

Agenda

- 1. Time for a Change SciFinder Web Version
- 2. Contenido
- 3. Explorar Referencias
 - ¡Para químicos!
 - ¡Para biólogos!
 - ¡Para farmacéuticos!

- ...

• 4. Explorar Sustancias-Ejemplo de búsqueda

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- 5. Explorar Reacciones
- 6. Ayuda y más información

1.1. *Time for a Change* – SciFinder Web Version

- CAS introdujo la nueva versión Web de SciFinder el pasado diciembre de 2008.
- SciFinder 2007 es la versión final de la versión cliente y será eliminada durante el 2011.
- Todas las nuevas funcionalidades, nuevos desarrollos y contenidos sólo serán accesibles desde la versión web de SciFinder.
- ¡La nueva versión Web de SciFinder es el futuro, ofrece únicas funcionalidades y posibilidades!

SCIFINDER

1.2. *Time for a Change* – Buenas razones

- SciFinder Web: acceso desde el navegador
 - No es necesario instalar un software.
 - No es necesario actualizarlo: ¡siempre se accede a la última versión de SciFinder!
 - Accesible desde cualquier ordenador.
 - Seguridad: protocolo https.
- SciFinder Web utiliza una arquitectura XLM con funcionalidades únicas Web 2.0
 - Guardar, conectar y combinar búsquedas es muy fácil.
 - Funiones personalizadas, como alertas, Tags y comentarios.
 - Es posible cooperar con colegas de profesión.
 - Preparado para futuras actualizaciones y nuevas funcionalidades.

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1.3. *Time for a Change* – Registro

Welcome to User Devictorian for OsiCiado @L	(bid' = requisit)
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2.1. Contenido - CAPLUS, REGISTRY, CASREACT, CHEMCATS y CHEMLIST

CAplus [™]	CAS REGISTRY SM	CASREACT®	CHEMCATS®	CHEMLIST®
 >32M bibliographic records >10,000 journals covered Patents from 60 patent offices Updated daily (~3K daily) Links to almost 300 publishers and 3 patent offices Literature back to early 1800s Cited articles from 1997 onward 	 55M small molecules >62M sequences Updated daily (>12K daily) Substances reported comprehensively in literature 1957- Includes nomenclature, spectra, and properties (experimental and predicted) 	 38.8M single and multi-step reactions Extracted from patents and journal articles Updated weekly (~30K weekly) Reactions back to 1840 Reaction conditions starting in 2003 	 41M comm. available chemicals >1100 suppliers >1200 chemical catalogs Updated when new or revised catalogs are available Contact/ordering information including quantity and pricing (when available) 	 >280K inventoried / regulated substances >100 inventories & regulated lists from 1979 to present Updated weekly (~50 additions) Contains regulatory requirements for substances REACH !

2.2. Contenido – Medline y MARPAT



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2.2. Contenido – CAS Editorial



3. Explorar Referencias

SF Web ofrece las siguientes novedades:

- Referencias guardadas: accesibles desde cualquier ordenador.
- Alertas: visibles en la página principal.
- Tags sus personales "Index Terms" ¡se pueden compartir con sus colegas!
- Es posible buscar por **DOI**s.
- SF Web incluye ahora casi todas las herramientas de búsqueda y refinar que SciFinder versión cliente 2007.
- Excepción: BLAST y Panorama (estas opciones no se utilizaban mucho en el pasado).

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SCIFINDER

3.1. Explorar referencias – Página principal

SciFinder®	Exp Re	ferences Explore Substances	Explore Reactions		Saved Answer Sets Help Keep Me Posted Results History My Connections Preferences
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3.2. Búsqueda por tema: ¡¡la nº 1!!

