Chuan-Che Liu Ph.D.
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0975765358

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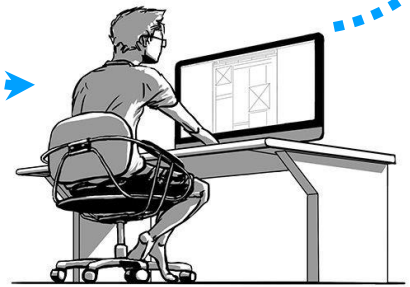

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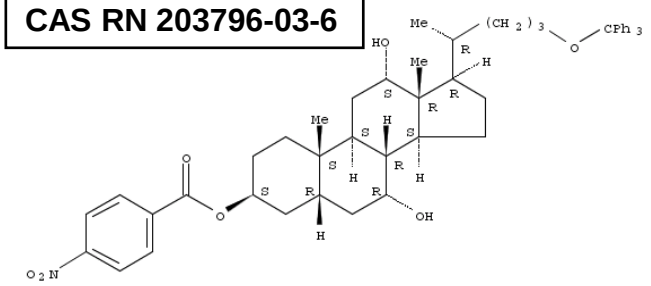
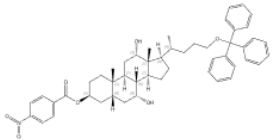
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 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, 64.22, 47.79, 46.79, 42.1 28.74, 27.71, 26.85, 26.3 (thioglycerol+Na^+ matrix

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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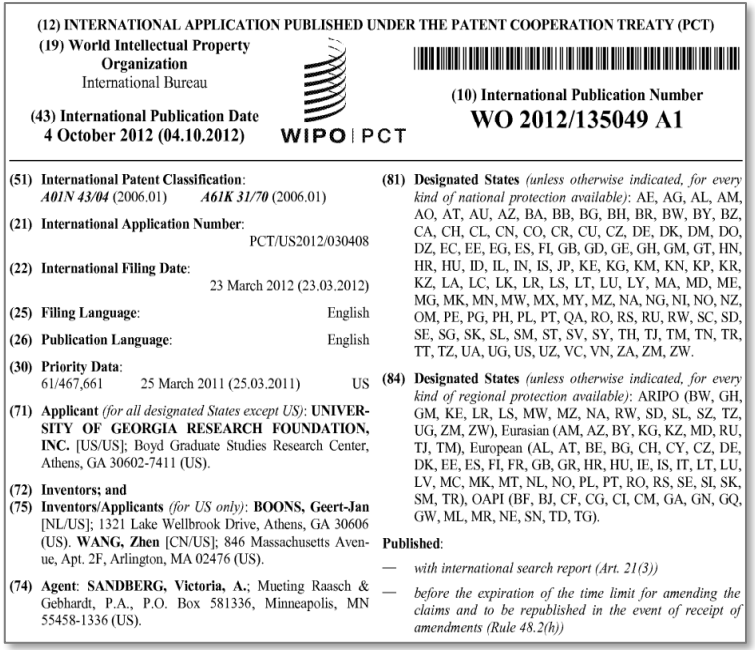

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(71) Applicant *(for all designated States except US)*: **UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC.** [US/US]; Boyd Graduate Studies Research Center, Athens, GA 30602-7411 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: **BOONS, Geert-Jan** [NL/US]; 1321 Lake Wellbrook Drive, Athens, GA 30606 (US). **WANG, Zhen** [CN/US]; 846 Massachusetts Avenue, Apt. 2F, Arlington, MA 02476 (US).

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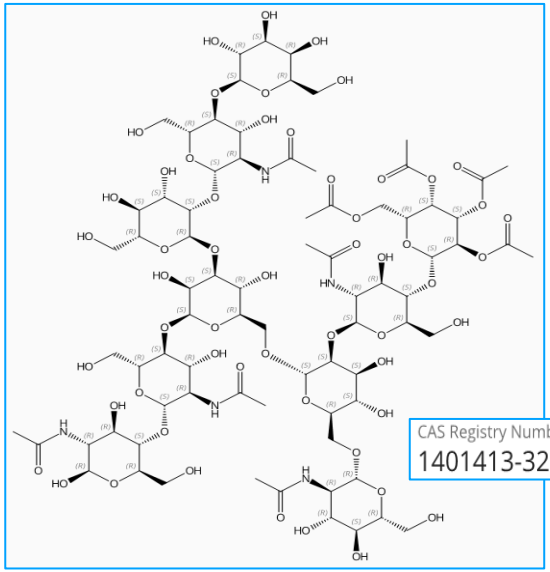

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- Reference searching
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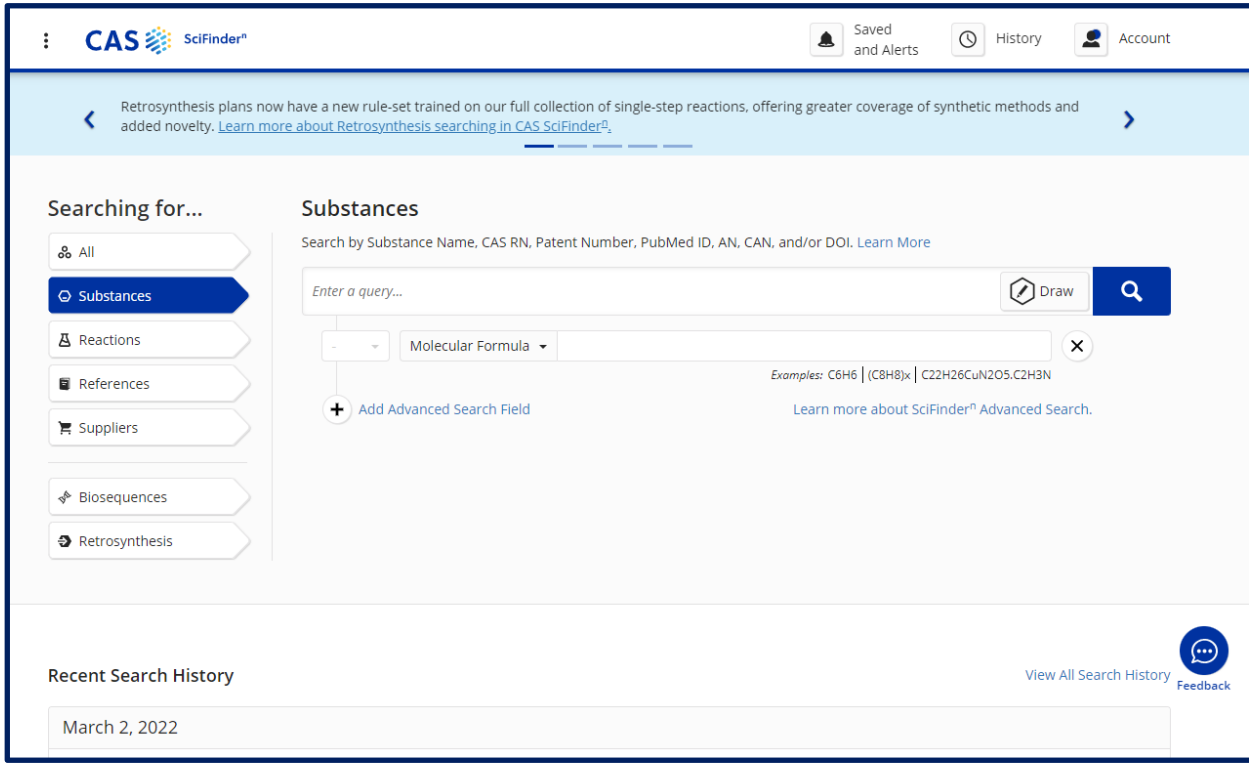

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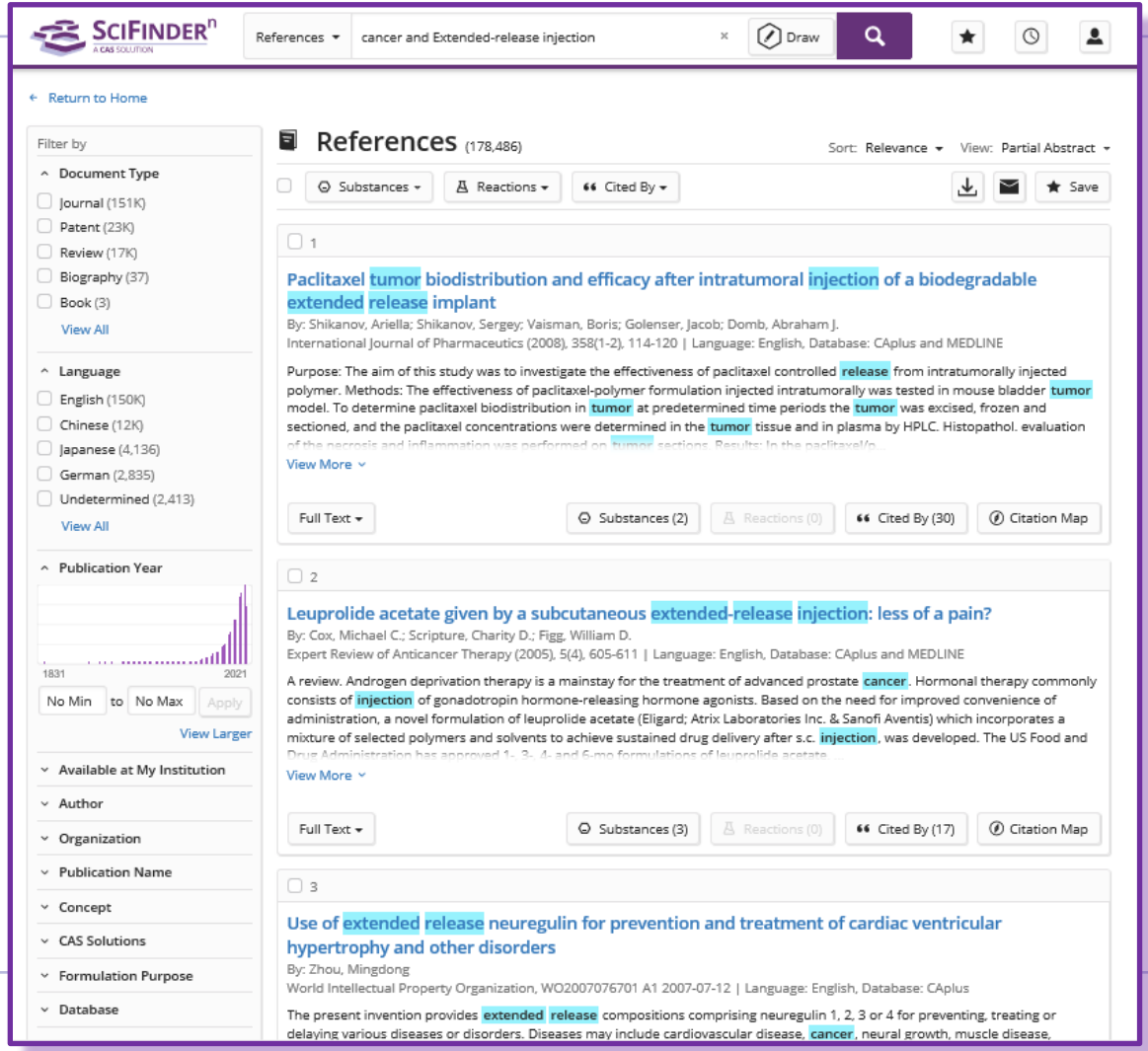

Reference Detail Page:

Reference Detail

Substances (6) | Reactions (0)

Patent

Patent Information

Patent Number
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Publication Date
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Application Number
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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

Use of ventric

By: Zhou,

The presen various dis muscular schizophre failure and reducing t differentia cytoskelet

Keywords:

PATENT

Patent F

Patent

WO2007

AU20063

CA26349

CA28413

US20070

EP19815

CN10139

Concepts

Alzheimer disease

Animal gene
Modifier: NRG1, NRG2, NRG3 ar

Role: Biological Study, Unclassif Activity; Therapeutic Use

Anti-Alzheimer agents

Antidiabetic agents

Antitumor agents

Cardiac hypertrophy

Cardiomyocyte
Modifier: growth and differentia

Cardioprotective agents

Cardiovascular disease

Cell differentiation
Modifier: cardiomyocyte

Cell proliferation
Modifier: cardiomyocyte

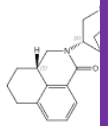
Controlled-release drug delive

Diabetes mellitus

Microspheres
Modifier: extended release neuregulin accomplished via

Substances (4)

135729-61-2

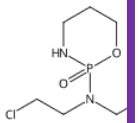


Absolute stereochemistry sh

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

Role: Pharmacological Activity Use, Biological Study, Uses

50-18-0



$C_7H_{15}Cl_2N_2O_2P$
Cyclophosphamide

Role: Adverse Effect, Includin Pharmacological Activity, The Biological Study, Uses

