CAS

The World's Chemical Information Authority

Dr. Míriam Plana

Regional Marketing Manager Spain & Portugal

mplana@acsi.info

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Today's discussion

- CAS is the world's authority for chemical information about CAS …
- … that speeds discovery by bringing together the broadest collection of scientific data …
  - CAS databases
- … with the most accessible and sophisticated suite of analysis tools and research services in the industry
  - SciFinder®
  - STN®
  - Science IP®

About CAS

"CAS is seen by the pharmaceutical industry as being the gold standard of chemical information both in numbers of compounds and quality."

Peter Murray-Rust
Unilever Centre for Molecular Information, Cambridge
petermr's blog: A Scientist and the Web

CAS is a division of the American Chemical Society

ACS Vision

Improving people's lives through the transforming power of chemistry.

ACS Chemistry for Life®

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CAS supports the mission of the ACS

ACS Mission

To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people.

CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.

Building the highest quality chemistry databases

Patents, journals, web, catalogs, etc.

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CAS Scientists

arXiv.org

Aldrichimica ACTA

ACS chemical biology

Beilstein Journal of Organic Chemistry

division of polymer chemistry, inc American Chemical Society

JACS Journal of the American Chemical Society

ACS Chemical Neuroscience

The Journal of Physical Chemistry Letters

Cornell University Library

U.S. Patent Office

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CAS is the leading global source of chemical information for scientific and patent research

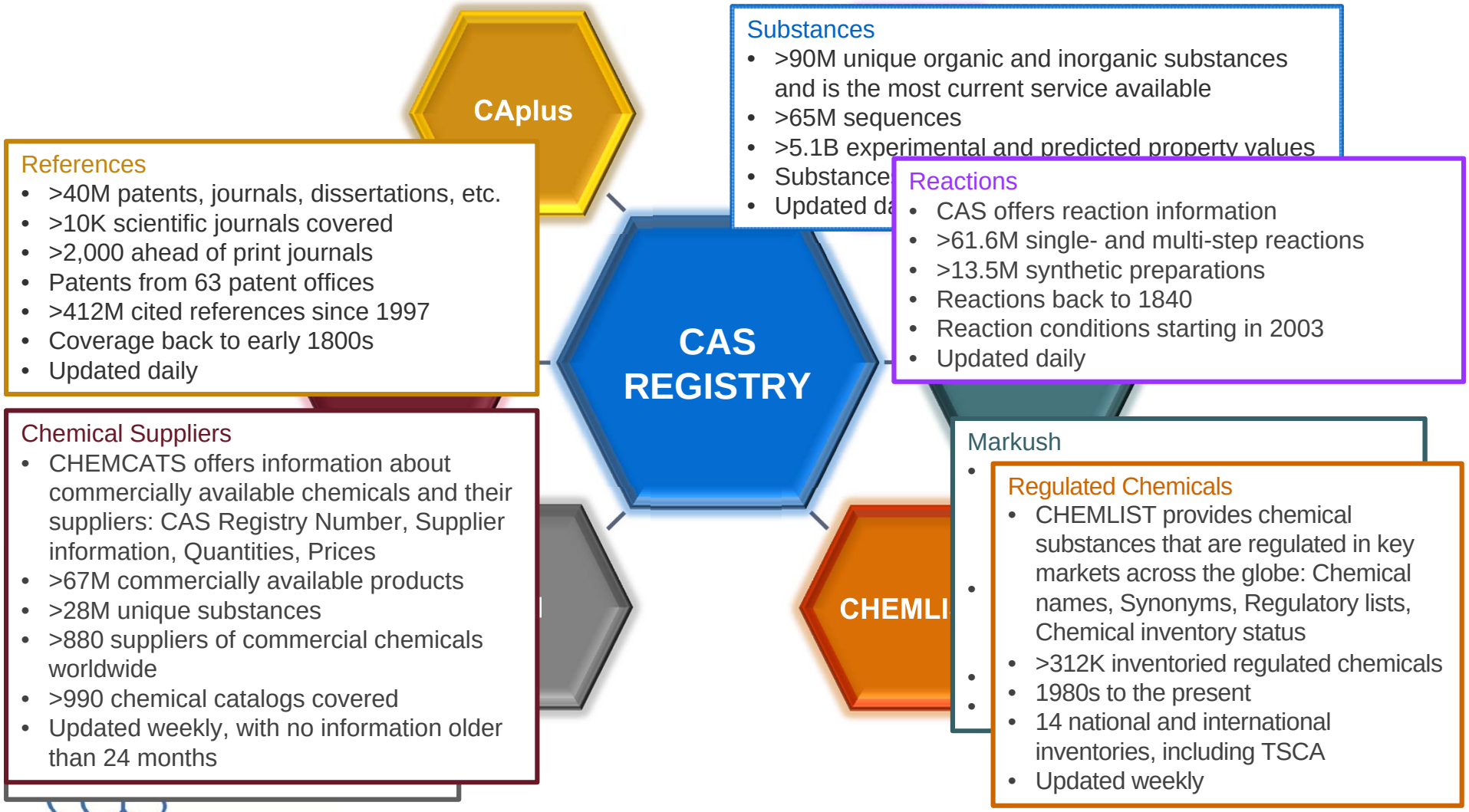
- Founded in 1907 to monitor, abstract and index the world's chemistry-related literature and make it available to the scientific community
- Work first published in *Chemical Abstracts*™
- Headquartered in Columbus, Ohio
- Approximately 1,400 staff members – including CAS scientists, speaking 50 languages among them
- More than 10,000 major scientific journals and patents from 63 patent authorities are reviewed and indexed
- Customers include more than 2,174 universities, top Fortune 500 corporations and all major patent offices

