CAS SCIFINDER[®] QUICK REFERENCE GUIDE



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Solution interface and References search

Main interface

The options below are found on the main interface in CAS SciFinderⁿ.



Search interface

CAS SciFinderⁿ features a streamlined search interface.

D. AN. CAN. and/or DOI. Learn More
Ø Draw
ie. X
Example: Schubert J A
Learn more about SciFinder" Advanced Search.
CAS General Thesaurus to find indexed concents and rith up to 1,000 indexed sear Launch the

References search result

Performing a References search provides you with access to a full result set in an easy-to-use interface where:

- References are default sorted by relevance with customizable sorting options.
- You can focus your answer set further using filters.
- You can save searches, send a link, set up alerts, or add results to a project list.
- You can quickly access full details for any of the references displayed.

menthol and (food or candy or "chewing gum")"	Save results, set up alerts
Combine current with saved set	Save and Alert
Filtering: Concept: Flavor Deselect applied filters Share answers Excluding: Concept: Antibacterial agents X Sort answers	Clear All Filters
391 Results Sort: Relevance	 View: Partial Abstract -
Click title to open reference detail	•••
By: Santos, Milla G. (a): Carpinteiro, Debora A.; Thomazini, Marcelo; Rocha-Selmi, Gial are displayed Christiane E. C.; Favaro-Trindade, Carmen S. Food Research International (2014), 66, 454-462 Language: English, Database: CAplus Coencapsulation of two or more core materials in one system can improve the functionality of individual or their performance. Xvlitol and menthol are cooling agents that are widely applied in the food industry, and Select Filter by or Exclude, then select filter categories Access full-text options	omponents and maximize d studies have reported ipsulated using the double to control the release of
Full Text Substances (2) Reactions (0) Citing (4) Search any text within this answer set Retrieve substance, reaction, or citation data for Confectionery composition including an elastomeric component, a cooked sacch	44) Ø Citation Map or this reference
	Immenthol and (food or candy or "chewing gum")" Filtering: Concept: Flavor X — Deselect applied filters Share answers Excluding: Concept: Antibacterial agents X Sort answers 391 Results Sort answers 1 Click title to open reference detail Coencapsulation of xylitol and menthol by double emulsion followed by complex and microcapsule application in chewing gum By: Santos, Milla G. © Carpinteiro, Debora A: Thomazini, Marcelo; Rocha-Selmi, Gi Change how answ are displayed Christina E. C; Favaro-Trindade, Carmen S. Food Research International (2014), 66, 454-462 Language: English, Database: CAplus Coencapsulation of two or more core materials in one system can improve the functionality of individual c their performance. Xviltol and menthol are cooling agents that are widely applied in the food industry, are select filter by or Exclude, then select filter categories Access full-text options Substances (2) Reactions (0) Citing (agence filter categories Full Text Substances (2) Reactions (0) Citing (agence filter categories

Reference detail and search operators

Reference detail

Access full details for each reference found in CAS SciFinderⁿ.