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

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Location: Article Page 3, 6

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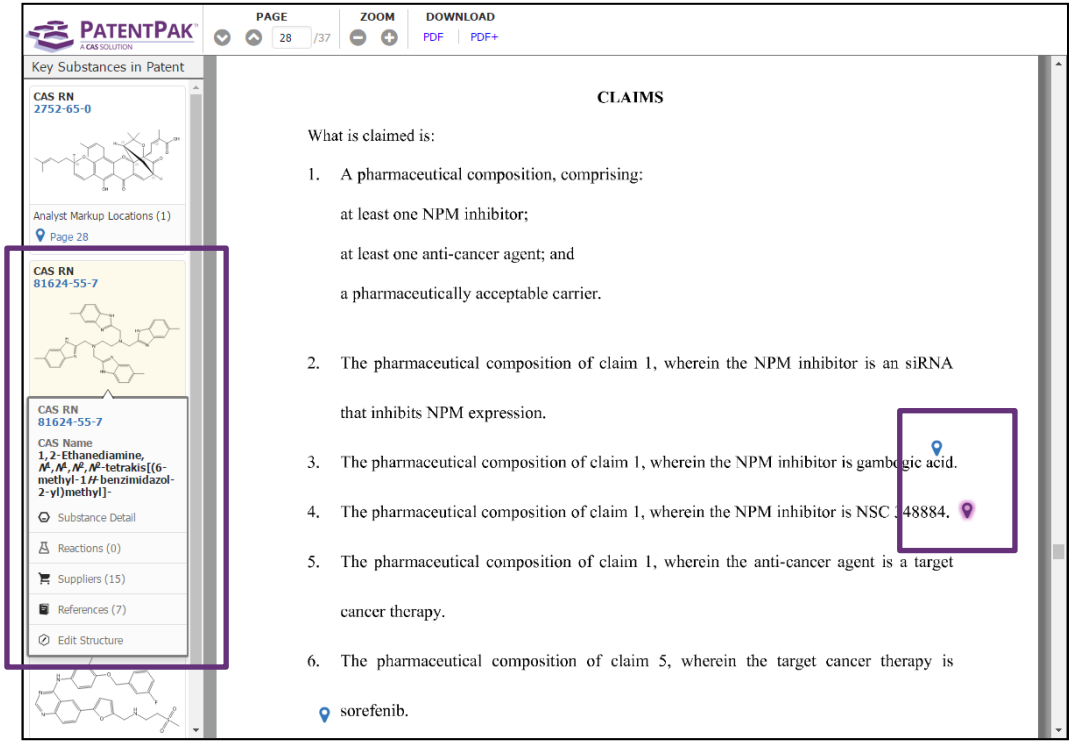

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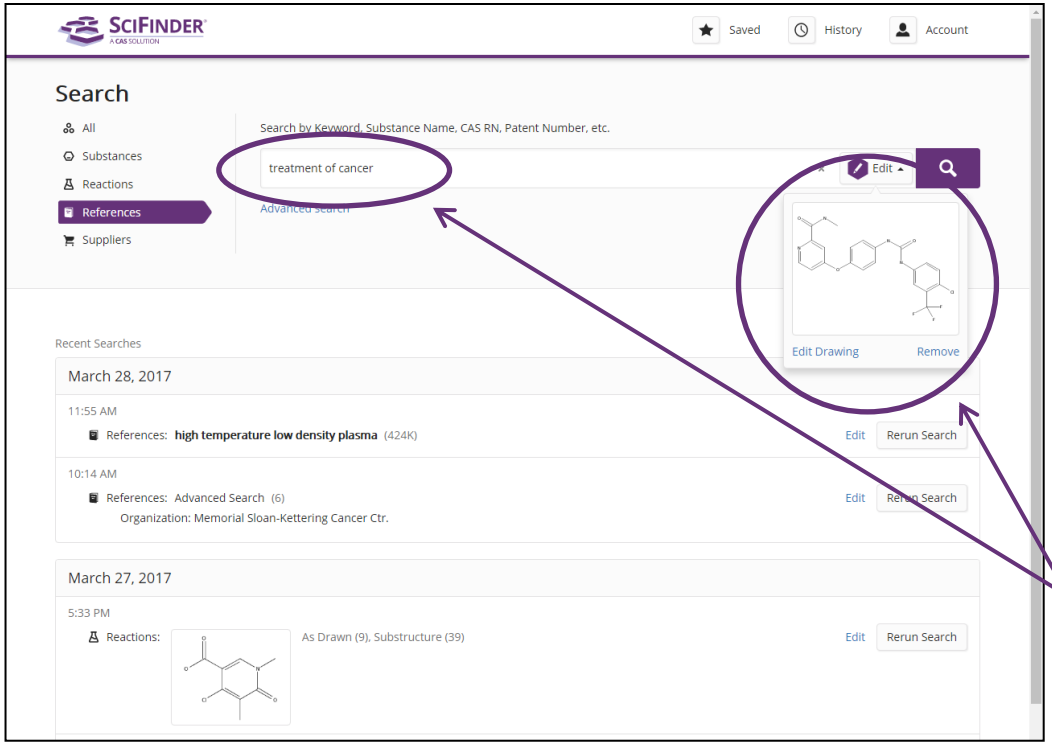

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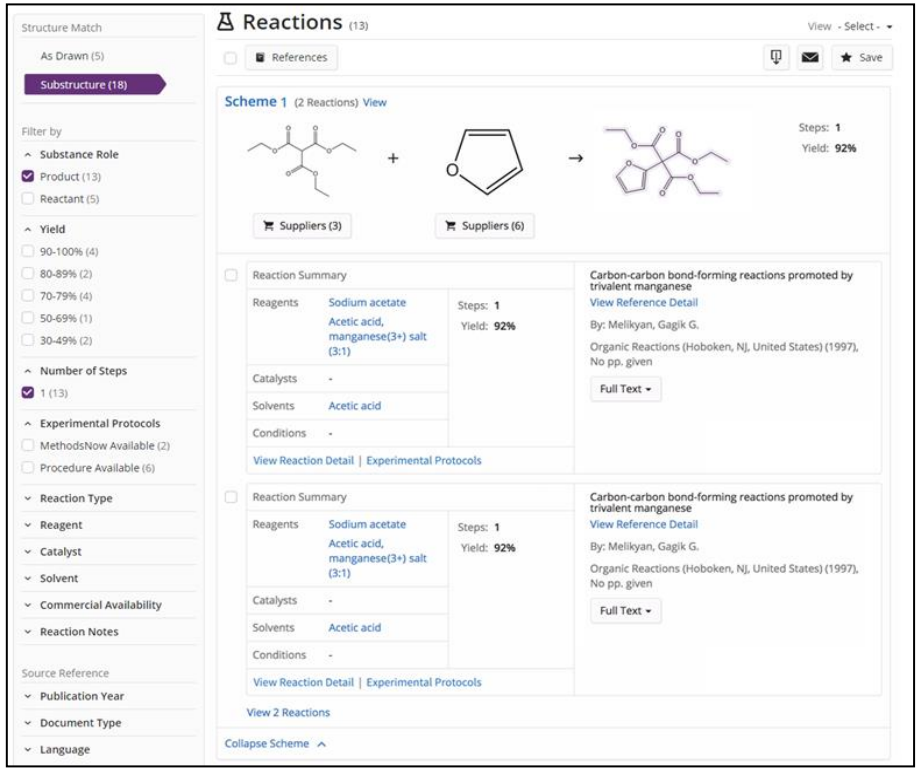

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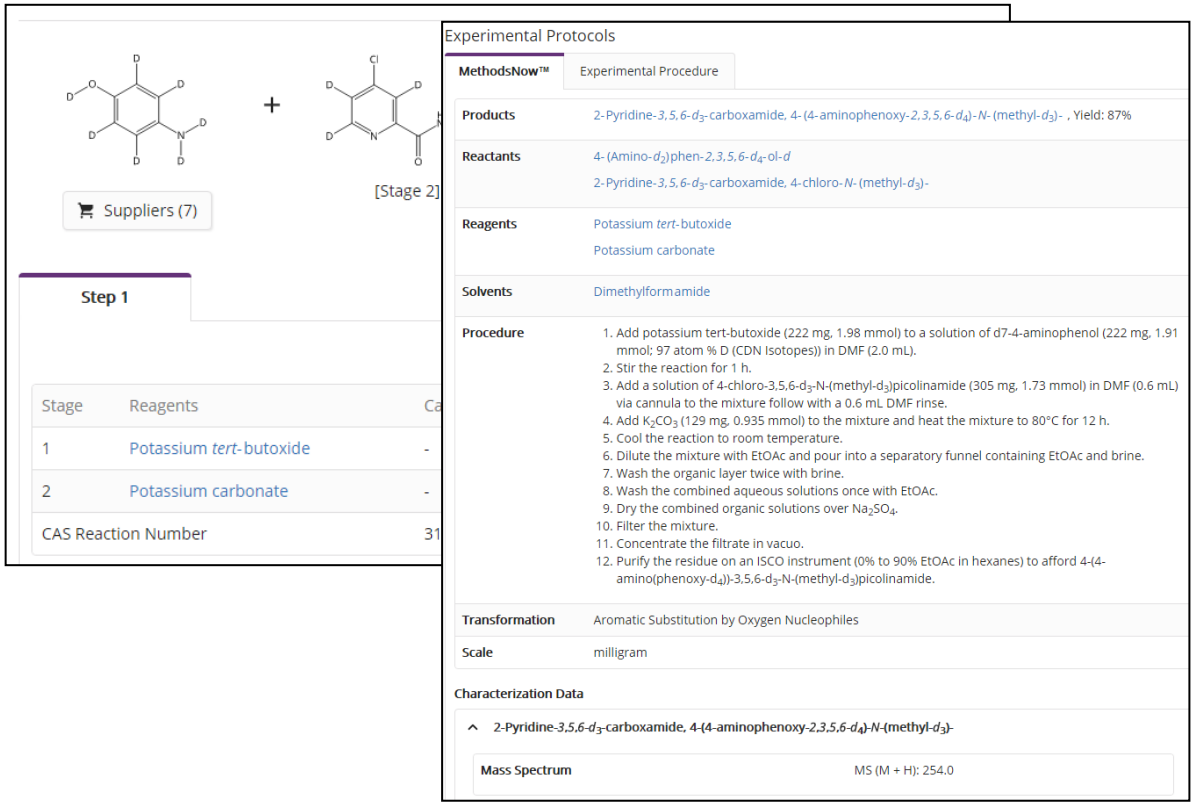
Go right to the lab with step-by-step synthetic procedures extracted and summarized from the literature



Key chemical components of the reaction are identified with links to additional information

