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Míriam Plana (mplana@cas.org)

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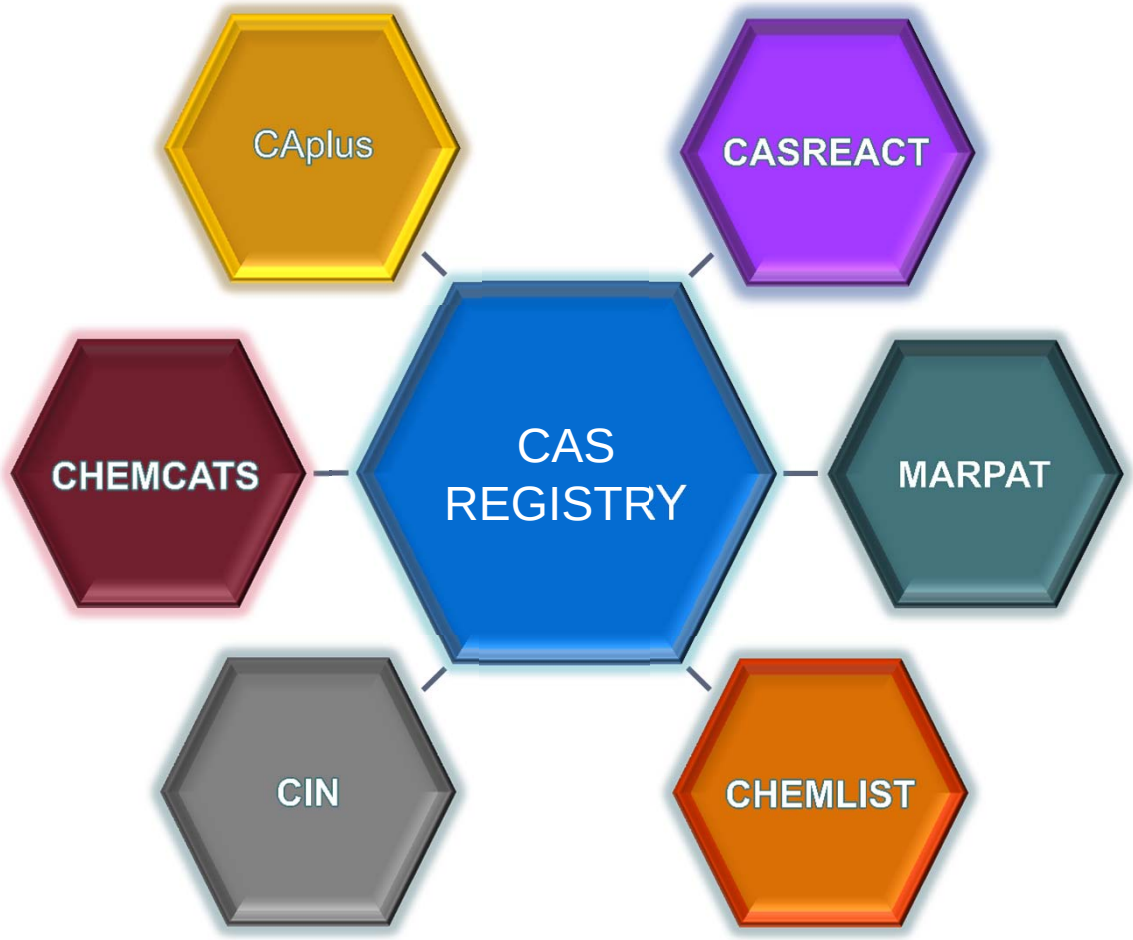
“Being able to rapidly search for important chemical information while an idea is fresh in your mind is almost priceless. CAS databases streamline the investigative process – allowing you to take an idea and rapidly find the important and necessary information before you forget about the idea or it loses its excitement. That really is invaluable.”

Dr. Robert H. Grubbs
Nobel Laureate
Victor and Elizabeth Atkins Professor of Chemistry
California Institute of Technology

CAS provides information to support scientists' and patent searchers' workflows



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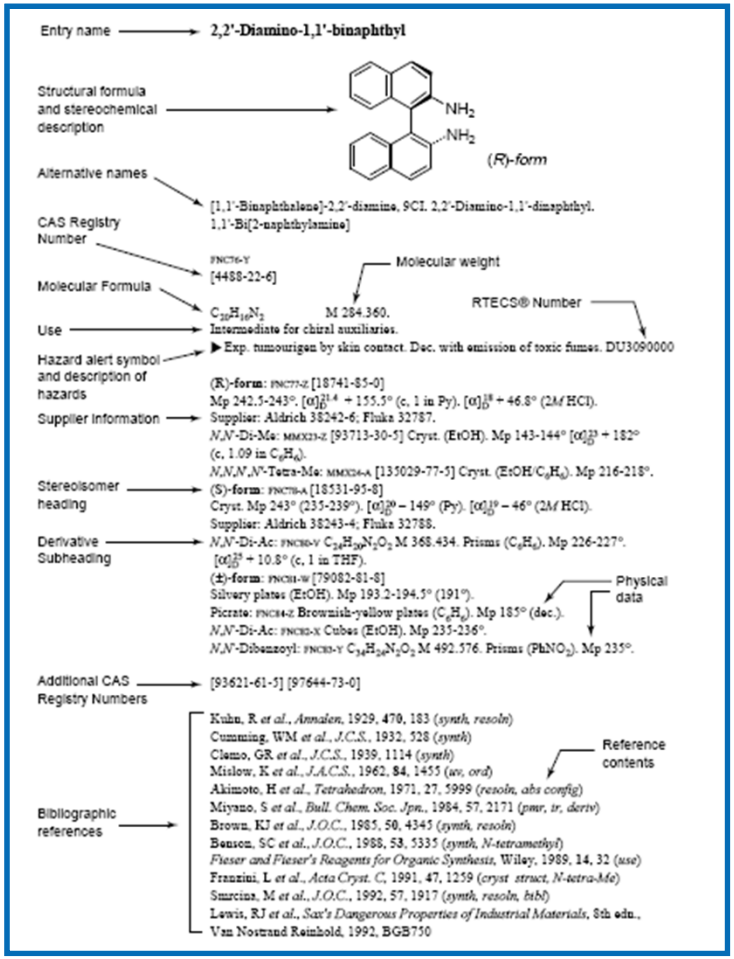

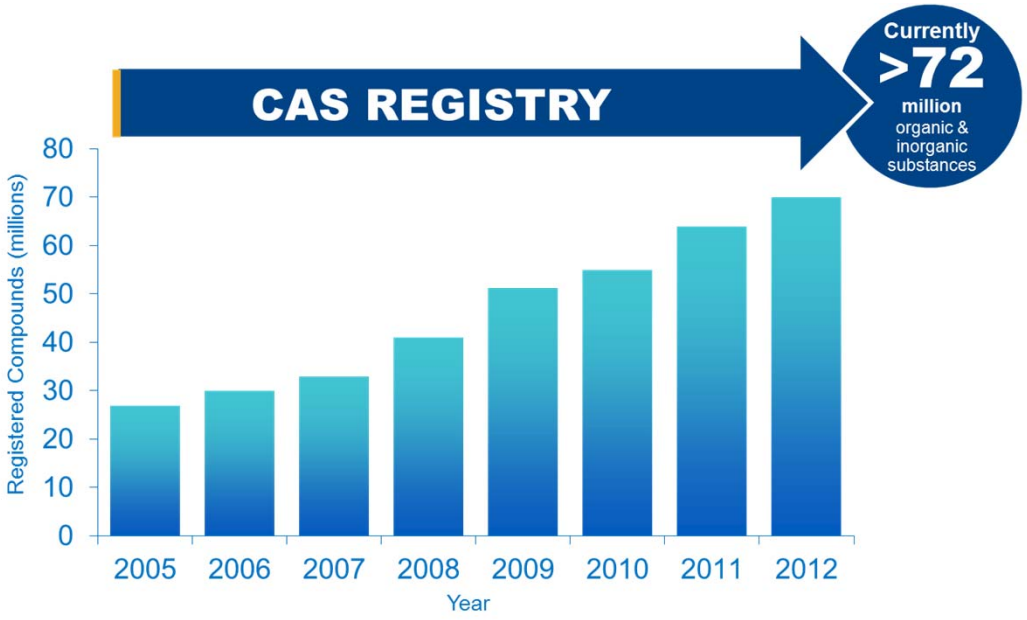

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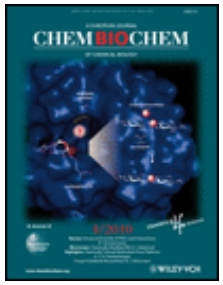
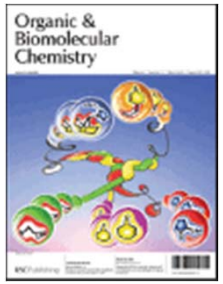
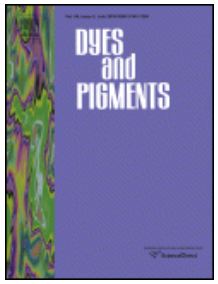
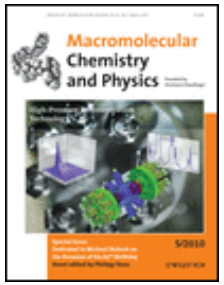
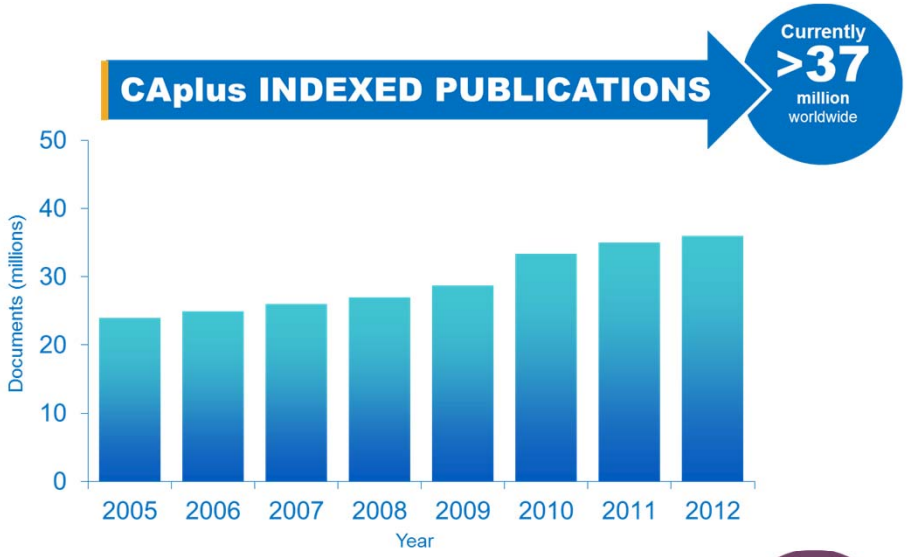
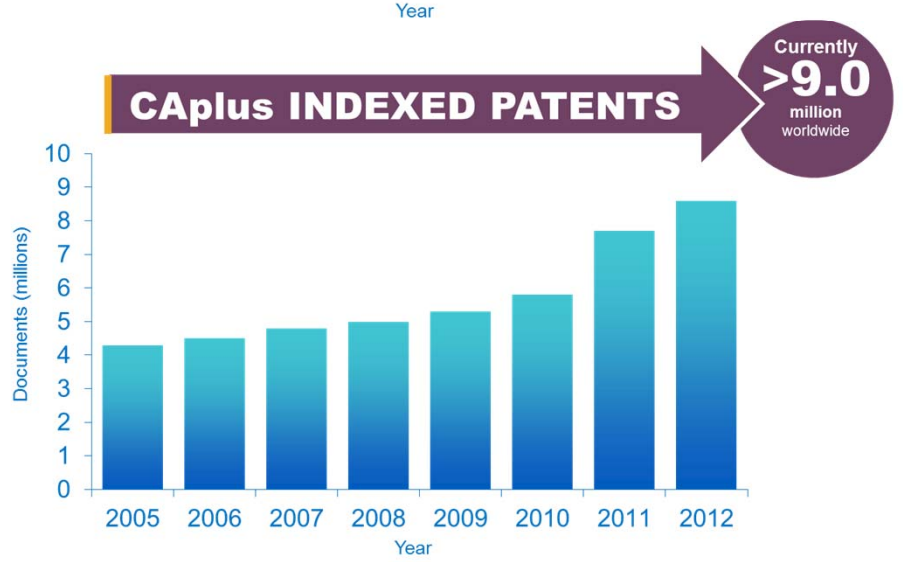