CAS Databases

"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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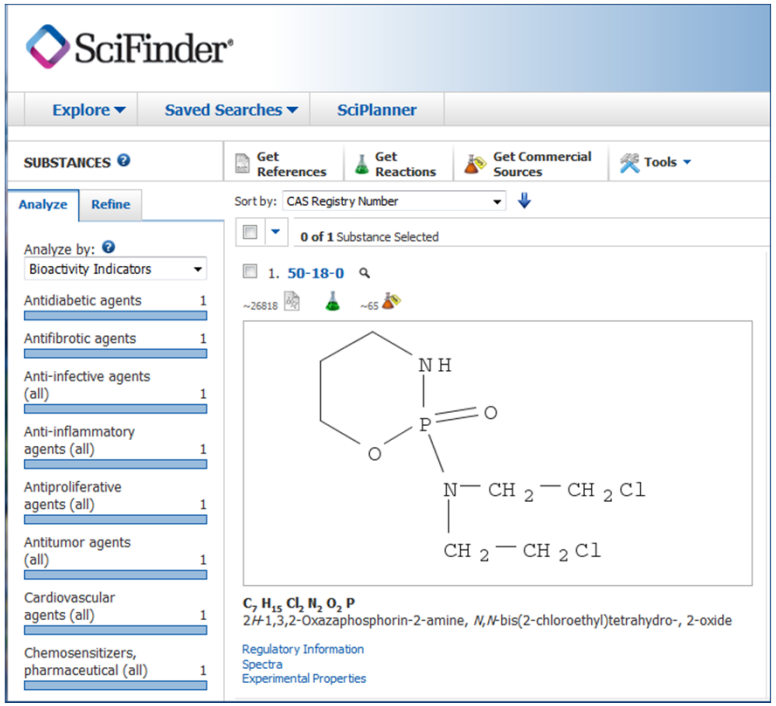
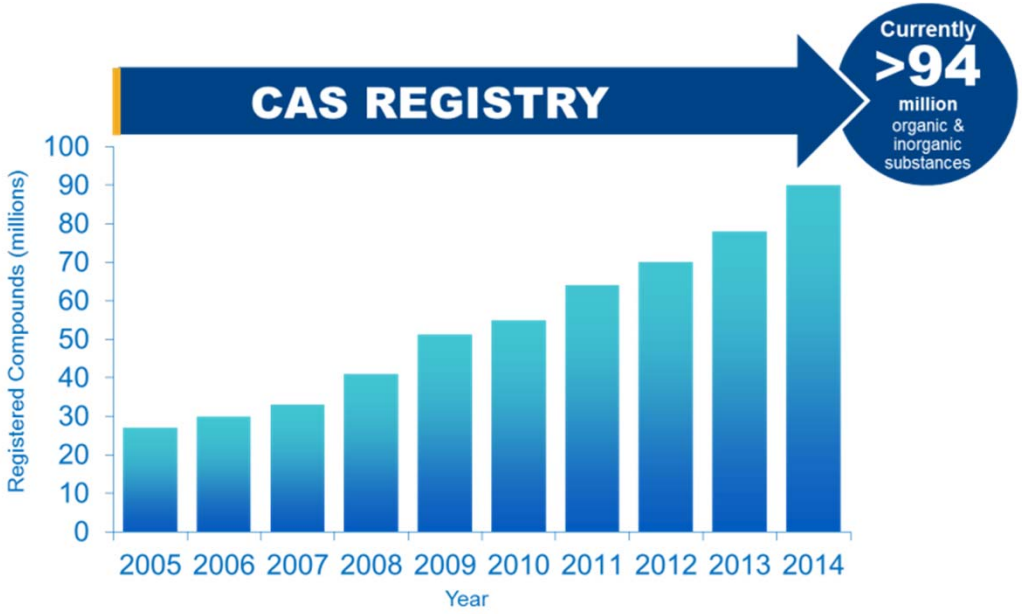
CAS REGISTRY^{SM} is the gold standard for chemical substance information





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CAS REGISTRY is the only integrated, complete source of chemical information

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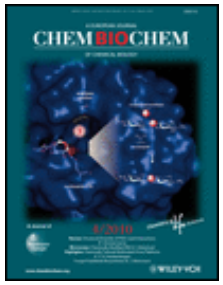
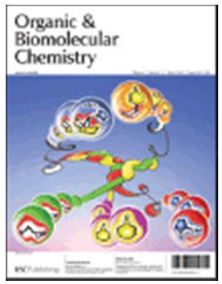
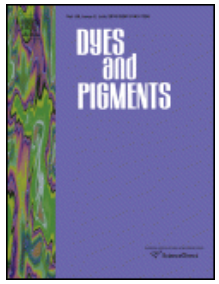
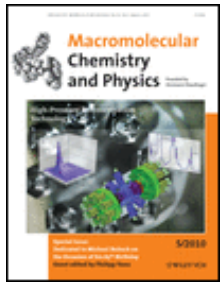
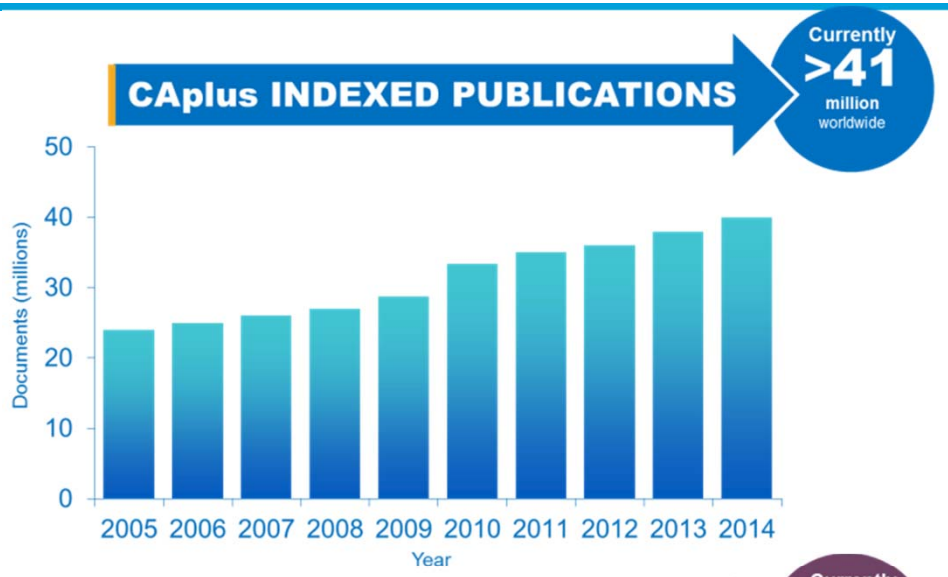
CAplus[SM] is your single source for chemistry and related scientific information

