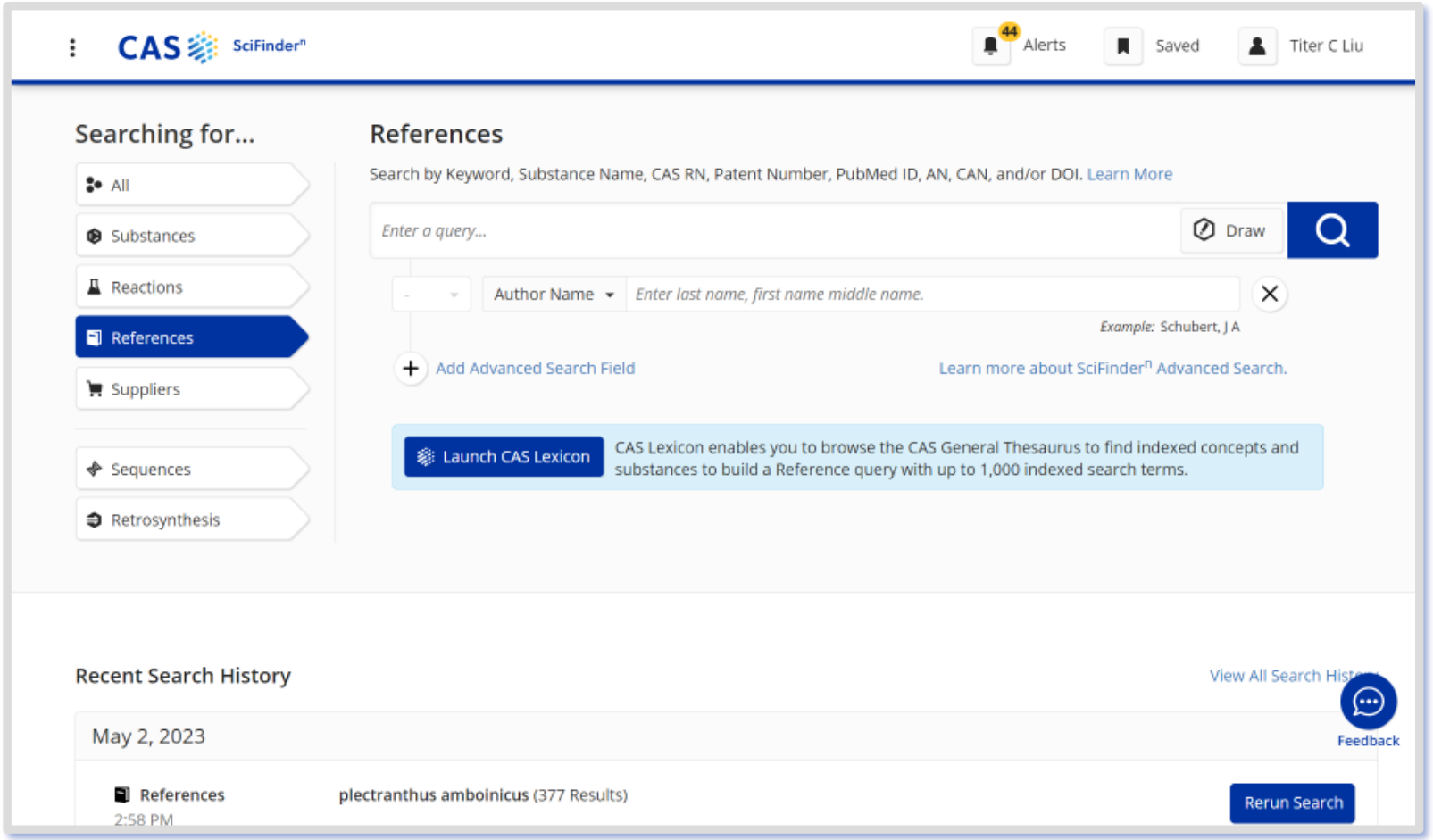
Scifinder^{n} Discovery platform

*SciFinderN

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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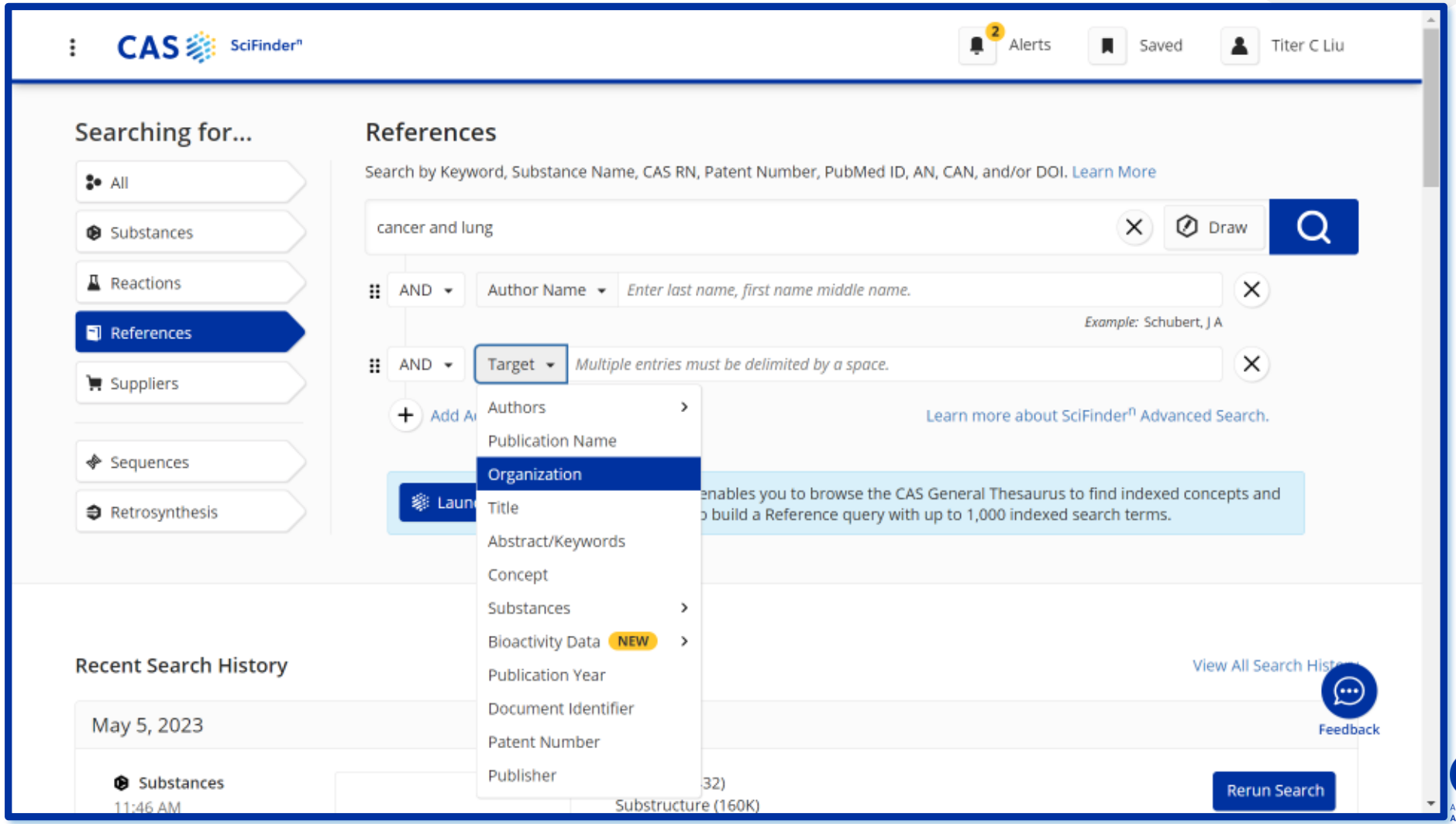
Perform Reference searching