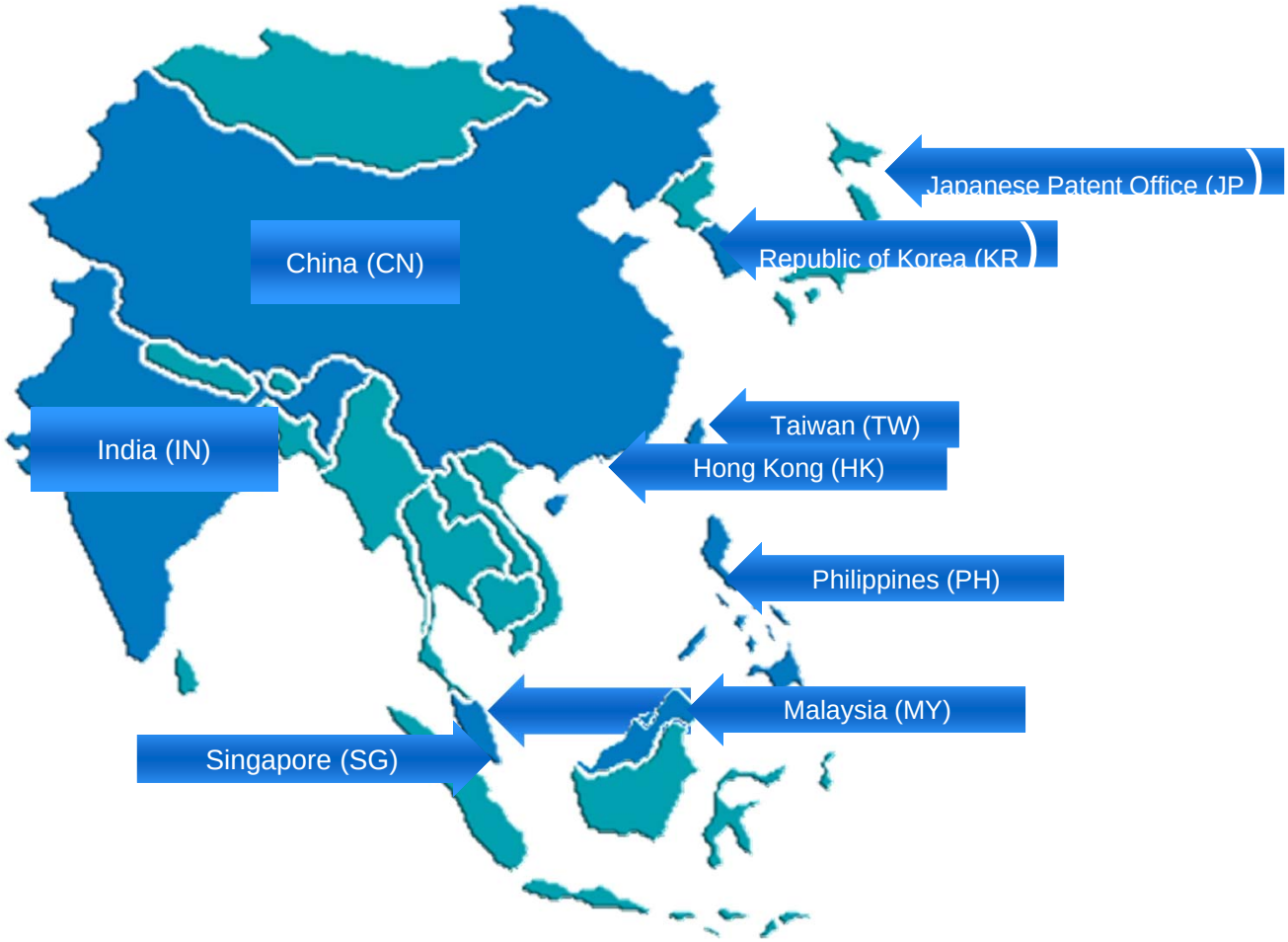








CAplus coverage of patents from Asia is unmatched



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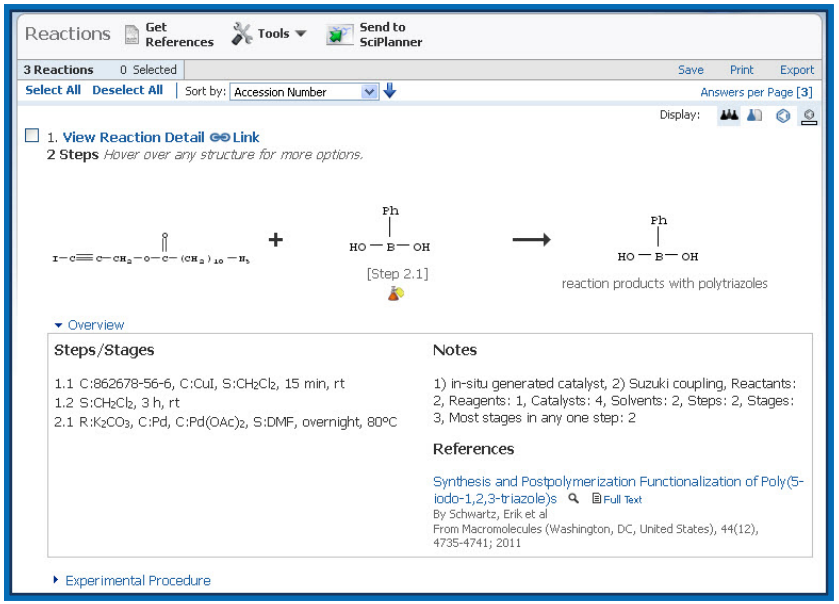
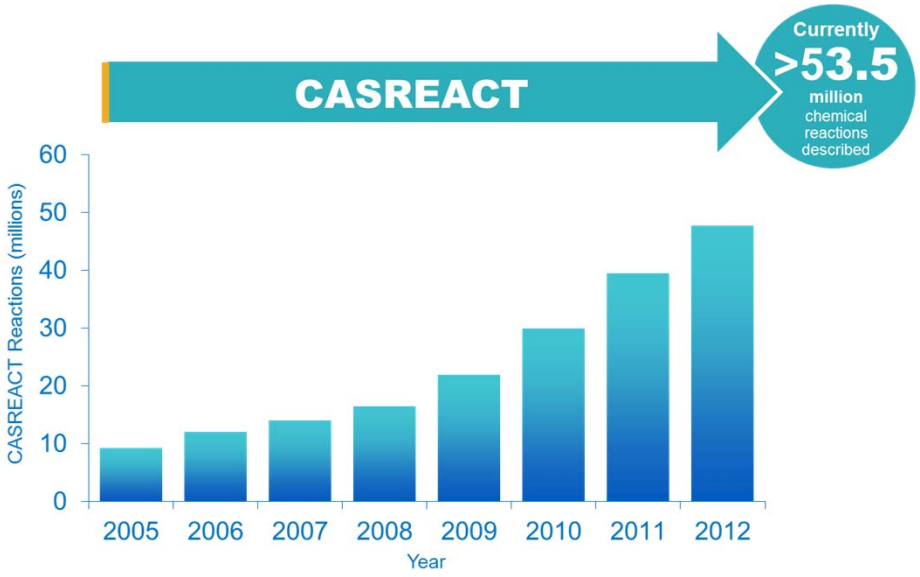
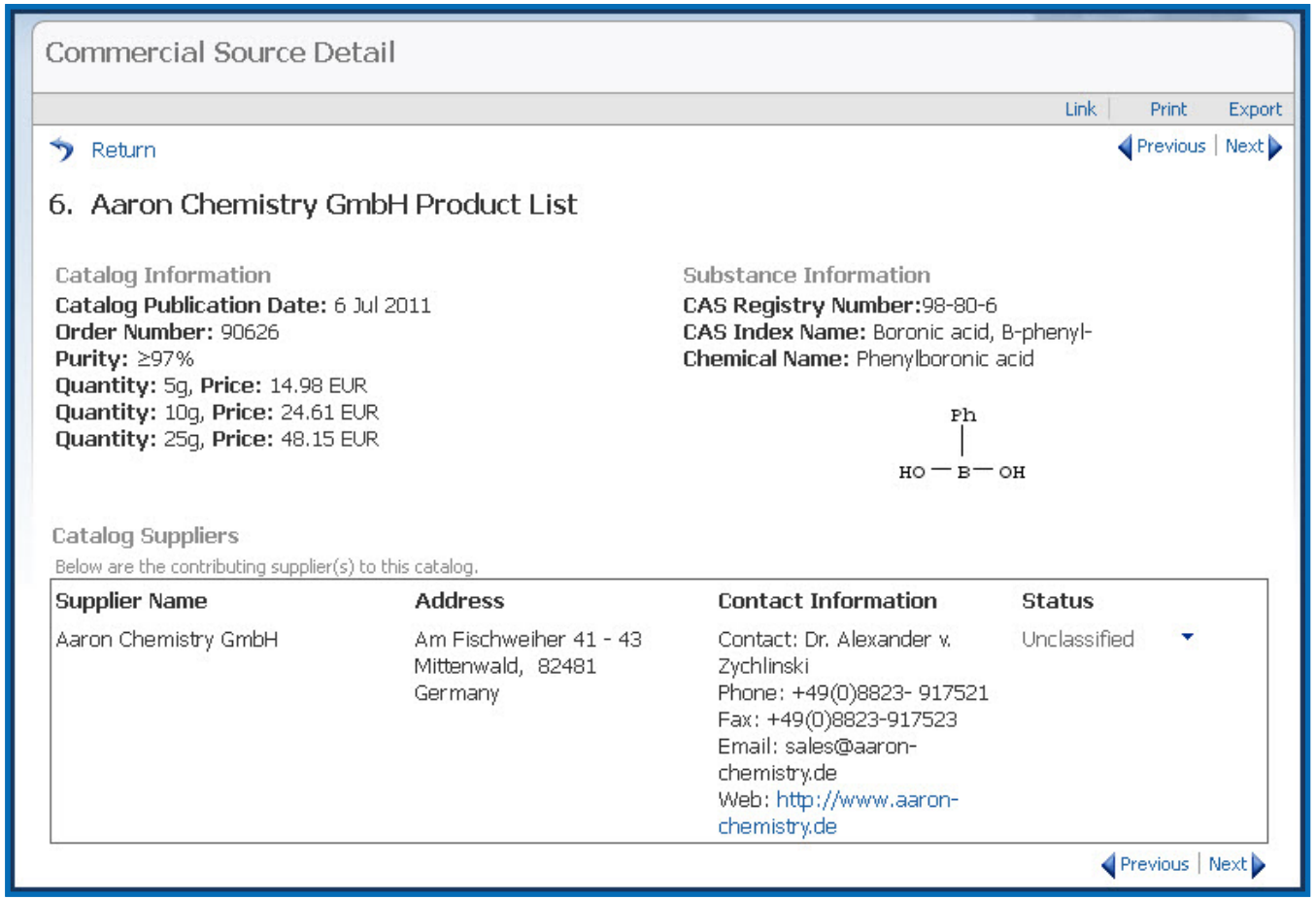




CASREACT answers your chemical reaction questions quickly, precisely, comprehensively

CHEMCATS® is the definitive collection of commercially available chemicals and suppliers



CHEMCATS provides fast access to chemical suppliers

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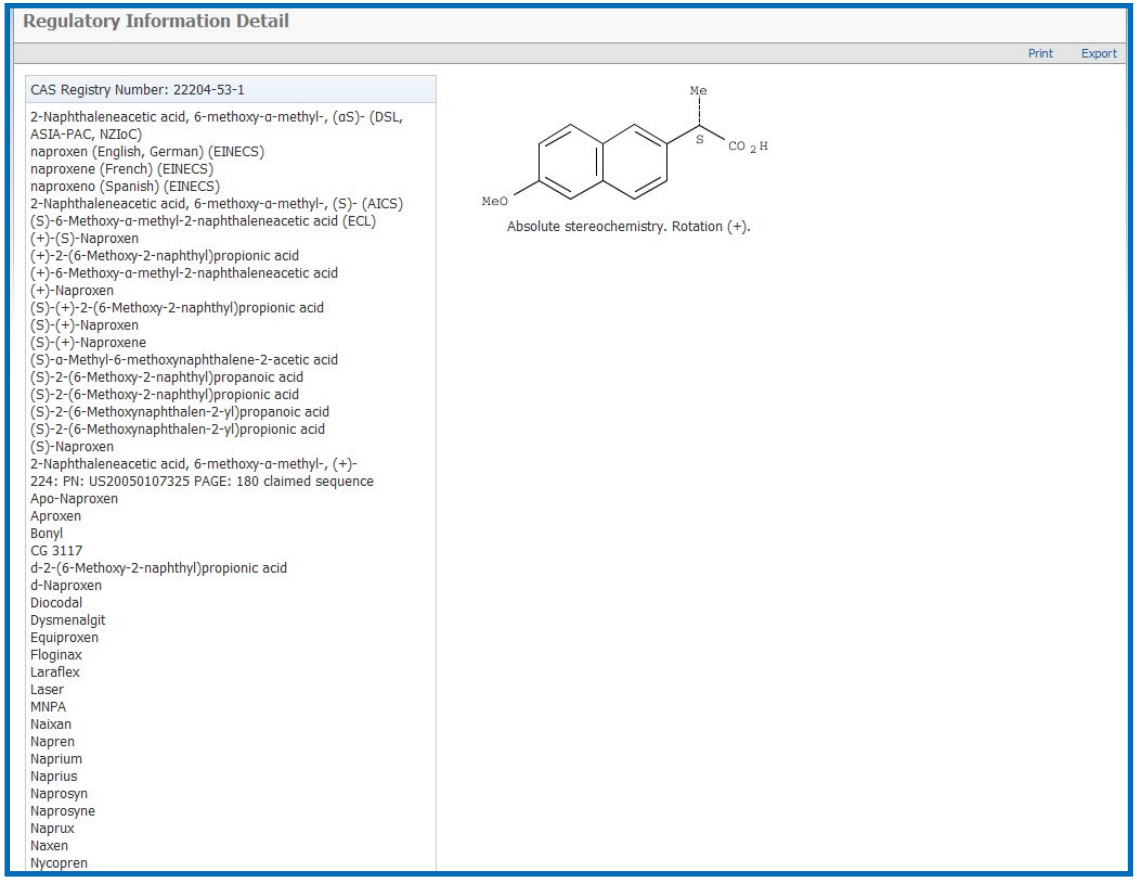


CHEMLIST enables you to discover how and where substances are regulated

MARPAT® is the leading collection of Markush structures from the world's patent literature

L1 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN

Full Text

AN **142:204619** MARPAT

TI Bioactive compositions for enhancement of drug comprising triazines

IN Sahouani, Hassan; Scherrer, Robert A.; Jumaa, Mouhannad; Zarraga, Isidro Angelo Eleazar; Vogel, Kim M.; Vogel, Dennis E.; Zou, Wei

PA 3M Innovative Properties Company, USA

SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2

DT Patent

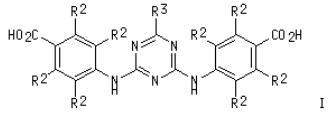
LA English

IC ICM A61K009-00

CC 63-5 (Pharmaceuticals)

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005011629	A1	20050210	WO 2004-US24515	20040729
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004261243	A1	20050210	AU 2004-261243	20040729
	CA 2533128	A1	20050210	CA 2004-2533128	20040729
	EP 1651185	A1	20060503	EP 2004-779530	20040729



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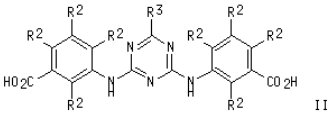
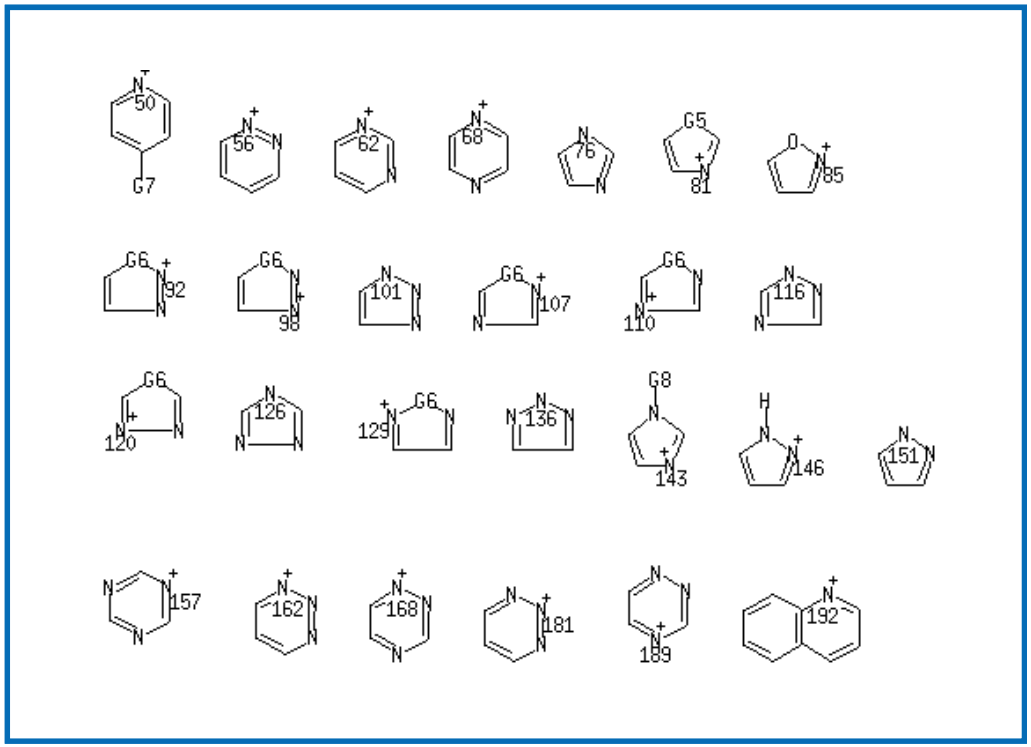


II

MARPAT supports maximum recall of patented information



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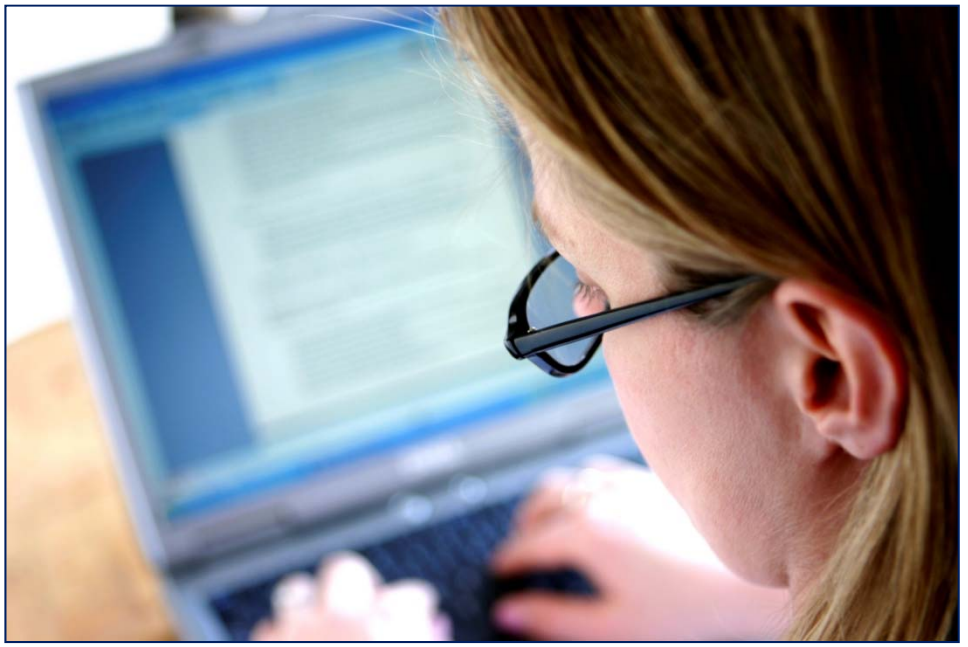

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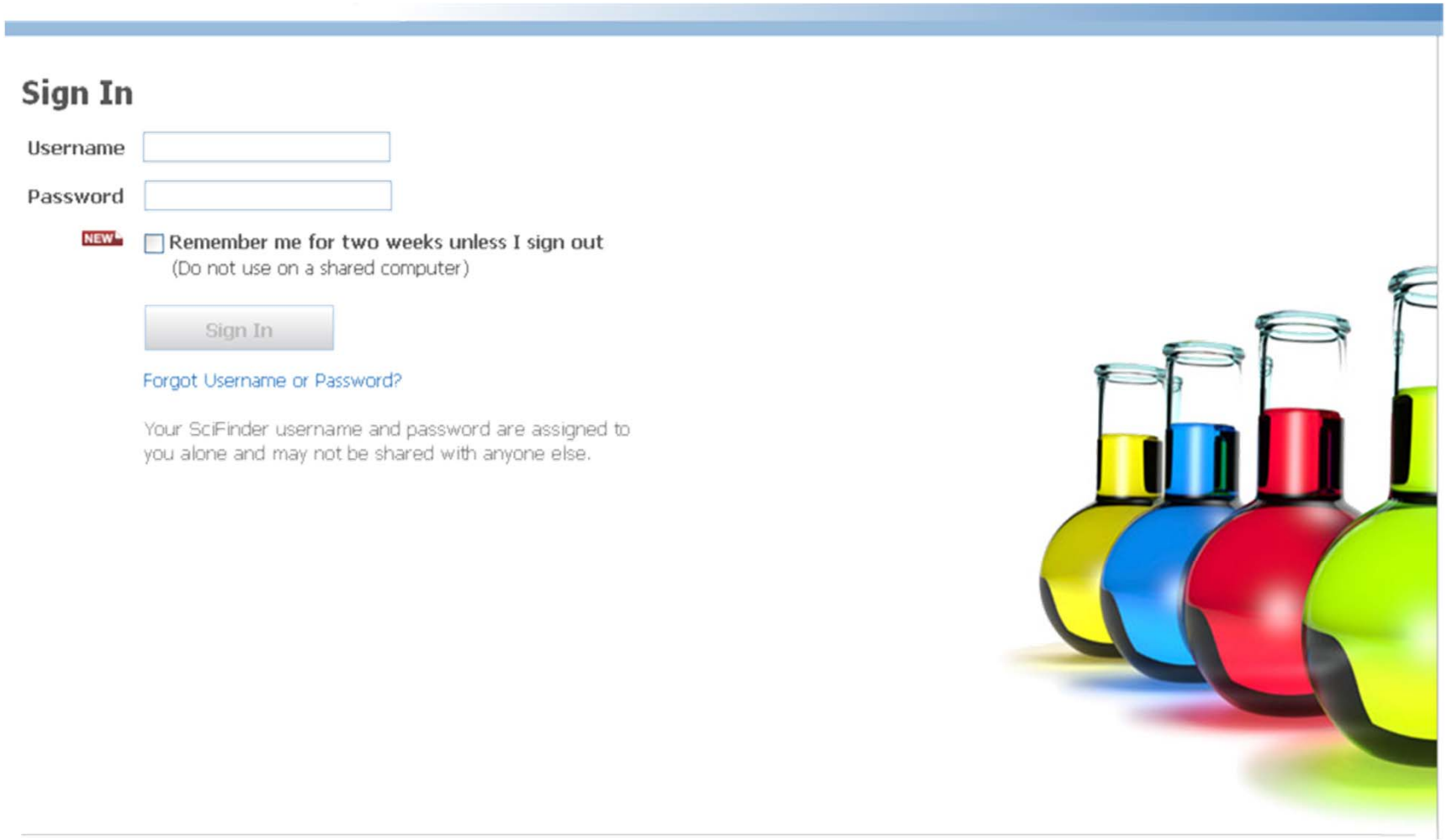
Dr. K. Barry Sharpless
Nobel Laureate
W.M. Keck Professor of Chemistry
Scripps Research Institute