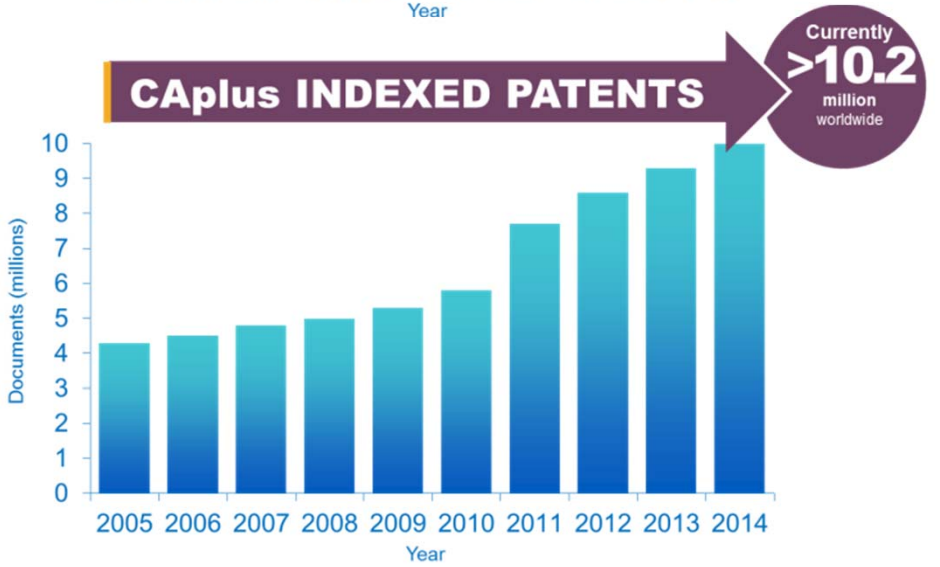












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CAplus coverage of patents from Asia is unmatched

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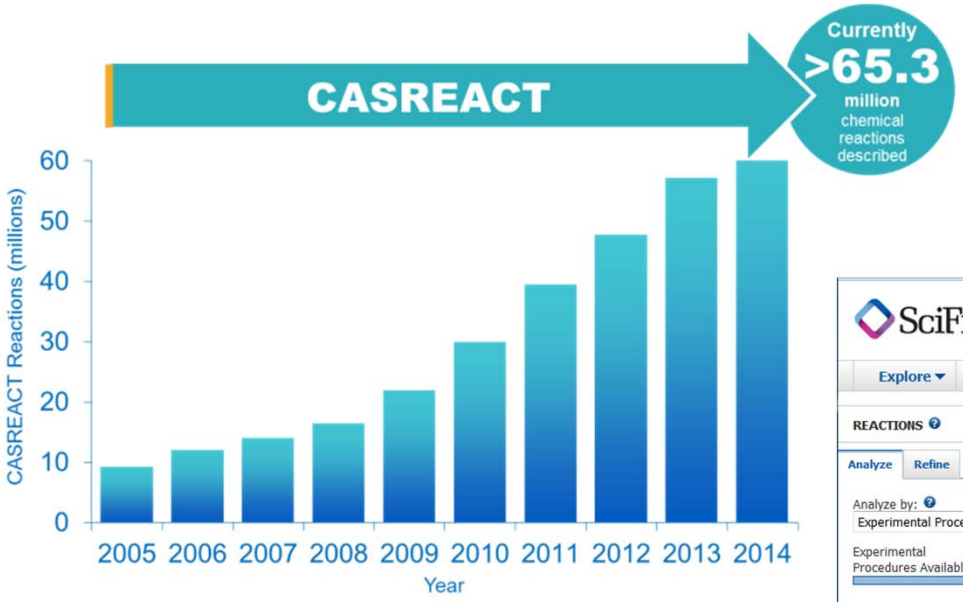
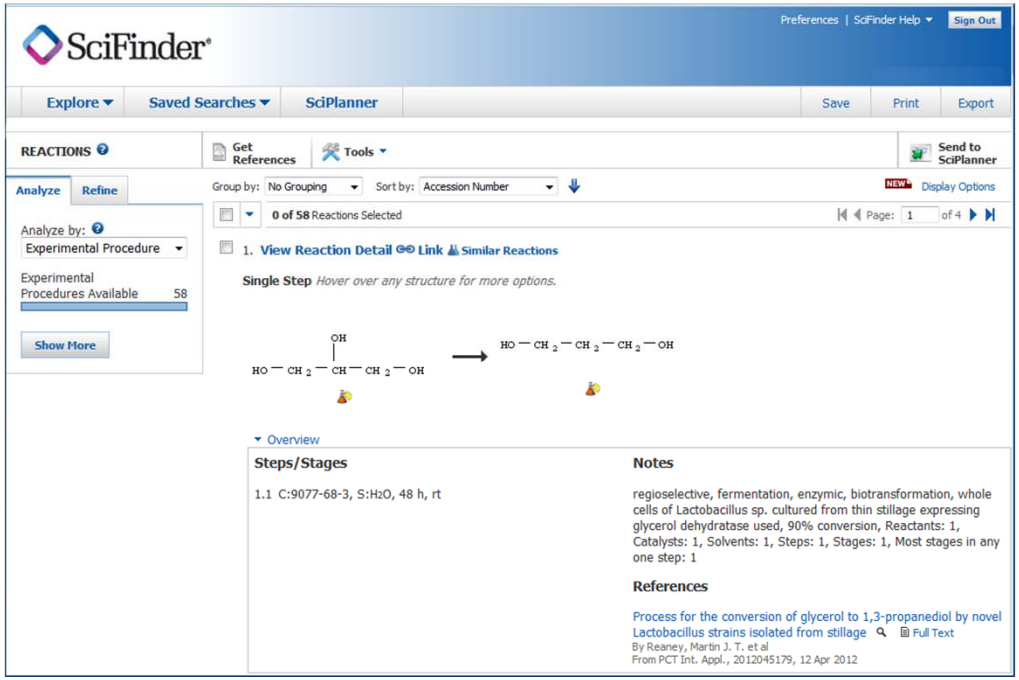
CASREACT® is the authoritative source for chemical reactions