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



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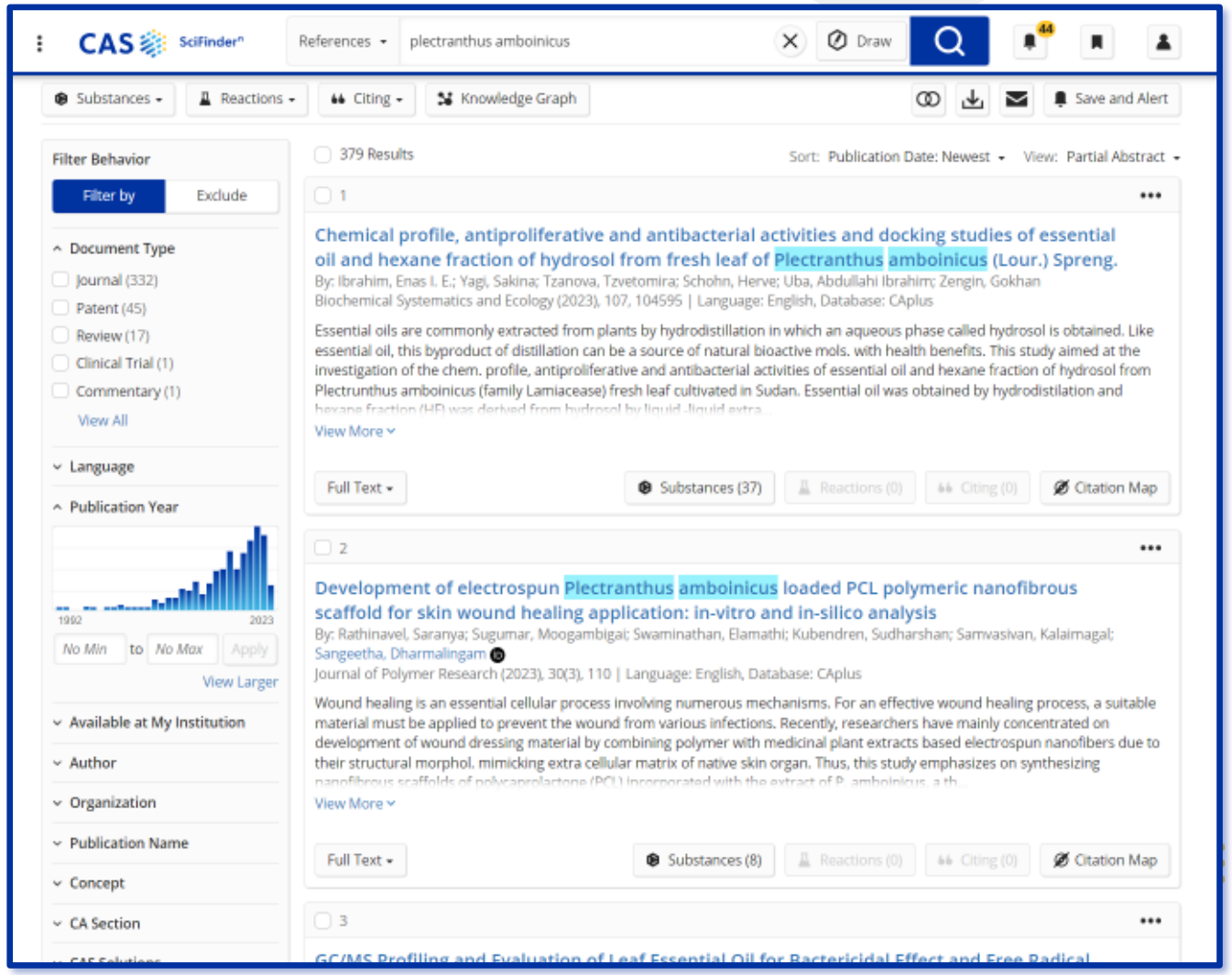
Perform literature reviews

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

Keep up to date with the world's published scientific patent and journal literature across multiple disciplines using the most advanced relevance engine for scientific research.

- An easy-to-read display lets user quickly browse reference
- Filters are available to further narrow results…by year, source type, and organization



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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 Effe
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

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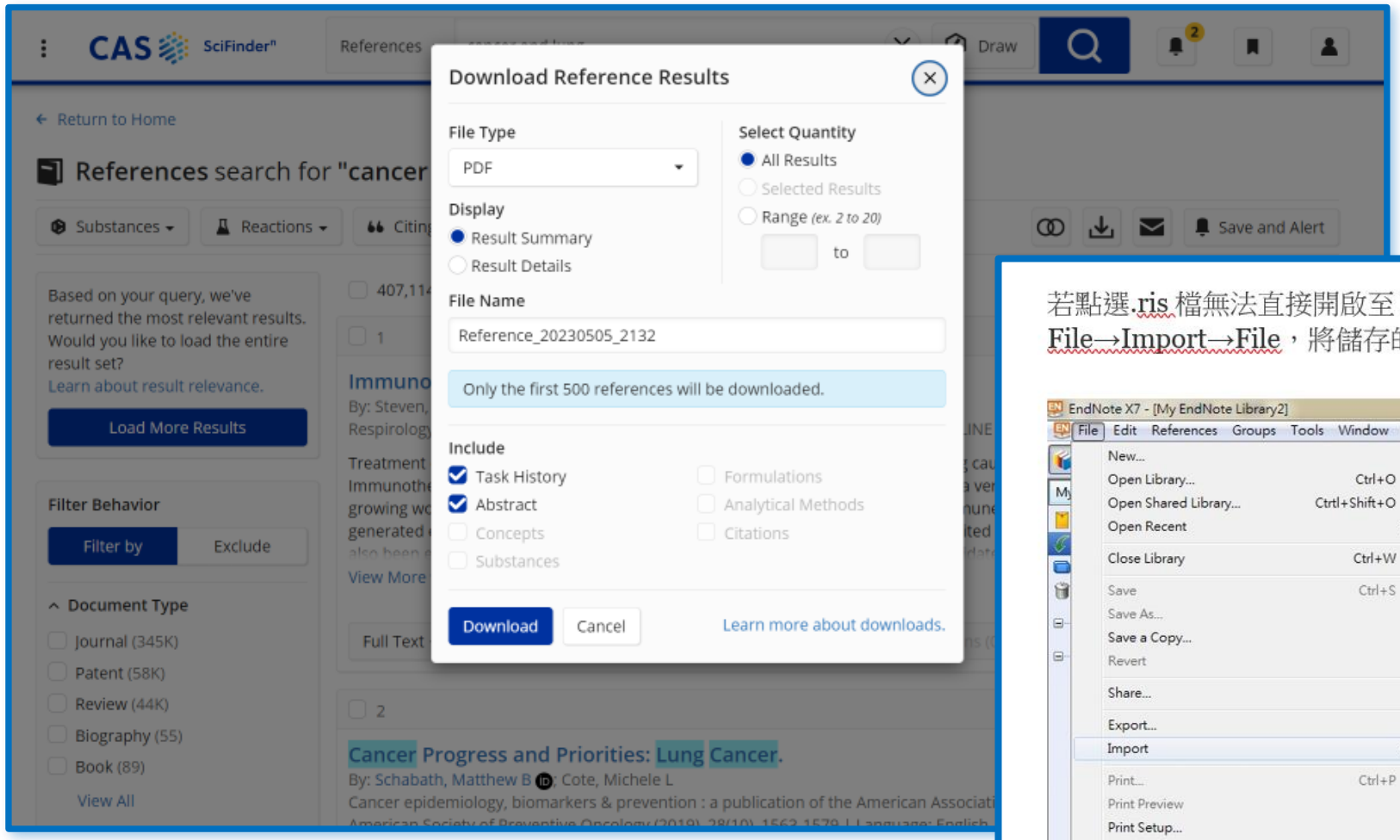
EndNote output



若點選.ris 檔無法直接開啟至 EndNote，也可另開啟 EndNote，在工具列點選 File→Import→File，將儲存的.ris 檔案匯入。↵

在 Import File 選擇檔案來源，Import Option 選擇 Reference Manager (RIS)，也可將 SciFinderN 的文獻檢索結果匯至 Endnote。↵

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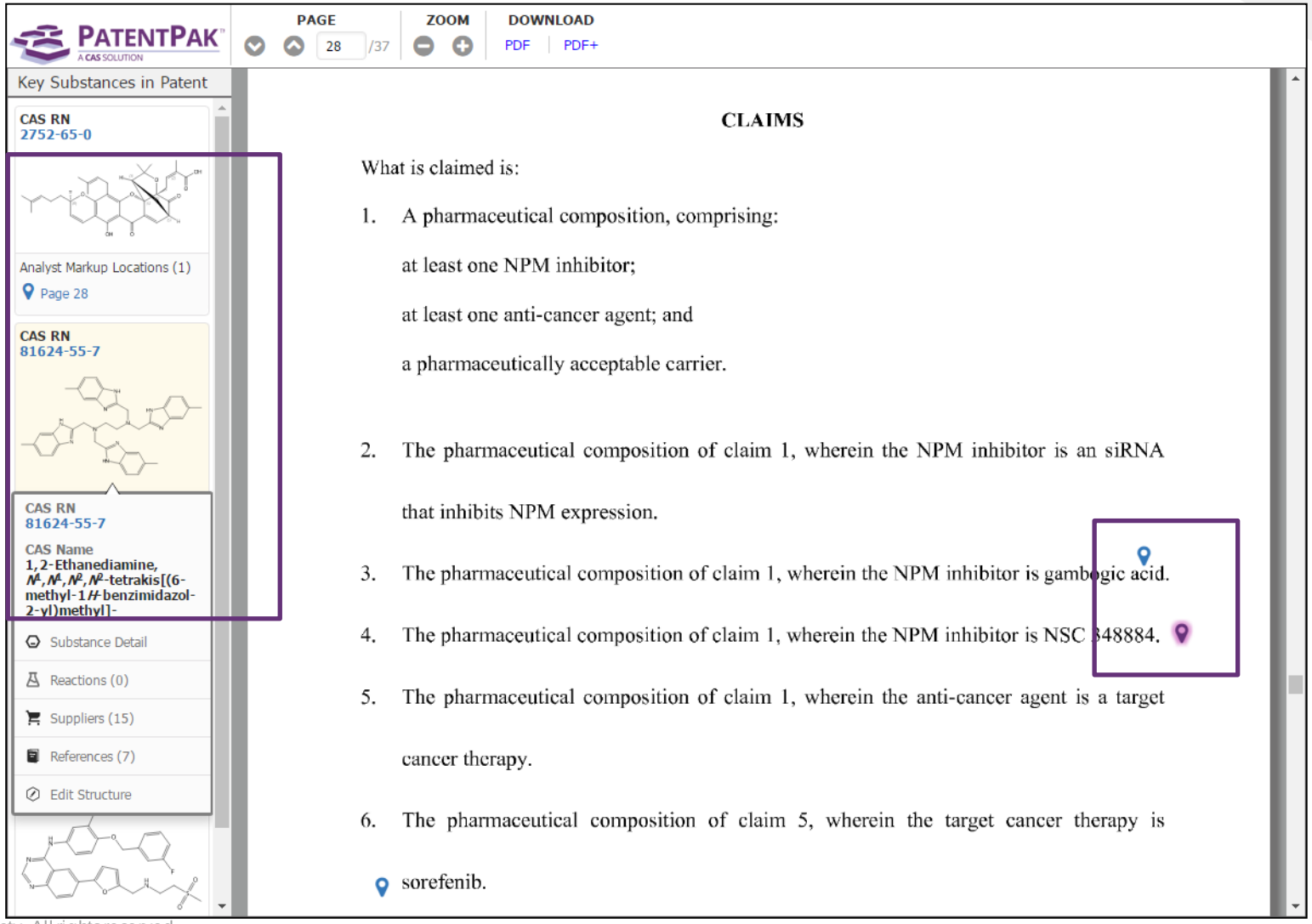
PatentPak:
Why waste time slogging through dense patent material with direct access to and understanding of the chemistry within the document