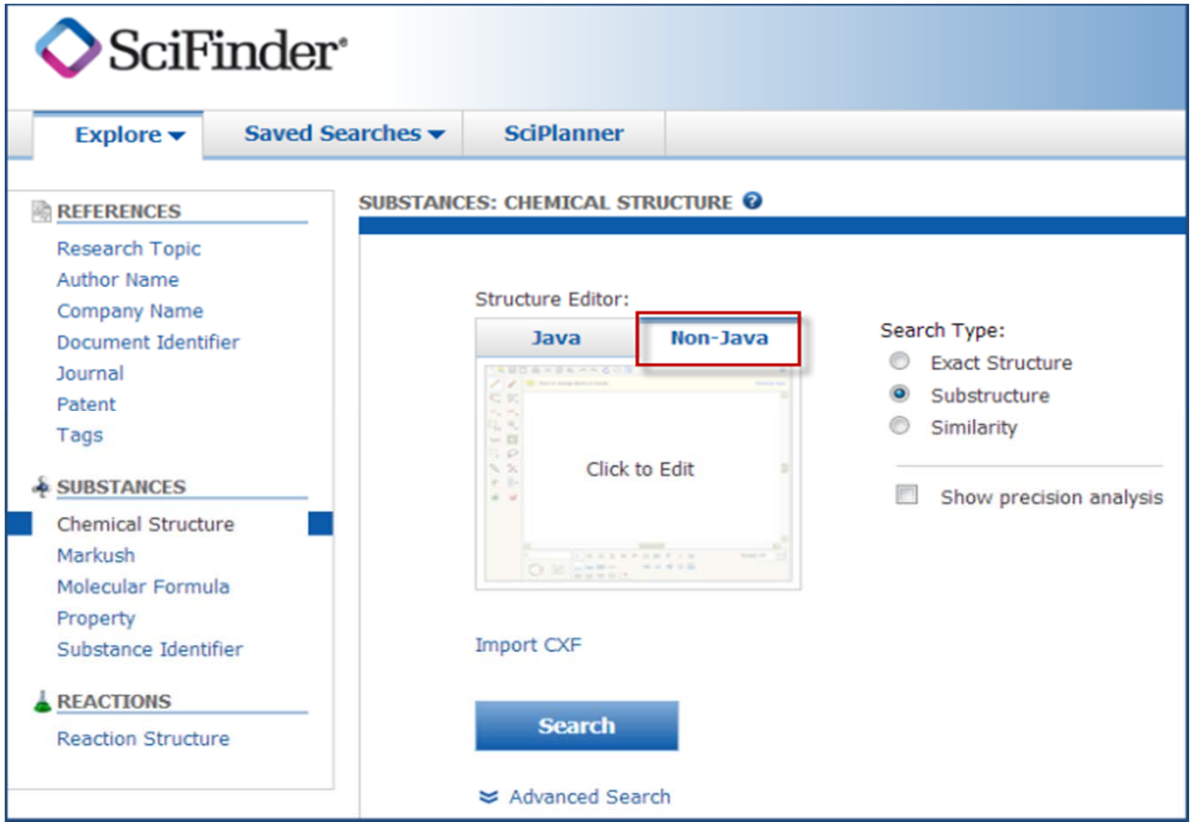
What's new on SciFinder



CAS

What's new on SciFinder

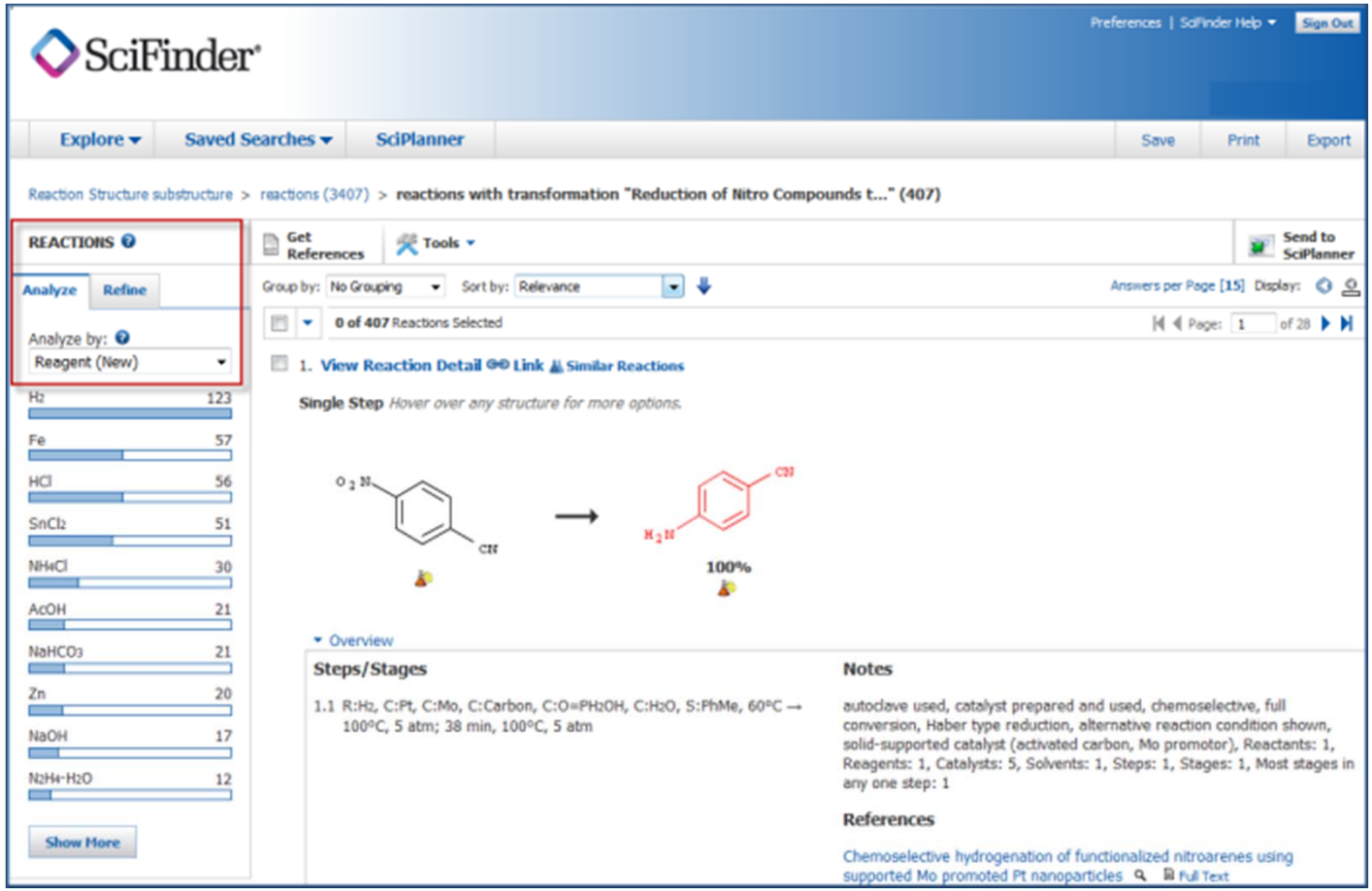
1.- New Non-Java CAS Structure Editor



CAS

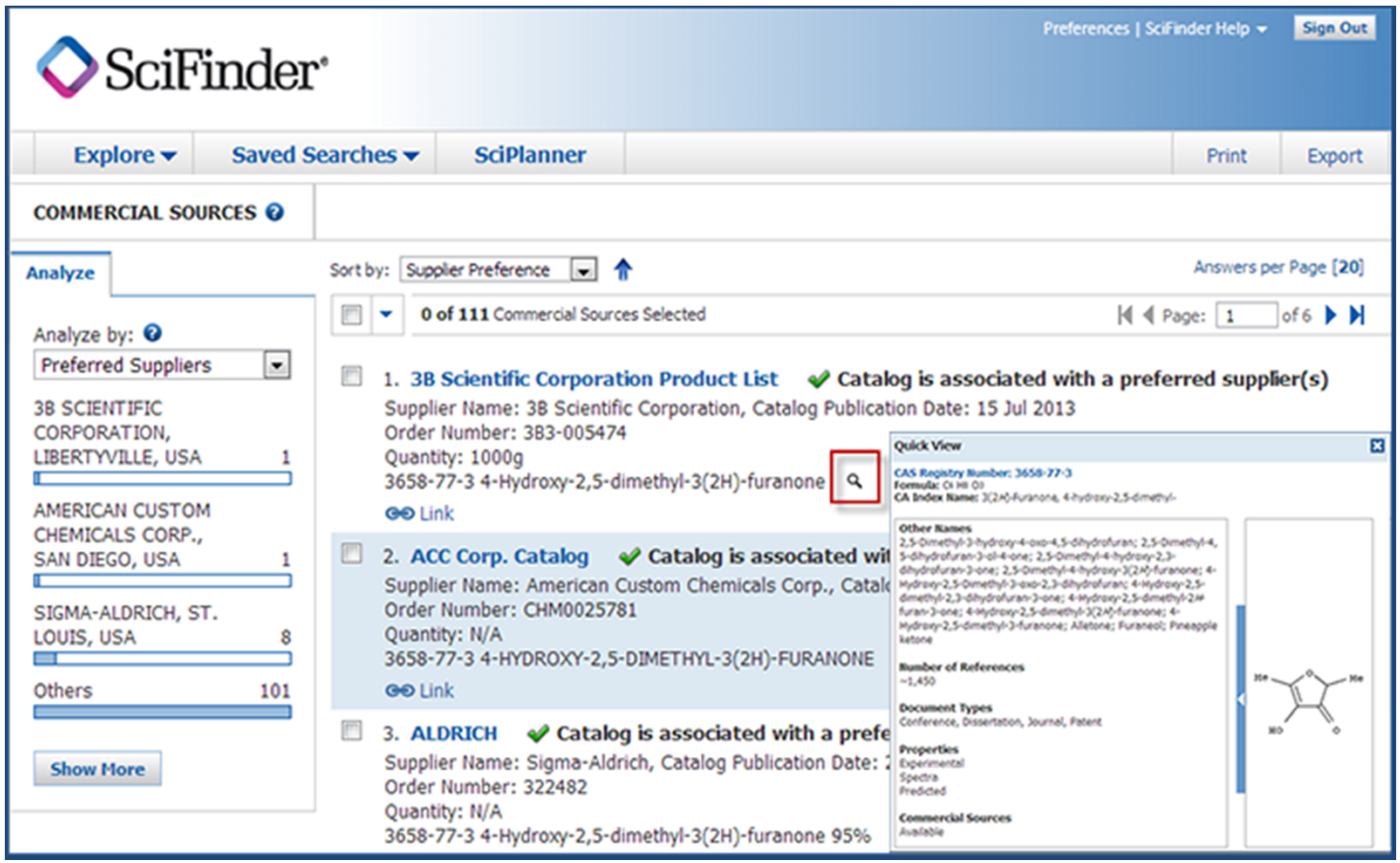
What's new on SciFinder

2.- Analyze by reagents



What's new on SciFinder

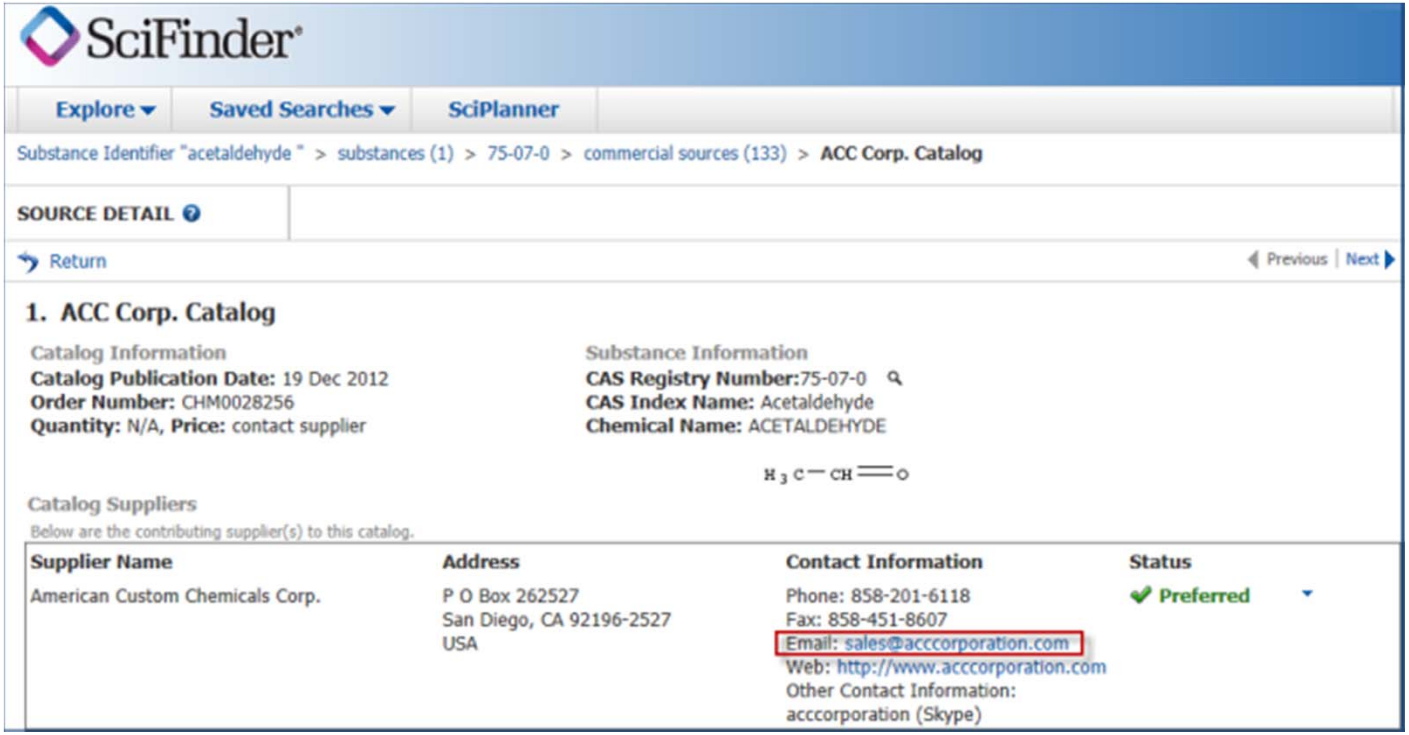
3.- Substance Quick View in Commercial Sources Answer Sets by reagents