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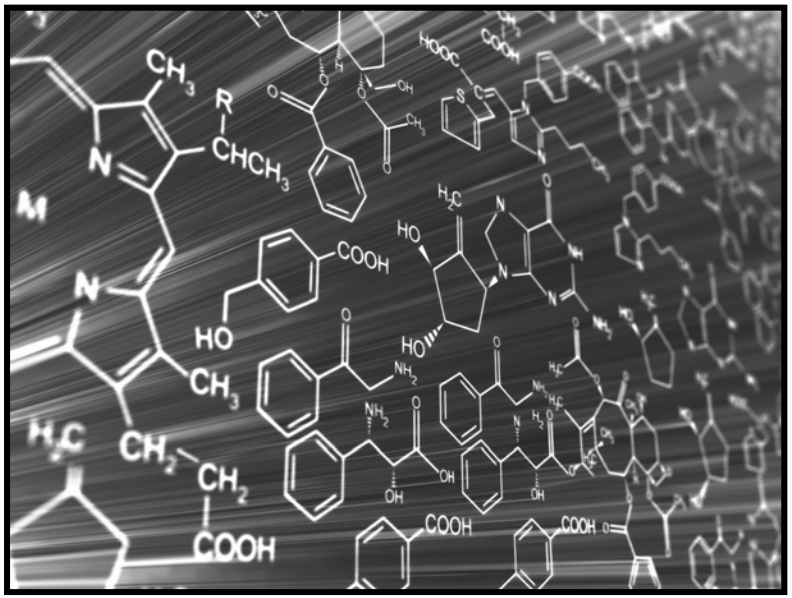
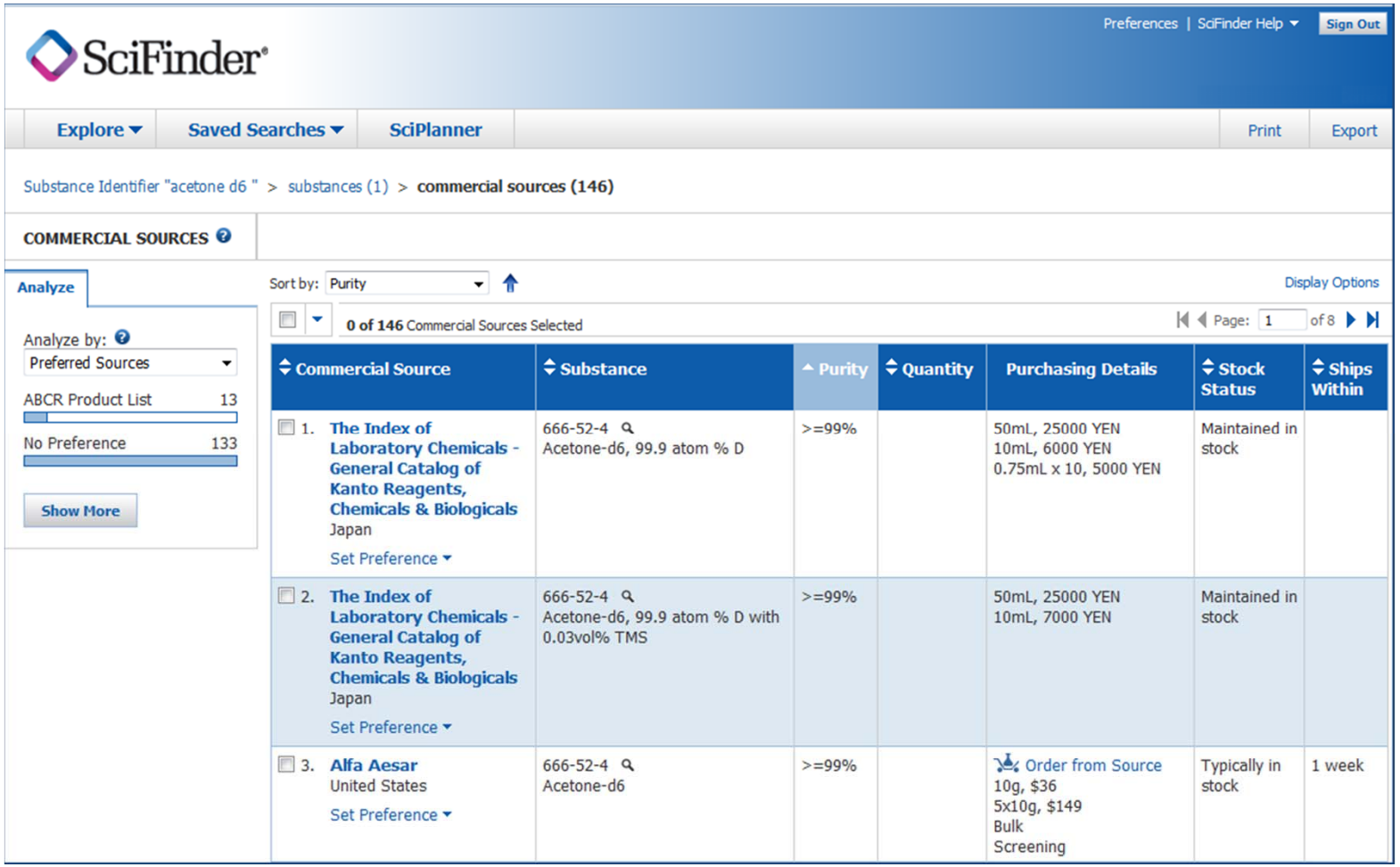
CASREACT answers your chemical reaction questions quickly, precisely and comprehensively