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



Important chemistry locations are identified by CAS expert scientists

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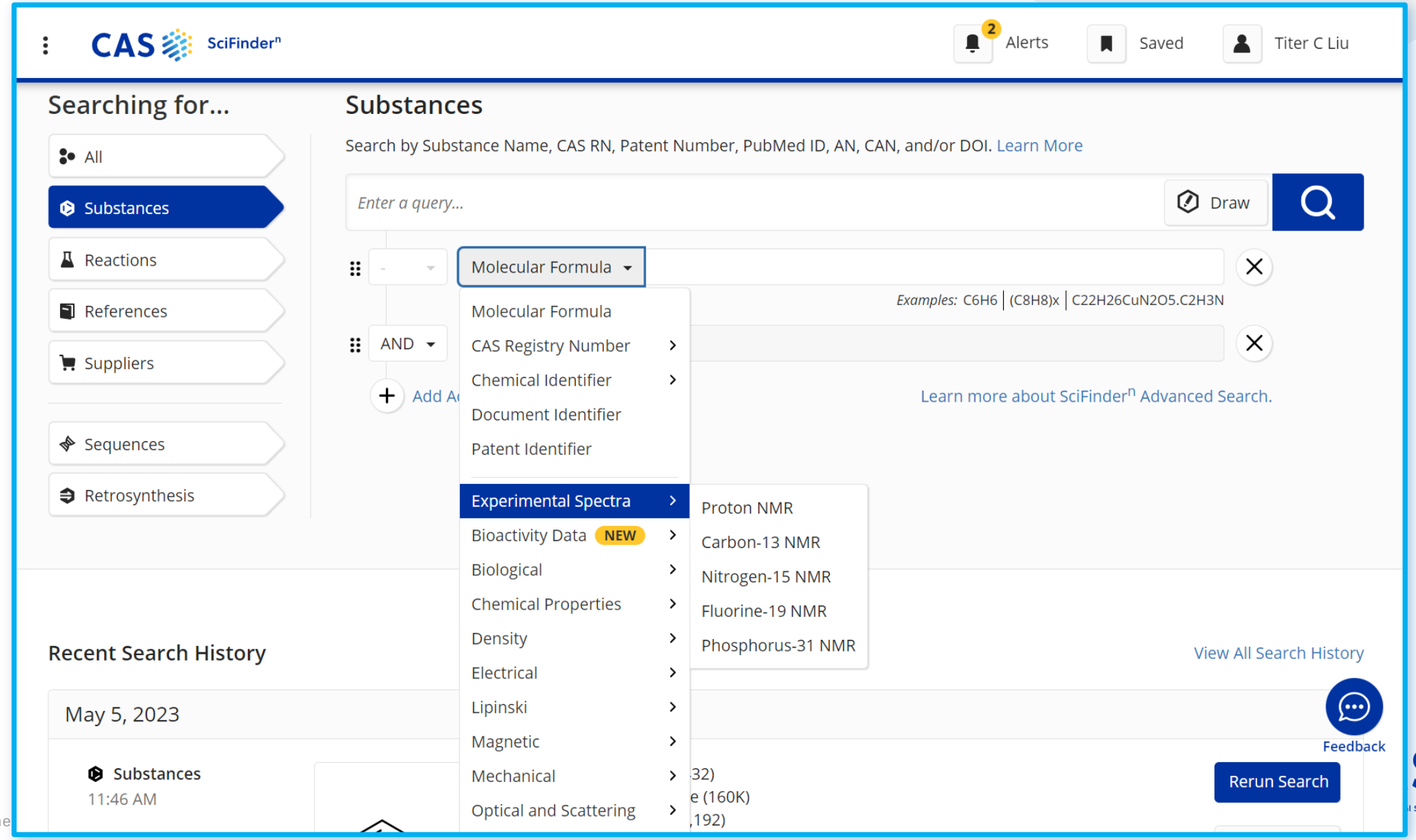
Substance searching



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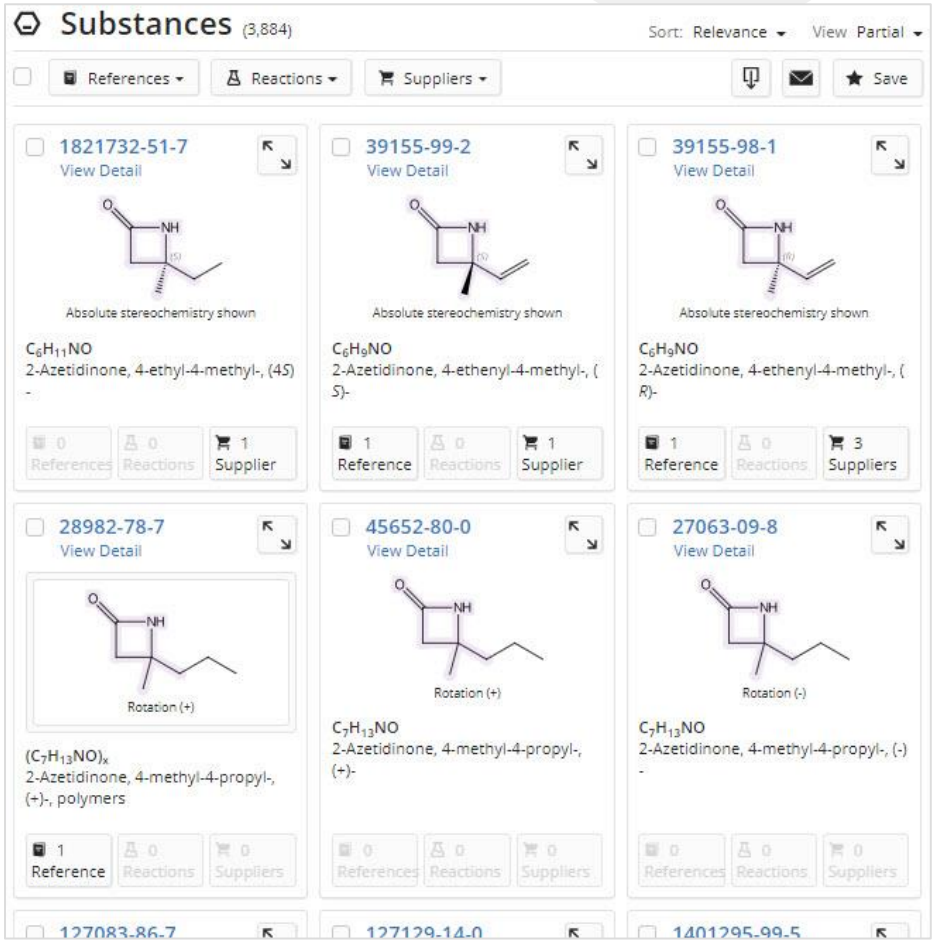
Mine substances and reactions

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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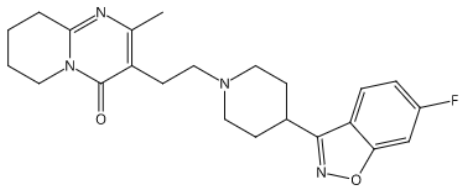
Substances information