CAS

What's new on SciFinder

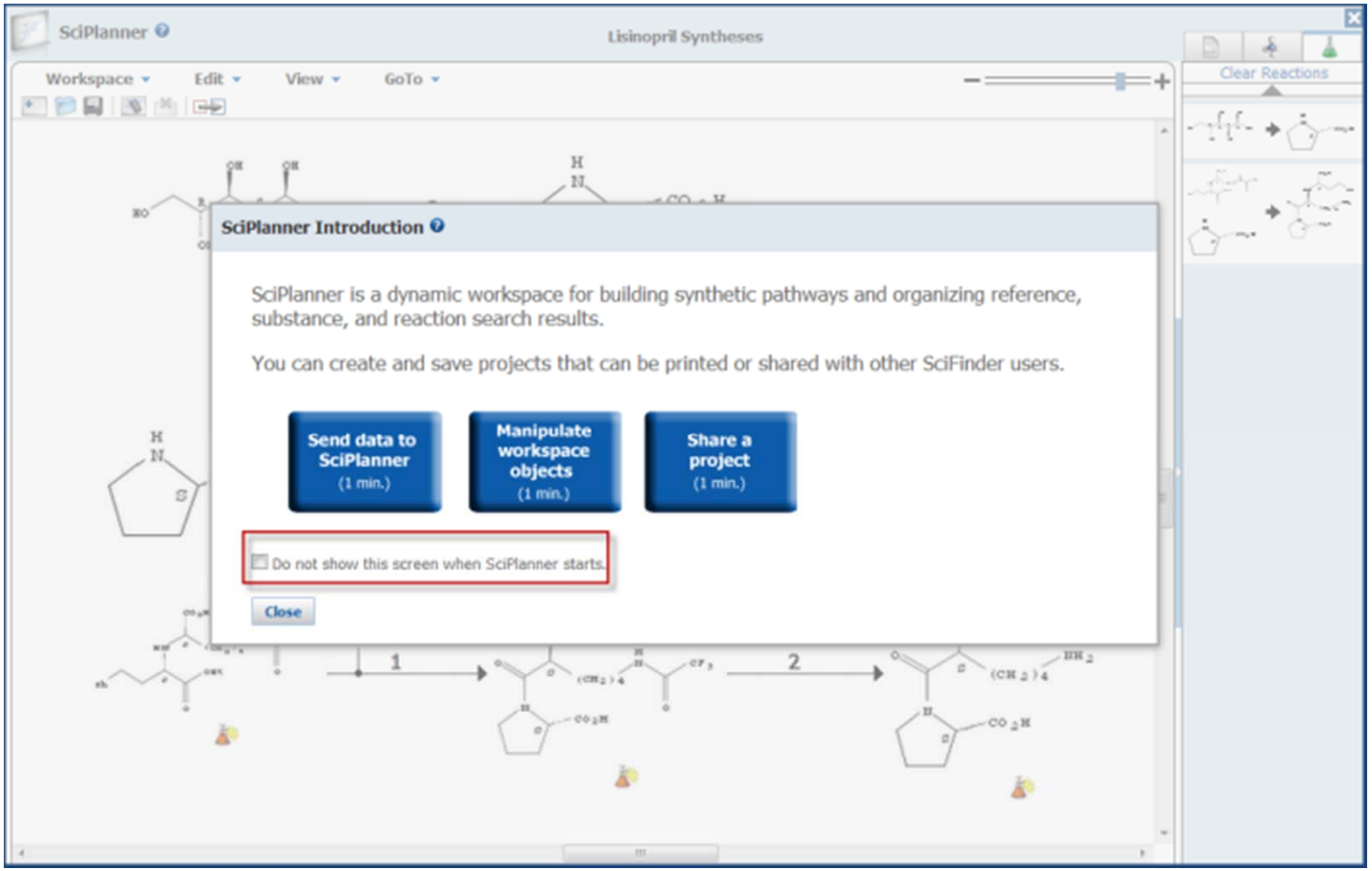
4.- Commercial Supplier Email Hyperlinks



CAS

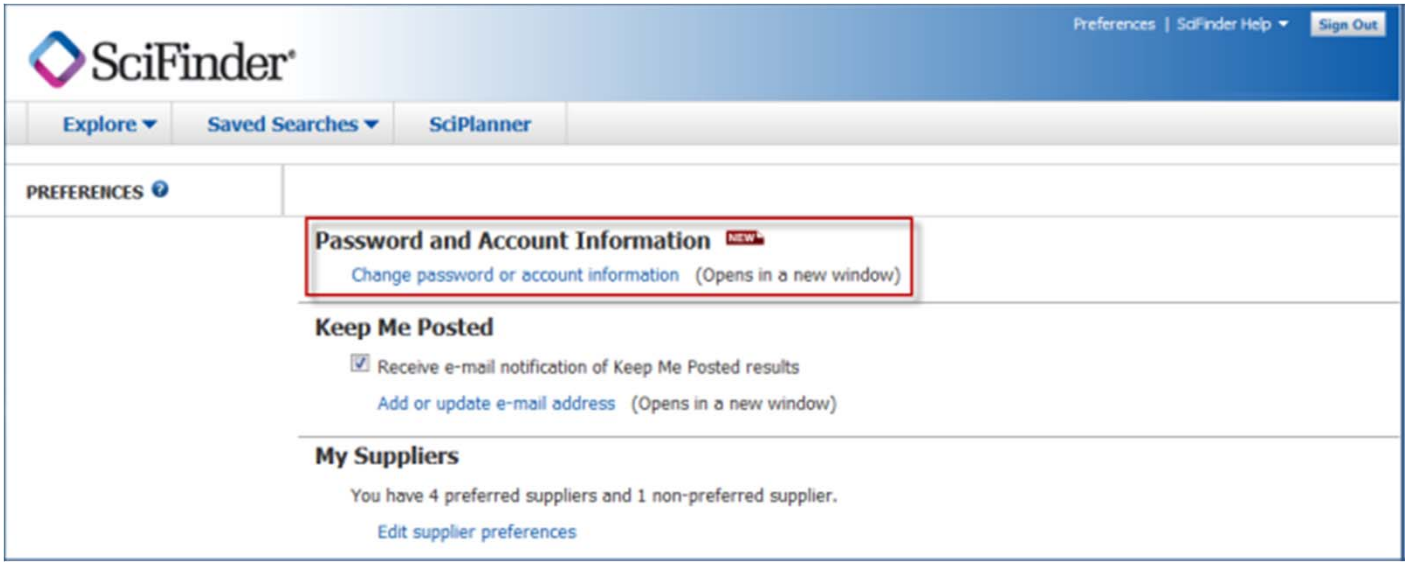
What's new on SciFinder

5.- Increased Availability of SciPlanner Tutorials



What's new on SciFinder

6.- Enhanced Account Management

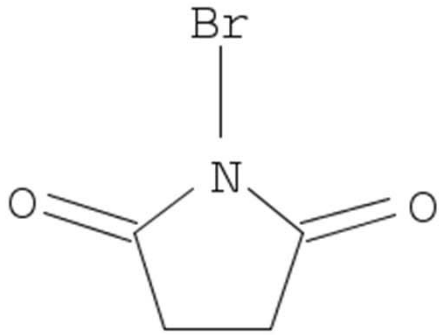


What's new on SciFinder

7.- Content Addition

CAS Registry Number:128-08-5

2,5-Pyrrolidinedione, 1-bromo- (TSCA, IECSC, DSL, ENCS, AICS, SWISS, PICCS, NZIoC)
N-Bromosuccinimide (English, French) (DSL, REACH, EINECS)
N-Bromsuccinimid (German) (EINECS, SWISS)
N-bromosuccinimida (Spanish) (EINECS)
1-Bromo-2,5-pyrrolidinedione (ECL)
SUCCINIMIDE, N-BROMO- (PICCS)
Bromosuccinimide
NBS
NSC 16



Regulatory List Number

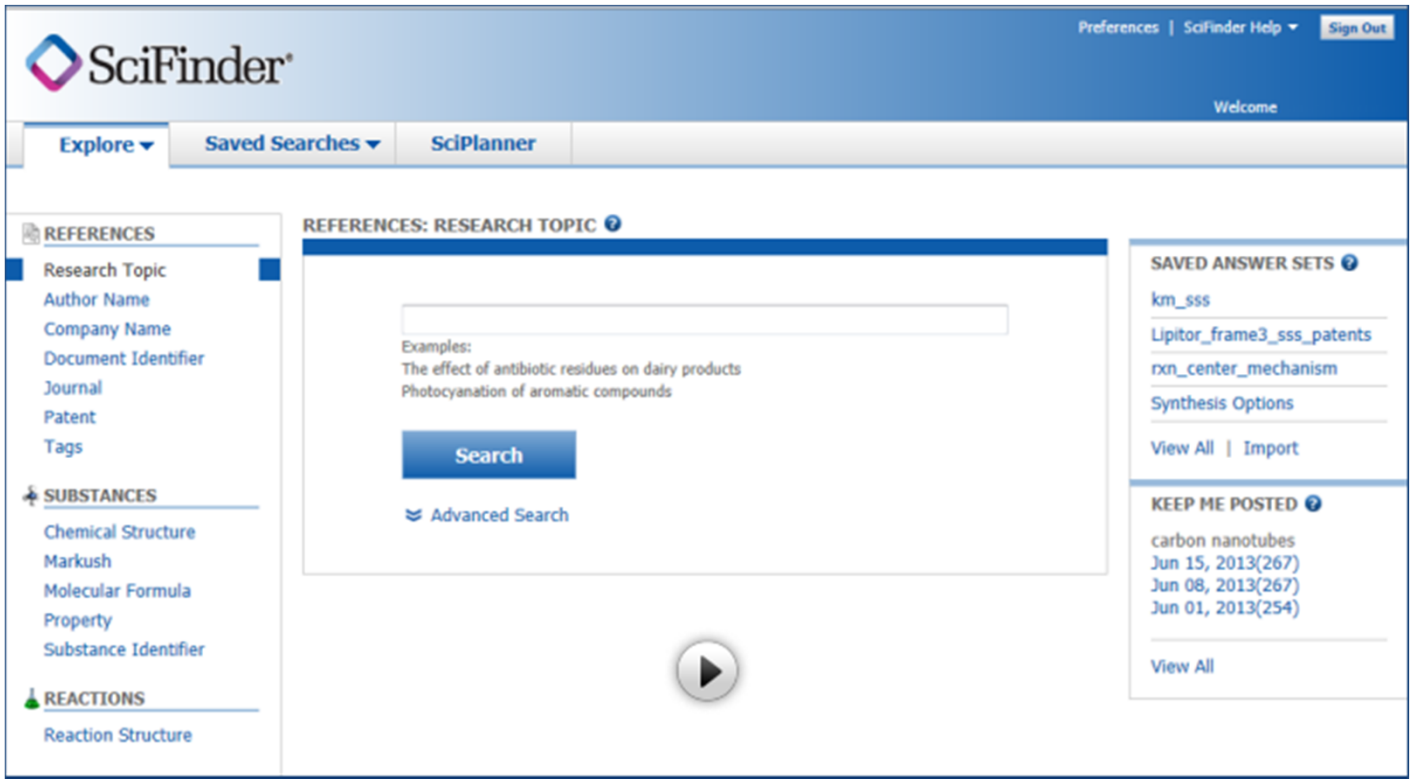
EC No.: 204-877-2
EINECS No.: 204-877-2
ENCS No.: 5-121X
ECL Serial No.: KE-03714
SWISS No.: G-8195

Harmonized Tariff Code NEW

Harmonized Tariff Code: 292519
EU Customs Code CN: 29251995

What's new on SciFinder

8.- New SciFinder Design



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Live demo

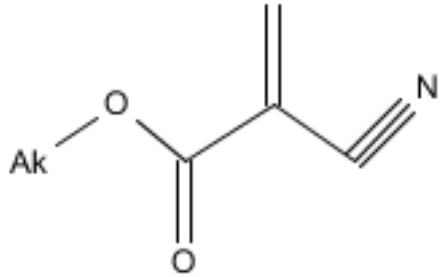
SciFinder options

Searches: topic, structure, reaction

Analysis tools

EJERCICIO

Buscar polímeros con esta estructura:



1.- No se permite fusión con otros anillos ni sustituciones adicionales al alquilo ni al carbono.

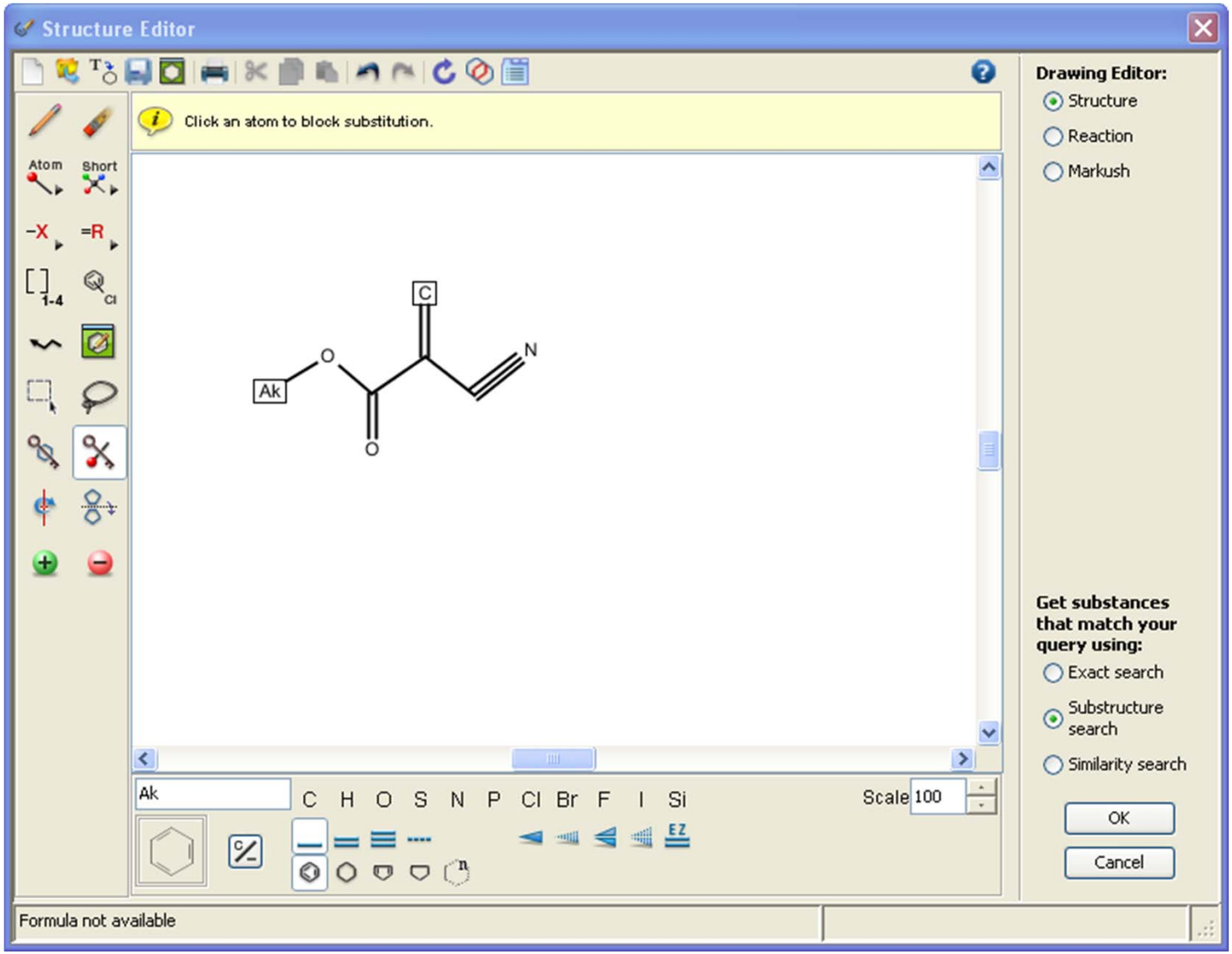
2.- Encontrar literatura que hable de aplicaciones magnéticas de dichos polímeros en el campo de la medicina. ¿Para qué se utilizan?

3.- ¿Quién trabaja sobre este tema?

4.- Encontrar algún artículo que hable específicamente de cápsulas de nanopartículas magnéticas.

