Chuan-Che Liu Ph.D. Senior Account Consultant tliu2@acs-i.org 0975765358

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((12) INTERNATIONAL APPLICATION PUBLISHED U (19) World Intellectual Property Organization International Bureau 43) International Publication Date 4 October 2012 (04.10.2012) WIPO P	NDE	R THE PATENT COOPERATION TREATY (PCT)
(51)	International Patent Classification: A01N 43/04 (2006.01) A61K 31/70 (2006.01)	(81)	Designated States (unless otherwise indicated, for eve kind of national protection available): AE, AG, AL, AM AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, B
(21)	International Application Number: PCT/US2012/030408 International Filing Date: 23 March 2012 (23.03.2012)		CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, D DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, H HR, HU, DJ, LL, IN, IS, JP, KE, KG, KM, KN, KP, K KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, M
(25)	Filing Language: English		MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, N OM, PE, PG, PH, PL, PT, OA, RO, RS, RU, RW, SC, SI
(26)	Publication Language: English		SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, T
(30)	Priority Data: 25 March 2011 (25.03.2011) US	(84)	Designated States (unless otherwise indicated, for eve
(71)	Applicant (for all designated States except US): UNIVER- SITY OF GEORGIA RESEARCH FOUNDATION, INC. [US/US]: Boyd Graduate Studies Research Center, Athens, GA 30602-7411 (US).		Kina (j) regional protection avaluate); AKN 50 (bW, G GM, KE, LK, LS, MW, MZ, NA, RW, SD, SL, SZ, T UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, R; TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, D DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, L'
(72) (75)	Inventors; and Inventors/Applicants (for US only): BOONS, Geert-Jan [NL/US]; 1321 Lake Wellbrook Drive, Athens, GA 30606		LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SI SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GG GW, ML, MR, NE, SN, TD, TG).
	(US). WANG, Zhen [CN/US]; 846 Massachusetts Aven- ue, Apt. 2F, Arlington, MA 02476 (US).	Pub	lished:
(74)	Agent: SANDBERG, Victoria, A.; Mueting Raasch & Gebhardt, P.A., P.O. Box 581336, Minneapolis, MN 55458-1336 (US).	_	with international search report (Art. 21(3)) before the expiration of the time limit for amending the claims and to be republished in the event of receipt amendments (Rule 48.2(h))







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PatentPak:

Patent

chemistry is

and more!

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



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Important chemistry locations are identified by CAS expert scientists



Export of marked up patents includes a summary of the key substances in a patent



Mark	Page #	CAS RN	Name	Structure
01	p.151	831203-13-5	Pyridine, 5-bromo-2-chloro-3-fluoro-	F C
02	p.151	57260-71-6	1-Piperazinecarboxylic acid, 1,1- dimethylethyl ester	
03	p.151	1289048-68-5	1-Piperazinecarboxylic acid, 4-(5-bromo-3- fluoro-2-pyridinyl)-, 1,1-dimethylethyl ester	* ŶO _{YX}
104	p.151	7547-97-9	Boronic acid, B-(1E)-1-propen-1-yl-	OH B
105	p.151	1416788-07-2	1-Piperazinecarboxylic acid, 4-[3-fluoro-5- (1£)-1-propen-1-yl-2-pyridinyl]-, 1,1- dimethylethyl ester	"Pays
106	p.151	1416788-08-3	1-Piperazinecarboxylic acid. 4-[5-[(1S,2S)- 1,2-dihydroxypropyl]-3-fluoro-2-pyridinyl]-, 1,1-dimethylethyl ester	rigova
107	p.151	1416788-09-4	1,2-Propanediol, 1-[5-fluoro-6-(1- piperazinyi)-3-pyridinyi]-, (1 <i>S</i> ,2 <i>S</i>)-	The Com
108	p.151	833491-50-2	1H-Imidazole-1-carboxamide, N-(6-methyl- 2-benzothiazolyl)-	CLITC
121	p.151	1416788-16-3	1-Piperazinecarboxamide, 4-[5-[(1 <i>S</i> ,2 <i>S</i>)- 1,2-dihydroxypropyl]-3-fluoro-2-pyridinyl]- <i>N</i> - (6-methyl-2-benzothiazolyl)-	the man
09	p.153	2536-91-6	2-Benzothiazolamine, 6-methyl-	S NH

This convenient summary is appended to the end of a patent.