Publication source information	(0) 46 Citing (6)	Ø Citation Map	View forward	and backward cita	ations	⊻ ≥	Save
PATENT	CAS Formulus®, the co	mprehensive formula m CAS Formulus® in	ations database and v	workflow solution, is	now available	for all SciFir	ider ⁿ
Patent Number WO2005048743	By: Shimizu, Toru; Shigeta, Yosl	ninari; Kunieda, Sator	ni				
Publication Date 2005-06-02	A fruit juice-containing food pr substances selected from the g	oduct contains, in ad roup consisting of <mark>m</mark>	dition to a fruit comp <mark>enthol</mark> , menthone, c	onent and a sweet t amphor, pulegol, iso	oase, (a) one o pulegol, puleg	r more refre gone, cineol,	shing mint oil,
Application Number NO2004-JP17524	peppermint oil, spearmint oil, e consisting of 3-(l-menthoxy)pro menthane-3,8-diol, 2-(l-mentho	eucalyptus oil, and fra pane-1,2-diol, N-ethy xy)ethan-1-ol, 3-(l-me	ctions thereof, and (k d-p-menthane-3-carb enthoxy)propan-1-ol,	o) one or more cool- oxamide, 3-(l-menth 4-(l-menthoxy)butar	tasting substa oxy)-2-methyl n-1-ol, cyclic ca	nces selecte propane-1,2 rboxamides,	d from the gro -diol, p- , acyclic
opplication Date 2004-11-18	carboxamides, N,2,3-trimethyl- group having 1-6 carbons), and menthol as the refreshing con	2-iso-Pr butanamide, a monthosy alkanod Get prior art for	a menthoxy alkanol (iol (allo) group having this patent paned	alkyl group having 2 g 3-6 carbons). Thus liol as the cool-tastir	!-6 carbons), a , an orange jui ng component	menthoxy a ice beverage	lkyl ether (alk may contain
ind Code 1	Keywords: fruit juice flavor for	d beverage mentho	l				
ssignee	PatentPak Viewer Ger	Prior Art Analysis	Full Text 🕶			Get simil	ar reference
akasago International orporation, Japan	Similar References	PDF displays	original patent PI s the full text with	DF table of indexed	substances	Get Sim	ilar Reference
iource Vorld Intellectual Property	Patent Family	Viewer displa	ays interactive vers	sion of annotated	full text	J	
Drganization	Patent Language	Kind Code P	atentPak Options	Publication Date	Application I	Number A	pplication Dat
atent family and priority polication information	WO2005048743 English	A1 P	DF PDF+ Viewer	2005-06-02)ata	
N: 2005:470226 AN: 143:25602	- Priority Application				~ Conc	epts	
Aplus	Priority Application Number	er	Appli	cation Date	y Subs	tancos	
anguage	JP2003-389758		IPC and inc	lexed	v Subs	ulations	
english	WO2004-JP17524		substance i	ndexing,	 V Form V Cited 	Documer	nts

Boolean operators

You can use logical operators to create precise text queries.

Use parentheses to group logical expressions, such as related terms using "OR", ex:



Wildcards allow for more comprehensive results in reference, substance, and filter searches. Internal and right-hand truncation is possible.

- * Replaces 0 to any number of characters ex: polymorph* | immunoglobulin*conjugate*
- ? Replaces 0 or 1 character ex: benzonorbornen?

Phrases containing double quotes will be searched as a precise phrase. Ex: a search for "Programmed cell death protein" only finds results that exactly match: "Programmed cell death protein."

Substance name and structure search

Substances search

You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

Streptomycin	Finds Streptomycin record
57-92-1	Finds Streptomycin record, uses CAS Registry Number [®] as identifier
Streptomycin sulfate	Finds three records: Streptomycin, Streptomycin sulfate, and Sulfate
"Streptomycin sulfate" Streptomycin	Finds two records: Streptomycin sulfate and Streptomycin
Sulfoximin*	Finds all names that start with the stem Sulfoximin
Sulfoximin*	Finds all names that start with the stem Sulfoximin
WO2019234160	Finds all indexed substances for this patent

Searching for	Substances	Click to draw new
S• All	Search by Substance Name, CAS RN, Patent Number, Pub	Med ID, AN, CAN, and/or DOI. Learn More
Substances	Enter a query Enter chemical name q	uery
Reactions	AND - Molecular Formula -	
References		Click query structure to edit
📜 Suppliers	Add Advanced Search Heid	
	Add more advanced search fields Change advanced s	search field Edit Drawing Remove
Sequences		Search Patent Markush
		Check to perform Markush search

Substances search result

Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search, including critical property information and high-resolution images.



Substance detail and structure editor

Substance detail

When you click a CAS Registry Number for one of your Substances search results, substance details including structure, molecular formula, properties, and further data are displayed.



CAS Draw editor

You can further define structure and reaction queries using the CAS Draw structure editor.