5.- ¿Cómo podríamos preparar algún polímero? Busca una posible vía de síntesis del polímero con el monómero cuyo CAS RN es 7085-85-0, que esté formada por más de 2 reacciones y que el procedimiento experimental

Example 1: Search for polymers with this structure

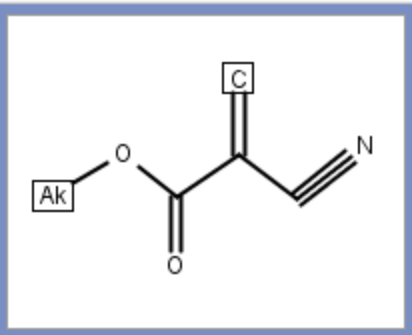


Substructure search limited to polymers only

Explore Substances

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

Chemical Structure



Click image to change structure or view detail

Search

Search type:
- Exact Structure
- Substructure
- Similarity

Show precision analysis

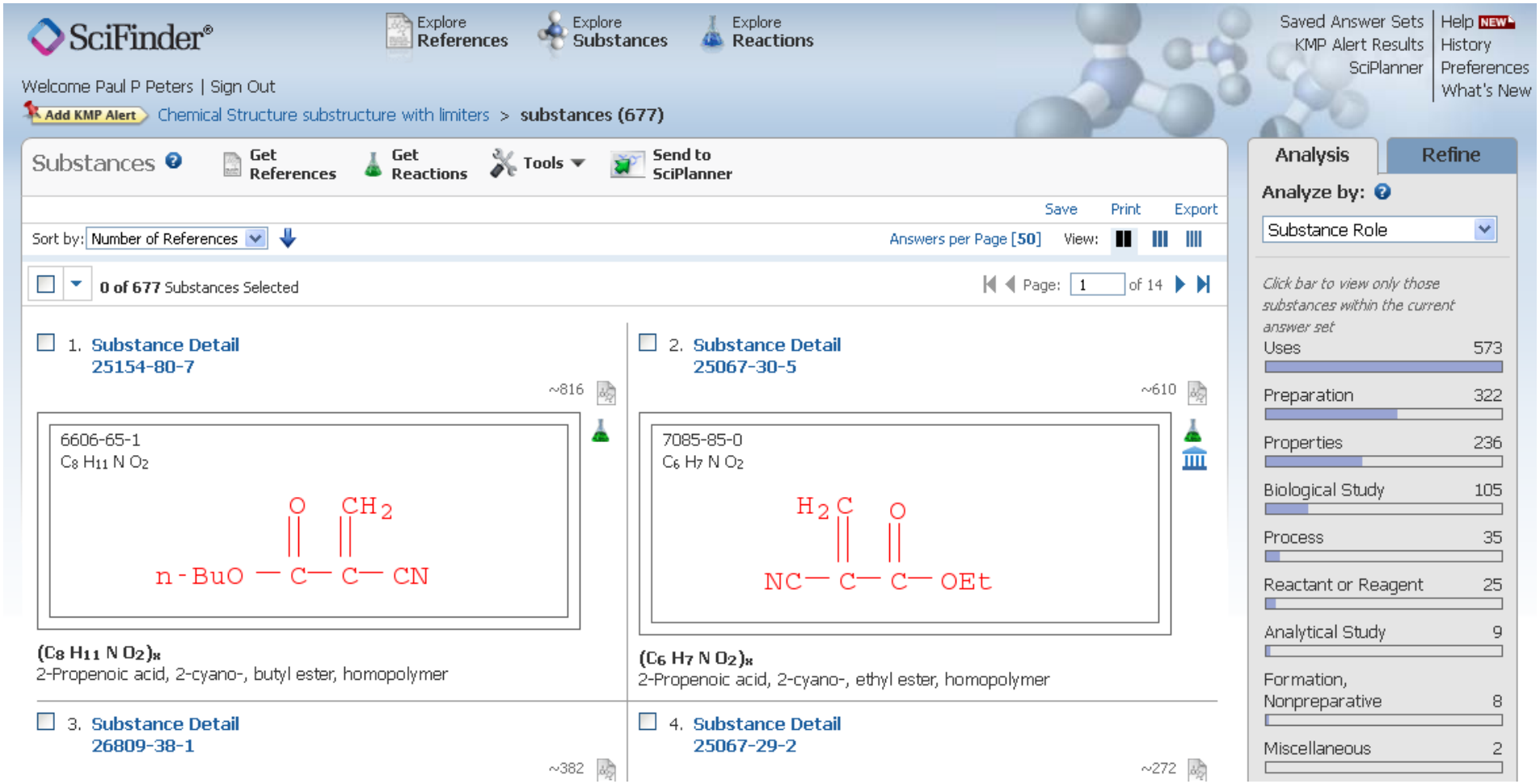
Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

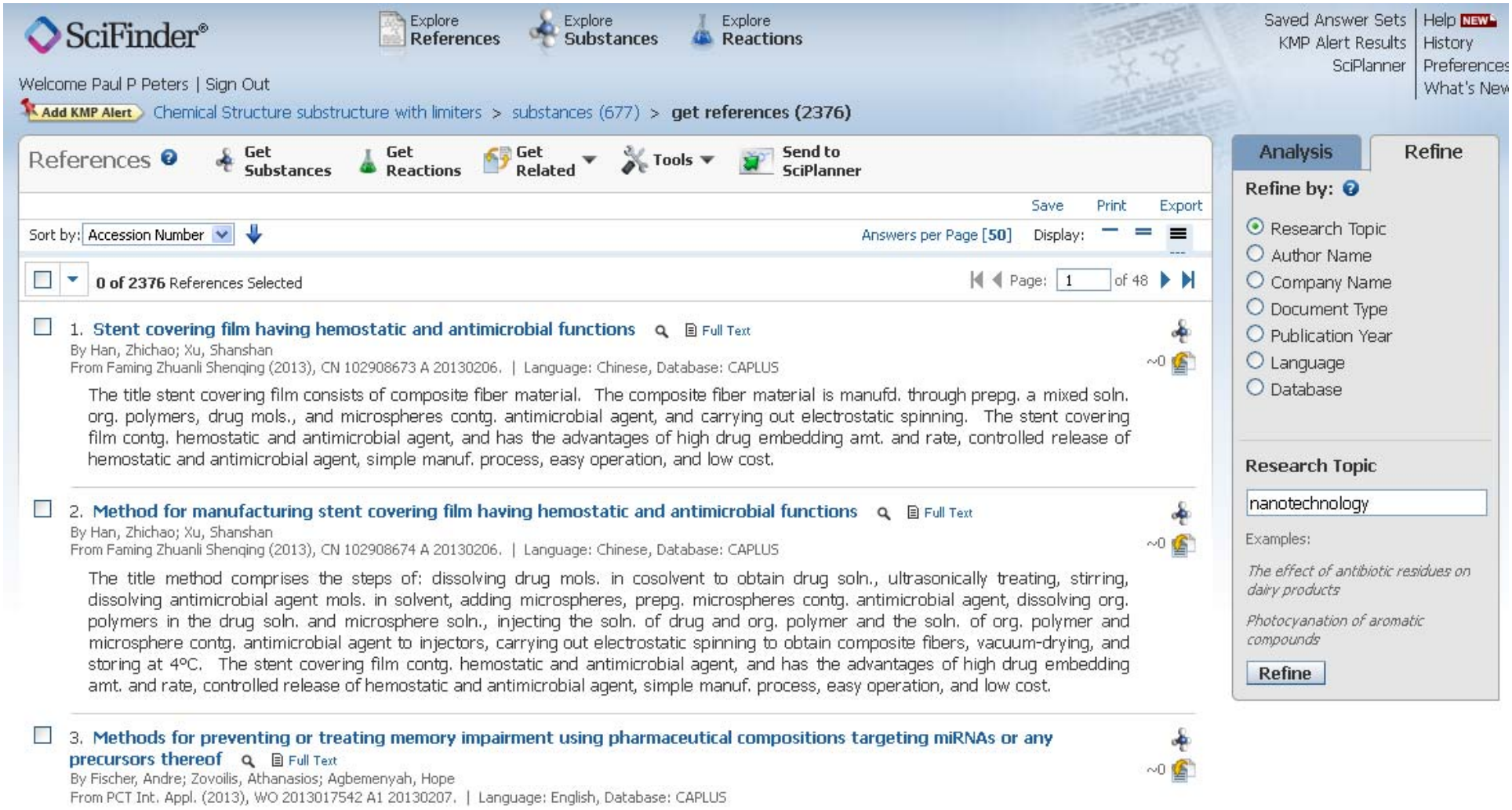
Class(es)

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

677 polymer structures sorted to most cited compound



Refine 2376 references to Nanotechnology including other nano-synonyms



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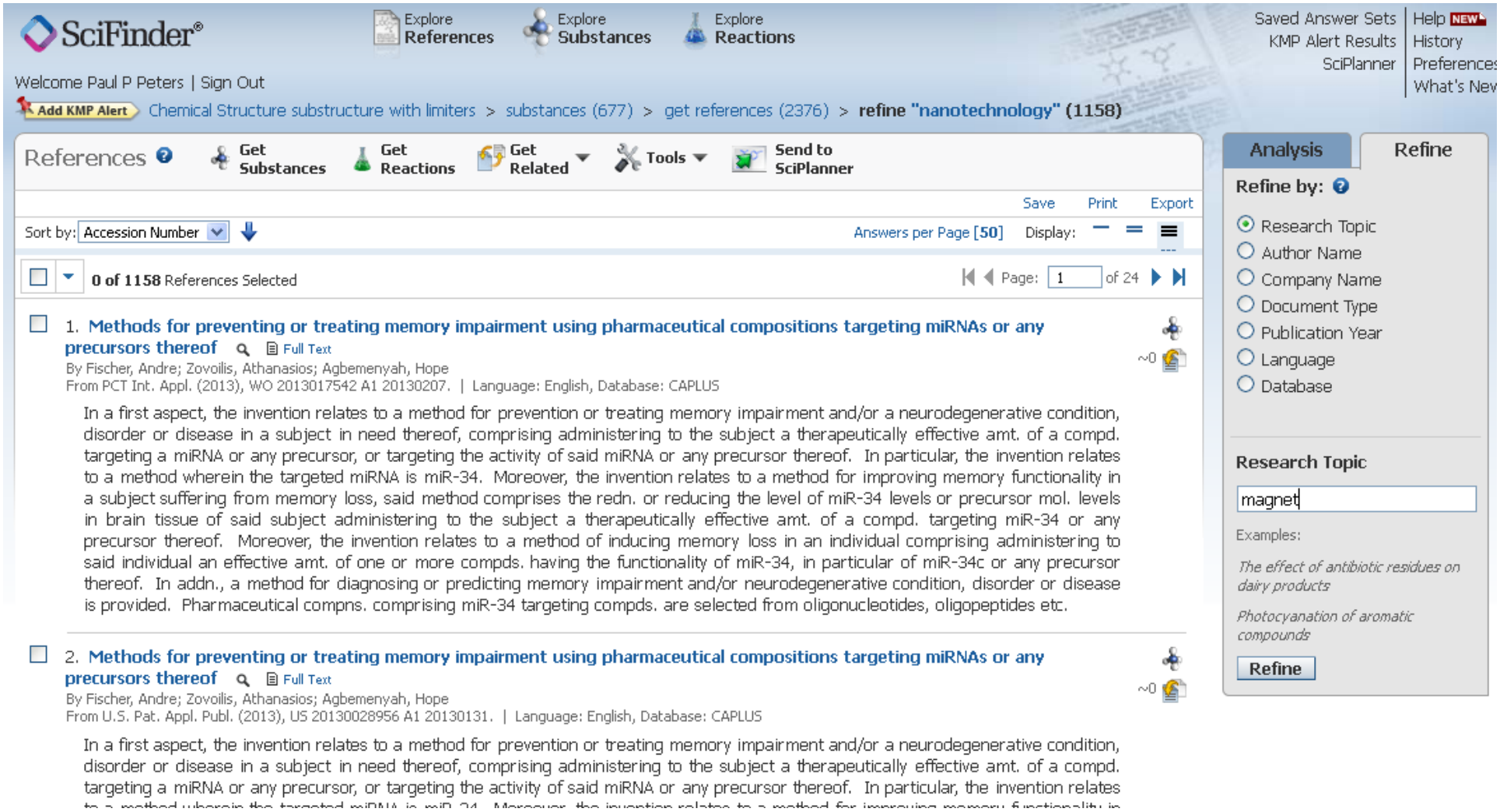
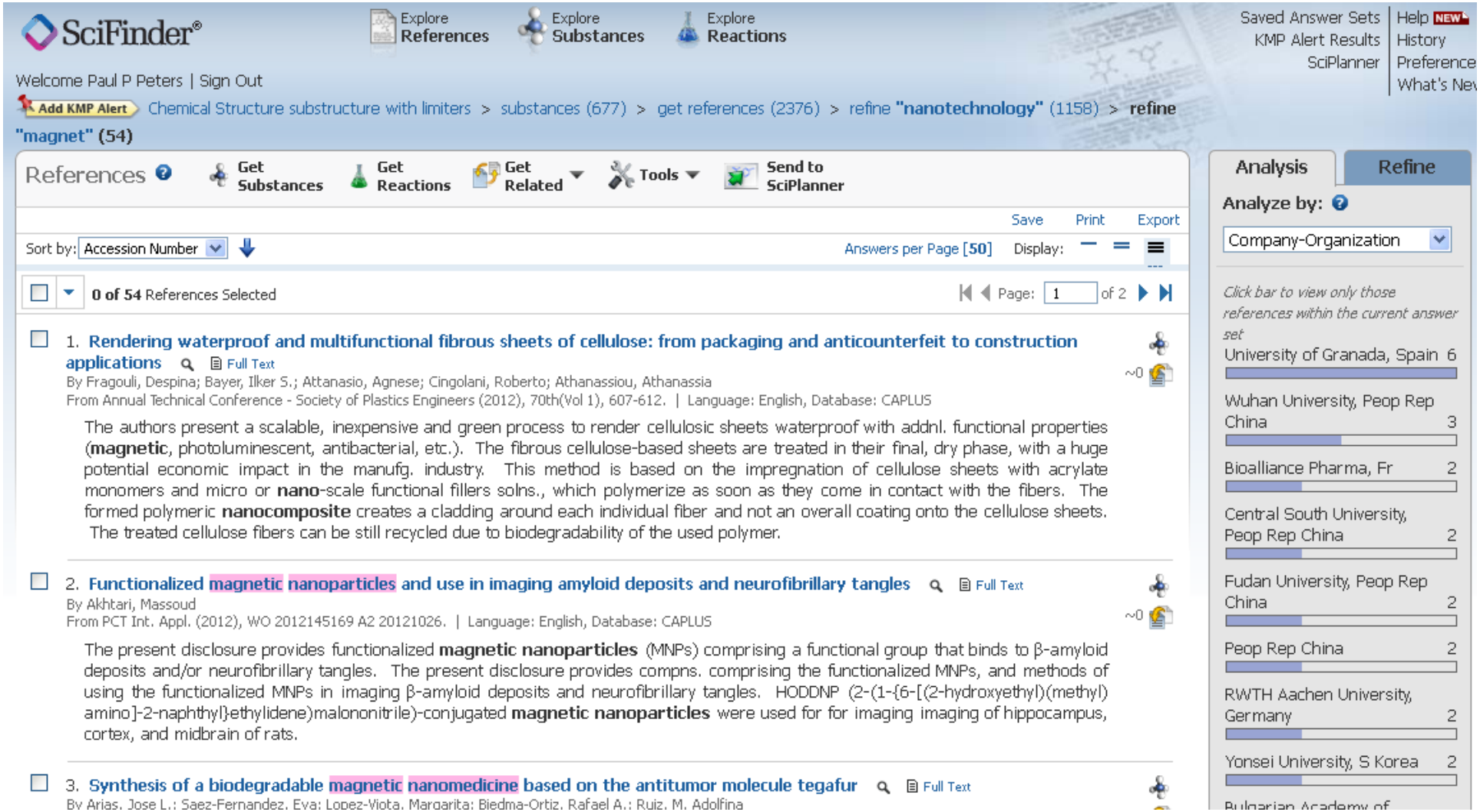
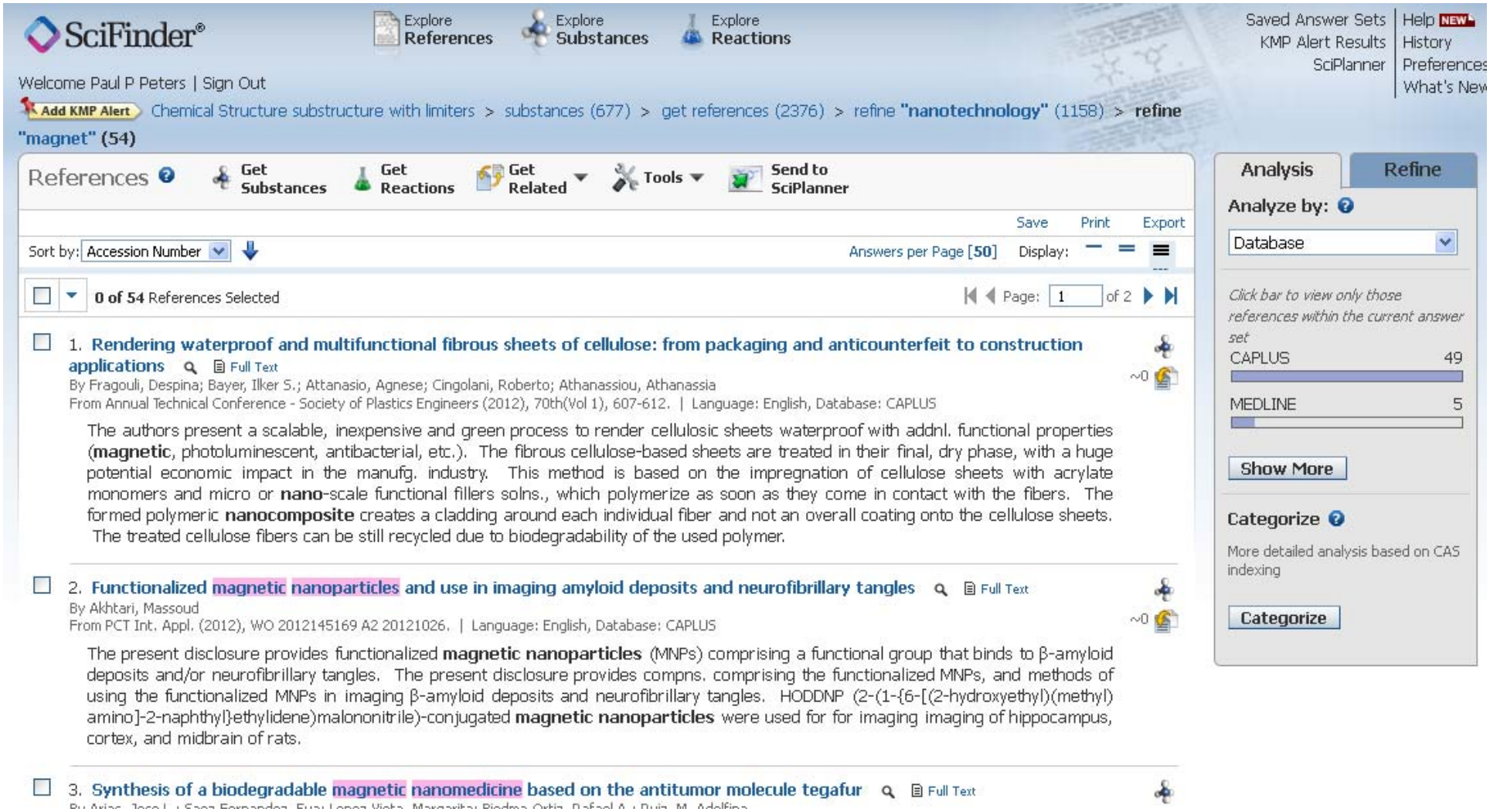
Refine 1158 reference to magnetic applications



54 references with University of Granada at the top



Pubmed (Medline) has only 5 references out of 54



CAS

Great advantage of CAS indexing of topics and compounds

Return

Previous | Next

3. Synthesis of a biodegradable magnetic nanomedicine based on the antitumor molecule tegafur

By: Arias, Jose L.; Saez-Fernandez, Eva; Lopez-Viota, Margarita; Biedma-Ortiz, Rafael A.; Ruiz, M. Adolfina

The introduction of magnetic nanocarriers in chemotherapy aims to enhance the anticancer activity of antitumor mols. whereas keeping their toxicity to a very min. Magnetite/poly(hexylcyanoacrylate) (core/shell) nanoplatforms were synthesized by an emulsion/polymn. procedure. An exhaustive physicochem. characterization (including IR spectrometry, electrophoresis, and thermodn. anal.) suggested that the magnetite nuclei were embedded into a polymeric nanomatrix. The very good magnetic responsiveness of such core/shell nanoparticles was defined by the hysteresis cycle. To improve the i.v. delivery of tegafur to cancer, the authors investigated its incorporation into the nanoplatform. Compared to surface adsorption, drug entrapment into the polymeric shell yielded higher tegafur loading values, and a much slower release profile. A high frequency alternating magnetic gradient was used to elucidate the heating characteristics of the nanoparticles: a stable max. temp. of 46 °C was successfully achieved within 32 min. Thus, the authors put forward that such kind of multifunctional nanomedicine hold very important characteristics (i.e., high drug loading, little burst release, hyperthermia, and magnetically targeted tegafur delivery), suggestive of its potential for combined antitumor therapy against cancer.