Go directly to the lab with step-by-step instructions

Additional useful information is included

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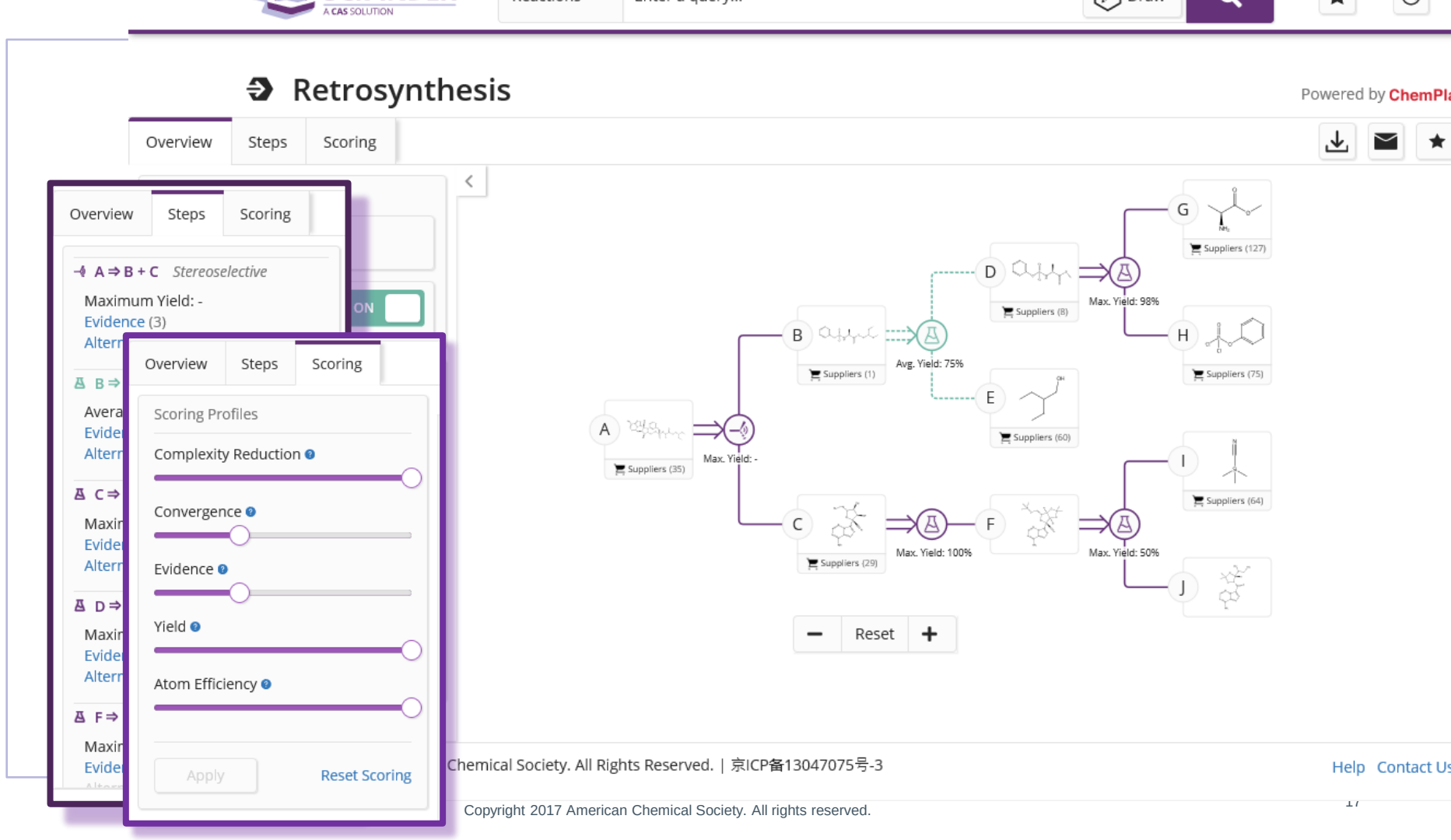
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Overview
Steps
Scoring
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Maximum Yield: -
Evidence (3)
Overview
Steps
Scoring
Scoring Profiles
Complexity Reduction
Convergence
Evidence
Yield
Atom Efficiency
Apply
Reset Scoring
A
Suppliers (35)
Max. Yield: -
B
Suppliers (1)
Avg. Yield: 75%
C
Suppliers (29)
Max. Yield: 100%
D
Suppliers (8)
E
Suppliers (60)
F
Max. Yield: 98%
G
Suppliers (127)
H
Suppliers (75)
I
Suppliers (64)
J
Max. Yield: 50%
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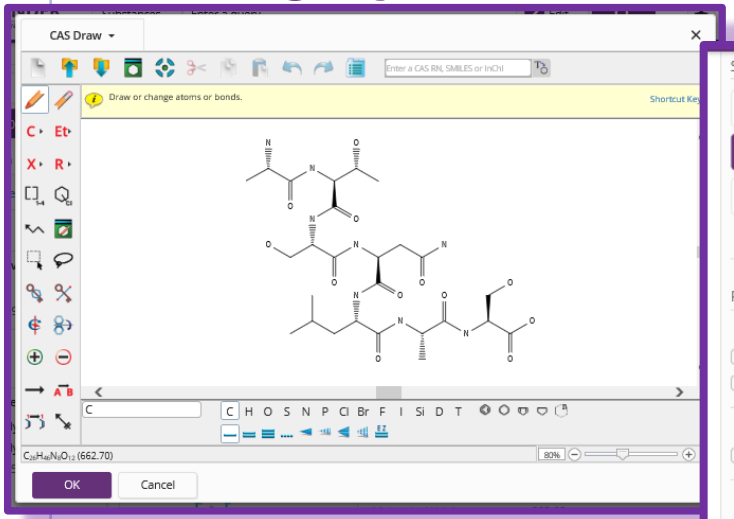

Structure Match

As Drawn (1)

Substructure (101)

Similarity (1.2M)

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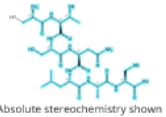


Absolute stereochemistry shown

$C_{26}H_{46}N_8O_{13}$

L-Seryl-L-threonyl-L-seryl-L-asparaginyl-L-leucyl-L-alanyl-L-serine

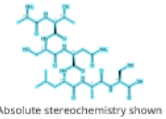
Protein/Peptide Sequence
Sequence Length: 7

247 References | 1 Reaction | 2 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	678.69	-
Boiling Point (Predicted)	1332.0±65.0 °C	Press: 760 Torr
Density (Predicted)	1.396±0.06 g/cm³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.02±0.10	Most Acidic Temp: 25 °C

2

192433-87-7



Absolute stereochemistry shown

$C_{26}H_{46}N_8O_{12}$

L-Alanyl-L-threonyl-L-seryl-L-asparaginyl-L-leucyl-L-alanyl-L-serine

Protein/Peptide Sequence
Sequence Length: 7

141 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	662.69	-
Boiling Point (Predicted)	1257.6±65.0 °C	Press: 760 Torr
Density (Predicted)	1.357±0.06 g/cm³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.02±0.10	Most Acidic Temp: 25 °C

3

167635-77-0

Key Physical Properties	Value	Condition

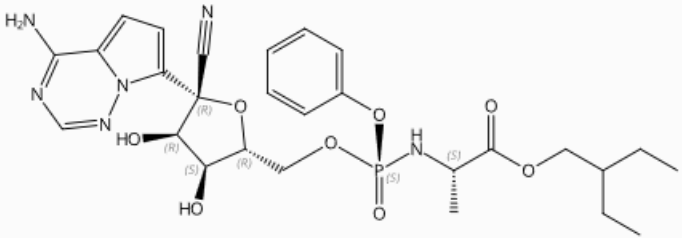
Substances Detail Page

Substance Detail (1 of 1)

← Prev Next →

References (488) | Reactions (325) | Suppliers (37) | Save

CAS Registry Number
1809249-37-3



Absolute stereochemistry shown

$C_{27}H_{35}N_6O_8P$

L-Alanine, *N*-[(*S*)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-*C*-(4-aminopyrrolo[2,1-*f*][1,2,4]triazin-7-yl)-2,5-anhydro-D-altrononitrile

Key Physical Properties	Value	Condition
Molecular Weight	602.58	-
Density (Predicted)	1.47±0.1 g/cm³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.00±0.70	Most Acidic Temp: 25 °C

Expand All |

- Other Names and Identifiers
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
  - Anti-infective agents
    - Antiviral agents (183)
- Target Indicators
  - Enzymes
    - Alanine aminotransferase (12)
    - Angiotensin-converting enzyme 2 (29)
    - Proteinase 3CLpro (11)
    - RNA-dependent RNA polymerase (30)
  - Glycoproteins
    - Viral spike glycoproteins (30)
  - Viral proteins
    - Viral spike glycoproteins (30)
- Regulatory Information
  - **Confidential Business Information:** Public
  - Regulatory Synonyms (2)
  - Details by Country/International & Other Lists
- Additional Details

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Patent Markush Match

As Drawn (71)

Substructure (1,314)

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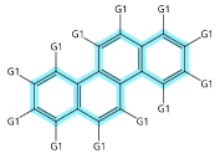
1

US20130214259



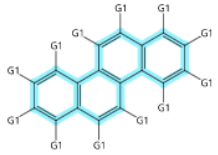
Patent claim 29

PATENTPAK | Full Text

There are no notes to display for this structure.

2

WO2009008352



Patent claim 1

PATENTPAK | Full Text

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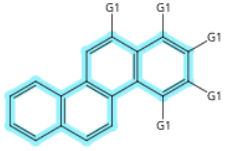
3

WO2002088025



Patent claim 2

PATENTPAK | Full Text

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PATENTPAK | PAGE 79 /100 | ZOOM | DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 5122-94-1

Analyst Markup Locations (2) Page 79 Page 82

CAS RN 591-18-4

Analyst Markup Locations (1) Page 79

CAS RN 1762-87-4

Analyst Markup Locations (1) Page 79

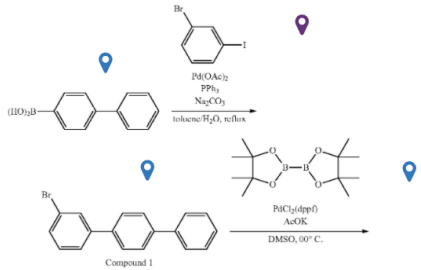
CAS RN 73183-34-3

Analyst Markup Locations (1) Page 79

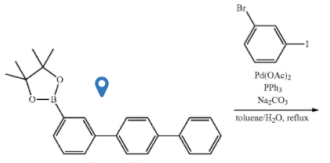
CAS RN 1401577-23-8

dures, and the like shown in the following Examples can be appropriately modified so far as the gist of the present inven-

[0281] A compound (H-1) was synthesized according to the following scheme.