CAS		CAS Draw - Import and export structure files Enter CAS Registry Number, SMILE or InChI to create structure	ES,	Acc
		🗈 👎 🛱 🛱 🛠 🖄 🖻 🖻 🗢 🗢 🛱 ? Enter a CAS Registry Number, SMILES, or InChI 🏹		
P		Click and drag to select objects. Ctrl-click to select or deselect individual objects.	с	H
		Draw atoms and bonds Eraser	0	s
, 💷	Et	Pick element symbol from periodic table Shortcuts	N	P
X	R	Variable selection Define own variables (R Groups)	ci'	SI
Fn	0	Add attachment point to fragment Select from templates Draw bonds. I indicate further options are available		EZ
Ð	Θ	Add positive charge Add negative charge		
E [] 1-4	~	Repeating groups Carbon chain tool	0	ŏ
	A B	Define variable point of attachment at ring Reaction role	0	Ċ
	۹	Atom mapping Lock rings/lock atoms		
`∕∗	\rightarrow	Bond mapping Draw reaction arrow		
ent Se	arch	С Zoom: 90% + OK Cancel w.	All Sea	irch Hi:

Advanced Search

Performing an Advanced Search

You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinderⁿ.

- Operators are processed in this order: OR, AND, NOT
- Operators are not available for a search using a single advanced search field
- Wildcards are allowed, e.g., peek*
- Use up to 50 Advanced Search Fields (49 if also using the main search field)

References

Advanced Search examples

Advanced References Search

Advanced Substances Search

"pollution monitoring" Operator to combine search fields	steel*
AND Chemical Name polyethylene	AND 👻 Tensile Strength (Mpa) 👻 >0
OR Chemical Name polypropylene	Experimental values only.
Query interpretation: "pollution monitoring" and (polyethylene or polypropylene)	Query interpretation: Steel with tensile strength property information
References - Edit Search "pollution monitoring	g" Click 'Edit Search' to modify the Advanced Search

Available Advanced Search fields

You can utilize many search fields and categories as part of an Advanced Search query, including:

References Search

- Author Name
- Publication Name
- Organization Name
- Title
- Abstract/Keywords
- Concept
- Substances
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Substances Search

- Molecular Formula
- CAS Registry Number/Component Registry Number
- Chemical Name
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

CAS Roles

CAS Roles overview

Roles are linked to substances, allowing you to find focused publications connecting a substance of interest to its specific role within the scope of the publication.

- Super roles are broad categories and comprise all related specific roles. Examples are Analytical Study, Preparation, or Occurrence.
- Specific roles are more precise. They relate to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in a plant (Natural Product Occurrence).

Roles in substance results

From a search on substance(s), the roles filter will indicate the types of roles that are connected to the substance(s) in the publications.

Reference Role				
By Count Alphanumeric	Example of 'reference roles' appearing in a substance answer set		Number of substance(s) in the	e
0 Selected			answer set with that role	
Adverse Effect (15)	Diagnostic Use (3)	Pharm	nacological Activity (10)	
Agricultural Use (29)	Food or Feed Use (120)	Physic	cal, Engineering, or	
Analyte (17)	Formation, Non-preparative	Chem	ical Process (888)	

Roles in reference results

Roles will appear as a filter in reference result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e., by retrieving substance names or performing a crossover after structure-based searches.

Example: I am interested in the subject of (marine) pollution, how can I find publications where polypropylene is specifically described as a pollutant?

The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3,217 publications that describe polypropylene as a pollutant. The Search Within function or concepts can be used to restrict results to marine pollution.