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

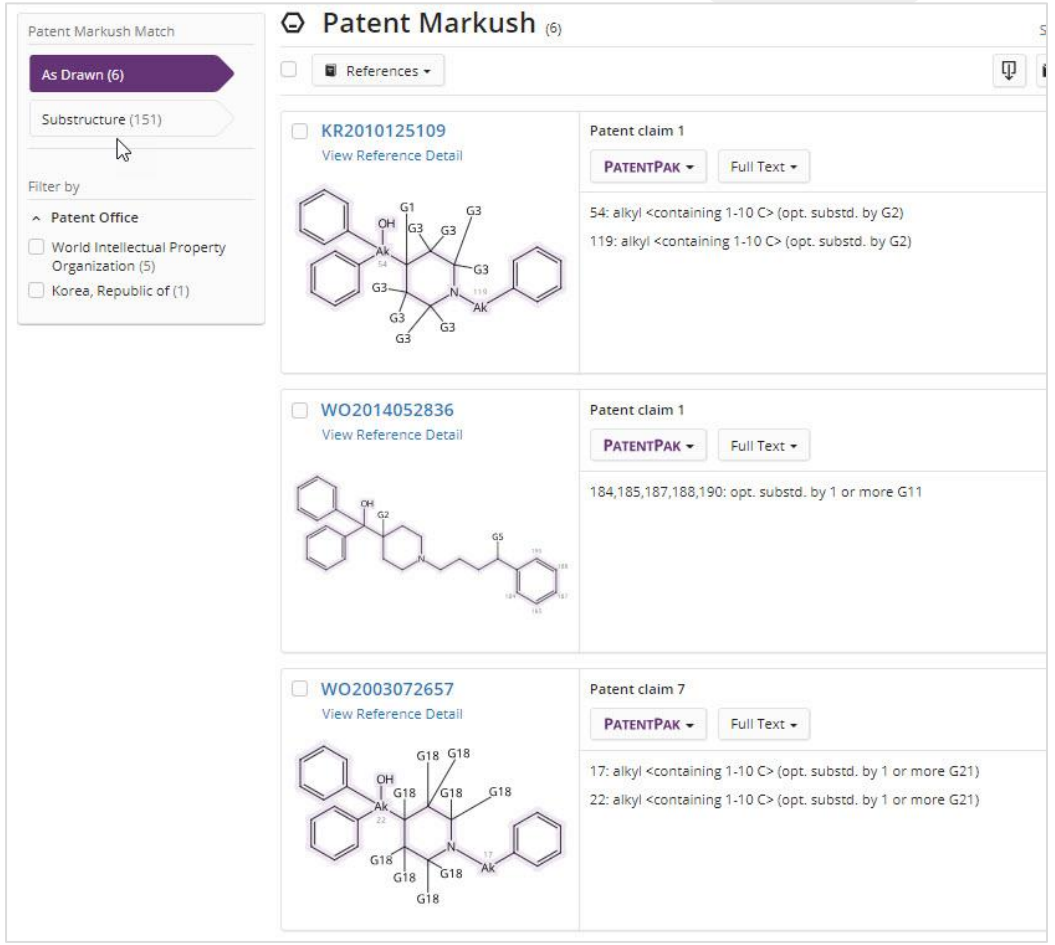
Target | Function | Parameter | Disease | Organism

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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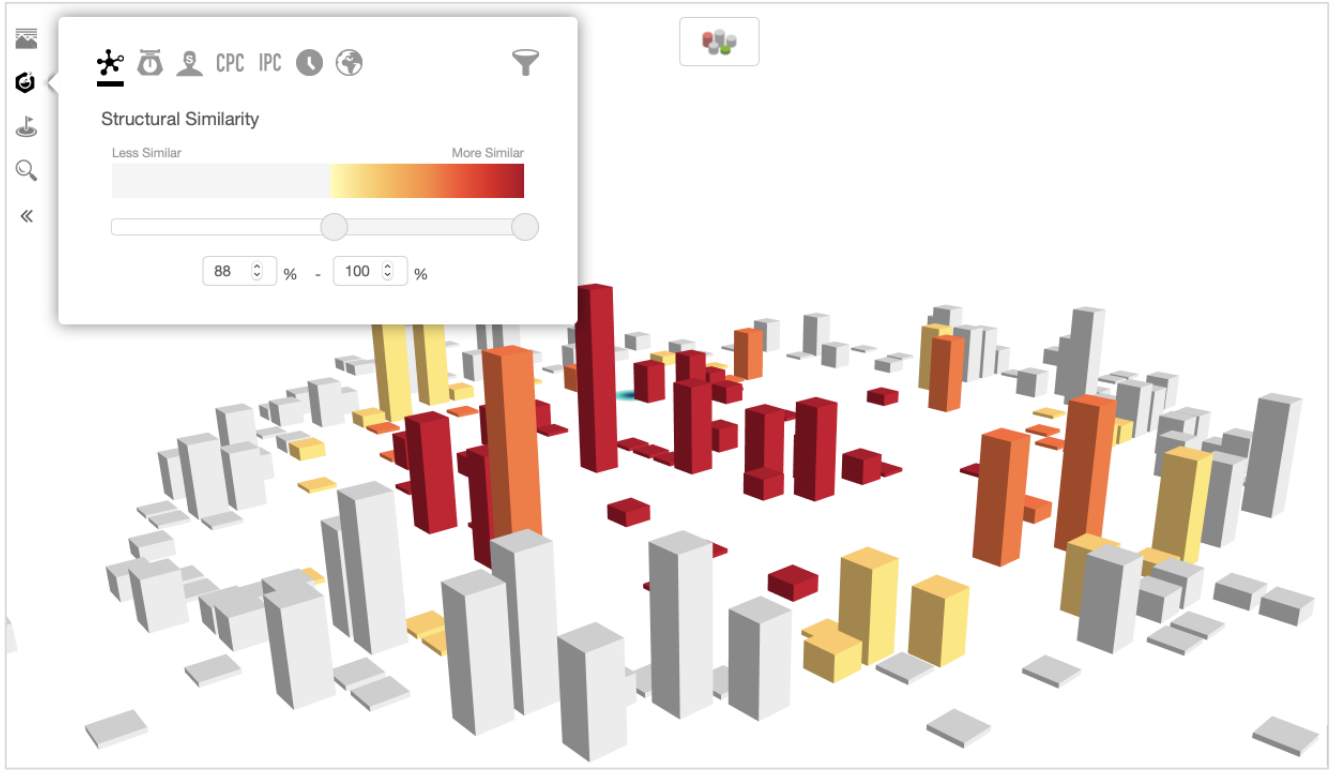
Visualize search results

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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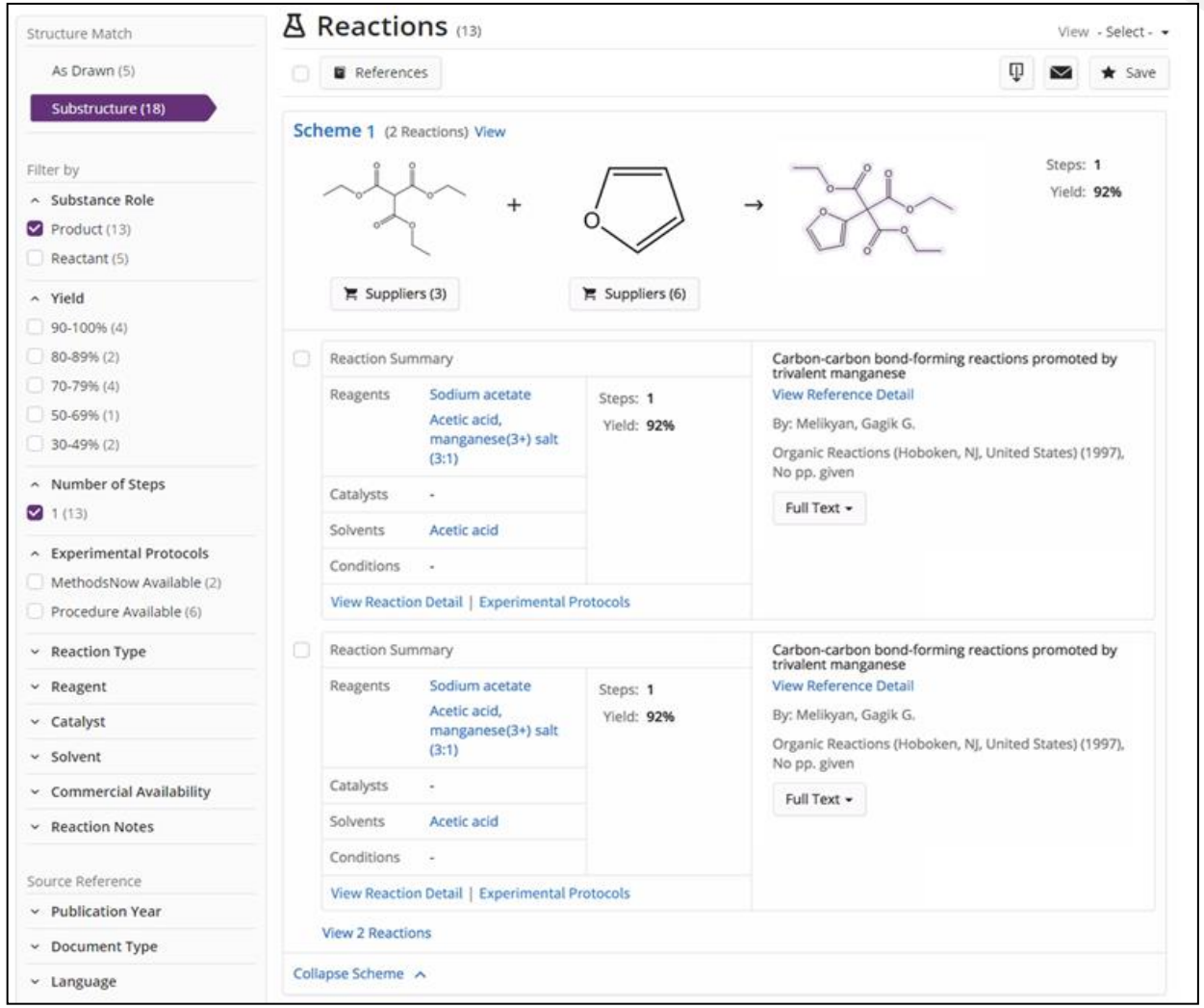
Reaction: Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus



Intuitive information layouts fosters quick comprehension

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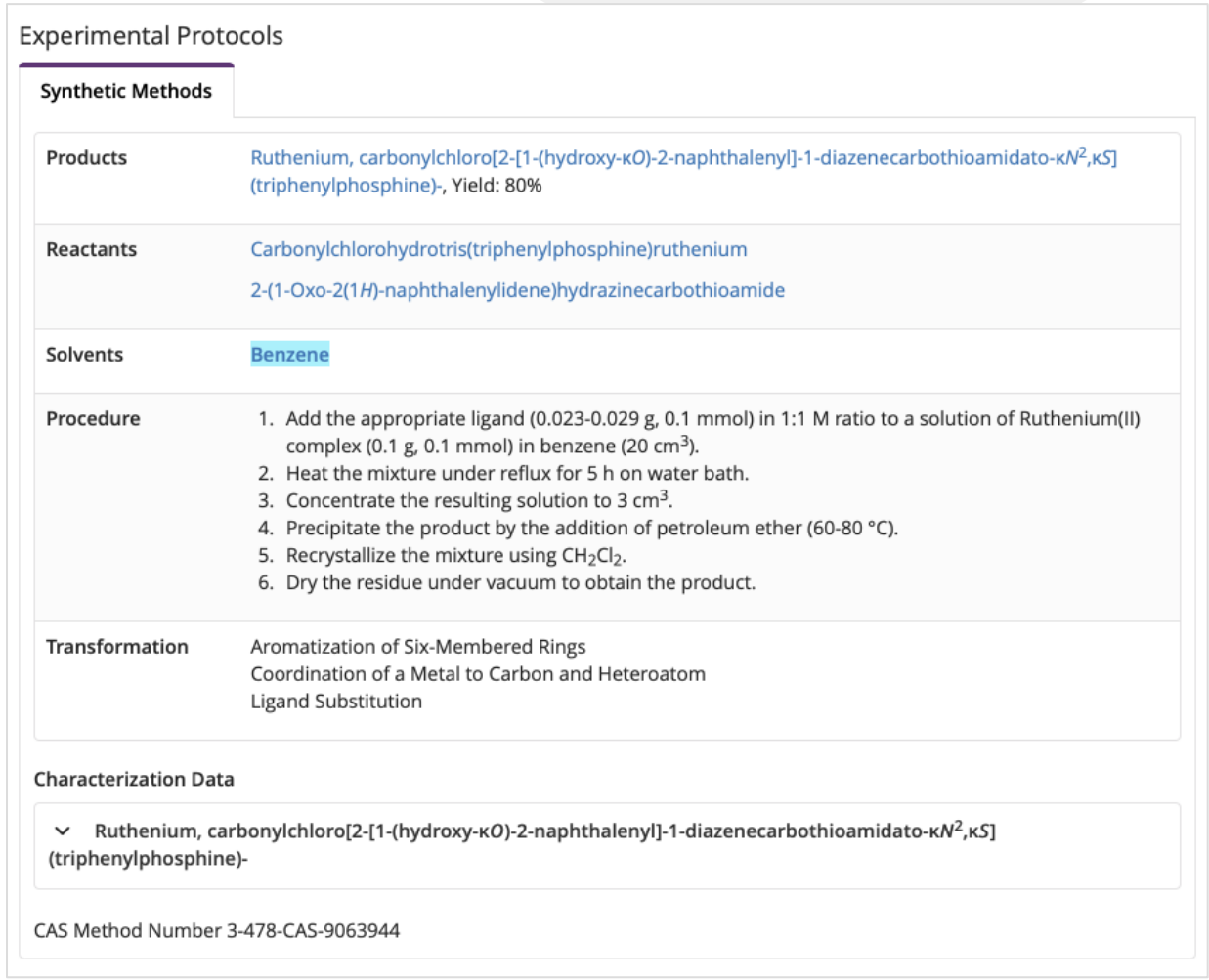
Design efficient bench strategies and work plans

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

Identify opportunities for new breakthroughs in synthetic methods.



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Retro-Synthetic Planning

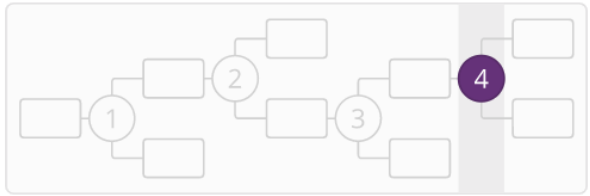
CAS SciFinder^{n} | Reactions | Enter a query... | Draw | 2

Retrosynthesis Plan Options for 106266-06-2

Powered by ChemPlanner®

Select Synthetic Depth Learn more.

- 1
- 2
- 3
- 4



Set Rules Supporting Predicted Reactions Learn more.

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

Set Starting Materials Cost Limit Learn more.

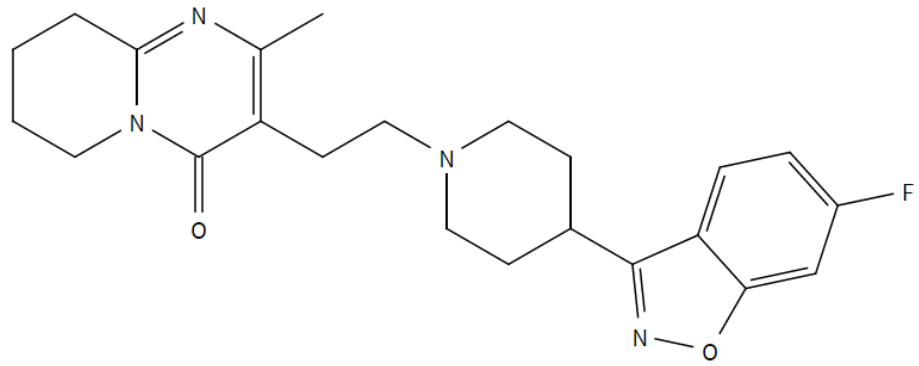
1000 USD/mol

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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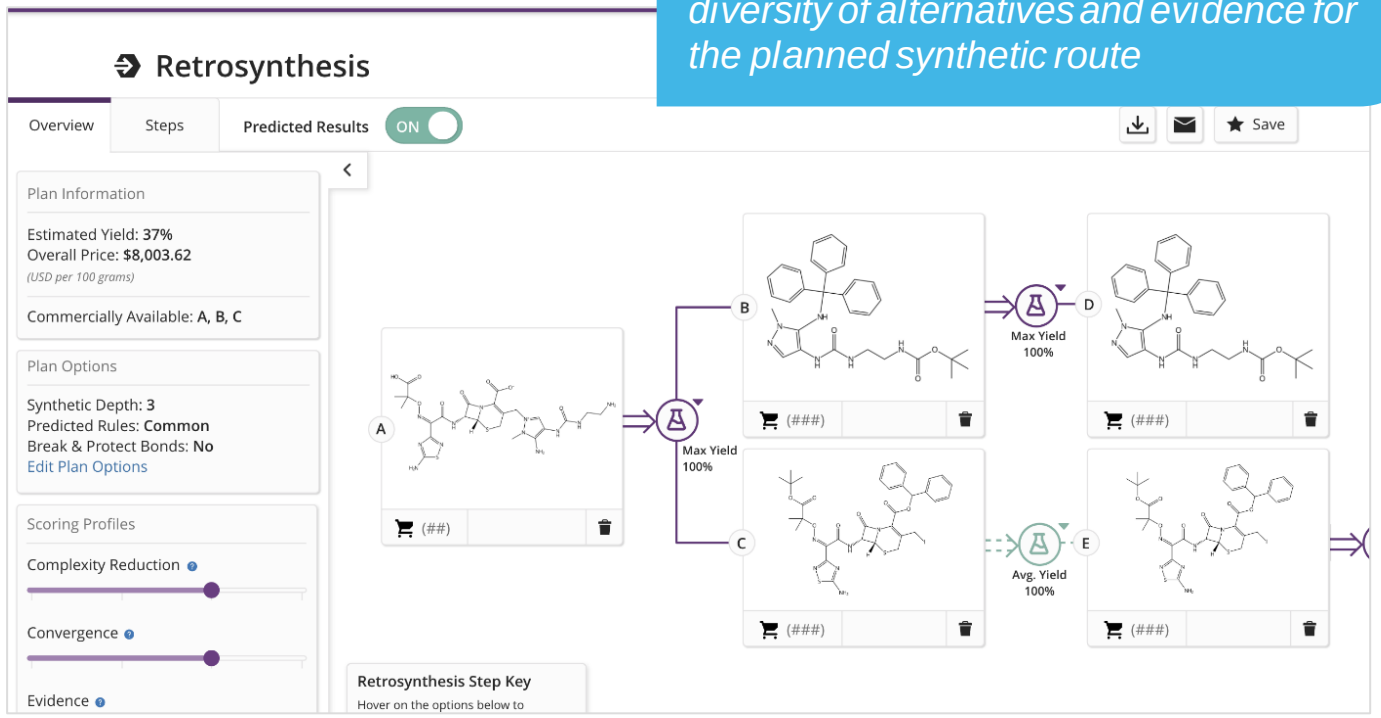
CAS SciFinder Discovery Platform for Synthetic Planning

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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CAS SciFinder Discovery Platform for Molecular Biologists