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

	Experimental Pro	ptocols	
	DD MethodsNow™	Experimental Procedure	
	Products	$2 - Pyridine - 3, 5, 6 - d_3 - carboxamide, 4 - (4 - aminophenoxy - 2, 3, 5, 6 - d_4) - N - (methyl - d_3) - , Yield: 87\%$	Key chemical components of
	Reactants	4- (Amino-d ₂)phen-2,3,5,6-d ₄ -ol-d	the reaction are identified with
Supeling (7)	[Stage 2]	2-Pyridine-3,5,6-d ₃ -carboxamide, 4-chloro- <i>N</i> - (methyl-d ₃)-	links to additional information
E Suppliers (7)	Reagents	Potassium tert-butoxide Potassium carbonate	
Step 1	Solvents	Dimethylformamide	
Step 1	Procedure	 Add potassium tert-butoxide (222 mg, 1.98 mmol) to a solution of d7-4-aminophenol (222 mg, 1.91 mmol; 97 atom % D (CDN Isotopes)) in DMF (2.0 mL). Stir the reaction for 1 h. Add a solution of 4-chloro.35 6-dN/methyl-d-bicolinamide (305 mg, 1.73 mmol) in DMF (0.6 ml.). 	Go directly to the lab
Stage Reagents	Ca	shad a solution of 4-chains (6.5, 3.6) generating a spectrum initial (3.5, ing. (7.5, initial) in the fold (1.6) via a chain (3.6) with a 0.6 mL DMF rinse. 4. Add K_2CO_3 (129 mg, 0.935 mmol) to the mixture and heat the mixture to 80°C for 12 h.	with step-by-step
1 Potassium <i>tert</i> -butoxide	-	 Cool the reaction to room temperature. Dilute the mixture with EtOAc and pour into a separatory funnel containing EtOAc and brine. Weak the accessic laws twice with bring. 	instructions
2 Potassium carbonate	-	 wash the organic tayer (where with brine) Wash the combined aqueous solutions once with EtOAc. Dry the combined organic solutions over Na-SO₄. 	
CAS Reaction Number	31	 b) Alter the mixture or game boddens or a trageoup Filter the mixture. Concentrate the filtrate in vacuo. Purify the residue on an ISCO instrument (0% to 90% EtOAc in hexanes) to afford 4-(4-amino(phenoxy-d₄))-3,5,6-d₃-N-(methyl-d₃)picolinamide. 	
	Transformation	Aromatic Substitution by Oxygen Nucleophiles	Additional useful
	Scale	milligram	information is included
	Characterization D	ata	
	▲ 2-Pyridine-3	5,6-d ₃ -carboxamide, 4-(4-aminophenoxy-2,3,5,6-d ₄)-N-(methyl-d ₃)-	
	Mass Spectrun	n MS (M + H): 254.0	
		CAS is a division of the American Chemical Society.	A CAS SOLUTION