Indexing

Pharmaceuticals (Section63-6)

Concepts

Medical goods

biodegradable; synthesis of biodegradable magnetic nanoparticle for antitumor tegafur delivery and hyperthermia

Pharmaceutical injections

i.v. injections; synthesis of biodegradable magnetic nanoparticle for antitumor tegafur delivery and hyperthermia

Magnetic particles Nanoparticles

magnetic nanoparticles: synthesis of biodegradable magnetic

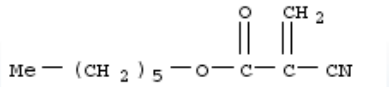
Substances

1309-38-2P Magnetite, biological studies

synthesis of biodegradable magnetic nanoparticle for antitumor tegafur delivery and hyperthermia

Physical, engineering or chemical process; Properties; Synthetic preparation; Therapeutic use; Biological study; Preparation; Process; Uses

26877-39-4 Poly(hexylcyanoacrylate)



Source

Medicinal Chemistry
Volume8
Issue4
Pages516-523
Journal
2012
CODEN:MCEHAJ
ISSN:1573-4064

Company/Organization

Department of Pharmacy and Pharmaceutical Technology,
Faculty of Pharmacy
University of Granada
Spain

Accession Number

2012:1072765
CAN157:474396
CAPLUS

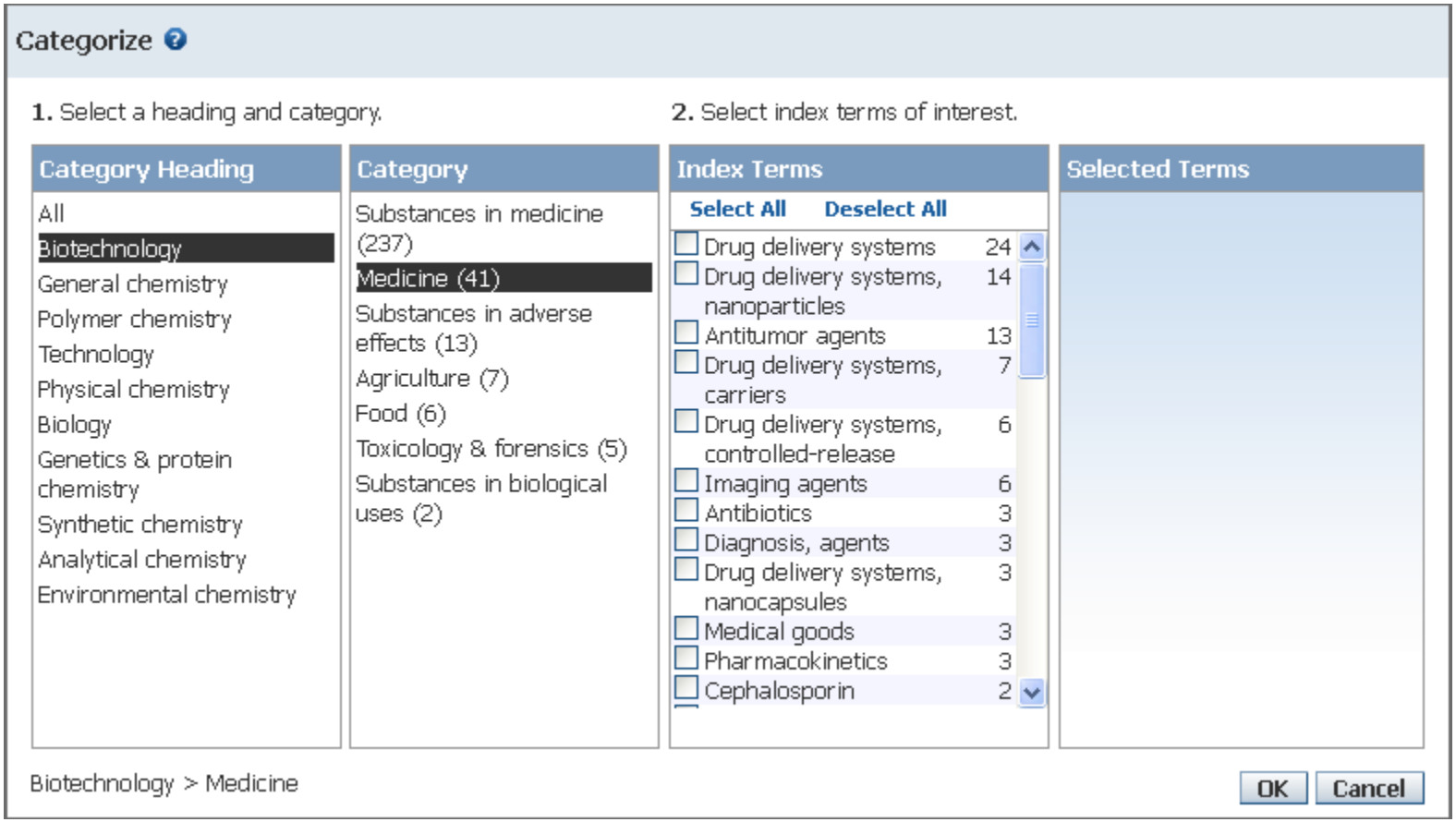
Publisher

Bentham Science Publishers Ltd.

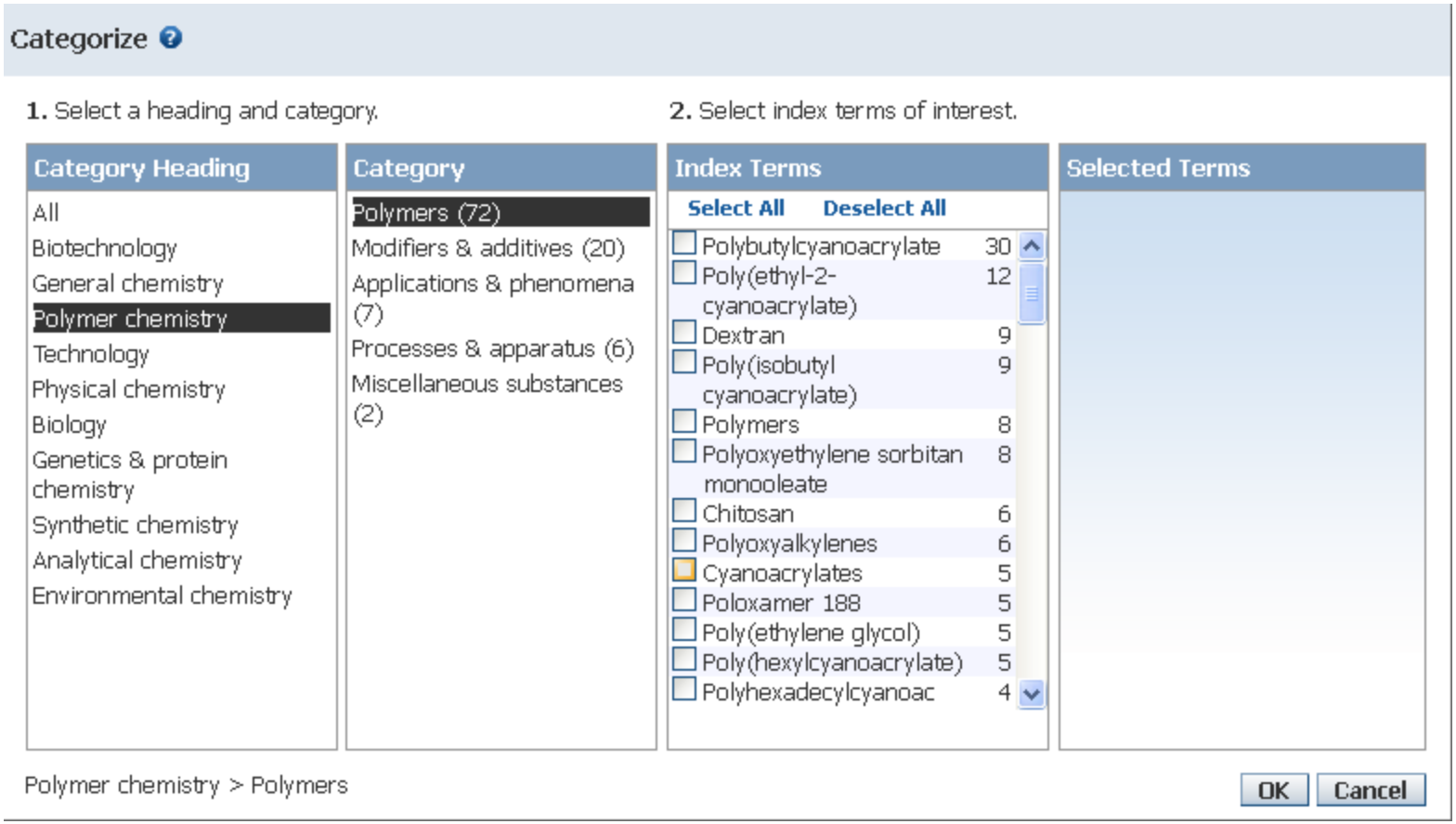
Language

English

SciFinder has advanced options for analysis by Medicine application



..or by type of polymers indexed



Míriam Plana

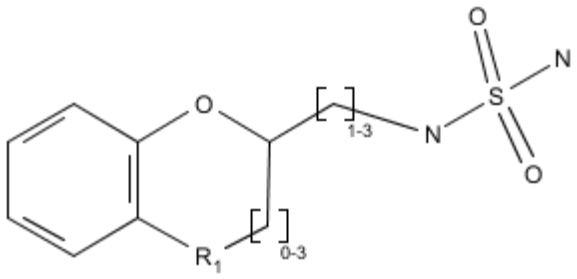
CAS Regional Marketing Manager, Spain & Portugal

mplana@cas.org

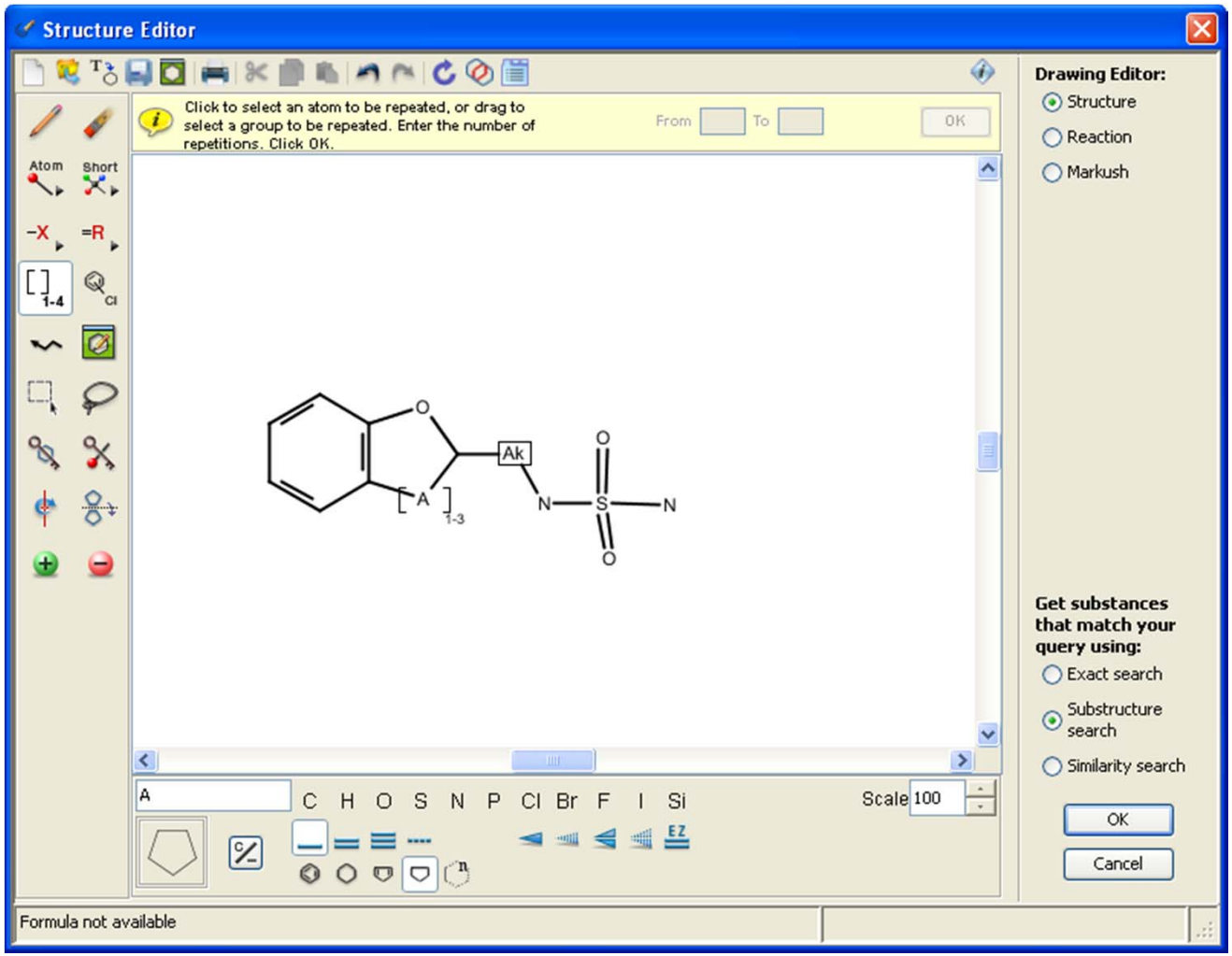
Example 2: Check novelty and design your synthesis

Research topic:

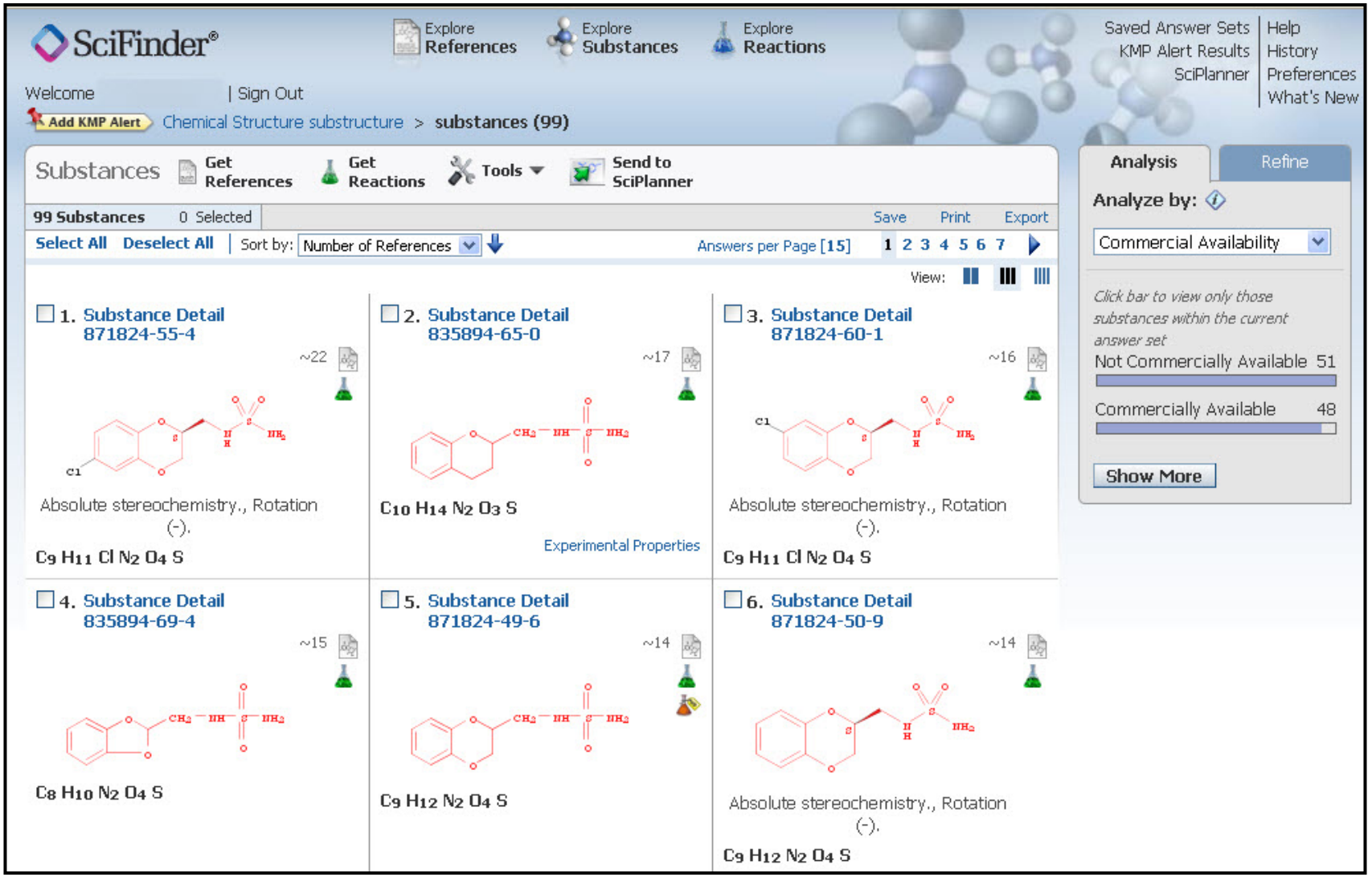
Looking for novelty on benzo-fused heterocyclic sulfamides, their possible pharmacological activity and synthesis pathway



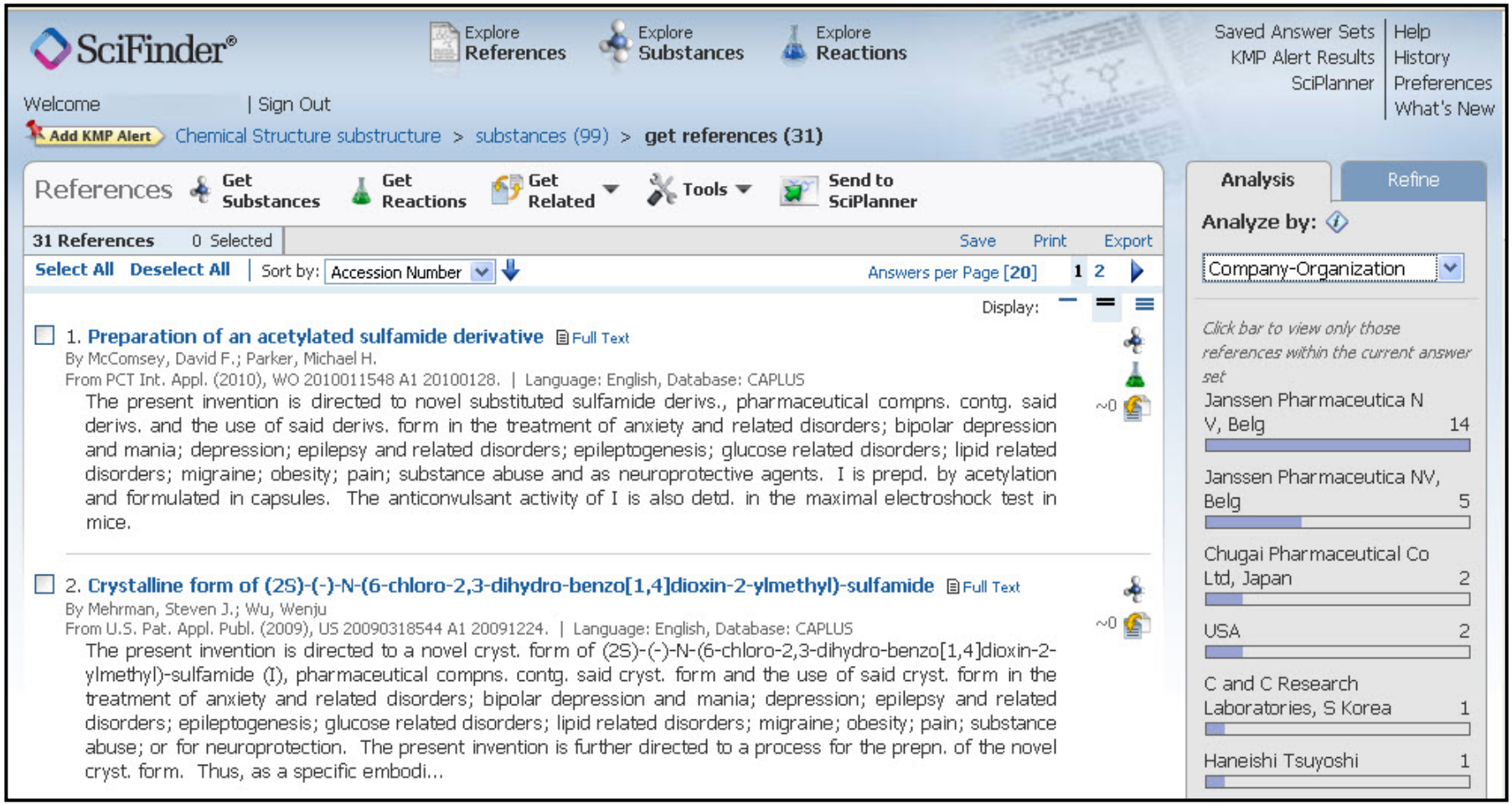
Search substances with chemical structures or other substance information to check novelty of substances



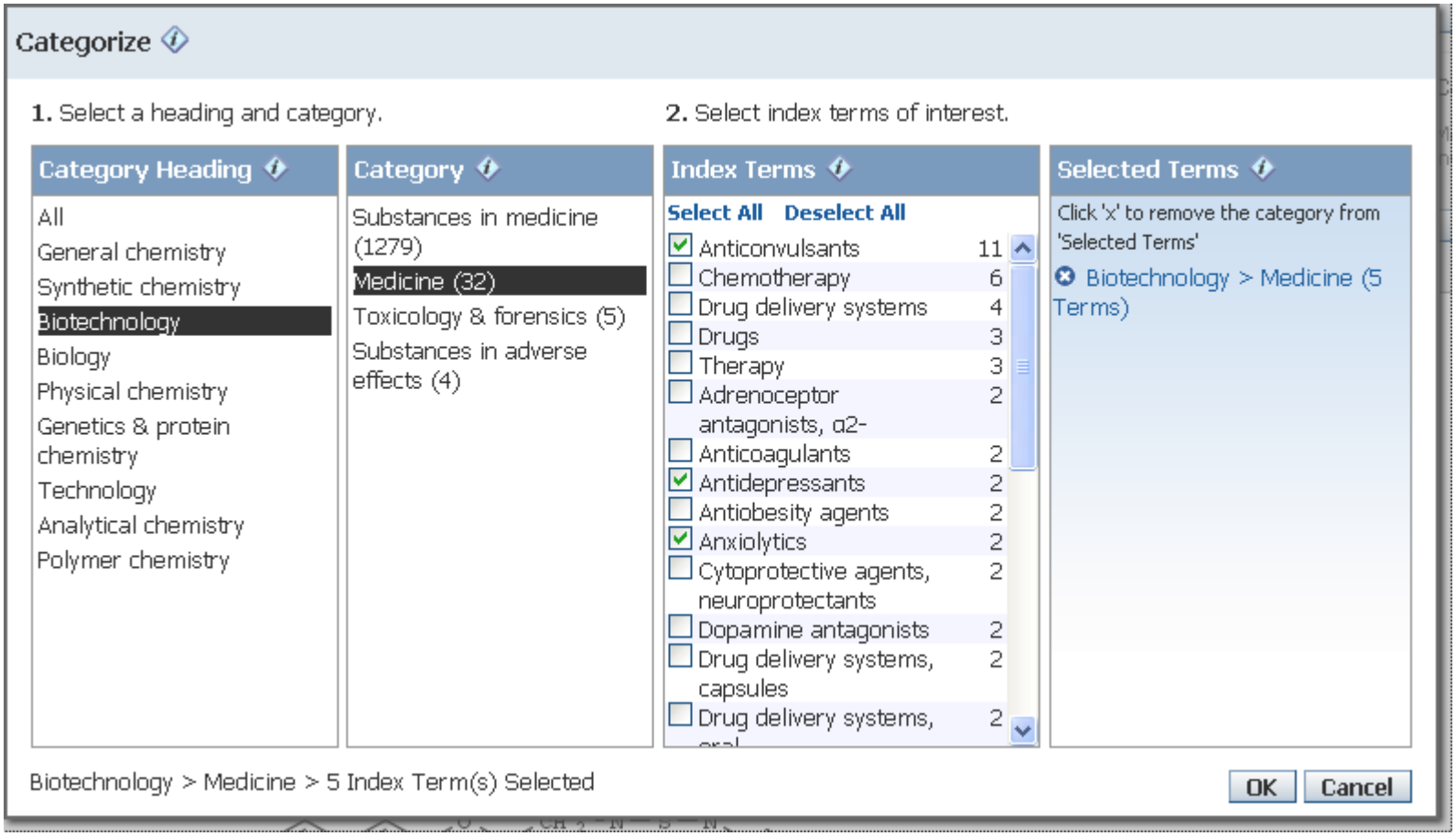
SciFinder produces 99 compounds from the journal and patent literature as well as from catalogs and libraries



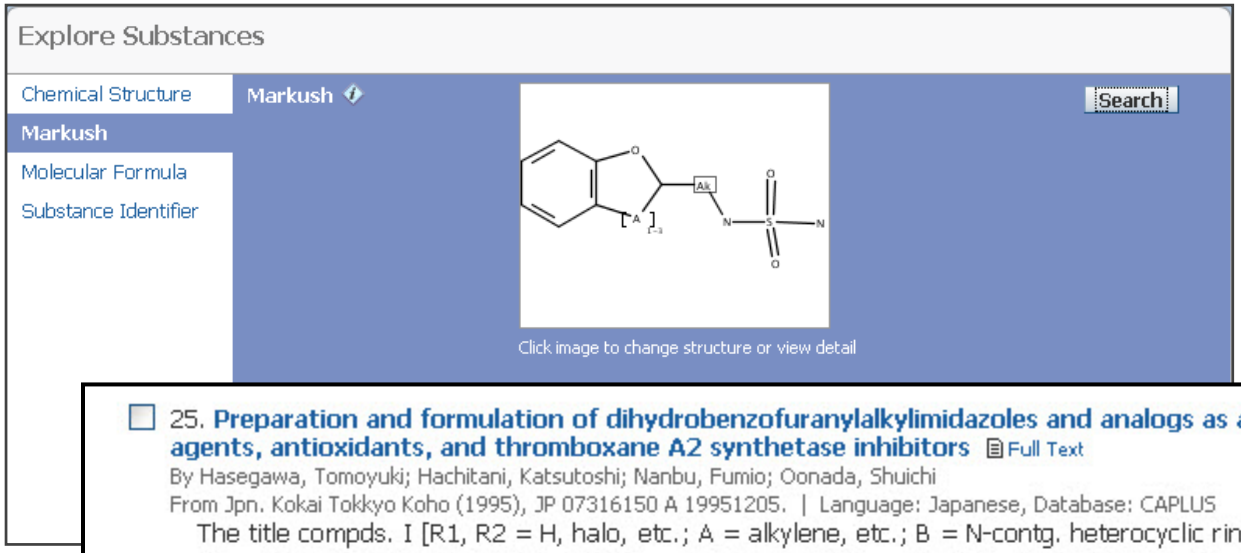
SciFinder retrieves 31 journal and patent references that disclose one or more of the 99 compounds



Categorize is a powerful tool to analyze the concepts and substances indexed in the retrieved answer set



A Markush search can produce additional patents matching the broad generic definition from the claim

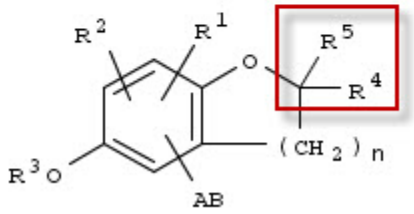


25. **Preparation and formulation of dihydrobenzofuranylalkylimidazoles and analogs as antiinflammatory agents, antioxidants, and thromboxane A2 synthetase inhibitors** Full Text

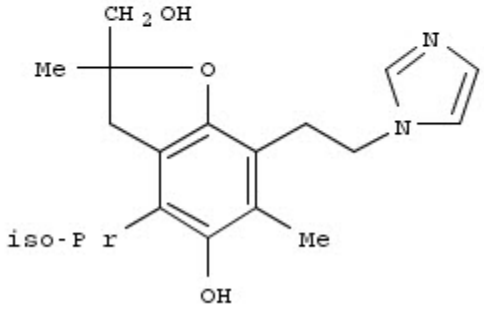
By Hasegawa, Tomoyuki; Hachitani, Katsutoshi; Nanbu, Fumio; Oonada, Shuichi

From Jpn. Kokai Tokkyo Koho (1995), JP 07316150 A 19951205. | Language: Japanese, Database: CAPLUS

The title compds. I [R1, R2 = H, halo, etc.; A = alkylene, etc.; B = N-contg. heterocyclic ring; R3 = H, acyl, etc.; R4 = H, alkyl, phenylalkyl; R5 = DE; D = alkylene, etc.; E = NR9R10, etc.; R9, R10 = H, alkyl, etc.; n = 1 - 3] are prepd. The title compd. II.HCl was prepd. in a multistep process starting from 2-(2-pivaloyloxyethyl)-3-methyl-4-acetyloxy-5-isopropyl-6-(2-methyl-2-propenyl)phenol. II.HCl in vitro at 10 μM gave 96% inhibition of thromboxane B2 formation.