Substances - poly 9003-07-0	rpropylene	Document Type Substance Role Uses (262K) Properties (60K) Process (50K) Biological Study (22K) Preparation (19K)	Recycling micro polyp By: Buruiana, Daniela Laura; Scientific Reports (2023), 13(One of the objectives of the (waste. The motivation of this such as plastic based polypr polypropylene based micro The morphol. and elemental SEM-EDX and the performan flow rate, solid-liquid report, After clicking "View All"	ypropylene in modified hot asphalt mixture a; Georgescu, Pulu Lucian; Carp, Gabriel Bogdan; Chisman, Viorica 3(1), 3639 Language: English, Database: CAplus and MEDLINE te circular economy is solving the world's plastic pollution crisis and recycling of materials by ensuring less his study was to demonstrate the possibility of recycling two types of wastes with a high risk of pollution, propylene and abrasive blasting grit wastes in asphalt roads. The effects of adding together roplastics and grit waste in asphalt mixture for wear layer performance have been shown in this study. tal composition of the hot asphalt mixture somples before and after freeze-thaw cycle were examined by ance of the modified asphalt mixture was determined with laboratory tests including Marshall sability, rt, apparent d., and water absorption. A hot asphalt mixture suitable for making wear layer in road bit mere, abrasive blasting grit waste and polypropylene based microplastics is also lif. more
(C ₃ H ₆) _x Polypropylene		View All View All	specific roles can be so polypropylene-modified hor changes.	selected entry and the sphalt mixture sample with 0.3% of based microplastics are bond with aggregates from mixture well, so the bot asphalt mixture can effectively decrease the appearance of cracks during sudden temperature
■ 278K References Reactions	₩ 20 Suppliers	 Publication Year Available at My Institution 	Full Text 👻	Substances (2) A Reactions (0) 64 Citing (0) Ø Citation Map
ubstance Role By Count Alphanumeric 1 Selected Uses (262K) Technical or Engineered Material Use (166K) Polymer in Formulation (7	с С	Biological Use, Unclassified (3.678) Occurrence (3.640) Pollutant (3.217)	Substance Role Uses (262K) Properties (60K) Process (50K) Biological Study (22K) Preparation (19K) Pollutant (3,217) View All Language	■ ** •** Comparison in marking environment review of methods for identification and quantification in the provide t
Properties (60K) Process (50K)		Miscellaneous (2.437) Biological Study, Unclassified (2.433)	Publication Year	22 Fut Tert - • • Substances (1) = ******* ** Crerc (2.03) @ Control Moo • Substances • • • • • • • • • • • • • • • • • • •

Sequences search

Search options

You can search sequences using three different modalities:

- BLAST: Search similar sequences
- CDR: Search antibodies and t-cell receptors via CDRs
- Motif: Search using variability symbols

BLAST similarity search

BLAST allows you to search for similar nucleotide and amino acid sequences. Alignment results are shown in an intuitive graphical layout with easy-to-use precision filtering for identity and coverage percentages. Reference results are linked to the sequence hits.

- To perform a BLAST search:
- Open the Sequences module from the main CAS SciFinderⁿ search page.
- Load a sequence from a file or paste a sequence.
- Take advantage of supported formats: Sequences containing residues represented by single-letter codes (e.g., in the FASTA format). Leading numbers are not allowed.
- Recognize that sequence input may contain a header line (starting with >).
 Sequences can be separated by (multiple) headers, thus allowing for batch processing.
- Adjust BLAST parameters as desired and start the sequence search.

Searching for	Sequences				
s• All	Enter a protein or nucleotide st	ring, or upload a .txt or .fasta f	ile. <u>Learn more about S</u>	equence Search	<u>).</u>
Substances	BLAST CDR M	lotif Sequence Search options	Upload Sequence	Clear Search	
References Suppliers	> human insulin sequence FVNQHLCGSHLVEAYLVCGERGFFY Paste sequence	TPKTGIVEQCCTSICSLYQLENYCN	ice from file w/o pred	ceding	Sequence Type: Nucleotide Protein Search Within: 1
Sequences	into this window	numbers or paste into	the BLAST pane		ONucleotides Proteins
Retrosynthesis	Advanced Sequence Search Alignment Identity % •	▲ Adjust Parameters Match with Gaps?	for Short Sequences ↓ Gap Costs ●	Reset All	Include NCBI Sequences Include NCBI sequences
Advanced BLAST	-		Existence 11 Exter	ision 1 👻	
parameters	Query Coverage % 💿	Word Size @	Scoring Matrix @		
	90	3 •	BLOSUM62	-	
	BLAST Algorithm BLASTp	E-Value • 10 •	Exclude Low Complexity Regions O Yes No	0	

BLAST results analysis

Access results

Sequence search results appear in the Recent Search History and general Search History (() History). Click 'View Results' to view sequence answers.