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



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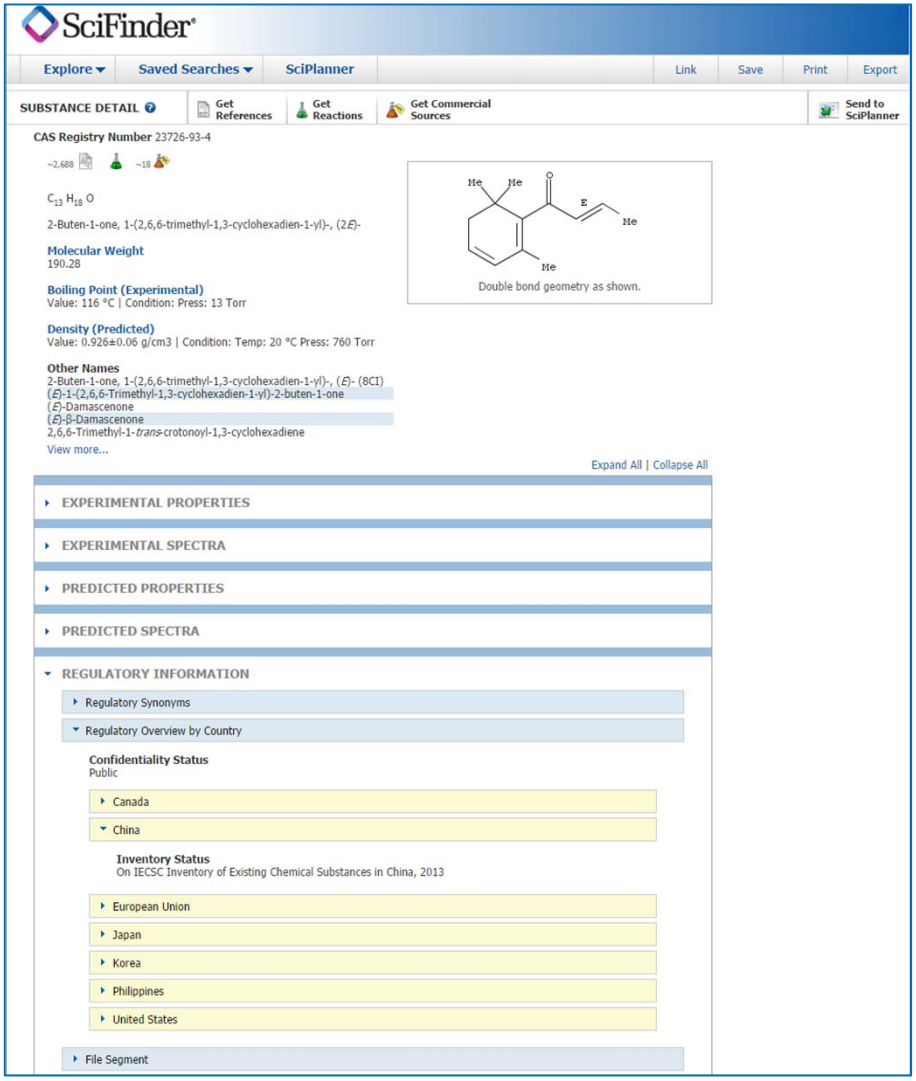
CHEMCATS provides fast access to chemical suppliers

CHEMLIST® is the comprehensive source for information on regulated chemicals



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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 2014 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
IPCI A61K0009-00 [ICM,7]
IPCR A61K0009-00 [I]; A61K0047-22 [I]
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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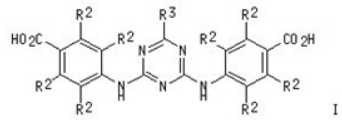

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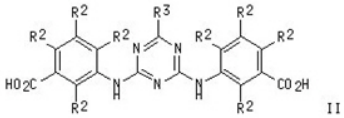

II

AB Compns. and methods includes a bioactive compd. and a triazine compd. comprising: formula I or formula II and proton tautomers and salts • • •