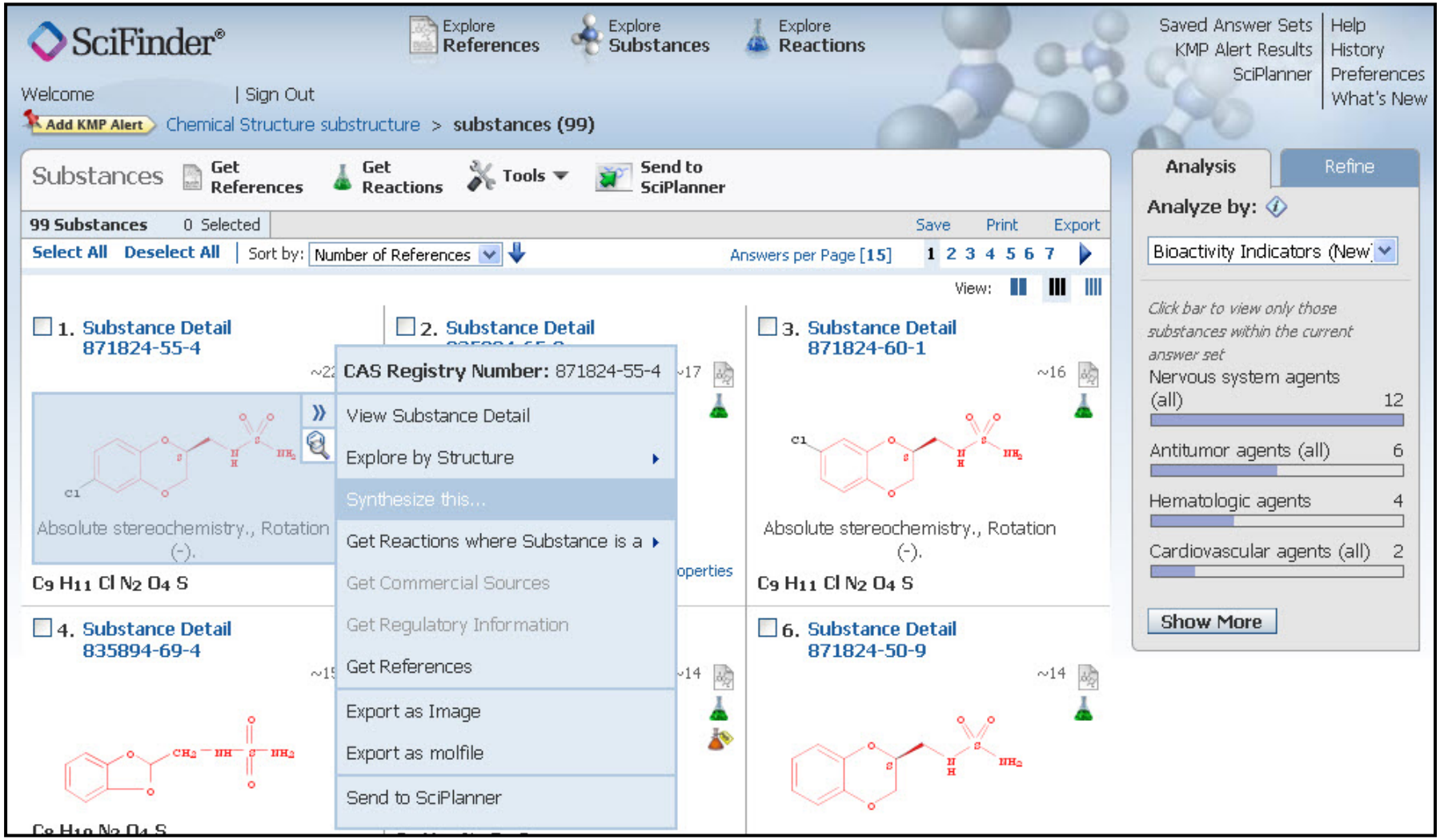


I

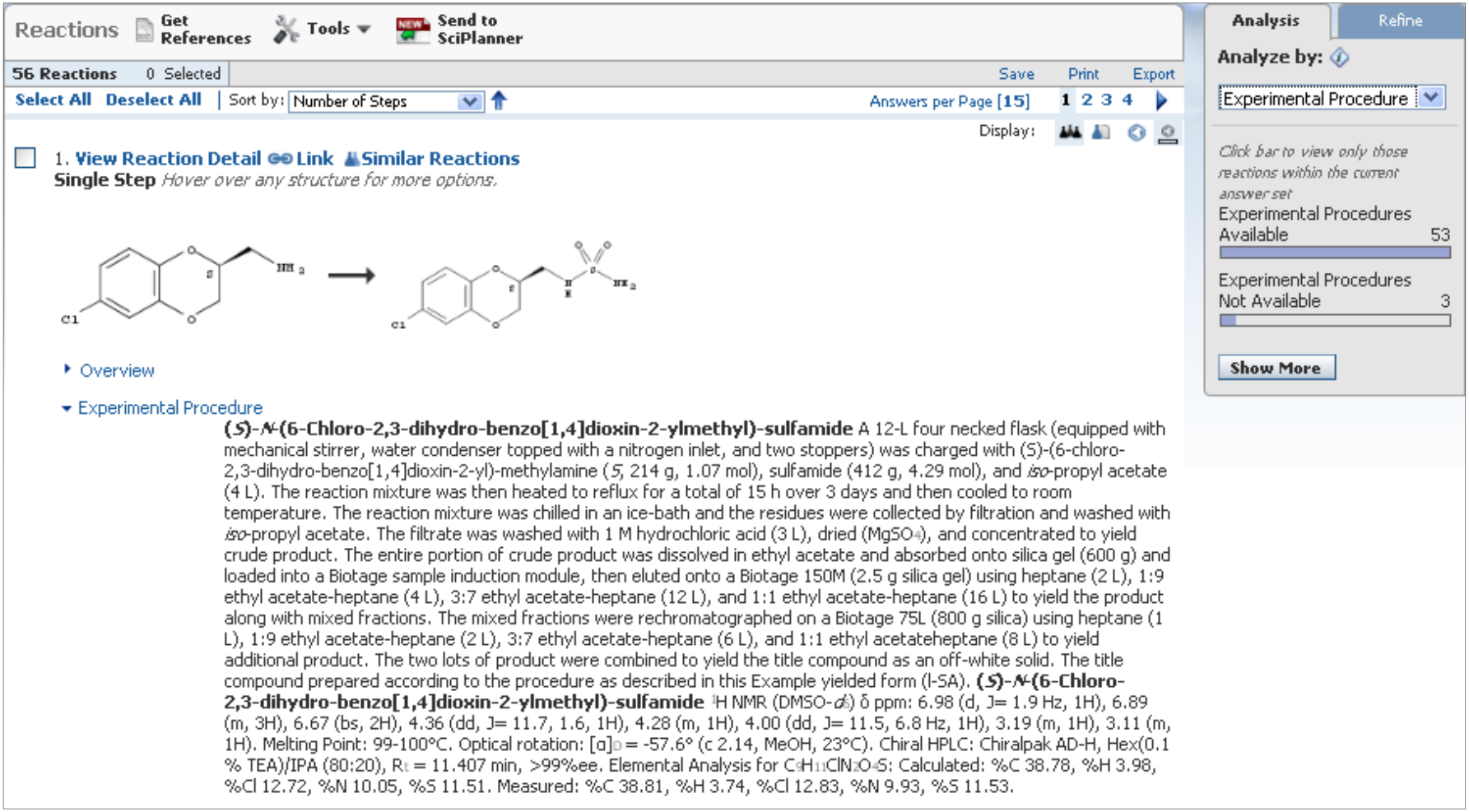


II

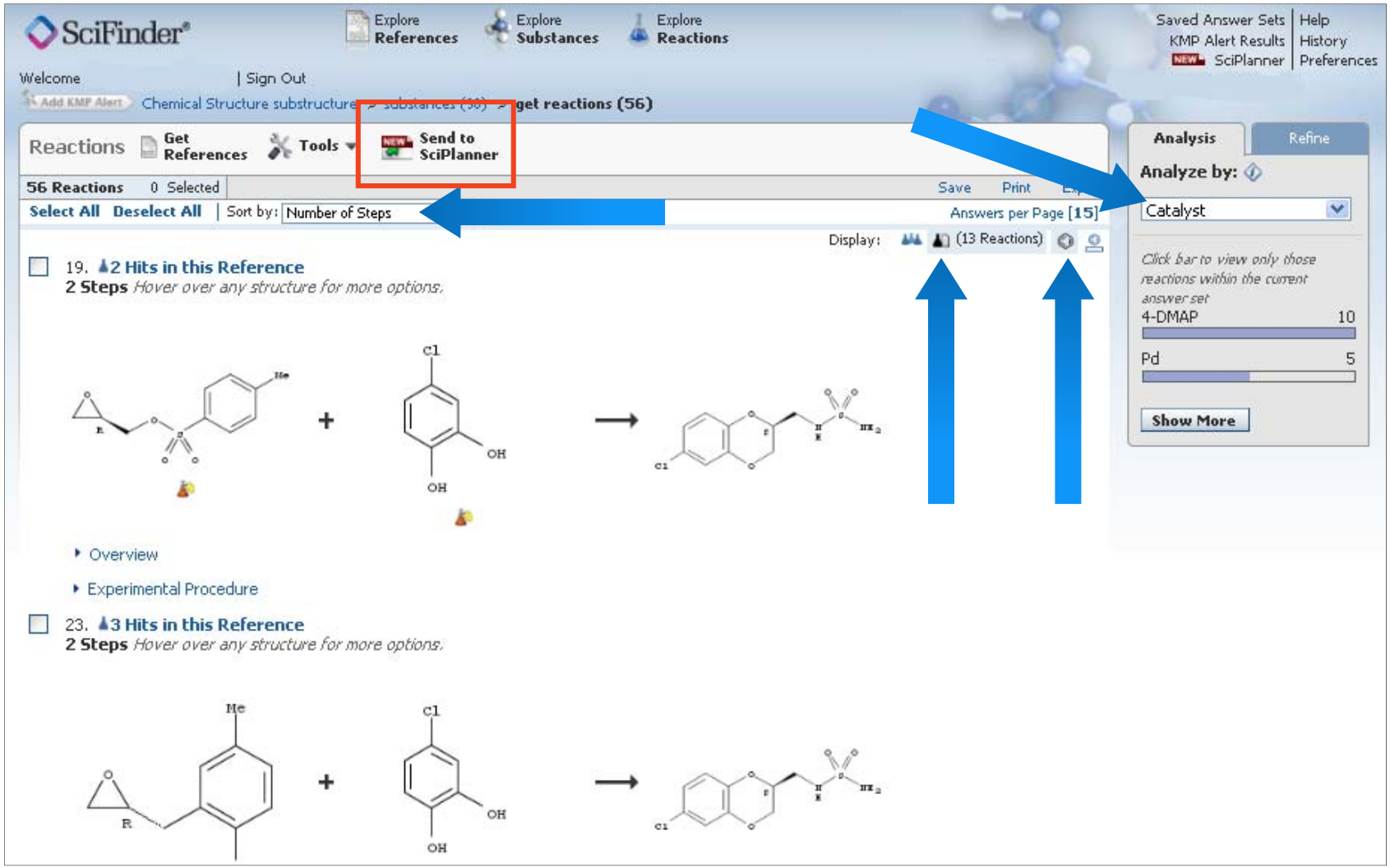
Let's create a synthesis plan for the compound in our set that has the most literature references



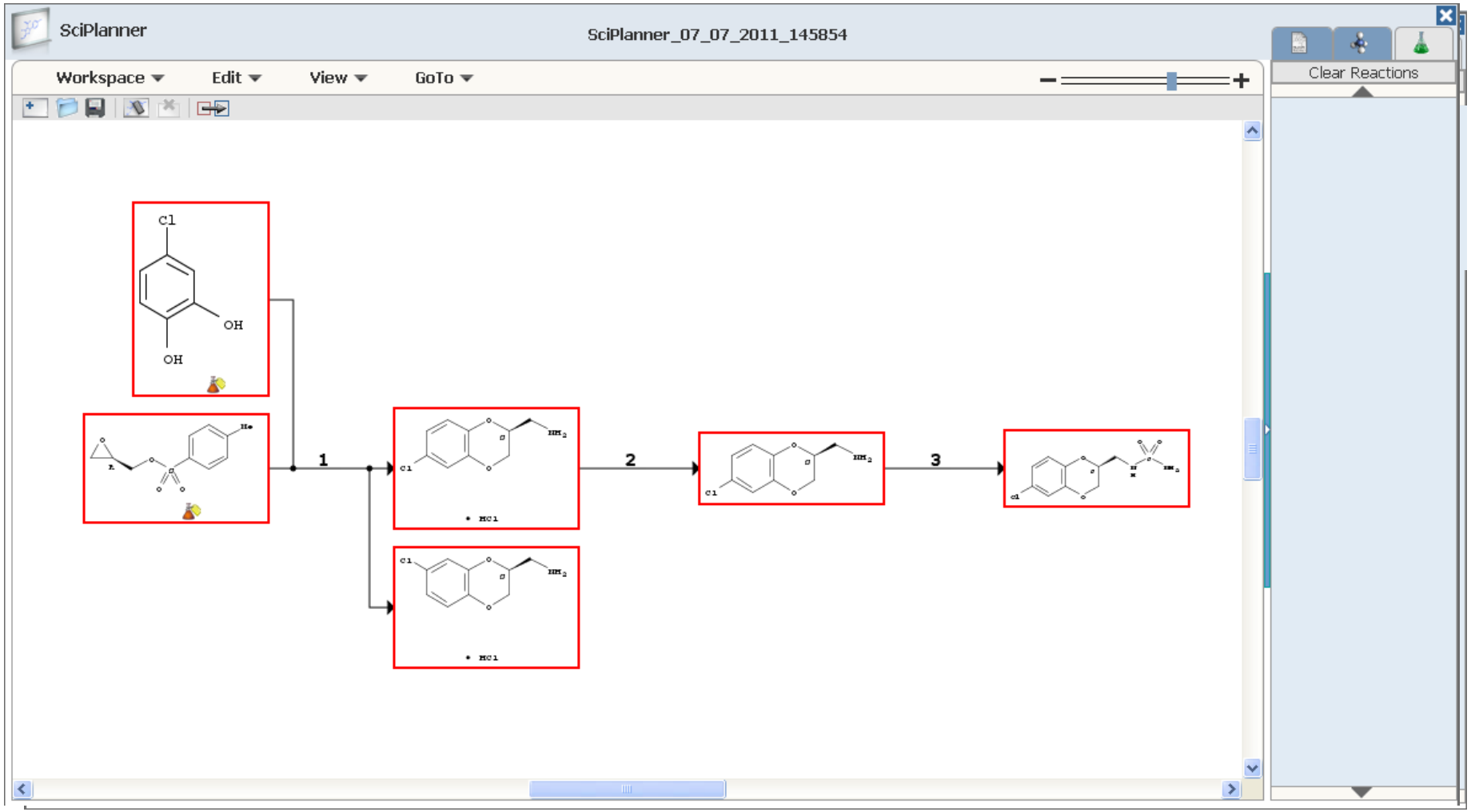
Almost 2 million reactions have experimental procedure text directly available for a detailed view on the synthesis



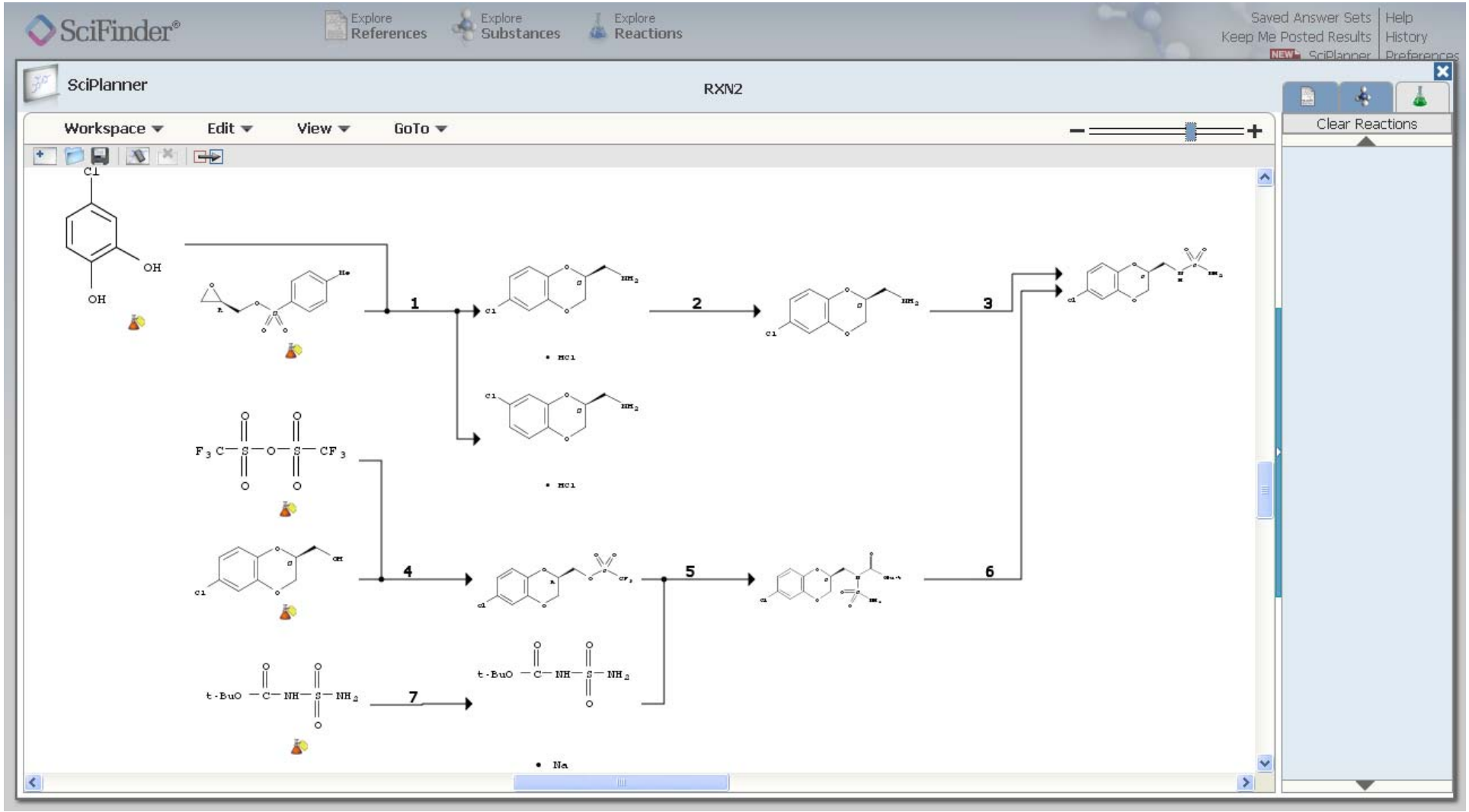
Sort, display and analyze options help make sense of larger reaction answer sets



Relevant reactions can be moved to SciPlanner



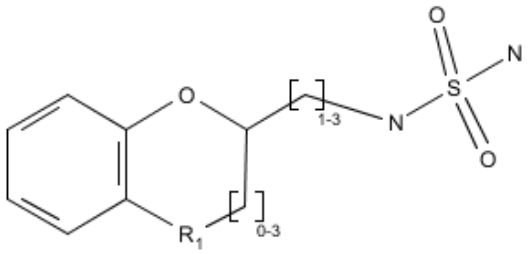
Two alternative pathways to our compound were constructed out of reactions from three publications



Example: Check novelty and design your synthesis

What did we learn?

- **There are 99 compounds already disclosed in 31 journal and patent references**
  - J&J seems to dominate the patent landscape
- **There are at least 24 additional patents that may influence our freedom-to-operate**
- **Compounds are used in oncology as well as in neurological diseases**
- **Two reaction pathways were constructed for the most frequently mentioned substance**



6.- Más información

Para cualquier duda: mplana@cas.org
help@cas.org

Estrategias de búsqueda
Soporte técnico

Propuestas, ideas, comentarios

Páginas web de interés:

http://www.cas.org
https://my.cas.org

¿Dudas? ¿Ideas? ¿Comentarios?

SciFinder®

¡Muchísimas gracias por vuestra atención!

Míriam Plana

CAS Regional Marketing Manager, Spain & Portugal

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