April 28, 2023			
Sequences 5:00 PM	Sequence Type: Protein Search Within: Proteins NCBI Included: Yes BLAST Algorithm: BLASTp	> human insulin sequence FVNQHLCGSHLVEAYLVCGERGFFYTPKTGIVEQC CTSICSLYQLENYCN	View Results Edit Search
	Query Coverage: 90% Results will expire on		Complete
	May 29, 2023.		

View results

When viewing BLAST sequence similarity results:

- Alignments are sorted by Sequence Identity.
- Simplified graphical overview shows alignment quality.
- Mismatches are indicated by red lines.
- Detailed alignments can be viewed in 'Alignment' tab.
- Subject details and patent previews are available in separate tabs.
- Click References to retrieve related references.
- XLSX result download dis available.

Sequences search for your query References Get references for all sequences 92 Alignment Identity: 89.09% Query (50) Query Length Matches: 49 Subject Length Mismatches: 6 Subject Alignment Length: 49+6=55 View Less Subject and links to NCBI and substance Reference previews information in CAS SciFinderⁿ References Alignment Alignment Subject References Details + Mismatch: Query aa aligned to functional Get References Match Mismatch equivalent subject aa for this sequence E-Value: 5.12823e-26 FVNQHLCGSH LVEA-YLVCG ERGFFYTPKT Q -GIVEQC CTSICSLYQL ENYCN 55 FVNQHLCGSH LVEALYLVCG ERGFFYTPKS DDARGIVEQC CTSICSLVQL ENVCN 55 S Gap in the query Start of alignment in query sequence and subject sequences

Filter results

Filtering dynamically changes your result set.



∧ s	equence Length
26	to 9521
^	Organisms
	Homo sapiens (25)
	Mus musculus (25)

Reactions search

Performing a Reactions search

Reactions queries can be performed using CAS Reaction Numbers, substance names, CAS Registry Numbers, document identifiers, or a chemical structure.

Searching for	Reactions		
S• All	Search by CAS Reaction Numbe	er, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN,	and/or DOI. Learn More
Substances	Enter a query		🖉 Edit 🔺 📿
L Reactions	Select reactions		
References		Click on reaction query to edit	
📜 Suppliers			Edit Drawing Remove
✤ Sequences			
Retrosynthesis			

Reactions search results

Reactions search results are grouped into schemes with identical reactants and products or into transformations. A robust panel of filters, including yield and steps, enables further refinement.

References 🗸		🔘 🛃 🔤 🖡 Save and Ale
View by structure match]	
ructure Match	26,932 Results	Group: By Scheme - Sort: Yield - View: Expande
As Drawn (0)	Scheme 1 (2 Reactions)	Steps: 1 Yield: 100% •••
Substructure (26K)	+ -	Yield for displa
Similarity (2,082)		
ter Behavior	Absolute stereochemistry shown, Rotation (+)	Absolute stereochemistry shown
Filter by Exclude	Suppliers (48) View supplier	s S
Search Within Results	31-614-CAS-27240963 Steps:	Yield: 100% Stereoselective process for preparing isoxazolo-quinoline- substituted cyclohexyl derivatives
Yield	1.1 Reagents: <u>Triethylamine</u> , <u>Diphenylphosph</u>	ioryl azide
Number of Steps	Solvents: <u>Toluene</u>	By: Barnett, Charles Jackson View reaction reference
New Deutisineting Functional	- View reac	tion details 2002-03-28
Groups	Experimental Protocols	PatentPak - Full Text -
Carboxylic ester (151) Halide (143)	31-614-CAS-27633989 Steps: •	Yield: 100% Preparation of N-(isoxazoloquinolinylcyclohexyl)carbox
Ether (125)	1.1 Reagents: Triethylamine, Diphenylphosph	ioryl azide
	Solvents: <u>Toluene;</u> 40 - 50 °C; 1 h, 110 °C;	110 °C \rightarrow 70 By: Bonjouklian, Rosanne; et al
Ketone (103)	Ϋ́C	world Intellectual Property Organization, WO2001046199 A1
Ketone (103) Carbamate (98) View All	1.2 70 °C; overnight, 70 °C \rightarrow 85 °C	2001-06-28