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& All S	As Drawn (5)	References	As Drawn (3,103)	Q Substances A Reactions	44 Cited By		ប្		k Save		
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A Reactions	Filter by	1 1		Multikinase inhibitors: a new	option for the treat	ment of thyroid cand	er				
E References	 Substance Role 		Filter by	By: Gild, Matti L.: Bullock, Martyn: Robi	nson, Bruce G.; Clifton-Blig	th, Roderick					
📜 Suppliers	Product (13)	0.000	 Document Type 	Nature Reviews Endocrinology (2011), 7(10), 617-624 Language: English, Database: CAplus View Reference Detail View Corresponding MEDLINE Reference							
	() Reactant (5)		(Journal (1.955)	Abstract: A review. Preclin. models ha	e shown that inhibition of	kinases in mitogenic and a	ngiogenic signali	ng pathways	can		
	∧ Yield	R Suppliers (3)	Patent (1,132)	have antitumoral effects. Starting with	a brief synopsis of a malig	mancy that responds well to	kinase inhibitio	(chronic m	yeloid		
and Country of	80-89% (2)	Reaction Summary	C Review (572)	leukemia) compared with one with less overcome in order to successfully tran	durable responses as yet slate small-mol. therapies t	(melanoma), this Review hi to thyroid cancer in the fut	ghlights challeng ure. Thyroid can	es that must cer, typically	has a		
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11:55 AM	(_) 30-49% (2)	(3:1)	. 1.0000.000	Full Text •	G Substances (7)	A Reactions IOI	Cited By (72)	@ Citation	n Map		
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Organization: Memorial Sloa	Procedure Available (6)	View Reaction Detail	C Korean (40)	Expert Opinion on Pharmacotherapy (View Reference Detail 1 View Correspo	Expert Opinion on Pharmacotherapy (2012), 13(3), 407-419 Language: English, Database: CAplus View Reference Datall L View Corresponding MEDI INF Reference						
	 Reaction Type 	Reaction Summary	French (24)	Abstract: A review. Introduction: was to	he first oral antiangiogenic	ntiangiogenic multikinase inhibitor (Raf kinases, VEGF receptors 1 - 3. PDGF-					
March 27, 2017	~ Reagent	Reagents Sodi	View All	beta. Fit-3, c-kit) for advanced renal cel	carcinoma (RCC) to be ap	proved. Since 2005, a total	of six drugs have	been appro	ved for		
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o	 Reaction Notes 	Solvents Acet	233	Full Text +	G Substance (1)	표 Reactions (0) 44	Cited By (11)	O Citation O	n Map		
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Information presented to facilitate rapid understanding $\int \underbrace{\|\mathbf{x}\|_{\mathbf{x}} + \|\mathbf{x}\|_{\mathbf{x}} + \|\mathbf{x}\|_{\mathbf{x}}$

Powerful filtering capabilities allow rapid focus Product (13) Reactant (5) Suppliers (3) Suppliers (6) ~ Yield 90-100% (4) 80-89% (2) **Reaction Summary** Carbon-carbon bond-forming reactions promoted by trivalent manganese 70-79% (4) Sodium acetate View Reference Detail Reagents Steps: 1 50-69% (1) Acetic acid, Yield: 92% By: Melikyan, Gagik G. manganese(3+) salt 30-49% (2) Organic Reactions (Hoboken, NJ, United States) (1997), (3:1) No pp. given Number of Steps Catalysts Full Text -1 (13) Solvents Acetic acid Experimental Protocols Conditions -MethodsNow Available (2) View Reaction Detail | Experimental Protocols Procedure Available (6) Reaction Summary Carbon-carbon bond-forming reactions promoted by Reaction Type trivalent manganese Sodium acetate View Reference Detail Reagent Reagents Steps: 1 Acetic acid. Yield: 92% By: Melikyan, Gagik G. Catalyst manganese(3+) salt Organic Reactions (Hoboken, NJ, United States) (1997), (3:1)~ Solvent No pp. given Catalysts Commercial Availability Full Text -Acetic acid Solvents Reaction Notes Conditions Source Reference View Reaction Detail | Experimental Protocols Publication Year View 2 Reactions Document Type Collapse Scheme Language