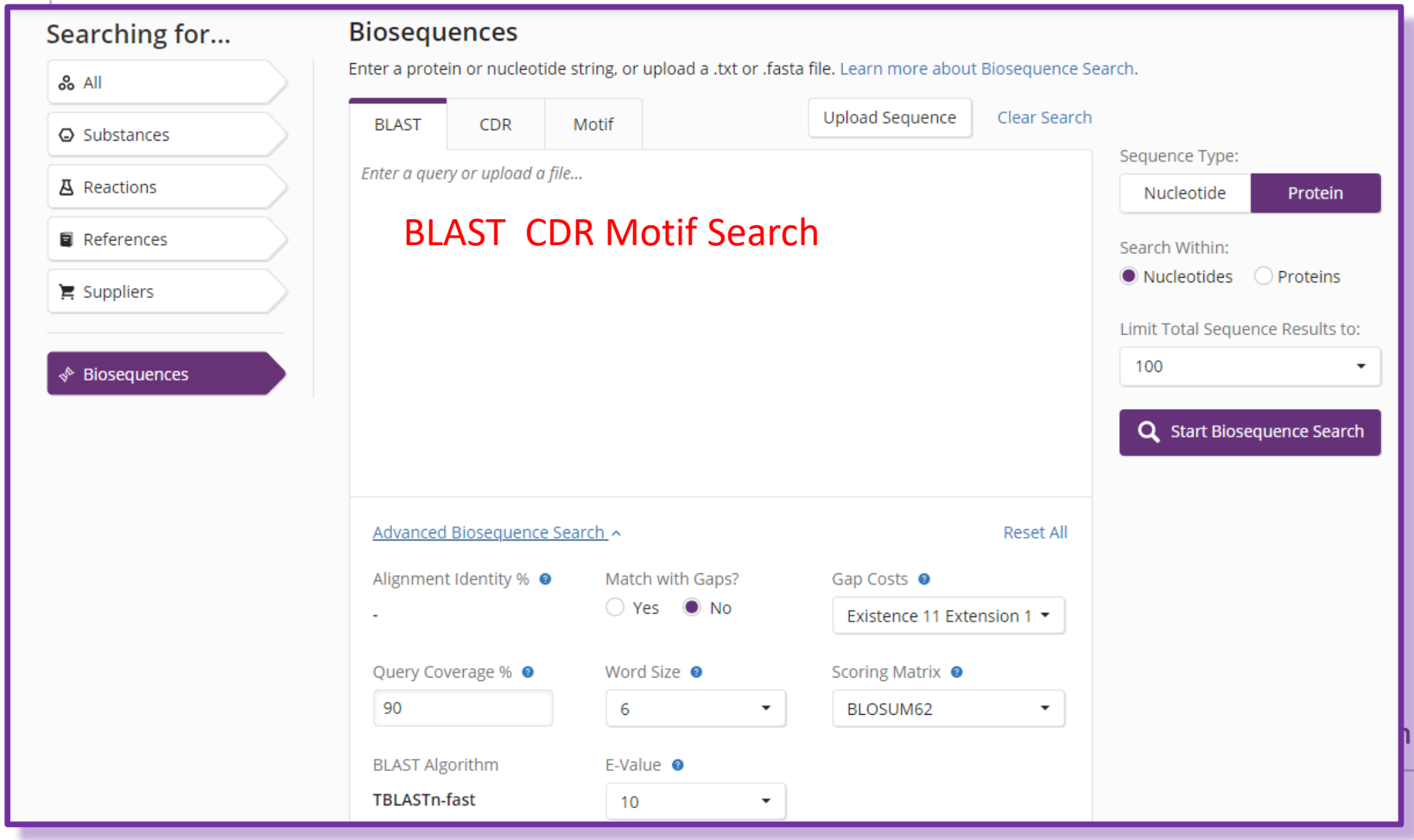


Compound 1



Compound 2

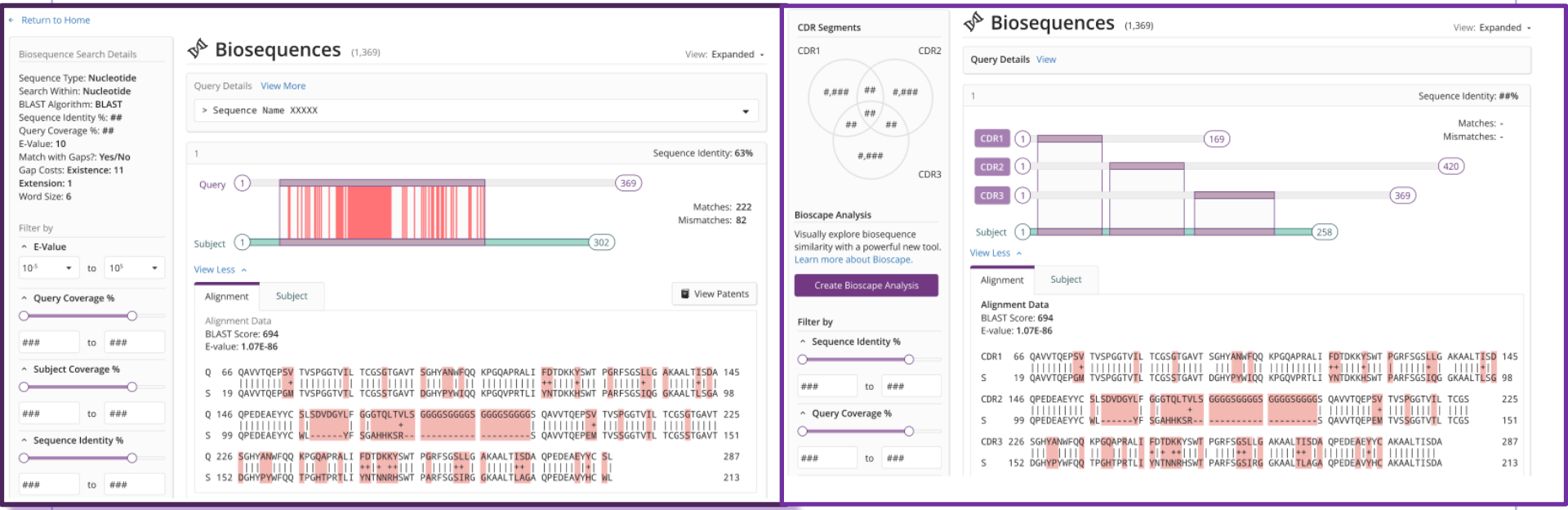
New Content & Capabilities - Sequence Search



New Content & Capabilities - Sequence Search

BLAST Display

CDR Display



SciFinder^n
A CAS SOLUTION

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Senior Account Consultant
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SciFinderN 文獻查詢

CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

Find References

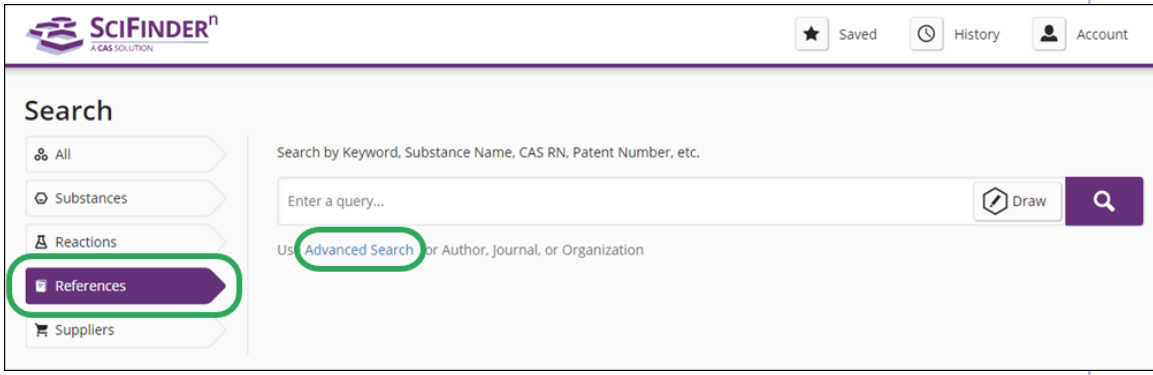
Find document references that match your query, which can be **search terms**, a **chemical structure**, or both:
•If you enter a search term **or** chemical structure query, SciFinder^n retrieves associated references, such as journal articles and patents.
•If you enter **both** a search term query and a structure query, the search results must match both criteria (queries are joined by the logical AND).

Find ADVANCED **References** by:
•**Author and Keywords**
•**A Specific Author**

Find **References Associated with a Company or Organization**

Find a **Reference Using Journal Information**

Find **Patent References** by:
•**Assignee**
•**Inventor**



SciFinder^n
A CAS SOLUTION

Find References Using Search Terms

Search terms may be:

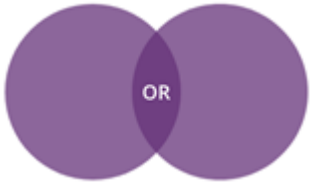
- **Research Topic/Keyword/Concept** (e.g., analgesics)
- **Substance Name** (e.g., ibuprofen, ß-amyloid)
  Note: If your search term contains a Greek letter, see Greek Letters Used in Searching to insert the correct character.
- **CAS Registry Number** (with dashes, e.g., 51146-57-7)
- **Accession Number** (e.g., 1986:230471)
- **PubMed ID Number** (e.g., 15980585)
- **Digital Object Identifier (DOI)** (e.g., 10.1093/nar/gki470)
- **Patent Number** (no spaces, e.g., US4571400)
- **Patent Application Number** (with dash, e.g., US1984-682902)

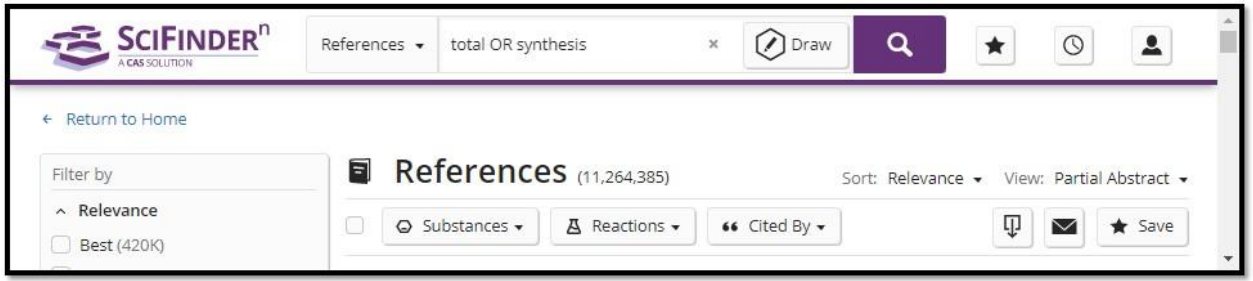
Note: You may enter multiple numbers separated by a space, no commas or other punctuation. The search field has a 2000-character limit.

SciFinder^n
A CAS SOLUTION

There are a total of five basic Boolean search operators:

- OR
  - The OR operator will provide results that contain either of the keywords
  - Will provide results that contain either of the terms
  - This is the default search when no operators are present in the search query
  - total OR synthesis





Examples:

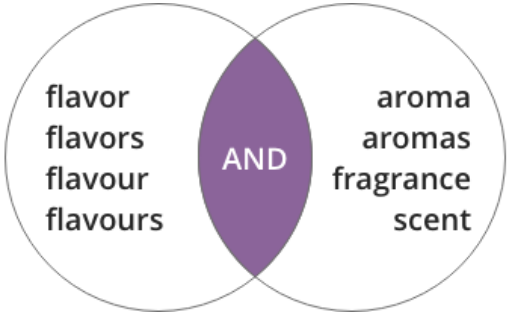
- ("flavor" **or** "extract") and ("turmeric" **or** "curcumin")
- (flavor not dye) **or** extract
- 13463-67-7 **or** 7664-41-7

SciFinder n
A CAS SOLUTION

•AND

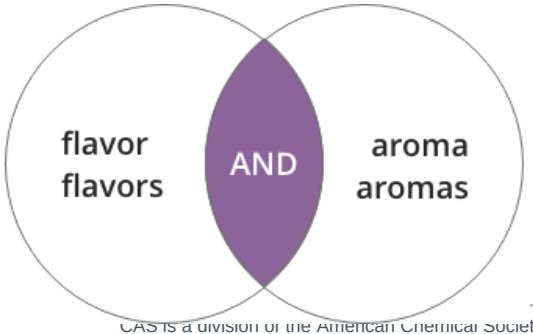
The **and** operator returns any combination of the terms' plurals, synonyms, or alternate spellings.

Example: The query **flavor and aroma** returns only results that **contain plurals/synonyms/alternate spellings of both terms**.



Entering terms in quotation marks to create a bound phrase **narrows the term to include**.

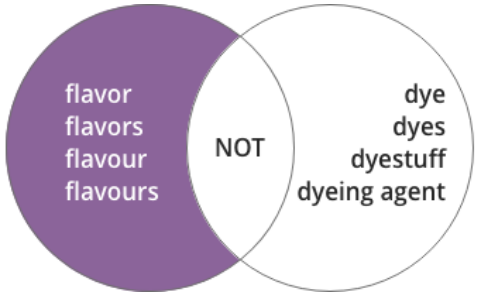
Example: The query **"flavor" and "aroma"** returns only results that **contain the exact spelling (includes plurals) of both terms**.



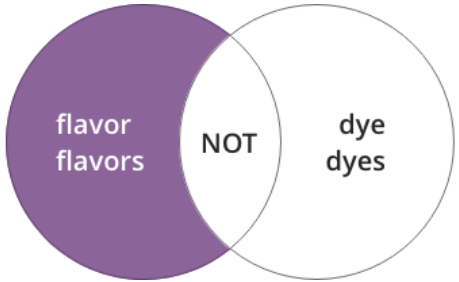
SciFinder^n
A CAS SOLUTION

•NOT

The **not** operator excludes any combination of the terms' plurals, synonyms, or alternate spellings.
Example: The query **flavor not dye** returns results that **contain plurals/synonyms/alternate spellings of flavor** but **excludes** those that **contain plurals/synonyms/alternate spellings of both flavor and dye**.



Entering terms in quotation marks to create a bound phrase **narrows the term to exclude**.
Example: The query **"flavor" not "dye"** returns results that **contain flavor(s)** but **excludes** those that **contain both flavor(s) and dye(s)**.

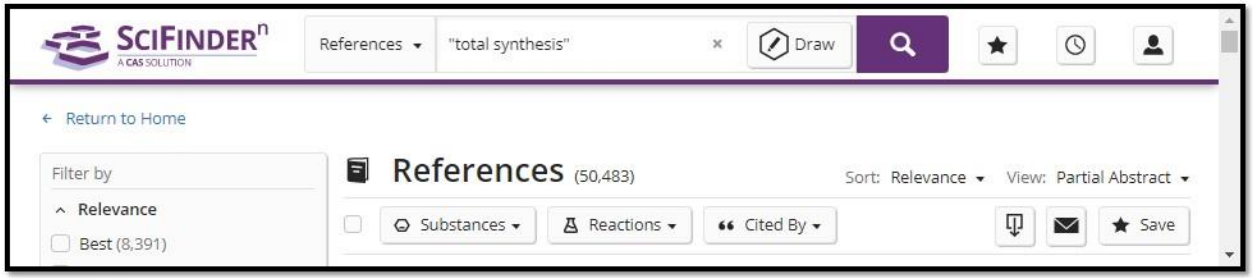


SciFinder^n
A CAS SOLUTION

- “”

  - Quotation marks means you are searching for a specific phrase
  - Will provide results that contain the exact phrase and will not return references with uses of these keywords on their own
  - “total synthesis”

"term"



Entering terms in **quotation marks** **creates a bound phrase that specifies an exact spelling** (plurals accepted, but no alternative spellings or synonyms) **and side-by-side relationship**.

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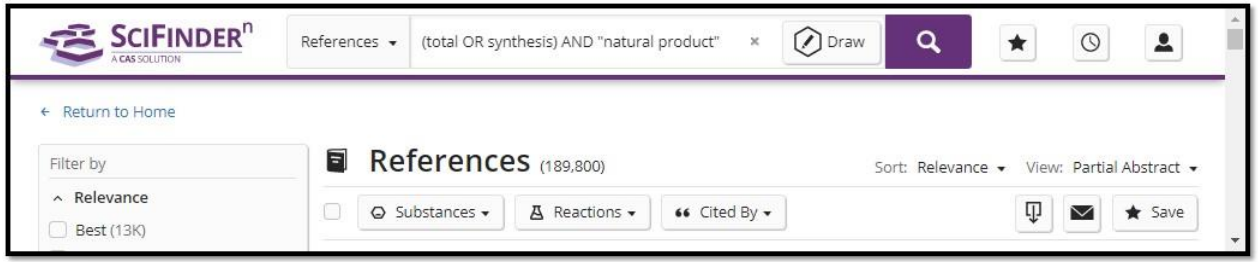
A CAS SOLUTION

• ()

- Parentheses can be added to allow the user to combine Boolean operators
- (total OR synthesis) AND “natural product”



Entering terms and operators in **parentheses** **creates an expression that functions as a single unit** that interacts with other terms.