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3.2. Búsqueda por tema – El sistema trabaja

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3.2. Búsqueda por tema – Seleccione opción

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SCIFINDER

3.2. Topic Search – explore Results

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3. The flavone, flavonol and flavan-3-ol content of the Greek traditional diet By Dils, Vards; Vasiopoulou, Effe; Trichopoulou, Antonia From Food Chemistry (2007), 105(2), 812-821, Language: English, Database: CAPLUS Flavonoids are an important category of plant antioxidants and evidence is accumulating on their favorable effects against the development of heart disease and certain forms of concer. The authors anal, devid. the flavonol (Quercetin, kaempferol, myricetin, isorharmetin), flavone (Uteolin, apigenin) and flavan-3- ol (catechin, epicatechin, epigallocatechin gallate, epicatechin gallate) content of a weekly menu representative of the Greek traditional diet. The overall daily av. content was found 79.01 mg of which flavonols contribute 47% (37.17 mg/day), flavan-3-ole 40% (31.6 +Sy chatopose Alegaritions Colling Delli Text Cepit & @ O Comments @ U Taos	PDF, RTF, EXCEL or RIS (jnuevo!)

3.2. Búsqueda por tema – ¡descubra los detalles!

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3.2. Búsqueda por tema- Analiza

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3.2. Topic Search – Refine



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3.2. Búsqueda por tema – KMP e Hipervínculos

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3.2. Búsqueda por tema – KMP e Hipervínculos

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3.2. Búsqueda por tema- Categorize



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3.3. Tags y Comments

- Los *Tags* y *Comments* se pueden añadir a las referencias encontradas.
- Los *Tags* se pueden añadir a referencias individuales o a un grupo de referencias.
- Los *Comments* sólo pueden añadirse a referencias individuales.
- Los *Tags* y los *Comments* son visibles sólo para uno mismo y (si tiene conexiones) a sus colegas que esten conectados.

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3.3. Referencia con *Tags* y *Comments*

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3.3. Referencia con *Tags* y *Comments*

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2 Tags Edit Tags heart disease(1); selenium(1)		
Comments		
1 Comment Sort by: Newer First Older First		
Describes the role of micronutrients such as selenium.		
Miriam Plana	Posted August 17, 2010 4:16 AM Last Modified August 17, 2010 4:16 AM	Edit Delete
Add Comment: Maximum of 1024 characters per comment; 50 comments per user. Reminder: Your comments and tags can be viewed by your connected colleagues	5.	<
Save	Char	acters Remaining: 1024
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	Contact Us Copyrights and Trademarks	
Copyright ©	2010 American Chemical Society. All Rights Reserved.	
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3.3. Tags asignados por su grupo



SCIFINDER

3.4. Más mejoras en la versión Web

- En las siguientes transparencias sólo se mostrará una imagen de la nueva funcionalidad. Para una información más detallada clique en HELP- ¡siempre disponible en su SciFinder!
- Estas funcionalidades son:
 - Links envielos vía e-mail a sus colegas.
 - Nuevas opciones KMP. ¡Esté al día!
 - Duplicados Elimine automáticamente los duplicados de CAplus y Medline.
 - Opción *Combine* combine sus sets de respuestas como prefiera.
 - Busque y vea los DOIs: ¡ahora es posible!

3.4. *Links*

SciFinder®	Explore References Explore Substances	Explore Reactions		Saved Answer Sets Help Keep Me Posted Results History My Connections Preference
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2 Vitamins minorals and	I flavonoids intake and the risk o	f cardiovascular diseases	https://scifinder.cas.org/scifind	er/view/link_v1/reference.tsf?l=Bn
		i cui diovascalai discuses	Create a bookmark, save in a docume	int, or e-mail to a colleague.
by related as, drive, resinver, sey A review. Diseases of heart and stro shown that numerous dietary risk fac that the naturally occurring antioxida Substantial lab, animal, and human of LDL cholesterol. B-carotene, a pre LDL cholesterol. B-carotene prevent batters. It is increasingly recognized LDL cholesterol. B-carotene prevent stress. It is increasingly recognized calcium and also vitamin D have prot have been shown to inhibit platelet a prevention of cardiovascular diseases Indexing	ke cause triv staffict data sugg in the initia cursor of i hat foldate and vitamin B6 may play a role in th a rodh. of a substantiation of the initia a redh. in playema homocytemic conch. byr active effect in blood pressure. Selenium is ar ggregation and adhesion, which may be anoth will be reviewed.	ara obtener el hipervículo que enviar a cualquier colega que esado en este artículo. e prevention of cardiovascular disease. The primary me important component of antoxidant defense and flavon er way they lower the risk of heart disease. In this articl	studies, and clin. trials have focused on the hypothesis promary heart disease. theroscientic lesions. Oxidn, kidant vitamins are vitamin E rotant in preventing oxidn. of protent levels during oxidative chanism proposed for their effect as like magnesium, Potassisum and pids which are derived from plants is the role of micronutrients in	Company Argentian States of States o
Mammalian Pathological Biochemist	ry (Section 14-0) 🚸			Accession Number
Section cross-reference(s): 18				2007:1343058 CAN 148:422910
Conconto 🔿		Substances 🚸		CAPLUS