Reaction details

Reviewing Reaction details

The details of a reaction provide you with access to information including solvents, catalysts, reagents, conditions, and experimental protocols extracted from the publication and its supplement.

Reaction Overview Steps: 1 Vield: 85% Reaction reference JOURNAL Development of a Scalable Synthesis of an AzaindolyI- Pyrimidine Inhibitor of Influenza Virus Replication	Absolute stereochemistry shown, Rotation (+)	Suppliers	OH	Absolute stereochemistry shown, Rotation (-)		
By: Liang, Jiangline and View All View all autho	rs Step 1					
Development (2016), 20(5), 965-969	Stage Reagents	Catalysts	Solvents	Conditions		
⊙ View Source Full Text -	1 <u>Triethylamine</u> <u>Diphenylphosphoryl azide</u>	-	<u>Toluene</u>	2 h, reflux; reflux \rightarrow 60 °C		
Company/Organization	2 -	-	-	overnight, 60 °C \rightarrow 80 °C		
Incorporated Boston, Massachusetts 02210 United States			View al	ternatives > Alternative Steps (5)		
Experimental Protoc	cols					
Synthetic Methods	View detailed procedures					
Products	Ethyl (1R,3S)-3-[(benzyloxycarbonyl)amin	<u>o]cyclohexanecar</u>	boxylate, Yield:	85%		
Reactants	<u>1-Ethyl (1R,3S)-1,3-cyclohexanedicarboxy</u> <u>Benzyl alcohol</u>	late				
Reagents	<u>Triethylamine</u> <u>Diphenylphosphoryl azide</u>					
Solvents	Toluene					
Procedure Characterization Data ^ Ethyl (1 <i>R</i> ,35)-3-	1. Add diphenylphosphoryazide (DPPA) 3R) -3-ethoxycarbonylcyclohexaneca View characterization data [(benzyloxycarbonyl)amino]cyclohexanec) (166 mL, 769 mm rboxylic acid (140 carboxylate	n ol) and triethyl g, 700 mmol) ir	amine (107 mL, 769 mmol) to (1S, n toluene (1.4 L).		
Proton NMR Spectrum	(300 MHz, CDCl ₃)), 5.11 (s, 2H), 4.67 6 Hz, 1H), 2.10-1.7	(s, 1H), 4.13 (q,J 9 (m, 3H), 1.50-1	= 7.1 Hz, 2H), 3.55 (s, 1H), 1.19 (m, 6H), 1.19-1.00 (m,		
Optical Rotatory Power	y =-33.3° (c = 1 in DCM).					
HRMS	(ESI) [M + H] ⁺ calculated for $C_{17}H_{24}$	NO ₄ 306.1700, four	nd 306.1700			
State	sticky solid					
CAS Method Number 3-451-CAS-15598720						
Transformations 1. Schmidt Reaction	Overview of transformations	Reaction Not scalable	es Fur	ther important notes		

Retrosynthesis planner

Launching the tool

There are two primary ways to launch the retrosynthesis tool within CAS SciFindern:

- 1. Draw or import a structure into the Retrosynthesis window accessed by selecting the Retrosynthesis option on the main page. The substance can be novel.
- 2. Choose the Start Retrosynthetic Analysis option found on the substance flyout window.