Examples:

- **(**extract not flavor**)** and **(**"turmeric" or "curcumin"**)**
- **((**turmeric or flavonoids**)** and immune cells**)** not inflammatory

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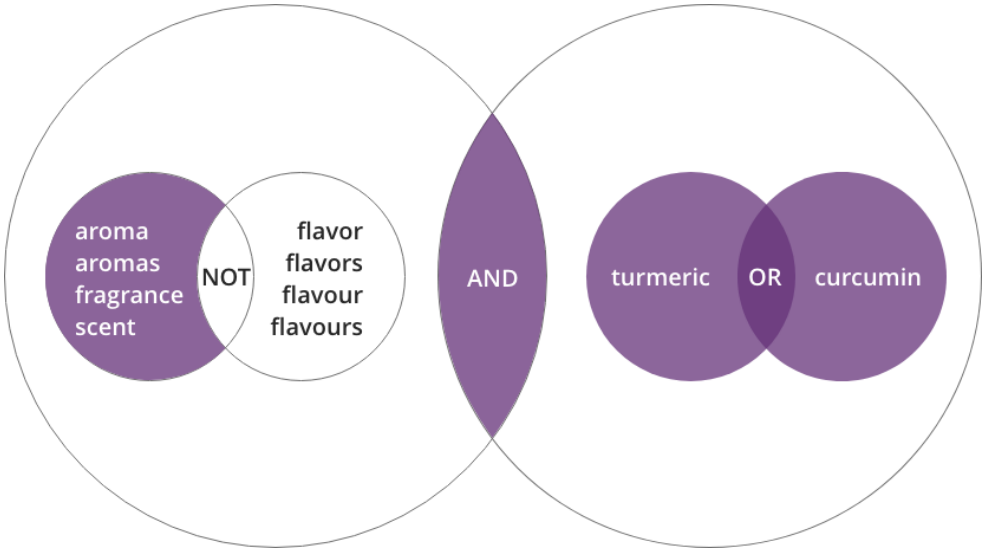
Boolean Modifier: ( )

Enclosing **terms and a Boolean operator within parentheses creates a Boolean expression that functions as a single unit/condition** that can interact with other terms, expressions, phrases, and operators.

Example: The query **(aroma not flavor) and ("turmeric" or "curcumin")** returns only results that **contain plurals/synonyms/alternate spellings of aroma, but not plurals/synonyms/alternate spellings of flavor and also contain turmeric, curcumin, or both**.



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A CAS SOLUTION

Syntactic Reference Text Wildcard Searching * ?

You may search references using the asterisk (* - match 0 or more characters) and question mark (? - match 0 or 1 character) wildcard characters.

Wildcard queries search a reference's:

•Title

•Abstract

•Keywords

•Substances/Medline Chemicals

•CAplus Concepts

Notes:

•Wildcards **contained within quotes are ignored**.

•Wildcards **do not find two terms that a separated by a space** (for example, *water?based* will find *water-based* but not *water based*).

The following wildcard characters will be supported:

- * - Used to match 0 or more characters
- ? - Used to match 0 or 1 character

Wildcard characters can be used within a term (infix) or at the end of a term (terminal).

- Leading wildcard characters are not supported and will be ignored in a query.

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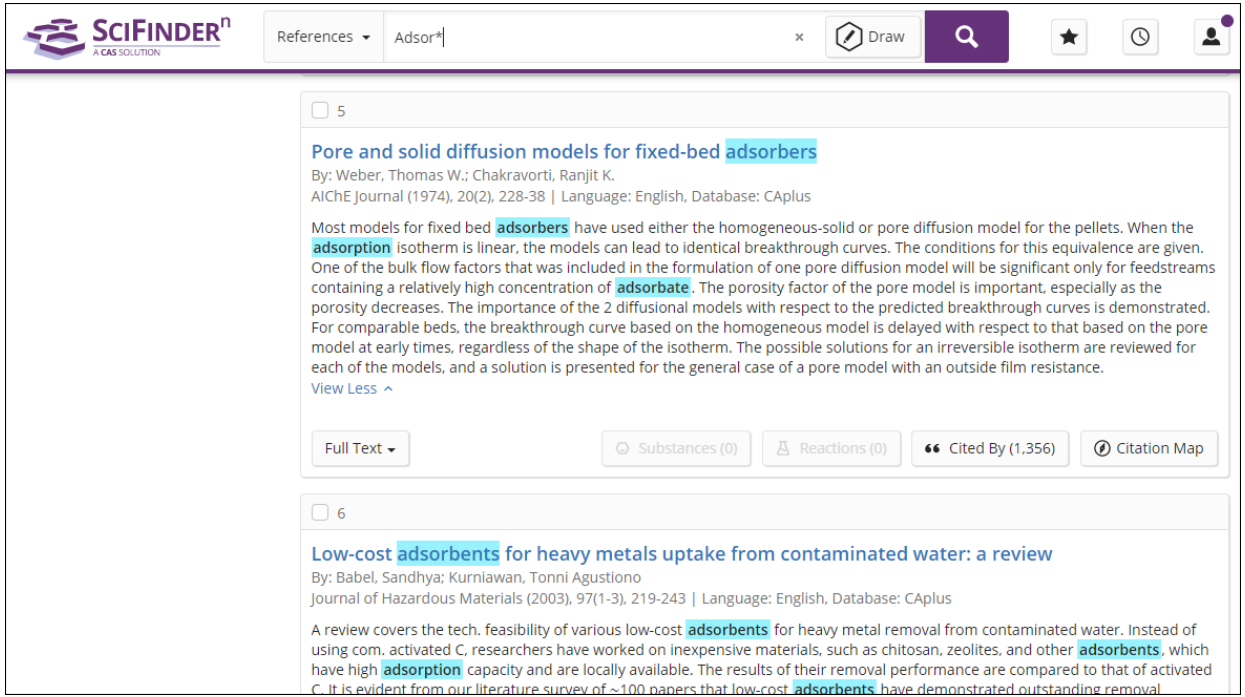
Examples

The query **Adsor*** will match terms such as:

- **Adsorbents**
- **Adsorbers**
- **Adsorption**



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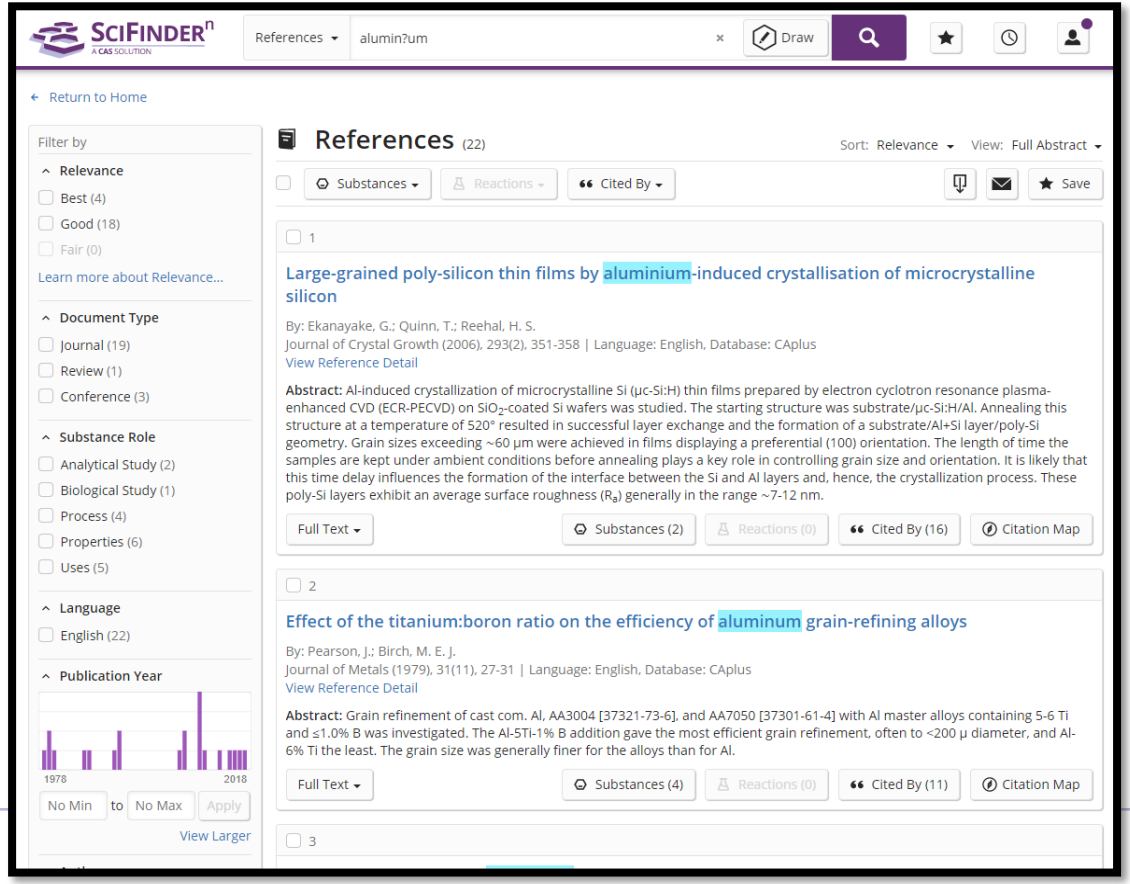
A CAS SOLUTION

Examples

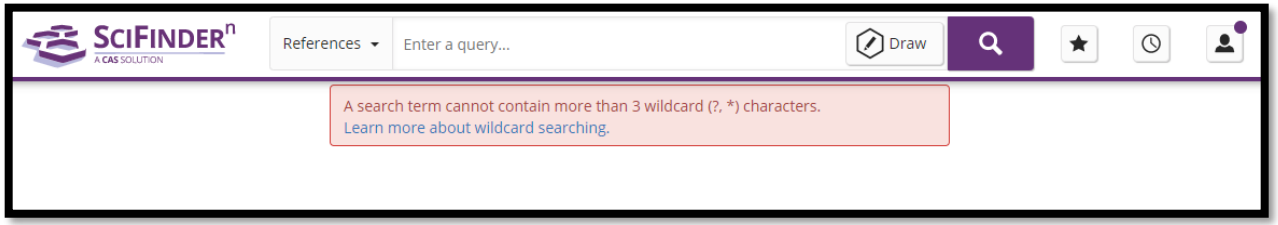
The query alumin?um will hit on terms such as

- Aluminum
- Aluminium
- Etc.



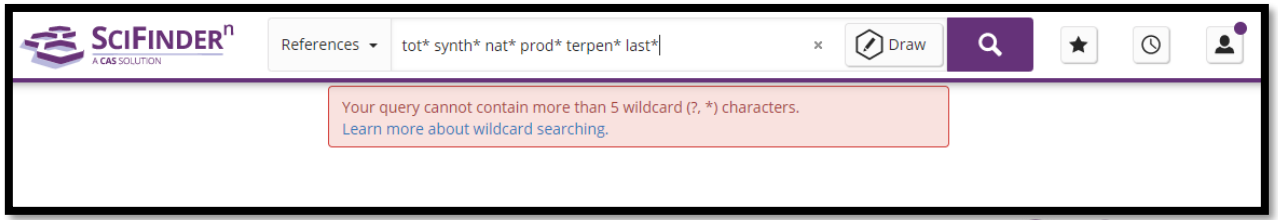
Exceptions:

- A term must have at least 3 non-wildcard characters for a wildcard to be searched
  - If a term has less than 3 non-wildcard characters, any wildcard terms will be searched literally.
- A search term cannot contain more than 3 wildcard characters
  - Currently, searchers will be provided with an error message for this scenario.



- In a subsequent build, terms with more than 1 wildcard character will be searched literally and the user will be provided with an informational message.

A search cannot contain more than 5 wildcard terms.