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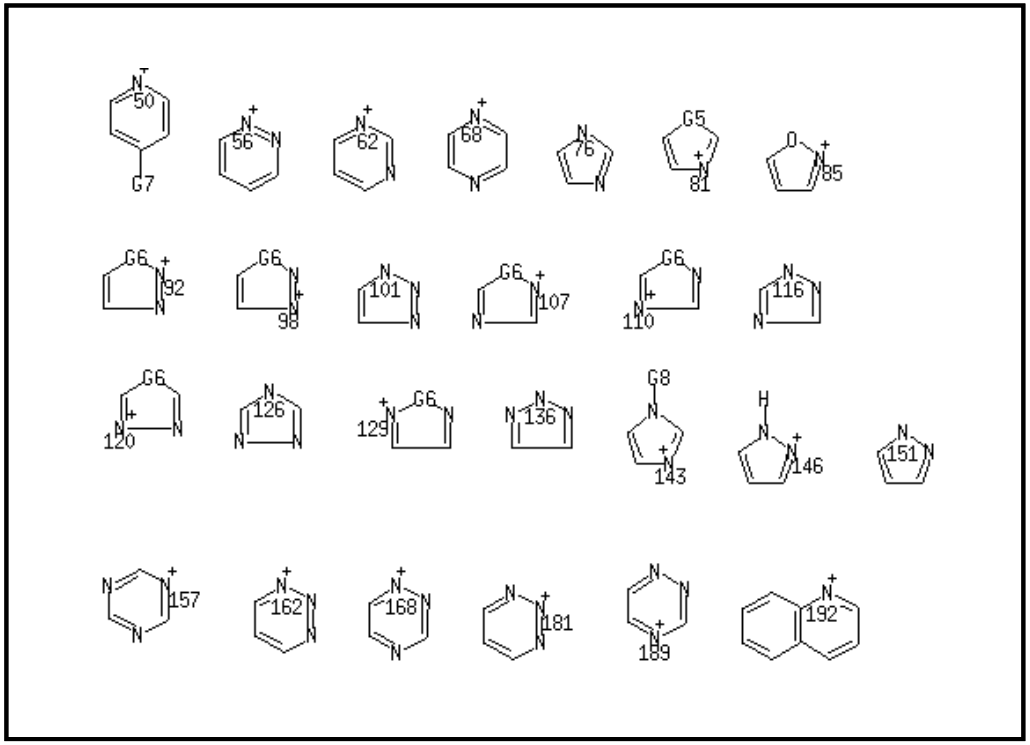
MARPAT supports maximum recall of patented information



CAS products streamline access to CAS databases to speed the pace of scientific discovery

SciFinder®
The choice for chemistry research.™

SciFinder is an intuitive discovery platform with flexible search and analysis options designed for scientists' workflows.

PatentPak™ now available

STN®
THE CHOICE OF PATENT EXPERTS™

STN combines industry-leading search and retrieval with unique and comprehensive content.

SCIENCE IP®
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The CAS information search service provides fast, comprehensive and accurate searches of the world's scientific and technical literature.

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News in SciFinder

"I am a big user and don't see how any researcher could hope to excel without daily, round-the-clock access. The speed and scope of its search power is amazing … In my case, SciFinder enhances my reactivity insights, making it easier to "see" those ill-defined boundaries where important new phenomena are lurking."

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

News in SciFinder

- New Substance Detail View Improves Readability and User Experience

CAS Registry Number 23726-93-4

~2,694 ~18

$C_{13}H_{18}O$

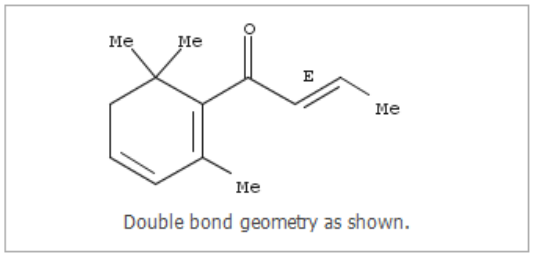
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2*E*)-

Molecular Weight
190.28

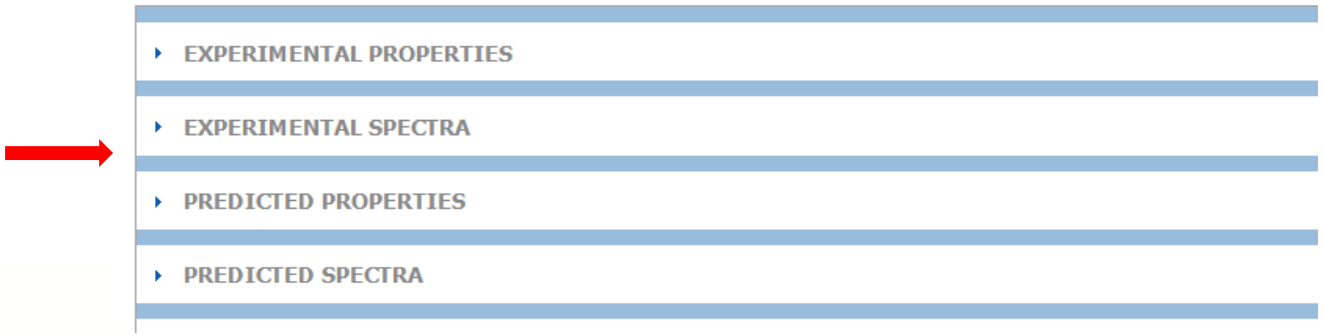
Boiling Point (Experimental)
Value: 116 °C | Condition: Press: 13 Torr

Density (Predicted)
Value: 0.926±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

Other Names
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- (8CI)
(*E*)-1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one
(*E*)-Damascenone
(*E*)-β-Damascenone
2,6,6-Trimethyl-1-*trans*-crotonoyl-1,3-cyclohexadiene
View more...