SCIFINDER

3.4. Links

SciFinder® Velcome Miriam Plana Sign Out	Explore References Substa	nces A Reactions				Saved Answer Sets Keep Me Posted Results My Connections	Help History Preference
Search Topies Saved Answer Sets	: "effect of plant flavonoids on" > refi Combine Answer Sets	erences (15) > Vitamins, minera	als, and flavon				
References (2)	ances (2) Reactions (2)						
Substance Answer S	et Details				Date Saved		
amb enllaç senzill i sen Chemical Structure sub	e bloqueig (924) structure > substances (924)		Edit	GO Link	Jun 3, 2010		
anell 3 bloquejat (2871	structure > substances (2971)		Edit	Ge Link	Jun 3, 2010		
ſ	También puede conse	guir el hipervícu	lo para co	ompartir			
	llink, podrán ver tod	as las referencia	as que gu	ardó.			
		Copyright © 2010 American Chemic	al Society. All Rights F	Reserved.			

3.4. Establecer un Keep Me Posted (KMP)



SCIFINDER

3.4. Resultados KMP – ¡SciFinder le envía un e-mail!



¡Tan sólo clique y SciFinder se abre!

3.4. Eliminar Duplicados



SCIFINDER

3.4. Combine resultados

SciFinder*	Explore References	Explore Explore Reactions	10 m	Saved Answer Sets Help Keep Me Posted Results History
Welcome Miriam Plana Sign Out Create Keep Me Posted Research Topic	Combine Answer Sets 🤇			
References & Get	Select saved answer set(s)	to combine with your current answer set (13):		Analysis Refine
13 References 0 Selected Keep	2 Answer Sets 1 Selected		El Combina on una ha	rromionto mun
2 duplicates were removed. To remove o	Reference Answ	er Set Details	El Combine es una ne	
Select All Deselect All Sort by: 1. Solution Structure of H By Robertson, Jan M.; U. Monica From Journal of Biological Chemist Heart muscle contraction Ca2+ is often albered. O protection against a varie ements and outport for	Autosaved Referer An answer set was EDT 2010. Research Topic "e climatic change (1 Research Topic "c	re Set (15) is automatically saved because the session ended due to inactivity on ffect of plant flavonoids on heart disease" > references (15) 145) limatic change" > references (1145)	útil: puede combina guardados y resulta Además, en la versión combinar más de do	r resultados dos activos. n web, ¡puede s resultados!
Substances AReactions			<u>.</u>	Serry Manuadaria 2
2. Vitamins, minerals, and By Tabatabai, Shiva; Keshavarz, From Journal of Tehran University A review. Diseases of h	Select an option for combin	ng the answer sets:		Vinson Joe A 2 Bolling Steven 1
clin, trials have shown th	Intersect	Include only answers that appear in both sets		Cai Songhuai 1
recently focused on the f infarction, progression of Substances Areactions	🔘 Exclude	Include only answers from current answer set (13) that are not in climatic change (1145)		Chang Soo Chul 1
3. The flavone, flavonol a By Dils, Vardis; Vasilopoulou, Effie From Food Chemistry (2007), 105	() Exclude	Include only answers from climatic change (1145) that are not in current answer set (13)		Dilis Vardis 1 Duthie Garry G 1
and certain forms of canc ol (catechin, epicatechin, The overall daily av. cont	ent was found 79.01 mg of wh	iich flavonols contribute 47% (37.17 mg/day), flavan-3-ols 40% (31	Combine Answer Sets Cancel	Elattar T M 1