SciFinder
A CAS SOLUTION

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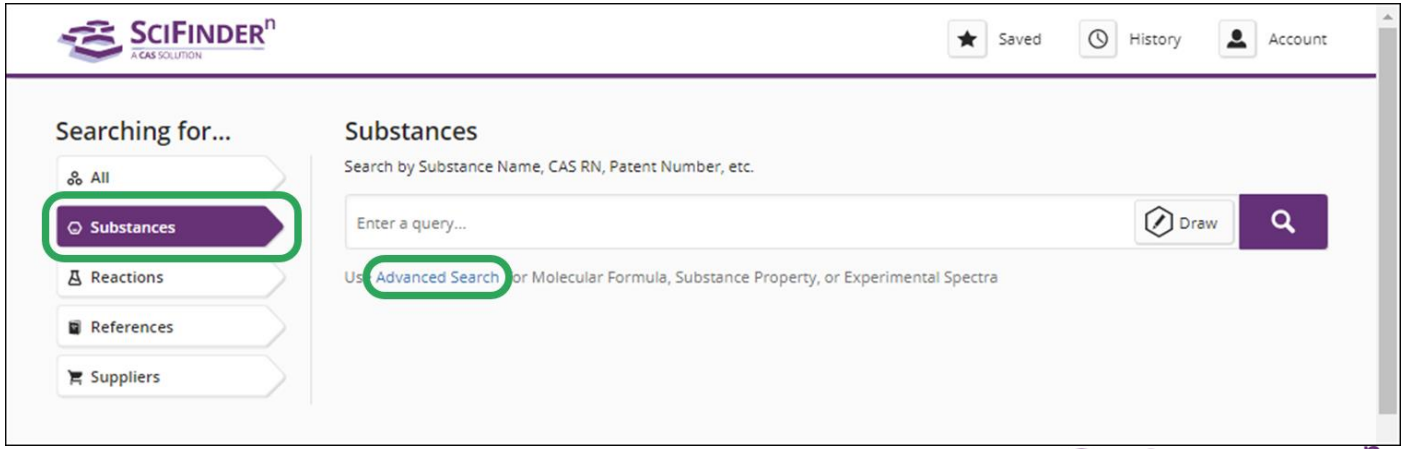
Senior Account Consultant
tliu2@acs-i.org

Substance Searching

CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

Find Substances

- Find substances that match your query, which can be substance names, CAS Registry Numbers, document identifiers, or a chemical structure:
- **Find Substances by Substance Name, Registry Number, or Document Identifier**
- **Find Substances by Chemical Structure**
- ***Note:*** If **both search term and chemical structure queries are present**, substances will **only match the chemical structure query (search term query is ignored)**.
- Click **Advanced Search** to find substances by **molecular formula**, **substance property**, and **experimental spectra**.



SciFinder n
A CAS SOLUTION

Find Substances by Name, Registry Number, or Document Identifier

Search terms may be:

•**Substance Name:**

- **Example:** benoxaprofen
  Note: Wildcard searching using an asterisk only works for single-search-term, single-word substance name searches (e.g., benoxa*). Partial substance names without a wildcard character will not return results.
- **Example:** methyl ethyl ketone
  Note: For an exact match, use double quotes around the substance name. Searching multiple word substance names without quotes also returns results matching part of the name. For example, searching the above example without double quotes returns methyl ethyl ketone, methyl, ethyl ketone, and ethyl.
- **Example:** ß-amyloid
  Note: If your search term contains a Greek letter, see Greek Letters Used in Searching to insert the correct character. to insert the correct character.

•**CAS Registry Number** (with or without dashes, e.g., 51146-57-7, 51146577)
Note: Square brackets are accepted around RNs (e.g., [51146-57-7], but not single or double quotes.

•**Document Identifier:**

- **Patent Number** (no spaces, e.g., US4571400)
- **Accession Number** (e.g., 1986:230471)
- **PubMed ID Number** (e.g., 15980585)
- **CAS Accession Number (CAN):** document number in CA Plus (e.g.,148:486341)

SciFinder^n
A CAS SOLUTION

Wildcard searching for substance (Lactobacillus*)

【常見益生菌乳酸菌中英文名對照表 / 市售益生菌乳酸菌中英文名對照】

乳酸桿菌屬 Lactobacillus	簡稱	關於
嗜酸乳桿菌（Lactobacillus acidophilus）	A菌	如優格等發酵乳製品就含有豐富的嗜酸乳桿菌。這種益生菌能協助免疫系統保持腸道細菌的平衡。女性多攝食嗜酸乳桿菌有助於抑制白色念珠菌造成的陰道炎。嗜酸乳桿菌還能調節體內的膽固醇濃度，能在小腸中產生可對抗病原微生物的有益物質。
乾酪乳桿菌（Lactobacillus casei ）	C菌	相當耐酸，能有效地通過胃酸膽鹼的考驗，而有規模的進入腸道定殖。
約氏乳桿菌（Lactobacillus johnsonii ）	LJ菌	健康新生兒之消化道中分離純化，屬人體原生菌種。Salivarius意指“腺體型”最初是由人類腺體中被發現，是人體消化道中的原生菌種，亦是美國食品藥品監督管理局（FDA）表列安全菌種之一。
副乾酪乳桿菌（Lactobacillus paracasei ）	LP菌	耐胃酸及膽鹽，在腸道中定殖效果良好，能促進體內Th1細胞激素分泌，抑制Th2細胞所造成的敏感免疫反應，達到免疫系統平衡。對於異位性皮膚炎等過症狀可能有療效。
鼠李糖乳桿菌GG株（Lactobacillus rhamnosus GG）	LGG菌	是當前世界上研究最多的益生菌，也是首批被證實能夠在人體腸道存活並定殖的益生菌之一。可在血清中增加足夠的細胞間白素-10，降低引起局部性敏感免疫反應的細胞激素形成。能促進益菌生長、降低對乳品或食物的過敏、治療不明原因或急性腹瀉功能等。
洛德乳桿菌（Lactobacillus reuteri ）	R菌	是少數在成人與嬰兒體內皆可發現到的乳酸菌之一，可幫助寶寶腸道細胞的生長，促進益菌繁殖。

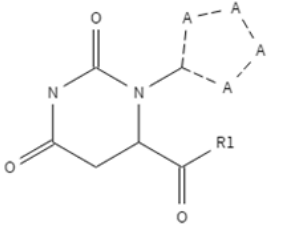
乳酸桿菌屬 Lactobacillus	簡稱	關於
發酵乳桿菌（Lactobacillus Fermentum）	LF菌	常見於發酵動物和植物材料，用作益生菌的商品化發酵乳桿菌菌株包括PCC， ME-3 和 CECT5716。

Find Patent Markush Structures

Use a **Patent Markush** search to find structures (including generic structures) matching your query within patent references.

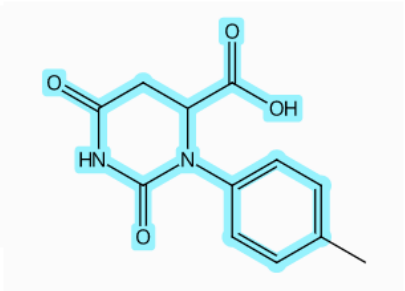
For example:

Query

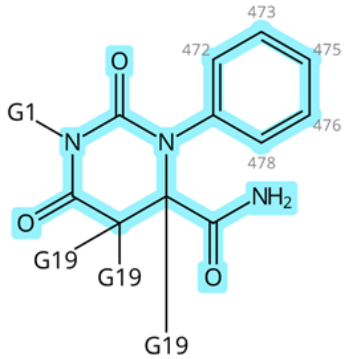


R1 = H, OH, NH_2

Substructure Match

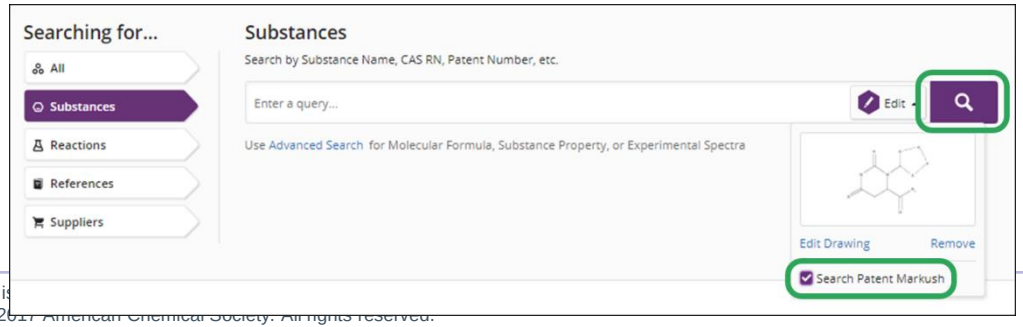


Markush Match

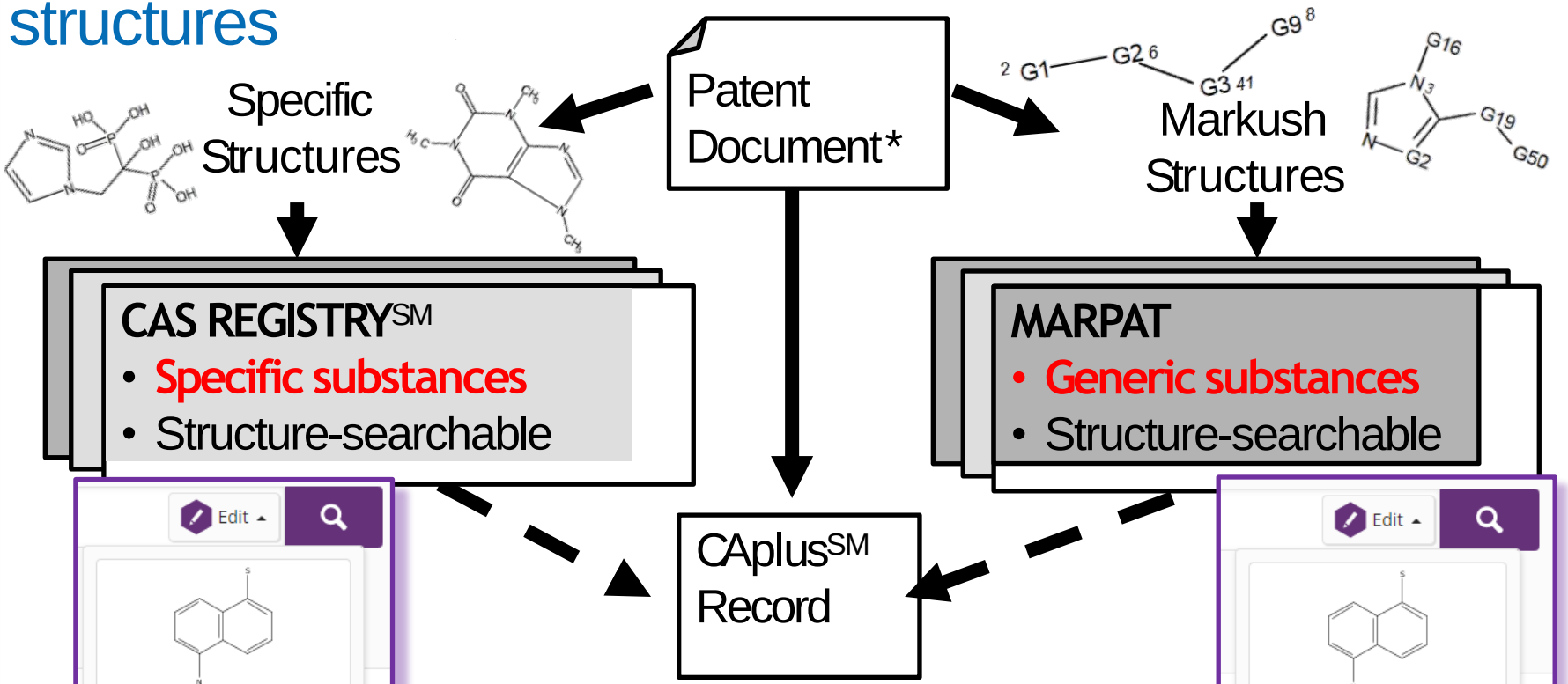


To conduct a Patent Markush search, click the **Substances** search type. Draw the query using a structure editor, and then check the box for **Search Patent Markush**.

Click the **magnifying glass** to submit the query.



Patent documents are evaluated for specific and Markush structures



Find Reactions by Name, Registry Number, or Document Identifier

Search terms may be:

•**Substance Name:**

- **Example:** benoxaprofen
  Note: Wildcard searching using an asterisk only works for single-search-term, single-word substance name searches (e.g., benoxa*).
- **Example:** methyl ethyl ketone
- **Example:** ß-amyloid
  Note: If your search term contains a Greek letter, see Greek Letters Used in Searching to insert the correct character.

•**CAS Registry Number** (with or without dashes, e.g., 51146-57-7, 51146577)

Notes:

- Square brackets are accepted around RNs (e.g., [51146-57-7], but not single or double quotes.
- You may enter multiple CAS RNs separated by a space, no commas or other punctuation. The search field has a 2000-character limit.