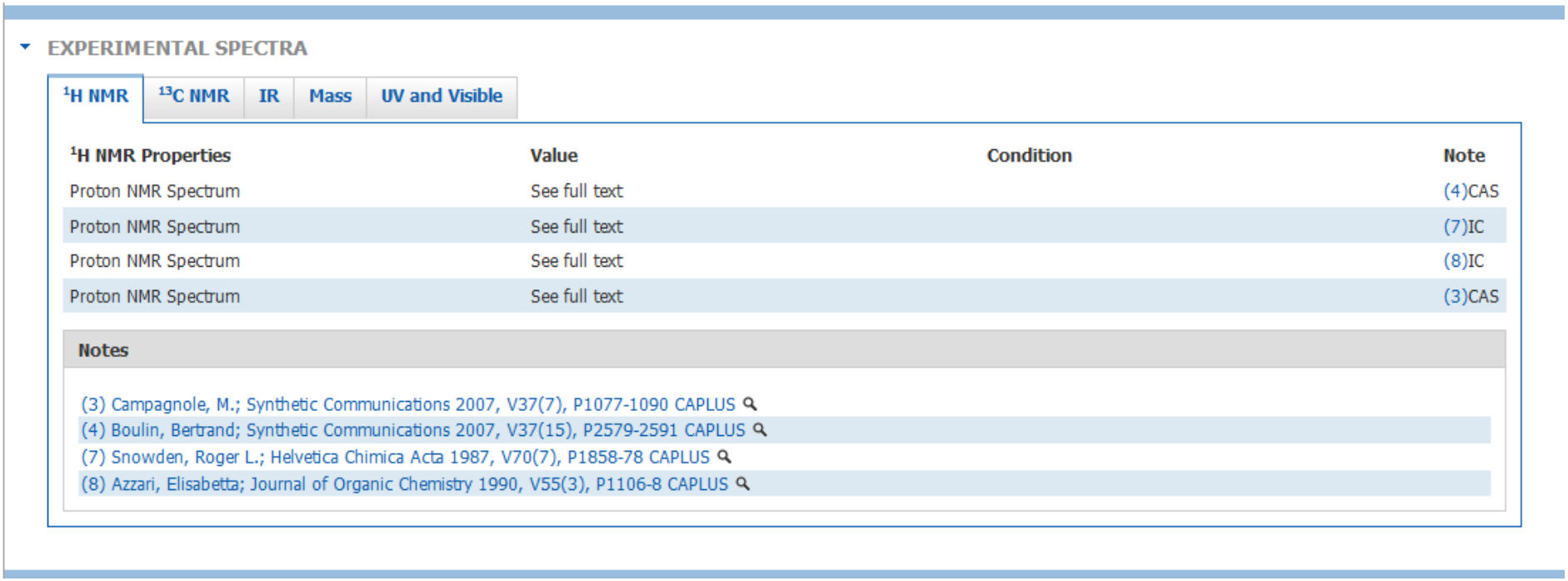


Double bond geometry as shown.