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Reference: Relevancy

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	Best (11)		
	Good (1.534)	Short communication: Ranid antibiotic screening tests detect antibiotic	residues
	C Este (222)	in powdered milk products.	residues
	Fair (333)		
	Learn more about Relevance	By: Kneebone, J: Tsang, P C W; Townson, D H	
	Pair (333) Learn more about Relevance Document Type	By: Kneebone, J: Tsang, P C W; Townson, D H Journal of dairy science (2010), 93(9), 3961-4 Language: English, Database: MEDLINE View Reference Detail View Corresponding CAplus Reference	
	Pair (333) Learn more about Relevance Occument Type Journal (1,441)	By: Kneebone, J: Tsang, P C W: Townson, D H Journal of dairy science (2010), 93(9), 3961-4 Language: English, Database: MEDLINE View Reference Detail View Corresponding CAplus Reference Abstract: Rapid antibiotic screening tests are widely used in the dairy industry to monitor mill	k for the presence
	Pair (333) Learn more about Relevance Occument Type Journal (1,441) Patent (374)	By: Kneebone, J: Tsang, P C W: Townson, D H Journal of dairy science (2010), 93(9), 3961-4 Language: English, Database: MEDLINE View Reference Detail View Corresponding CAplus Reference Abstract: Rapid antibiotic screening tests are widely used in the dairy industry to monitor mill of antibiotic residues above regulated levels. Given the persistent concern over contamination with antibiotic residues, we investigated the utility of (IDEX) Span test devices (IDEX) (Span)	k for the presence



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Identification and characterization of a Pantoea citrea gene encoding glucose dehydrogenase that is essential for causing pink disease of pineapple By: Cha, Jae-Soon: Pujol. Catherine: Kado, Clarence I. Applied and Environmental Microbiology (197), 63(1), 71-76 [Language: English, Database: CAplus			Abstract: Pantoea citre symptom is characteriz pineapple fruit cylinde responsible for this fru and fruit discoloration, activities was isolated h	bstract: Pantoea dtrea, a member of the family Enterobacteriaceae, causes pink disease of pineapple, whose ymptom is characterized by the formation of pink to brown discolorations of the infected portions of the aineapple fruit cylinder upon canning. Mol. genetic approaches were applied to elucidate the mechanism esponsible for this fruit discoloration. A P. citres mutant strain, CMC6, defective in its ability to cause pink disease and fruit discoloration was generated by introsoguandine mutagenesis. A DNA fragment that restored these relatives was caused these new discoloration. Was generated by introsoguandine mutagenesis. A DNA fragment that restored these relatives was character by created these new discoloration.					vhose disease nese		
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15. A process according to any one of the preceding claims wherein the organoboron compound is a compound of formula (II) or (III):



wherein:

Ar is an aryl ring or a heteroaryl ring;

each R^A group is the same or different and is a group selected from substituted or unsubstituted C_{1-20} alkyl, substituted or unsubstituted C_{2-20} alkenyl, substituted or unsubstituted C_{2-20} alkynyl, substituted or unsubstituted C_{3-20} cycloalkyl, substituted or unsubstituted heterocyclyl, substituted or unsubstituted aryl, substituted or unsubstituted heteroaryl, cyano, amino, C_{1-10} alkylamino, di(C_{1-10})alkylamino, arylamino, diarylamino, arylalkylamino, amido, acylamido, hydroxy, halo, carboxy, ester, acyl, acyloxy, C_{1-20} alkoxy,





aryloxy, haloalkyl, sulfonic acid, thiol, C_{1-10} alkylthio, arylthio, sulfonyl, phosphoric acid, phosphate ester, phosphonic acid and phosphonate ester, wherein two or more R^A groups may be bonded together to form one or more rings;

R^B, R^C, and R^D are each independently selected from H, substituted or unsubstituted C₁₋₂₀ alkyl, substituted or unsubstituted C₂₋₂₀ alkenyl, substituted or unsubstituted C₂₋₂₀ alkynyl, substituted or unsubstituted C₃₋₂₀ cycloalkyl, substituted or unsubstituted heteroaryl, cyano, amino, C₁₋₁₀ alkylamino, di(C₁₋₁₀)alkylamino, arylamino, diarylamino, arylalkylamino, amido, acylamido, hydroxy, halo, carboxy, ester, acyl, acyloxy, C₁₋₂₀ alkoxy, aryloxy, haloalkyl, sulfonic acid, thiol, C₁₋₁₀ alkylthio, arylthio, sulfonyl, phosphoric acid, phosphate ester, phosphonic acid and phosphonate ester, wherein two or more of R^B, R^C, and R^D may be bonded together to form one or more rings;

Z is group selected from a boronic ester group, a boronic acid group, a borate group or a trifluoroborate group; and

x is an integer from 0 to 5.