Searching for	Retro	synthesis	CA	S RN	
\$• Al	Draw or import a structure to perform a retrosynthetic analysis. Learn more about Retrosynthesis searching.		24	08121-76-4	
Substances	P 🖪	🗅 ∓ 🛱 🛱 🛠 👘 🖻 🦘 🗢 😫 ? Enter a CAS Registry Numbers, SMILES 🏹	CA	S Name	
A Reactions	11	Draw or change atoms or bonds.	2-[Methoxy[5-[5-(trifluoromethyl)-	F
References	с н		me	ethyl]-5-meth	r - F
The Suppliers	O S				
	N P	F			
✤ Sequences	ci, si		6	Get Substance Details	
Retrosynthesis	Et				N=0
	~ 0	N			20
		/*	л	Get Reactions (1)	
	 N ≦ A A 			Synthesize (1)	
	00				
	00		¢	Start Retrosynthetic Analysis	2
	00	Molecular Formula: C+dH+3FtN+Q>S (355.34)		Get References (1)	
		c Zaorr: 100% + 1 -Start Retrosymmetic Analysis	1		Edit Structure – Reset +

Selecting plan options

You can edit plan options to:

- Increase the synthetic depth.
- Protect bonds through the entire synthetic route.
- Define bonds to be broken in the first disconnection.
- Change the starting material cost limit.
- Create a predictive plan with more meaningful alternatives, (such as poly- or heterocyclic molecules).

Once you have completed your option selections, choose the Create Retrosynthesis Plan button.



Retrosynthesis plan and alternative steps

Open the plan

An Experimental plan is typically available within a few seconds. The calculation of a Predictive Retrosynthesis Plan can take a bit longer.



Alternative steps

Get an overview of all experimental and predicted disconnections along with the evidence reactions displayed as a reaction answer set. You can access these evidence reactions from either the (1) link in the steps overview or (2) alternative reaction scheme.

Overview Steps	Filter by	1 of 15		Predicted Ste
view step specific evidence and alternate	 Alternative Step Type Predicted (49) 			
teps below or select the node between teps on the plan.	^ Stereochemistry		X - X	+
A⇒B+C	Non-Selective (49)		I OH	N I
Average Yield: 47% Evidence (16) Alternative Steps	Grouped similar	reactions	View 4 similar Alternatives 2	- View Evidence (1,580) Average Yield: 59%
	Reactions from Retr	osynthesis Plan Evidence		
B⇒D+E	References •	🗑 References 🗸 🔘 💆 📕 Save		
Average Yield: 59% Evidence (23)	Filter Behavior	Filtering: Experimental Protocols: 2 S	elected • ×	Clear All Filters
Alternative Steps (34)	Filter by Exclude	727 Results	Group: By Scheme 👻	Sort: Relevance - View: Expanded -
C⇒F+G	 Search Within Results 	Scheme 1 (1 Reaction)		Steps: 1 Yield: 72% •••
Average Yield: 59%	 Yield Number of Steps 	но		ta
Alternative Steps (49) — 1	Non-Participating Functional Groups		F J J F	, , , , , , , , , , , , , , , , , , ,
D⇒H+I	 Reaction Mapping Mapping Data Available (727) 	🐂 Suppliers (81)	🐂 Suppliers (77)	🐂 Suppliers (65)
Maximum Yield: 79% Evidence (1) Alternative Steps (11)	 Reaction Scale Milligram (130) Gram (20) No Scale Provided (577) 	31-614-CAS-24629063 1.1 Reagents: Triethylamine, Hydro Solvents: Dimethylformamide, reflux 1.2 0.5 h, reflux	Steps: 1 Vield: 72% <u>sylamine</u> <u>tetrahydrofuran</u> ; 2 h, By: Yang, Zihui 🚱 et. Chemistry & Biodiver	I Activity, DFT Study and Molecular of Novel 4(1,2,4-Oxadiazol-3yl)-N-(4- amide Derivatives al sity (2021), 18(12), e2100651
	 Experimental Protocols Synthetic Methods (286) Experimental Procedure (467) 	Experimental Protocols Collapse Scheme A	Full Text •	Evidence reactions for (predicted) disconnection

Retrosynthesis scoring options

Scoring options

For plans with predicted steps, you may increase or decrease the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- Each scoring profile may be set to Off (extreme left), Low, Medium, or High (extreme right).
- The default setting for each profile is "Medium" as shown below.
- Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor in step selection or alternative ranking.