•**Document Identifier:**

- **Patent Number** (no spaces, e.g., US4571400)
- **Accession Number** (e.g., 1986:230471)
- **PubMed ID Number** (e.g., 15980585)
- **CAS Accession Number (CAN):** document number in CA Plus (e.g.,148:486341)

SciFinder^n
A CAS SOLUTION

Biosequence Searching: New Data, New Options

- New biosequence search option:
  - BLAST Search nucleotides and proteins
  - CDR: Search complementarity-determining regions of antibodies and T-Cell receptors and antibodies
  - Motif: sequence matching with wild cards and other features
- Over 550 M sequence-patent relationships and ~ 23 M sequences linked to non-patent literature
- Displays sequence alignment with filters and links to literature references
- Export sequence answer sets into Excel, including alignments
- Bioscape visualization tool provides additional analysis options

SciFinder^n
A CAS SOLUTION

Find Biosequences

There are three biosequence search types:

- **BLAST (Basic Local Alignment Search Tool):** Search for proteins as well as nucleotides using a set of local alignment algorithms (BLASTn, MegaBlast, BLASTp, tBLASTn, BLASTx).

- **CDR (Complementarity-Determining Region):** Search for antibody and t-cell receptors.

- **Motif:** Search for short patterns in DNA, RNA, or proteins with queries enabled for additional variability.

SciFinder^n
A CAS SOLUTION

Find Biosequences - BLAST

Find biosequences that match your query, which can be a protein/nucleotide string or a .txt/.fasta file.

1.Enter or copy and paste a protein/nucleotide string, or upload a sequence file:

- **Single sequence:** .txt file
- **Multiple sequences:** .fasta file

Note: The **maximum number** of sequences is **100**.

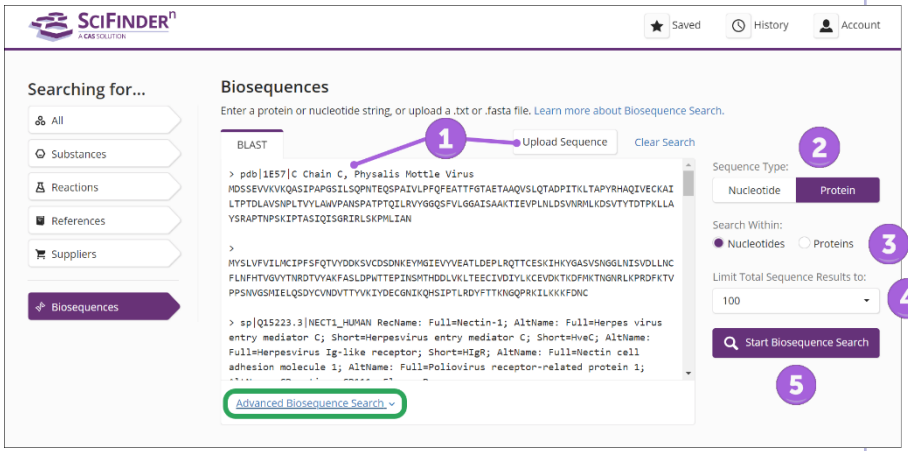
2.Select the appropriate **Sequence Type** based on your query.

3.Select the relevant **Search Within** option.

4.You may a select **total sequence result limit** of 10 to 20,000 (default is 100).

5.Click the **Start Biosequence Search** button.

Click **Advanced Biosequence Search** to find sequences using parameters such as sequence identity percentage, gap costs, and BLAST algorithm.



SciFinder n
A CAS SOLUTION

Coverage and Sequence Identity percentages

Query Sequence QQLLVVEEGG

Subject Sequence QQLLVVEEIGS

Alignment

$$\text{Query Coverage (100\%)} = \frac{Alignment\ Length}{Query\ Length} = \frac{10}{10}$$

$$\text{Subject Coverage (91\%)} = \frac{Alignment\ Length}{Subject\ Length} = \frac{10}{11}$$

$$\text{Sequence Identity (90\%)} = \frac{Number\ of\ Matches}{Alignment\ Length} = \frac{9}{10}$$

SciFinder^n
A CAS SOLUTION

Find Biosequences - BLAST

Advanced Biosequence Search has default values based on the selected **Sequence Type** and **Search Within** options.

Sequence Type / Search Within	Options (Default Value Shown)										
	Adjust Parameters for Short Sequences	Sequence Identity %	Match with Gaps	Gap Costs	Query Coverage %	Word Size	Reward for Match, Penalty for Mismatch	Scoring Matrix	BLAST Algorithm	E-Value	Exclude Low-Complexity Regions
Nucleotide / Nucleotides	Available	80	No	Existence 5, Extension 2	90	11	2, -3	—	BLASTn	10	No
Nucleotide / Proteins	N/A	—	No	Existence 11, Extension 1	90	6	—	BLOSUM62	BLASTx-fast	10	—
Protein / Nucleotides	N/A	—	No	Existence 11, Extension 1	90	6	—	BLOSUM62	TBLASTn-fast	10	—
Protein / Proteins	Available	—	No	Existence 11, Extension 1	90	3	—	BLOSUM62	BLASTp	10	No

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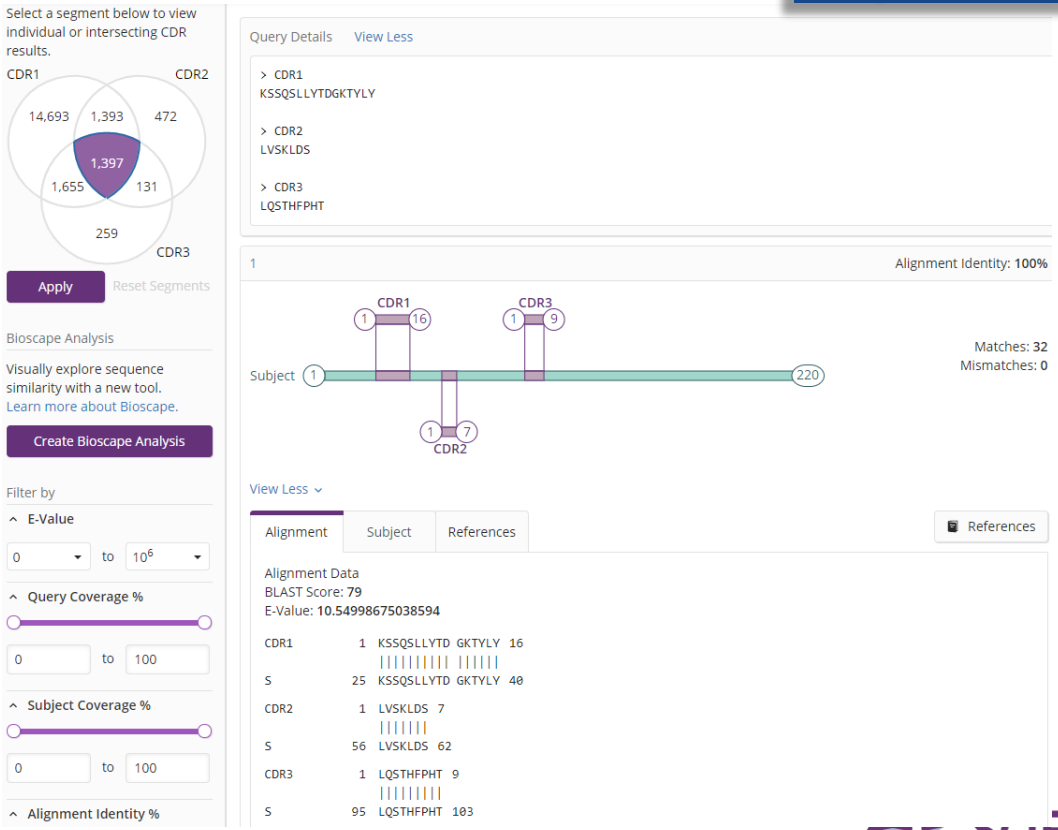
CDR Search

CDR
Complementarity-**D**etermining **R**egion



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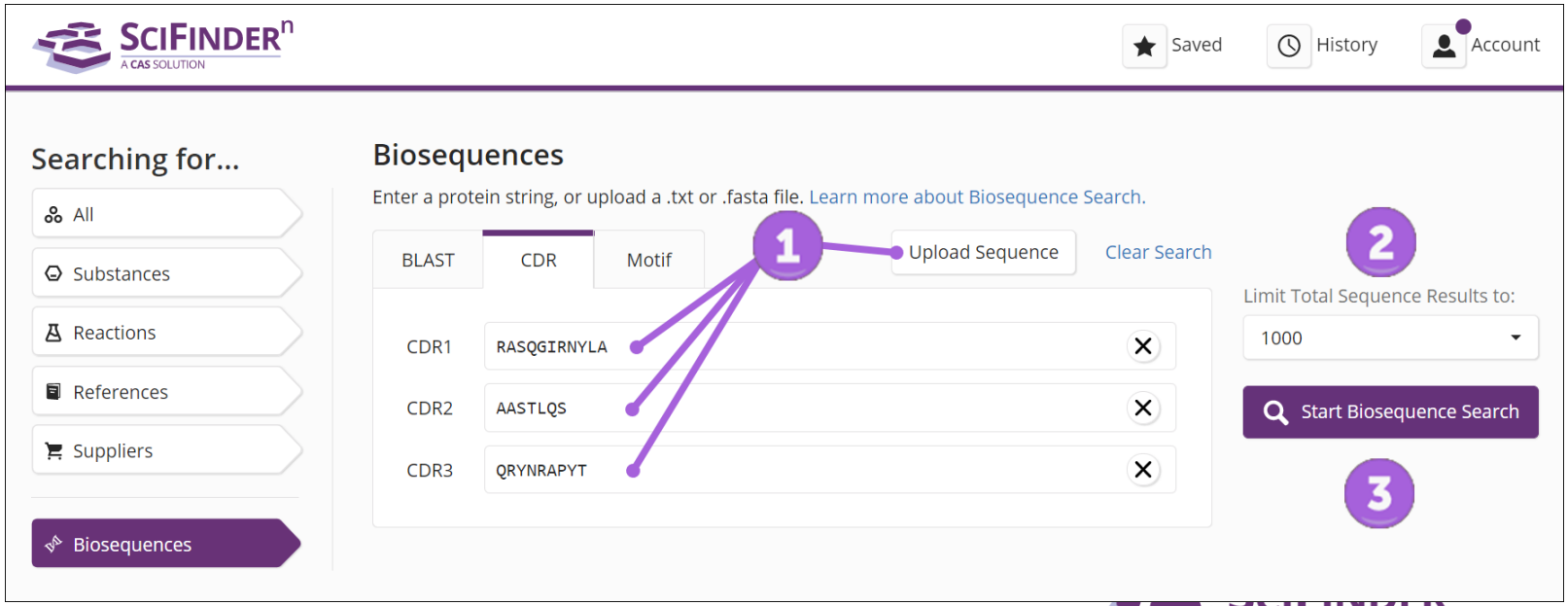
Find Biosequences - CDR

Find biosequences that match your query, which can be a protein string or a .txt/.fasta file.

1.Enter, **copy and paste**, or **upload** a file for **up to three CDRs**.

2.You may a select **total sequence result limit** of 10 to 20,000 (default is 100).

3.Click the **Start Biosequence Search** button.



Find Biosequences - Motif

Find biosequences that match your query, which can be a protein/nucleotide string.

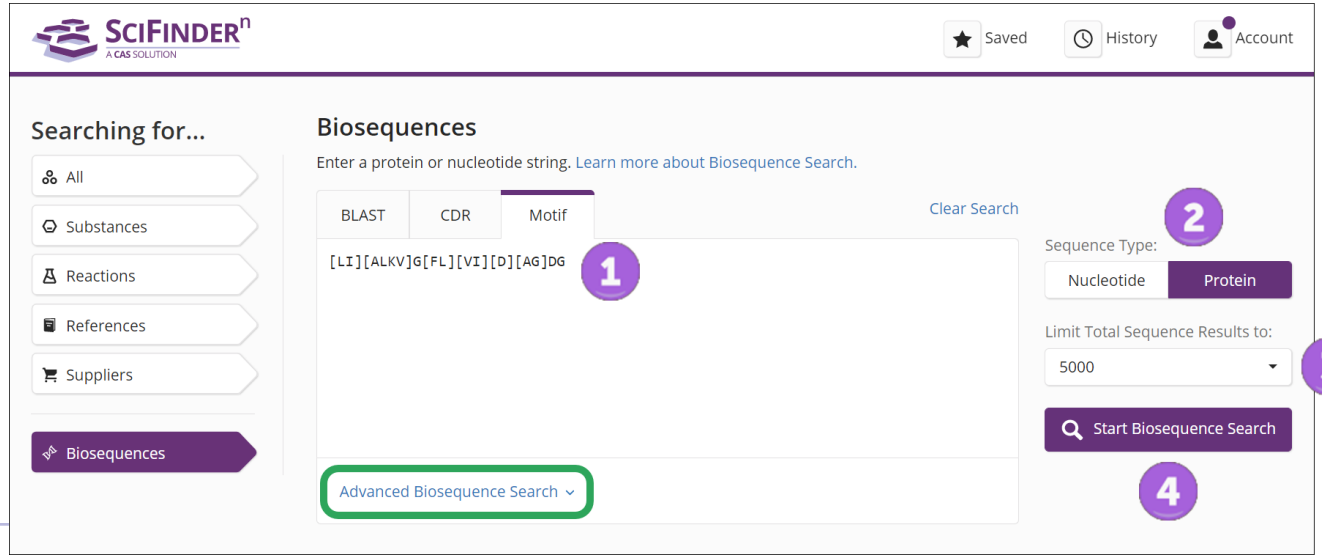
1.Enter or copy and paste a protein/nucleotide string.