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Retrosynthesis

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NMR SPECTRA SEARCH

NMR peak \rightarrow Molecular Weight \rightarrow Fragments structure \rightarrow Identify Structure

 $(500 \text{ MHz}): \delta 6.84 \text{ (br s, 1 H)}, 6.10 \text{ (br s, 1 H)}, 6.02 \text{ (s, 1 H)}, 5.15 \text{ (br s, 1 H)}, 5.05 \text{ (s, 1 H)}, 4.98 \text{ (m, 1 H)}, 4.50 \text{ (br d, 1 H, J = 11 Hz)}, 3.19 \text{ (t, 1 H, J = 12 Hz)}, 2.72 \text{ (dd, 1 H, J = 12, 4.5 Hz)}, 2.40 \text{ (dd, 1 H, J = 14.5, 3.0 Hz)}, 2.36 \text{ (t, 1 H, 11 Hz)}, 2.07 \text{ (m, 1 H)}, 2.04 \text{ (s, 3 H)}, 1.99 \text{ (br s, 3 H)}, 1.89 \text{ (br s (OH)}, 1 \text{ H)}, 1.79 \text{ (br s, 3 H)}, 1.66 \text{ (m, 1 H)}, 0.89 \text{ (td, 1 H, J = 13.5, 3.5 Hz)}$

Removing the info in brackets you can search with: 6.84, 6.10, 6.02, 5.15, 5.05, 4.98, 4.50, 3.19, 2.72, 2.40, 2.36, 2.07, 2.04, 1.99, 1.89, 1.79, 1.66, 0.89



NMR peak \rightarrow Molecular Weight \rightarrow Fragments Structure \rightarrow Identify Structure

AND Substance Property Select Property - Select One -	Enter Value	
Add Another Property AND Experimental Spectra Select Spectrum Proton NMR	Enter Value 5, 2.07, 2.04, 1.99, 1.89, 1.79, 1.66, 0.89	
Add Another Spectra	(Search includes allowance of ± 0.2 ppm) Example: 8.03, 7.2, 2.63 5.95, 7 to 8.5 6.3	
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NMR peak \rightarrow Molecular Weight \rightarrow Fragments Structure \rightarrow Identify Structure

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	 Commercial Availability Available (3) 	References •• 🛽 Reactions ••	😲 💌 ★ Save				
	Not Available (22)	0 16846-24-5	Key Physical Properties	Value	Condition		
 Stereochemistry 	 Reaction Role 	View Detail	Molecular Weight	827.99	-		
 Number of Components 	Product (9) Reactant (6)	1 the	Melting Point (Experimental)	131.5 °C			
 Substance Class Isotopes 	 Reference Role 	Jani	Boiling Point (Predicted)	877.8±65.0 °C	Press: 760 Torr		
 Metals 	Adverse Effect (1)	Absolute stereochemistry shown Double bond geometry shown	Density (Predicted)	1.20±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr		
 Molecular Weight 	 Analytical Study (2) Biological Study (23) 	C ₄₂ H ₆₉ NO ₁₅ Josamycin	pKa (Predicted)	13.06±0.70	Most Acidic Temp: 25 °C		
No Min to No Max Apply Available Range: 328 to 1291	Formation (1) Miscellaneous (2) View All	■ 2,065 ▲ 53 ₩ 34 References Reactions Suppliers	Experimental Properties	Spectra			
 Experimental Spectrum 	Δt this time v	ou can enter the mo		Value	Condition		
 Regulatory Information 	 Number of Components 		Molecular Weight	593.75			
 Bioactivity Indicator 	weight or trag	ment.	Boiling Point (Predicted)	780.4±60.0 °C	Press: 760 Torr		
 Target Indicator 	 Isotopes 	- String -	Density (Predicted)	1.085±0.06 g/cm³	Temp: 20 °C; Press: 760 Torr		
Search Within Results	 Metals 	Absolute stereochemistry shown, Rotation (+)	pKa (Predicted)	13.61±0.70	Most Acidic Temp: 25 °C		
Ø Draw	 Molecular Weight 	Double bond geometry shown $C_{35}H_{47}NO_7$	Experimental Properties Spectra				
	 Experimental Property 	2 3:11 12-Dideepoxy-2 3 11 12-tetradebyd					