Enhancing biological research with biosequence searching in SciFinder^n

UNMATCHED CONTENT

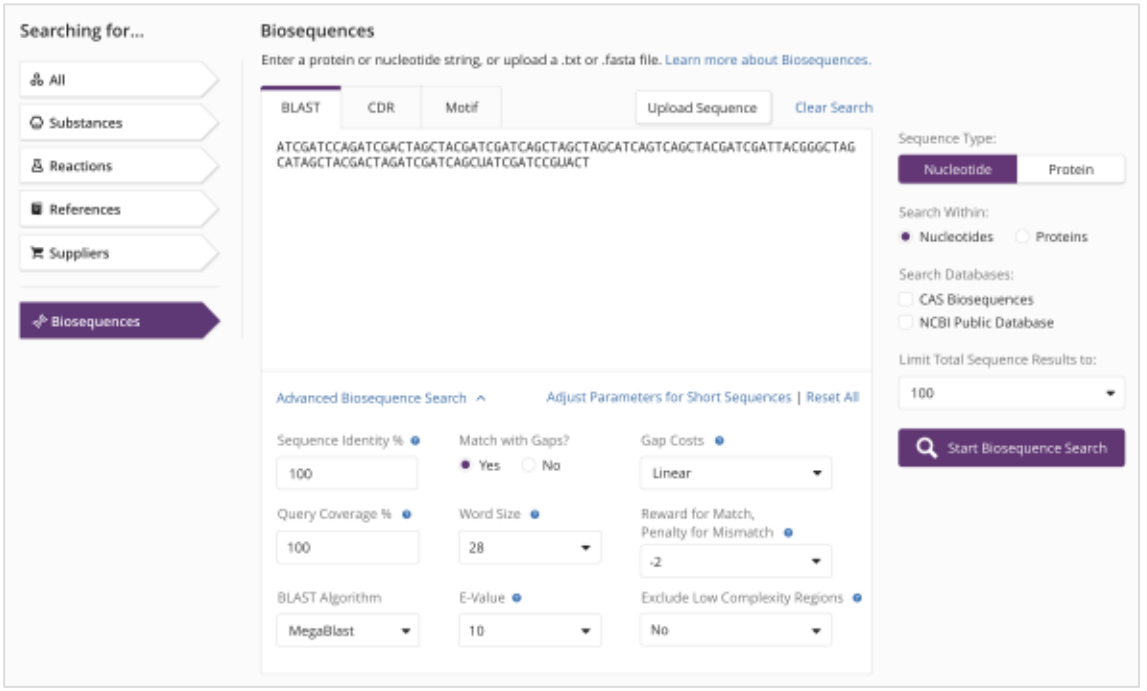
Newly enhanced collection of 500M+ proteins and nucleotides from 60+ patent authorities dating back to 1957

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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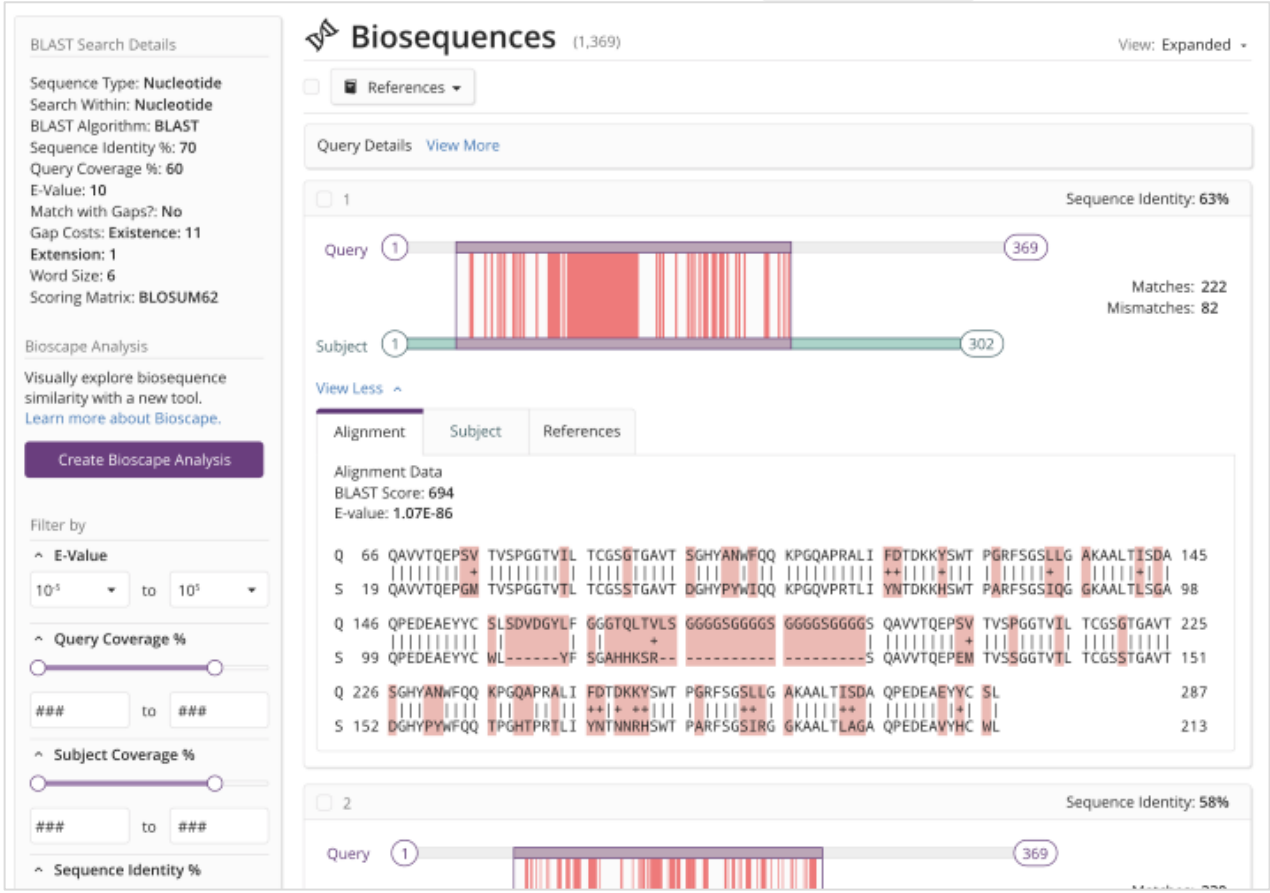
Conduct comprehensive biologics research

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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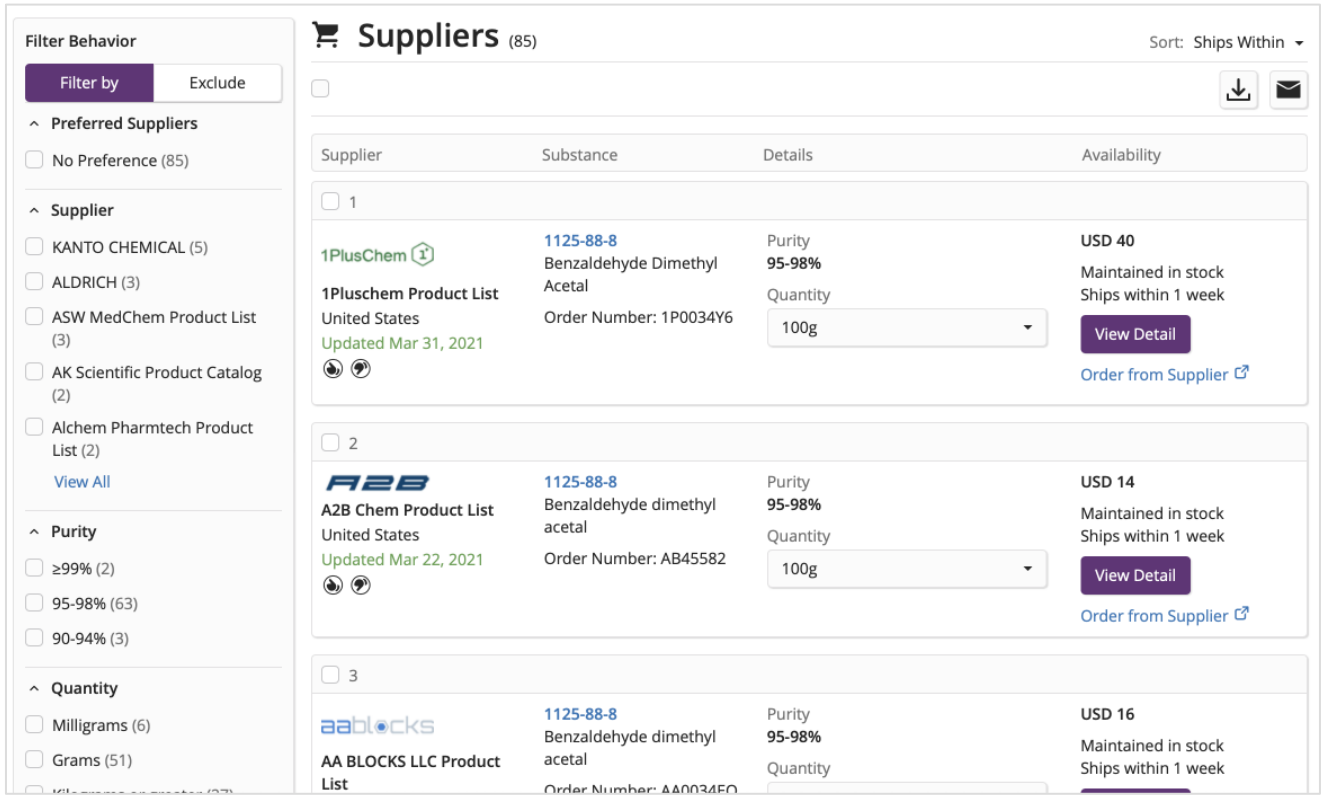
Find commercially available chemicals