3.4. Búsqueda por Digital Object Identifier (DOI)

Research Topic Author Name Company Name	Document Identifier(s) 🤄	10.1021/ol1007907 10.1021/jo100454m 10.1021/np050327j		Search
Document Identifier Journal Patent		Enter one per line. Examples: 1983:4296 102:12825	<u> </u>	
Tags	[10.1021/hp050327j		
	/			
	Los DOI's en un ic universal. los usuar	 (Digital Object Ide lentificador de refe CAS ha respondio ios incluyendo est referen 	entifier) se han conve rencias literarias a ni lo a los requerimiente a nueva forma de bu cias.	rtido vel os de scar
	Más	información en es	te link: www.doi.org	

SCIFINDER

3.4. El DOI es visible en la referencia bibliográfica

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Reference Detail & Get Substances & Get Reactions	Get Get Full Text	Quick Links
	Link Save Print Export	0 Tags, 0 Comments
Return I. Synthesis and Evaluation of 2,5-Linked Alternatin By: Rocha, Silvia V.; Finney, Nathaniel S. image omitted] The first iterative access to alternating 2,5-linked pyridine ligomers exhibit strong absorption and emission, even in the solid state (p large red shifts in emission and, unlike most known thiophene-contg. olig pecies represent a promising new class of materials for further study and	Previous Next G Pyridine-Thiophene Oligomers thiophene (Py-Th) oligomers is presented. These icture of the longest oligomer, above). Protonation leads pomers, they are readily reduced but not oxidized. These potential application.	Source Organic Letters Volume 12 Issue 11 Pages 2598-2601 Journal 2010 CODEN: ORLEF7 ISSN: 1523-7060 DOI: 10.1021/ol1007907
		1

3.5. Exporte referencias en distintos formatos

Reference Detail 🖌 Get 🚽 Get Substances 🚽 Reactions	Export 🚸	* Denvised		Quick Links
Return Turmeric extracts containing curcuminoids By: Funk, Janet L; Oyazo, Janice N; Frye, Jennifer B; Cher Turmeric has been used for centuries in Ayurvedic medicine supplements contg. Turmeric rhizome and turmeric exts. are are available regarding antarthritic efficacy of complex turn here were undertaken to det. the in vivo efficacy of well-cha wall (SCW)-induced artitrits, avell-described animal mode for assessing the effect of exts. on pint inflammation. An exploit inflammation when reatment was started before, burr point inflammating compds. In the crude turmeric ext. may Indexing Pharmacology (Section 1-7)	For: Citation Manager Quoted Format (*.ris) Quoted Format (*.tkt) Tagged Format (*.tkt) Offline review Portable Document Format (*.pdf) Rich Text Format (*.rtf) Answer Keys (*.tkt) Saving locally Answer Key eXchange (*.akx)	Petalis: File Name: * Reference <u>8</u> <u>17</u> <u>2010</u> <u>12039</u>	Save Print Export	Source Journal of Natural Products Volume 69 Issue 3 Pages 351-355 Journal 2006 COCEN: INPROF ISSN: 0163-3864 DOI: 10.1021/hp050327) Company/Organization Arizona Center for Phytomedic Research Department of Medi Department of Cell Biology and Anatomy and Department of Pharmacology University of Arizona Tucson, Az, USA 85724
Concepts 🖗 Antiarthritics Curcuma longa Rheumatoid arthritis	Substances @ 459-37-7P. Curcun 22609-11-3P. Dem 33171-05-0P. Bis-c	Exporte a gestore formato .pdf, word más se adapte a	es de referenc ¡Escoja el for a sus necesid	ias, en er rmato que ades!
				35

SCIFINDER

4. Búsqueda de Sustancias

- Cuando se buscan sustancias, se consulta en REGISTRY y ahora (02/08/2010) ¡también en MARPAT!
- La opción de búsqueda de estructuras de MARKUSH no es posible en SciFinder 2007.
- REGISTRY es la mayor base de datos de substancias del mundo (más de 54 millones de sustancias y más de 61 millones de secuencias).