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Search History Screen									
		Substances • Enter a query Celit • Q	Delete search						
	Filter by Search Type All (58) Substances (81) Reactions (18) References (115) Suppliers (4) Date	© Search History (276) October 16, 2017 1:20 PM & All:	Rerun Search						
Specified date range	Start Date End Date mm/dd/yyyy to mm/dd/yyyy Coctober, 2017 SU MO TU WE TH FR SA 1 2 3 4 5 6 7 8 9 10 11 12 14	Substances: As Drawn (263) Reactions: As Drawn (1,136) References: As Drawn (38K) Suppliers: (0) October 6, 2017	Return search for new result						
	6 9 10 11 12 13 14 15 16 47 18 19 20 21 22 23 24 25 26 27 28 29 30 31 1 2 3 4	 10:02 AM References: polyimide manufacture (1.3M) 10:00 AM Substances: risperidone (1) 	Rerun Search Rerun Search						
		9:57 AM	Rerun Search						



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Senior Account Consultant tliu2@acs-i.org

SciFinderN 文獻查詢

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Find References

Find document references that match your query, which can be <u>search terms</u>, a <u>chemical structure</u>, or both: •If you enter a search term **or** chemical structure query, SciFinderⁿ 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
- <u>A Specific Author</u>

Find References Associated with a Company

or Organization

Find a Reference Using Journal Information

Find Patent References by:

Assignee

•<u>Inventor</u>

			★ Saved	() History	Account
	Search				
	& All	Search by Keyword, Substance Name, CAS RN, Patent Number, etc.			
2	O Substances	Enter a query			raw Q
	A Reactions	Us Advanced Search or Author, Journal, or Organization			
	References				
	🐂 Suppliers				



Find References Using Search Terms

Search terms may be:

- •Research Topic/Keyword/Concept (e.g., analgesics)
- •Substance Name (e.g., ibuprofen)
- •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)



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



•AND

•The AND operator combines two keywords in a search to get results that contain both of them

Will provide results that contain both terms anywhere in the document
total AND synthesis



Examples:

•flavor **and** extract •3463-67-7 **and** 7664-41-7

> SCIFINDERⁿ A CAS SOLUTION

•NOT

- •The NOT operator will eliminate keywords from the search
- Will provide results that contain the term total but not the term synthesis
 total NOT synthesis



Examples:

- •electrolysis not haptens
- •1,5-Di-2-naphthalenyl-3-pentanone **not** Dibenzylideneacetone



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"



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



• ()

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



Entering terms and operators in <u>parentheses</u> 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



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.



Syntactic Reference Text Wildcard Searching * ?

This epic will allow users syntactically search references with wildcards.

Syntactic searching is limited to:

- Title
- Abstract
- Keywords
- Concept Modifiers

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.



Examples

The query synth* will hit on terms such as

- Synthesis
- Syntheses
- Synthetic
- Synthesizing
- Etc.