Scoring profiles

For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

Each scoring profile may be set to **Off** (extreme left), **Low, Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.

Plan Options	
Synthetic Depth: 3	
Predicted Rules: Commo	n
Break & Protect Bonds: N	10
starting Material Cost Lin	nt: \$1,000.00/mol
Edit Plan Options	
Scoring Profiles	
Complexity Reduction •	
	Medium
convergence •	All Colored
	0
Evidence O	
Cost 😐	
Vield a	
tietu 🗸	
Atom Efficiency O	
	~
	Recent Freedom

Complexity Reduction

Reduces the complexity of a step's reactants compared to its product.

In retrosynthesis plans, you typically want high complexity reduction.

Convergence

Determines how "branched" the plan is; you typically want the plan to be as branched as possible (high convergence), rather than linear.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

Increasing Convergence displays steps/alternatives with more reactants.

Evidence

Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type.

More evidence examples for a step means that the reaction type has more applications and is more versatile in terms of conditions and substrates, and hence predictions made based on it are probably more reliable.

Increasing Evidence displays steps/alternatives with more supporting examples.

Cost

Weighs the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.

Yield

Applies to the yield of each step in the plan, which contributes to the yield of the target molecule.

Increasing the Yield displays a higher yield target molecule and steps/alternatives.

Atom Efficiency

Reduces reactant parts not included in a plan step's product.

Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.

Clicking the Apply button redraws the retrosynthesis plan with the revised scoring profiles; clicking Reset Scoring restores the "Medium" default.



Reset Scoring

Markush search and CAS PatentPak

Markush search

Markush structure searches can be performed using the Search Patent Markush option while in Substances search mode.



CAS PatentPak

There are three CAS PatentPak options for viewing a patent PDF:

- **PDF**: Full-text patent PDF only; text-searchable PDF
- PDF+: Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- Viewer: Patent PDF with linked markups of Key Substances (see below)



Supplier search and ChemDoodle®

Suppliers search

Using Suppliers search allows you to directly access chemical catalog information based on chemical structure, names, or other identifiers.



ChemDoodle

The ChemDoodle structure editor is available in addition to the standard CAS Draw editor. ChemDoodle is useful for tablets and mobile devices.



Prior Art Analysis

Reviewing Prior Art

When viewing a patent Reference Detail page, an option to "Get Prior Art Analysis" is available. Results will also appear in the search history. This functionality:

- Provides an AI-based relevance prediction.
- Is based on a single patent document as the starting point.
- Includes analysis of CAS concepts, indexed substances, IPC codes, and additional full-text.
- Generates a list of relevance-ranked previously known documents, comprising patent and non-patent literature.

Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)						
Substances (13)	Reactions (0) 44 Citing (1) 📮 💋 Citation Map	⊥ I Save -				
PATENT	By: Wang, Shaofeng; Li, Hairong; Seow, Swee How					
Patent Number WO2017135893	The present invention relates to a water based emulsion coating composition, e.g. paint composition dendritic poly(amido)amir Initiate the analysis from agent, at least one isothiazolone bioc	The present invention relates to a water based emulsion coating composition, e.g. paint composition, comprising a hyper- branched or dendritic poly(amido)amir Initiate the analysis from the detailed record				
Publication Date 2017-08-10	Keywords: aqueous dendhae coaang rownen poryannaoannine PatentPak Viewer Get Prior Art Analysis Full Text +					
Application Number						
References 8:57 AM	Prior Art Analysis (198) Aqueous dendritic amine coatings containing dendritic	View Results				
	poly(amido)amine (PAMAM)	Complete				
	View Res	ults from the search history				

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