4.1. Búsqueda de Sustancias - Página principal



SCIFINDER

4.2. El nuevo Editor de Sustancias



4.2. Editor de estructuras: Import

SciFinder*	Ø Structure Editor	×	d Answer Sets Help Posted Results History
Welcome Miriam Plana Sign Out Explore Substances	Draw or change stoms or bonds. Shortout Keys	Structure Reaction	Answer Sets 📀
Chemical Structure Markush Molecular Formula Substance Identifier Characteristic (s) Class (es) Studies	Import Import from Import from	Markush	Import Cancelar

SCIFINDER

4.3. Una gran novedad: ¡MARPAT en SciFinder!

- Esta nueva opción busca en la base de datos MARPAT producida por CAS.
- Es una búsqueda de Markush real: es decir, no es sólo una una búsqueda SSM con display de Markush
 - Hablaremos de esta diferencia en las siguientes transparencias.
- Los resultados de una búsqueda por estructuras de Markush son Patentes, no estructuras.
 - Necesitará explorar el texto completo de la patente si desea identificar algún obstáculo para su FTO, por ejemplo.



SCIFINDER

4.4. Ejemplo de búsqueda en SciFinder por fórmula de Markush

- ¿Se ha descrito el siguiente compuesto en la literatura o en patentes?
- Si no, ¿es un compuesto nuevo?
- ¿Tengo la libertad para operar (FTO) con esta sustancia?



4.4. Editor de estructuras de Markush



SCIFINDER

4.4. Búsqueda subestructural

SciFinder* Welcome Miriam Plana Sign	Out	re Explore Explore Explo rences Substances Explo	re tions		Saved Answer Sets Help Keep Me Posted Results History My Connections Preference:
Explore Substances Chemical Structure Che Markush Structure Molecular Formula Substance Identifier	emical Structure 🗘	Mo Search type: • Exact Structure • Substructure • Substructure • Similarity	Búsqueda SSM	Search	Saved Answer Sets SSM Patents 31 SSM patents Sativex SSM patents Sativex SSM patents UV amb enlias senzill i sense bloqu eig anell 3 bloquejat Lactroe blocked positions o-c=o Lactroe Non participating funct ional group climatic change Autosaved Reference Set View All Import. Keep Me Posted Results Climatic Change Aug 21, 2010 (8)
Ch	aracteristic(s)	Single component Commercially available Included in reference(s)			View All My Connections ② No invitations to connect
Cla	ass(es) 🚸	Alloys	Mixtures		No outstanding sent invitations You have 4 connections

SciFind	er°	Explore References	Explore Substances	Explore Reactions		Saved Answer Sets Help Keep Me Posted Results History	
alcome Paul P Pet	ers Sign Out				1	My Connections Preferences	
eate Keep Me Posted	Chemical Structure subst	ucture > substances	(0)	0	20-	200	
Substances	Combine Answer Sets					Analysis Refine	
Substances () Selected					Analyze by: 🕢	
xplore Substa	esulted in 0 substances Retu	m				No substances available	

Ahora es posible recuperar patentes adicionales con la búsqueda de Markush. No es necesario volver a dibujar la estructura.



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Hay 12 referencias donde la estructura coincide con fórmulas de Markush



SCIFINDER

Si el abstract tiene una estructura (gráfico) puede dar pistas sobre nuestra estructura– ¡consulte la patente para más detalles!

4. Naphthalene derivatives for the treatment of gastrointestinal disorders By Lehmann, Anders

From PCT Int. Appl. (2005), WO 2005058292 A1 20050630. Language: English, Ratabase: CAPLUS The invention discloses the use of compds. I [X = S, S(O), C(O), NH, etc.; R1 = aryl, heteroaryl; R2 = H, OR4, NR5R6; R3 = H, cyano, heteroaryl, etc.; <u>R4 = C1-8 alkyl</u>, *C2-8 alkenyl*; R5, R6 = H, C1-8 alkyl; C(O)C1-8 alkyl; for the inhibition of transfert lower esophageal sphincter relaxations. A further aspect of the invention is directed to the use of I for the treatment of gastroesophageal reflux disease, as well as for the treatment of regurgitation.