References 👻 synth*	× 🖉 Draw 🔍 🖈 🔇 💵
Full Text 🗸	Image: Substances (0) Image: A Reactions (0) Image: A Reaction State of the sta
5	
A planning strat	tegy for diversity-oriented <mark>synthesis</mark>
By: Burke, Martin D.; Angewandte Chemie View Reference Deta	: Schreiber, Stuart L. e, International Edition (2004), 43(1), 46-58 Language: English, Database: CAplus ali
Abstract: A review. In precise or dense reg diverse structures. Th collections of small n also yield compound post-screening, mat multiple orientations the development of and thinking, these f forward-synthetic a	n contrast to target-oriented synthesis (TOS) and medicinal or combinatorial chem., which aim to access jons of chem. space, diversity-oriented synthesis (DOS) populates chem. space broadly with small-mols., having he goals of DOS include the development of pathways leading to the efficient (three- to five-step) synthesis of mols. having skeletal and stereochem. diversity with defined coordinates in chem. space. Ideally, these pathways 5s having the potential to attach appendages site- and stereoselectively to a variety of attachment sites during a wration stage. The diverse skeletons and stereochemistries ensure that the appendages can be positioned in s about the surface of the mols. TOS as well as medicinal and combinatorial chemistries have been advanced by retrosynthetic anal. Although the distinct goals of DOS do not permit the application of retrosynthetic concepts foundations are being built on by using parallel logic, to develop a complementary procedure known as anal. This anal. facilitates synthetic planning, communication, and teaching in this evolving discipline.
Full Text 🗸	
6	
Zeolite and mol	lecular sieve <mark>synthesis</mark>
By: Davis, Mark E.; Lo Chemistry of Materia View Reference Deta	obo, Raul F. als (1992), 4(4), 756-68 Language: English, Database: CAplus ail
Abstract: A review, w and phosphate-base The ability to plan ze demonstrate the cur	with 107 references, of zeolite and mol. sieve syntheses. The syntheses of Al-rich zeolites, high-silica zeolites, 2d mol. sieves are evaluated. Unresolved mechanistic issues are outlined, and areas for exploration suggested, 2olite and mol. sieve syntheses is discussed, and a strategy for synthesizing a chiral zeolite is used to rrent limitations in designing new mol. sieves.
Full Text 🗸	Substances (0) A Reactions (0) G Citation Map
7	
Recent develop	pments in the stereoselective synthesis of α-amino acids
By: Duthaler, Rudolf	°0.

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.

Referer	nces 👻	tot* synth* nat* prod* terpen* last*	×	Draw	٩	*	0	L
	Your qu Learn r	uery cannot contain more than 5 wildcard (?, *) characters. nore about wildcard searching.						
						2 S	CIF	IND
						AC	AS SOLUTI	ON

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Senior Account Consultant tliu2@acs-i.org

Substance Searching

CAS is a division of the American Chemical Society. Copyright 2017 American Chemical Society. All rights reserved. CAS° A DIVISION OF THE AMERICAN CHEMICAL SOCIETY **Find Substances by Name, Registry Number, or Document Identifier** Search terms may be:

•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)



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*).

• 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.



Find Substances Using Multiple Search Terms

You may search for substances using multiple substance names, CAS Registry Numbers (RNs), and document identifiers like patent, accession, and PubMed ID numbers.

For example, the query **methyl ethyl ketone 15687-27-1 "phenyl bromomethyl sulfone" 98113** returns the following results:

1.15687-27-1: CAS RN in the query.

2.98-11-3: CAS RN matched to 98113 in the query.

3.Phenyl bromomethyl sulfone: quoted substance name in the query.

4.Methyl ethyl ketone: substance name in query. Since the name does not appear in quotes, each word may be matched to a substance:

- 5. Methyl
- 6. Ethyl ketone
- 7. Ethyl

8.Mg: substance indexed in a MEDLINE reference with a PubMed ID matching 98133 in the query.

9.F: substance indexed in a MEDLINE reference with a PubMed ID matching 98133 in the query.



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	簡稱	關於	1
登酵乳桿菌 (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。	



Enable Structure Searching with Deuterium and Tritium

Explicit structure searching of deuterium (D) and tritium (T) atomshas been enabled.

In CAS Draw, the D and T atoms are accessed via the bottom toolbar asshown in the screenshot below, and are selected and used in the editorthe same as any

other atom.



Thank you!



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