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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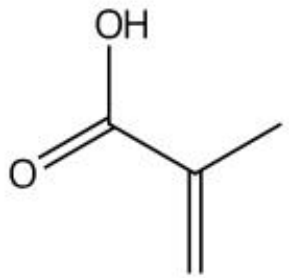
GHS Hazard Statements

CAS Registry Number: 79-41-4

References (105K) | Reactions (51K) | Suppliers (69) | Save



GHS Hazard Statements

Code	Hazard Statement	Source
H402	Harmful to aquatic life	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, Expert Curated, Japan GHS Classifications (Japanese), Merck Life Science OY (Sigma-Aldrich), Redox Pty Ltd, Sigma-Aldrich (as MiliporeSigma, Merck), Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H400	Very toxic to aquatic life	Pfaltz&Bauer
H373	May cause damage to organs through prolonged or repeated exposure	Expert Curated, New Zealand Hazardous Substances and New Organisms (HSNO) Act - Classification of Chemicals, Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H372	Causes damage to organs through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, Expert Curated, Japan GHS Classifications (Japanese), Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H370	Causes damage to organs	Expert Curated, Japan GHS Classifications (Japanese)
H350i	May cause cancer by inhalation	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H350	May cause cancer	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H341	Suspected of causing genetic defects	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria

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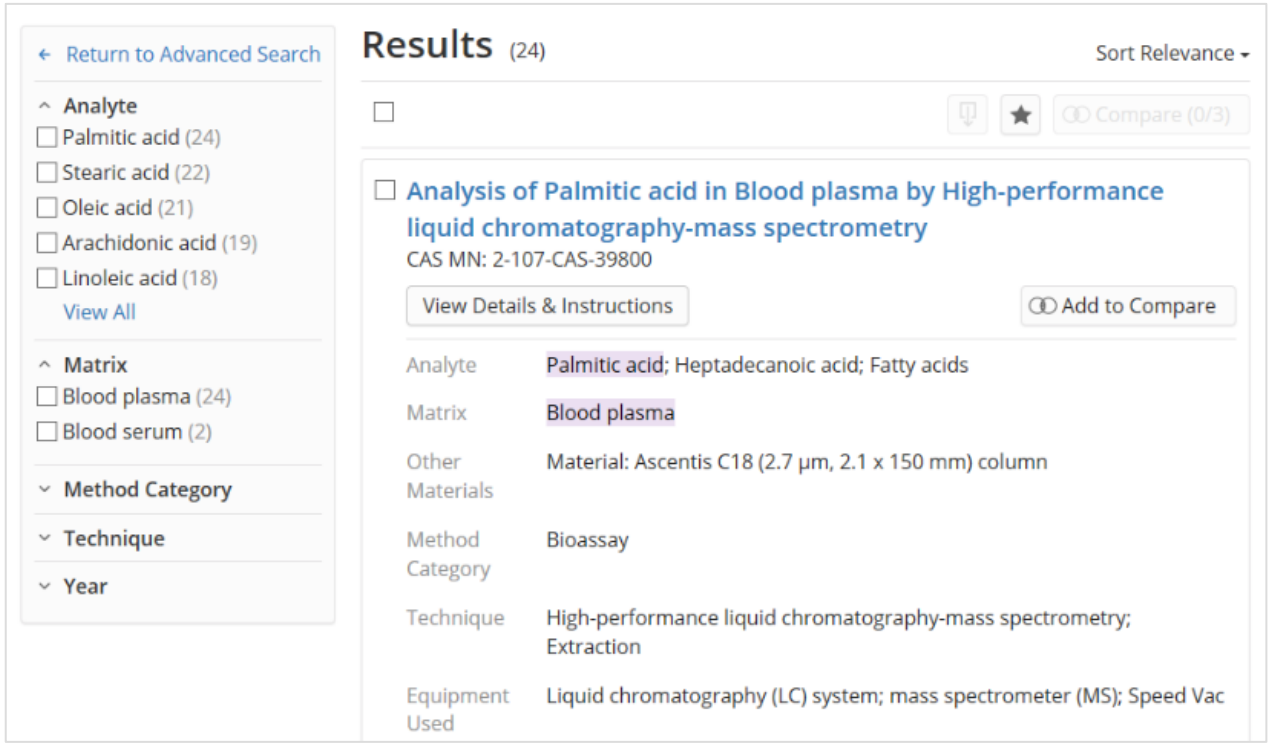

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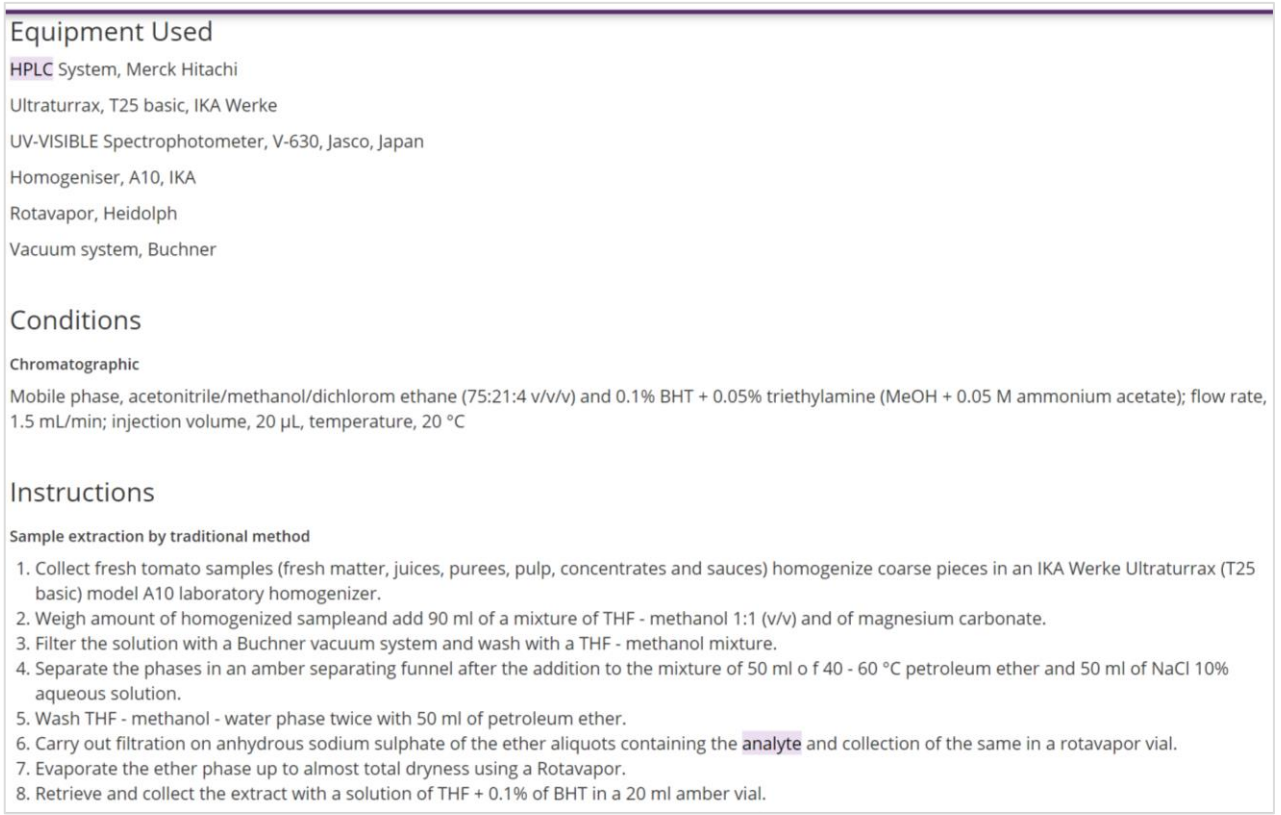

Equipment Used

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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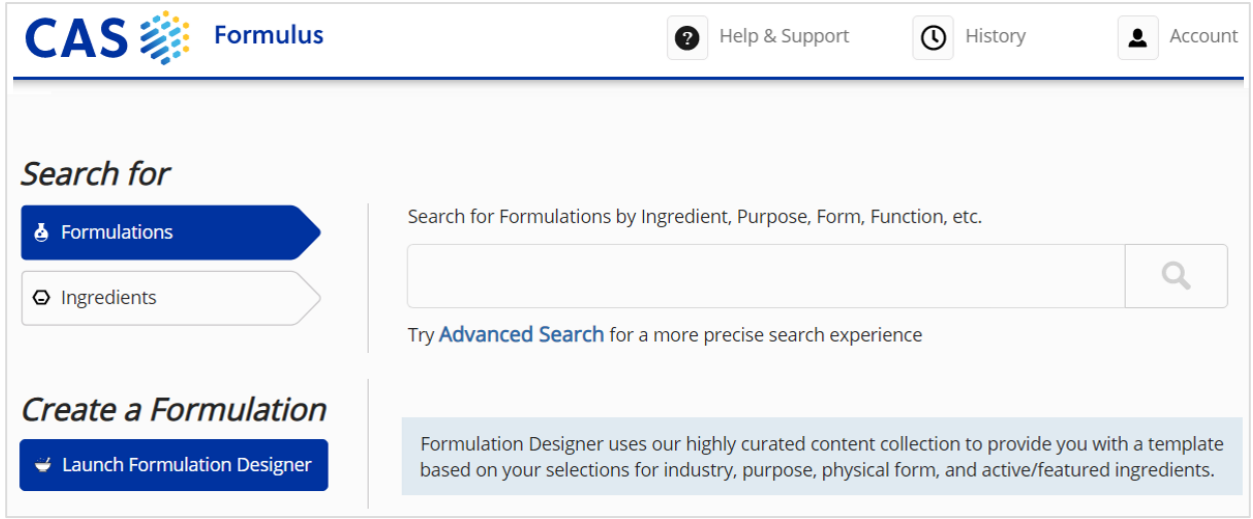