♣Substances ▲Reactions ௴Citing DFull Text 👄 Link 🗭 0 Comments 💷 0 Tags



A tener en cuenta.... Opciones en las búsquedas de Markush

- Sólo considera las variables de la estructura especificadas
 - No hay sustitución adicional: las posiciones abiertas serán hidrógenos
- Para resultados grandes de búsquedas de Markush: refine por "topic" con palabras clave como aplicaciones (pesticidas, etc)
- Utilice la opción combine para eliminar las estructuras repetidas de los resultados de búsquedas SSM o exactas.
- Analice por Sección CA para encontrar áreas de aplicación más generales
- Utilice la opción Categorize para revisar la terminología de sus resultados (medicina, agro, alimentación, etc)
- Considere una búsqueda Structure Similarity search como una alternativa o complemento a sus búsquedas de Markush

¿Cuáles son las limitaciones de las búsquedas de Markush?

- No todas las patentes tienen fórmula de Markush, la mayoría sólo describen compuestos específicos
 - De las 486.700 patentes cubiertas en las bases de datos de CAS en 2009, 17.222 conetnían una estructura de Markush
- Cualquier anillo que busque está específicamente dibujado o mencionado en la fórmula de Markush como una opción.
- Patentes que sólo describen el anillo genéricamente (un arilo) no se encuentran.
- Sus anillos son automáticamente aislados (dibujar un fenilo no recupera un naftilo)
- Los profesionales de las búsquedas (STN) pueden hacer búsquedas más genéricas en MARPAT
- Los compuestos organometálicos no se pueden buscar en SciFinder. Contacte a un profesional (STN)
- Los compuestos inorgánicos y los polímeros no se encuentran en la base de datos de fórmulas de Markush

SCIFINDER

5. Búsqueda de Reacciones

- La búsqueda de reacciones en la versión Web de SF ofrece nuevas funcionalidades y opciones (¡ y muy interesantes!):
 - Restricción a determinados disolventes. Puede escoger uno (o más) disolventes a partir de una jerarquía de disolventes real.
 - Puede fijar grupos que no reaccionen desde el principio.
 - Reacciones adicionales a partir de Similar Reactions
 - Más reacciones adicionales a partir del contenido de CA(*Half reactions*)
 - ¡Y más novedades!

5.1. Búsqueda de Reacciones-Página principal

plore React	ions				Saved Answer Sets 🚸
eaction Structur	e Reaction Structure 🕈		Search		SSM patents Sativex SSM patents UV amb enllaç senzill i sense bloqu eig
Selecci Non-part para limi	one Solvents y cicipating Groups tar su búsqueda	Click to Edit	Clique el edi (Re	e aquí para activar tor de Estructuras quiere Java 1.6)	anelli 3 bioquejat Lactone blocked positions o-c= Lactone Non participating funct ional group climatic change Autosaved Reference Set View All
					Import
	Solvent(s) 🚸 🎽	⇒Select Solvents			Keen Me Dosted Results
	Non-participating 🚸 Functional Group(s)	⇒Select Groups			Climatic Change No results
	Number of Steps 🚸				View All
	Classification(s)	Examples: 1, 1 - 3, 1 -, - 3			My Connections 🚸
		Catalyzed	Gas-nhase		No invitations to connect
			Non-catalyzed	Stereoselective	No outstanding sent invitations
		Combinatorial	Photochemical		You have 4 connections
Más o	pciones para limi	tar la			
púsqueda	(también se pue	de hacer			53
ousqueda	(también se pue	de hacer			53

SCIFINDER

5.2. Editor de Reacciones



5. Ayuda y más información

- SciFinder Web es realmente una herramienta única e imprescindible
- Su Login ID y password son válidos para la versión web. No es necesario hacer nada tan sólo empezar a utilizar SciFinder en https://scifinder.cas.org
- Puede encontrar información adicional sobre SciFinder en varios formatos en: http://www.cas.org/support/scifi/index.html

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• ¡Preguntenos!

mplana@cas.org o help@cas.org