2.Select the appropriate **Sequence Type** based on your query.

3.You may a select **total sequence result limit** of 10 to 20,000 (default is 100).

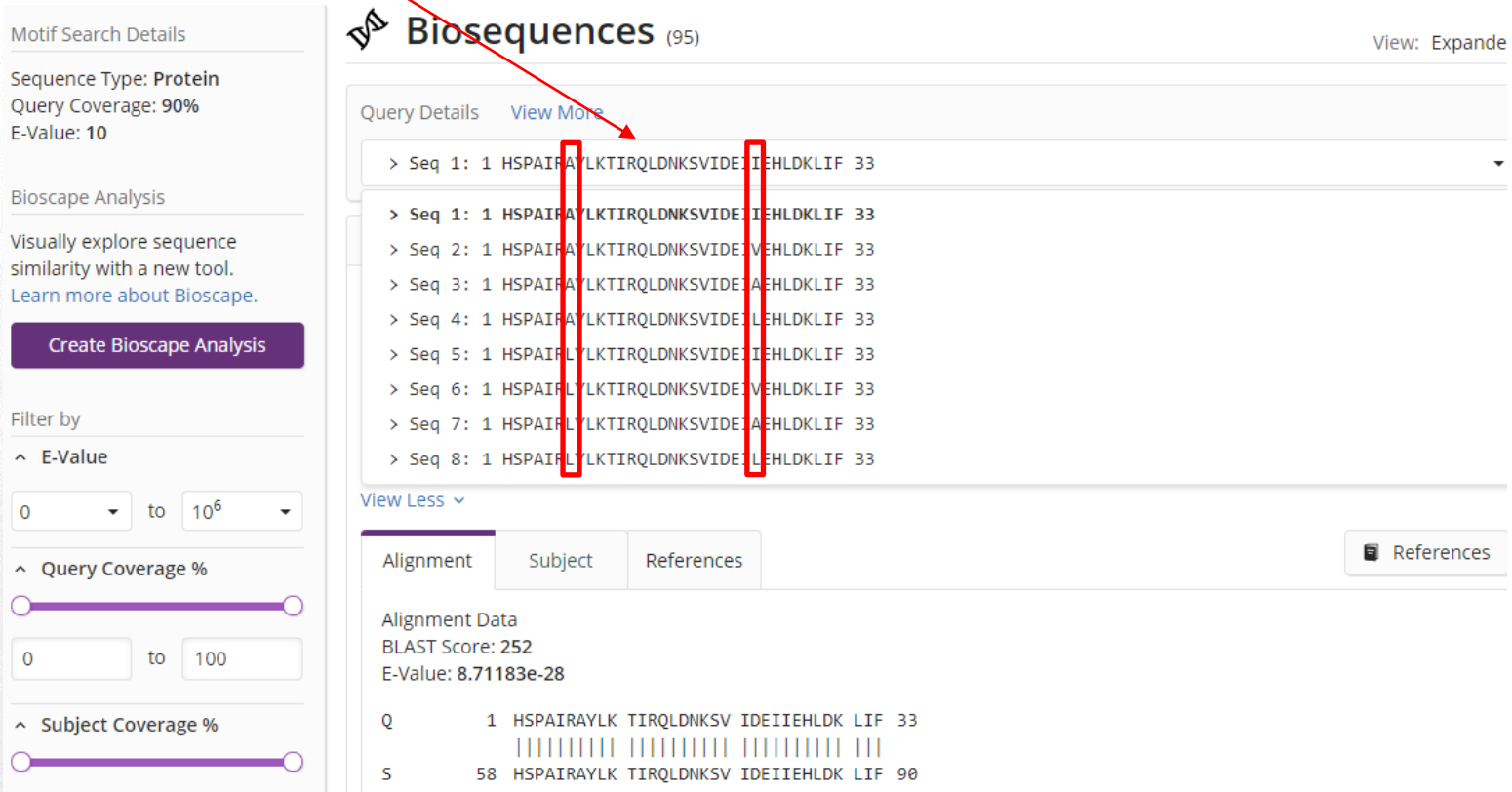
4.Click the **Start Biosequence Search** button.

Click **Advanced Biosequence Search** to find sequences using query coverage % and e-value.



HSPAIR[AL]YLKTIRQLDNKSVIDEI[IVAL]EHLDKLI
F

Motif Search



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Biosequence Motif Codes

Degenerate Code	Meaning
X	any amino acid
B	D or N (aspartic acid or asparagine)
Z	E or Q (glutamic acid or glutamine)
J	I or L (isoleucine or leucine)

Degenerate Code	Meaning
N	A or C or G or T
R	A or G
Y	C or T
M	A or C
K	G or T
S	C or G
W	A or T
H	A or C or T
B	C or G or T
V	A or C or G
D	A or G or T

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Biosequence Motif Codes

Degenerate Code	Meaning
[XYZ]	Any nucleotide or amino acid listed within the square brackets
{m,n}	at least m and maximum n residues length
{n}	exactly n length
^XYZ$	Search for the exact sequence XYZ

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Thank you!

SciFinder[n]
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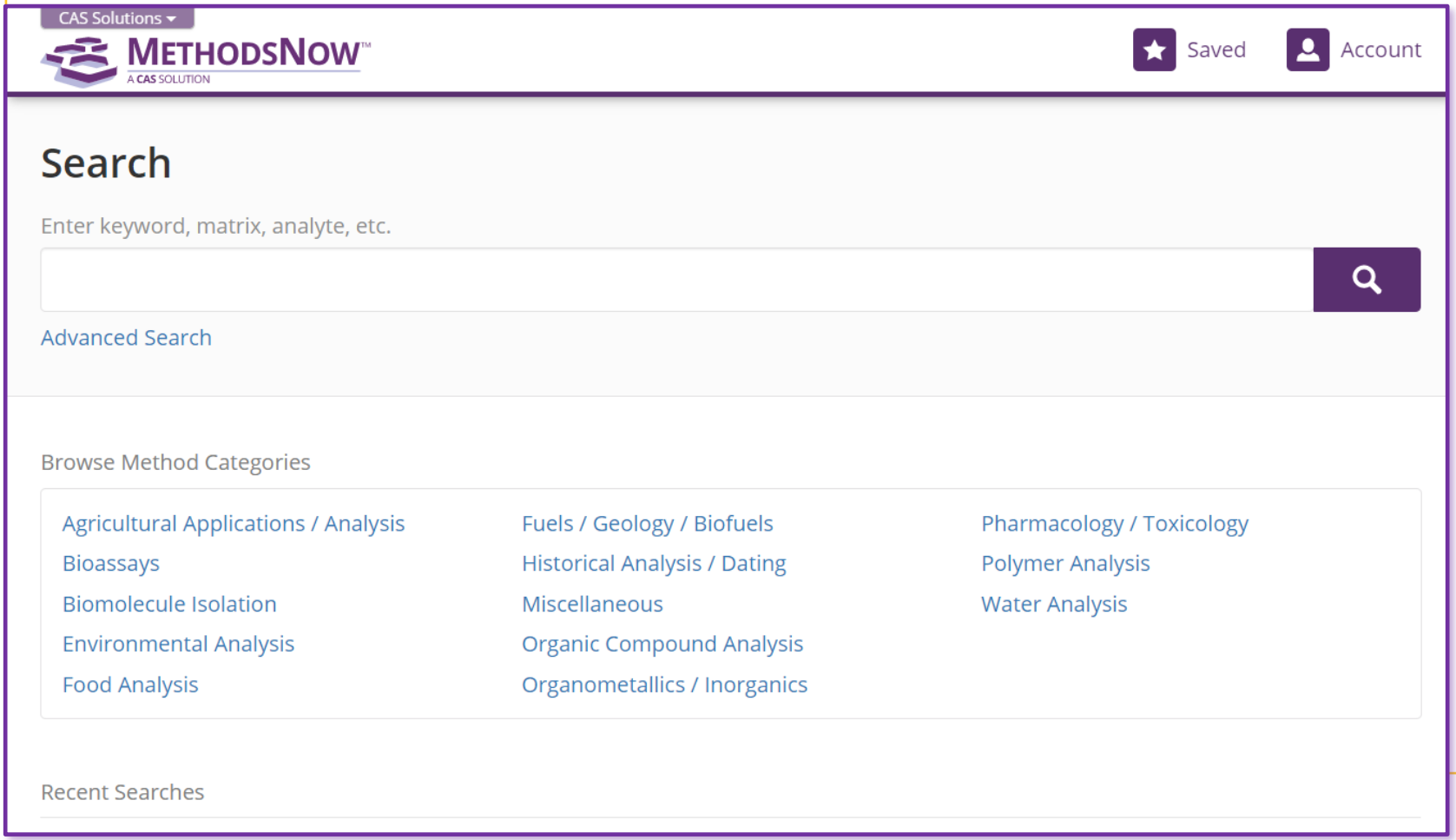
High valued function – MethodesNow Search



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Method Detail (1 of 43)

Analysis of Gemcitabine hydrochloride in Blood plasma by Pr

CAS MN: 1-101-CAS-65250

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Precipitation; Liquid chromatographic UV detectors; HPLC

Materials	Role	Image
Gemcitabine hydrochloride	analyte	View Structur
Blood plasma	matrix	
Phenomenex C_{18} (250 mm x 4.6 mm, 5 µm)	material	
Filter (0.4 µm)	material	
Methanol	reagent	View Structur

Source

Bioanalytical method development and validation of gemcitabine hydrochloride by RP-HPLC method

Rajesh, V.; Anupama, B.; Jagathi, V.; Varaprasad, K.

Asian Journal of Chemistry (2011), 23 (9), 3961 - 3963. Asian Journal of Chemistry

CODEN: AJCHEW | ISSN: 09707077

Full Text

CAS Solutions

METHODSNOW™ A CAS SOLUTION

"gemcitabine hydrochloride"

Full Text

Abstract

A simple, accurate, precise and sensitive HPLC method with UV detection was developed and validated to sep. and detect gemcitabine hydrochloride in human plasma using capecitabine hydrochloride as an internal standard Gemcitabine hydrochloride and capecitabine hydrochloride (internal standard) were extracted from human plasma using methanol protein precipitation and were chromatographed on a phenomenex C_{18} (250 mm × 4.6 mm. 5µm) column using 20 µl injection volume and detection at 270 nm. An isocratic mobile phase consisting of methanol: water (85:15 % volume/volume) was used to sep. these drugs. The retention times of gemcitabine hydrochloride and internal standard were 4.6 and 6.2 resp. The method was validated over the range of 406.10-4020.05 ng/mL. The limit of detection was 200 ng/mL and the limit of quantification was 400 ng/mL. Within and between-day precisions are less than 6.5 % for all quality control samples. The absolute recoveries of gemcitabine hydrochloride was greater than 90 % were achieved. The described method can be readily utilized for anal. of pharmaceutical products.

Equipment Used

High-performance liquid chromatography system, Shimadzu scientific instruments

Conditions

Chromatographic

Mobile phase, methanol and water (85:15% v/v); flow rate, 1.0 mL/min; total run time, 10 mins; detection wavelength, 270 nm.

Instructions

Preparation of standard solutions

1. Prepare stock standard solutions of gemcitabine hydrochloride and the (Capecitabine hydrochloride) internal standard by dissolving appropriate amounts of compounds in a known volume of methanol and water.
2. Store the prepared solutions at 4 °C.

Precipitation

1. Collect blank human blood with heparin from healthy and drug free volunteers.
2. Centrifuge the samples at 5000 rpm at room temperature.
3. Collect the plasma and store at -30 °C until analysis.
4. Prepare the blank plasma sample by adding 1 mL of plasma and 1 mL of methanol and vortex for 30 s.
5. Then centrifuge the solution at 4 °C, 5000 rpm for 5 min.
6. Take the supernatant liquid and transfer to HPLC vials.

High-performance liquid chromatography analysis

1. Perform the analysis on Shimadzu scientific instruments consisting of LC-20 AT pump and SPD-20 AT variable wavelength detector.
2. Carry out separation of compounds using a phenomenex C_{18} (250 mm x 4.6 mm, 5 µm).
3. Use the mobile phase consisting of methanol and water (85:15% v/v).
4. Filter the mobile phase through 0.4 µm filter and then degas ultrasonically for 15 min.
5. Set the flow rate at 1.0 mL/min and total run time to 10 mins.
6. Monitor the eluent at a wavelength of 270 nm for gemcitabine hydrochloride.

Validation

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