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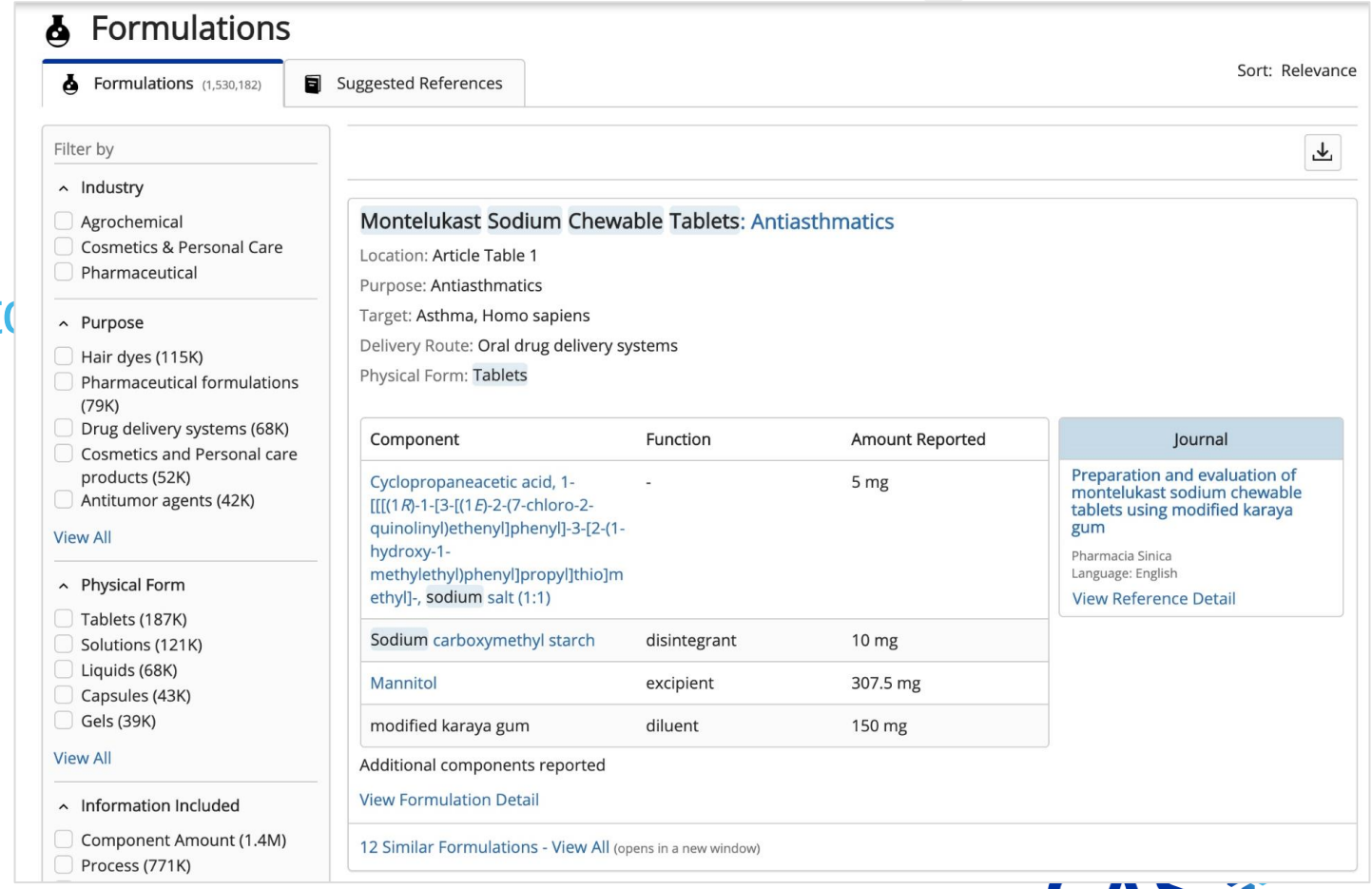

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Case:

1. Revlimid →multiple myeloma

2. Humira

藥品	2022 銷售額 (美元)	2021 銷售額 (美元)	成長率	公司	適應症
Comirnaty (tozinameran)	408億	403億	1.2%	Pfizer/BioNTech	COVID-19 mRNA疫苗
Spikevax (elasomeran)	218億	177億	23.2%	Moderna	COVID-19 mRNA疫苗
Humira (adalimumab)	216億	212億	1.9%	AbbVie	類風濕性關節炎
Keytruda (pembrolizumab)	210億	172億	22.1%	Merck & Co.	癌症免疫療法
Paxlovid(Nirmatrelvir/Ritonavir)	190億	1億	18900.0%	Pfizer	COVID-19口服抗病毒藥物
Eliquis (apixaban)	118億	108億	9.3%	BMS / Pfizer	抗凝血劑
Biktarvy (bictegravir, emtricitabine, tenofovir alafenamide)	104億	86億	20.9%	Gliead	HIV-1抗反轉錄病毒複方製劑
Eylea (aflibercept)	103億	99億	4.0%	Bayer/Regeneron	黃斑部退化病變
Stelara (ustekinumab)	101億	96億	5.2%	Janssen Biotech	中至重度斑塊性乾癬
Revlimid (lenalidomide)	100億	129億	-22.5%	BMS	多發性骨髓瘤 (MM)

資料來源：《Nature》、Statista、生策會/生策中心彙整

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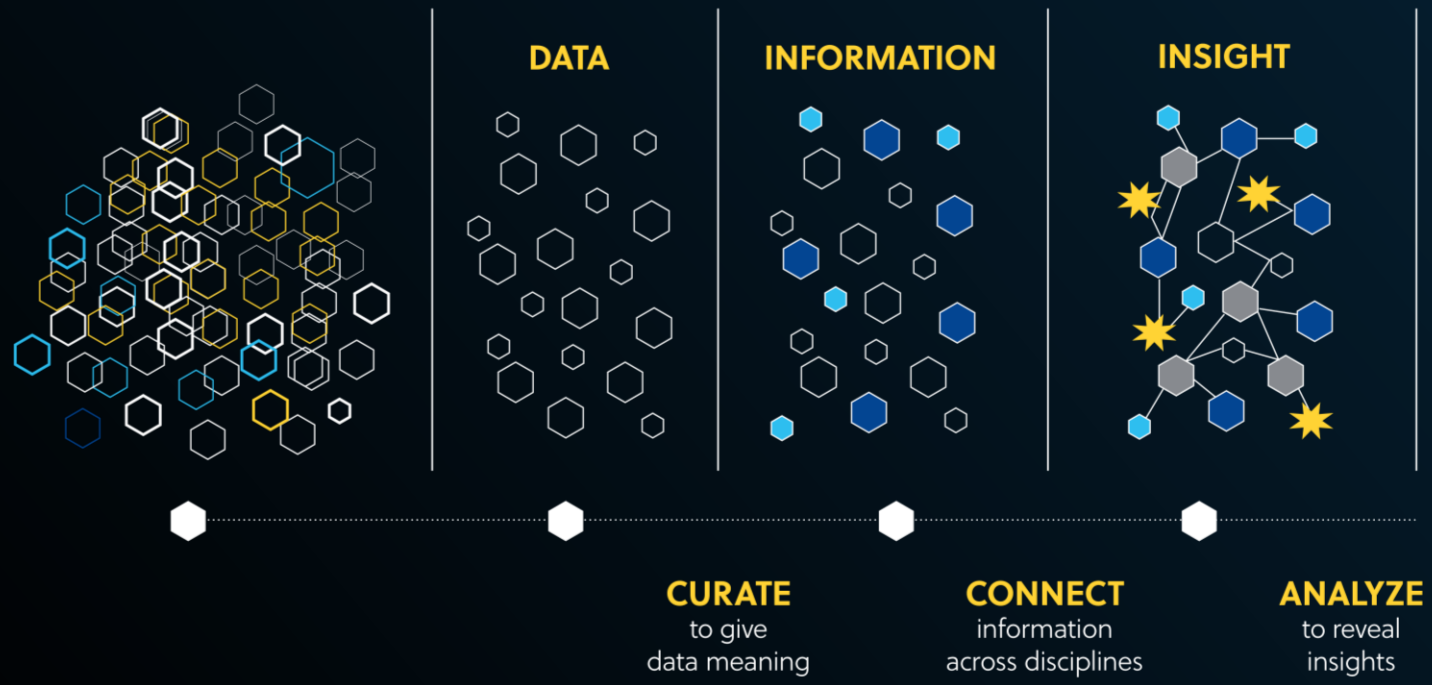

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