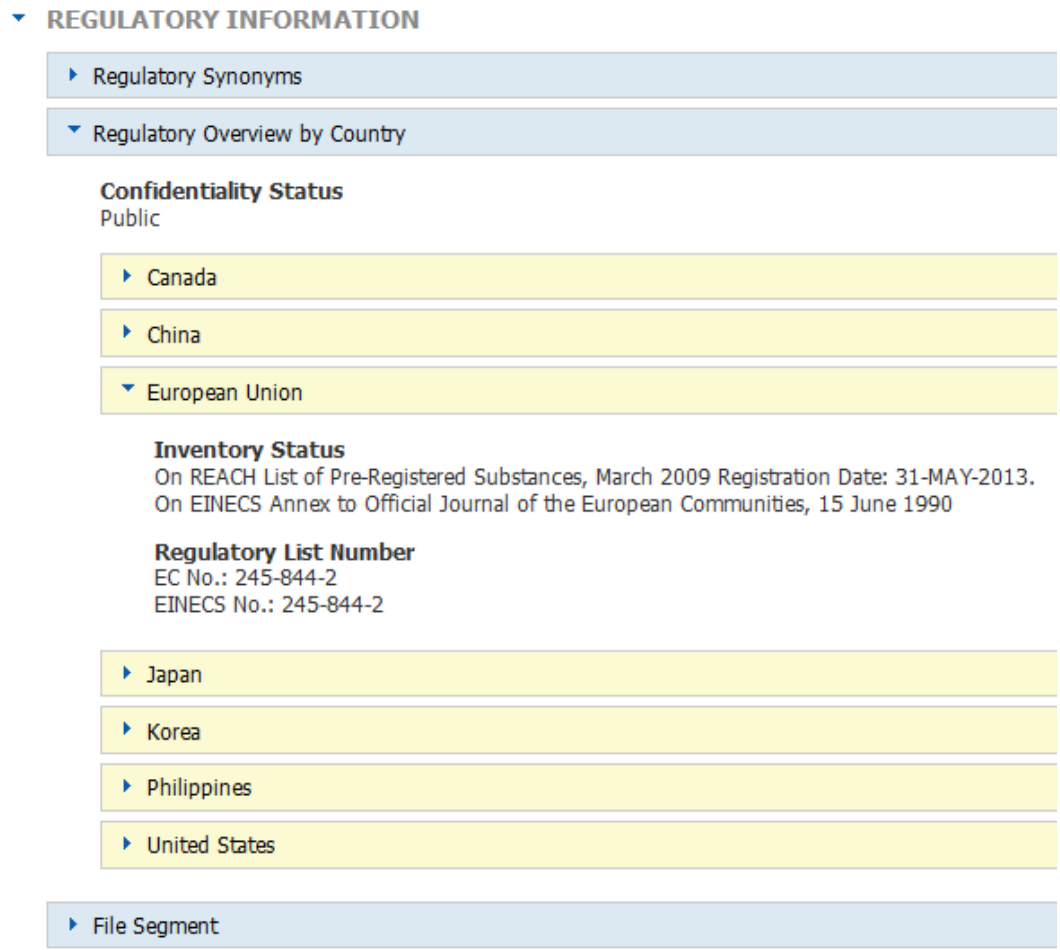
News in SciFinder

- New Substance Detail View Improves Readability and User Experience



News in SciFinder

- New Substance Detail View Improves Readability and User Experience



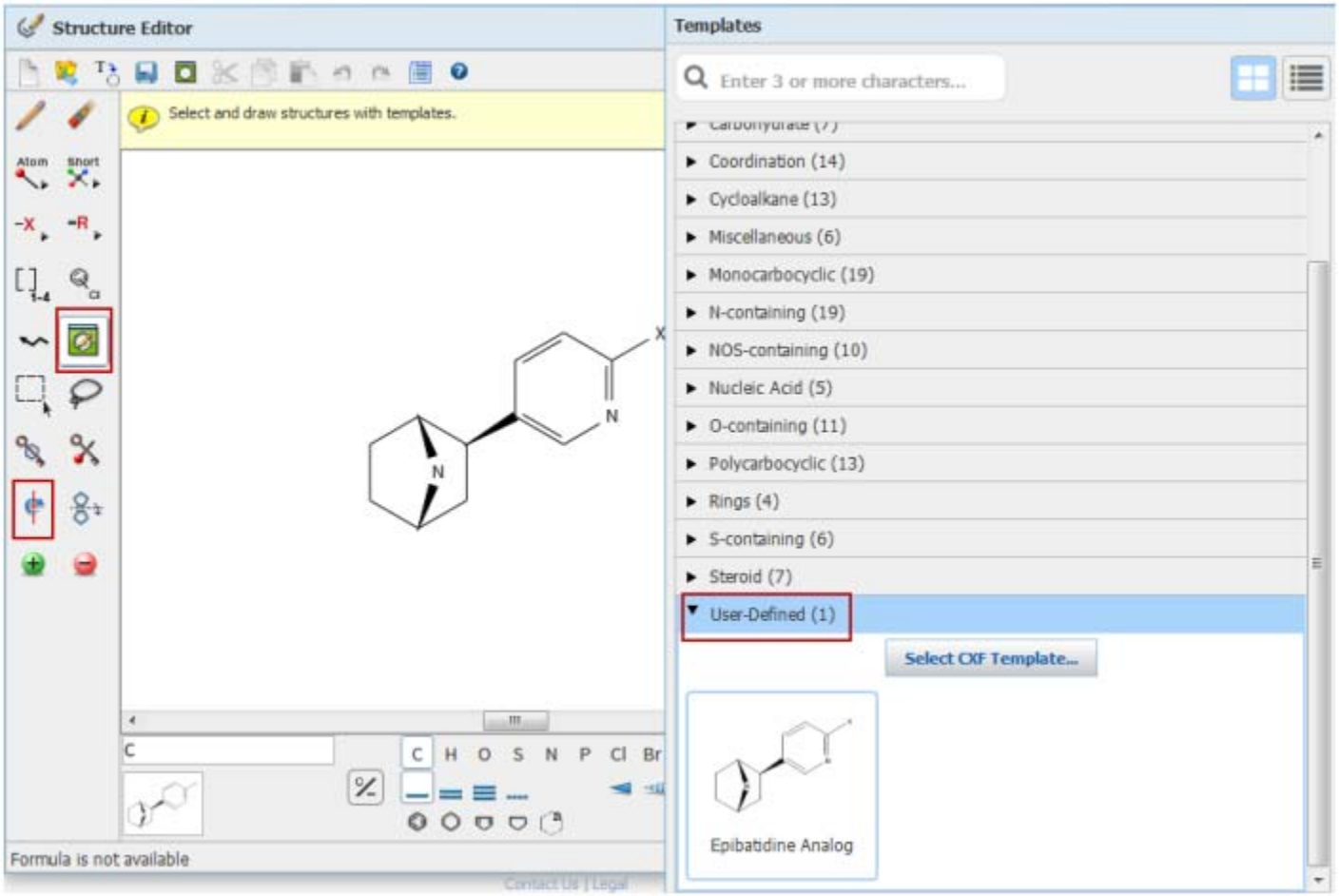
News in SciFinder

- Table View Presentation of Commercial Sources Answer Sets

Commercial Source	Substance	Purity	Quantity	Purchasing Details	Stock Status	Ships Within
1. **Chemieliva Pharmaceutical Product List** China Preferred	23726-93-4 beta-Damascenone	>=99%		Bulk Screening	Maintained in stock	2 weeks
2. **A.S. Chemical Laboratories Product List** Canada Set Preference	23726-93-4 (2E)-1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one			N/A, contact source		
3. **ACC Corp. Catalog** United States Set Preference	23726-93-4 (E)-1-(2,6,6-TRIMETHYLCYCLOHEXEN-1-YL)BUT-2-EN-1-ONE			10MG, contact source 100MG, contact source 500MG, contact source		
4. **AKos Building Blocks Product List** Germany Set Preference	23726-93-4 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)-				Typically in stock	2 weeks
5. **Allicon Pharmaceuticals Product List** China Set Preference	23726-93-4 beta-Damascenone			Bulk	Maintained in stock	1 week
6. **Ambinter Stock Screening Collection** France Set Preference	23726-93-4 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)-	90-95%	Milligrams	Screening	Typically in stock	4 weeks
7. **Ark Pharm Product List** United States	23726-93-4 1-(2,6,6-Trimethylcyclohexa-1,3-dien-1-yl)but-2-en-1-one	95-98%	Grams	Order from Source 1 g, $120 5 g, $380	Synthesis on demand	4 weeks

News in SciFinder

- Non-Java CAS Structure Editor enhancements



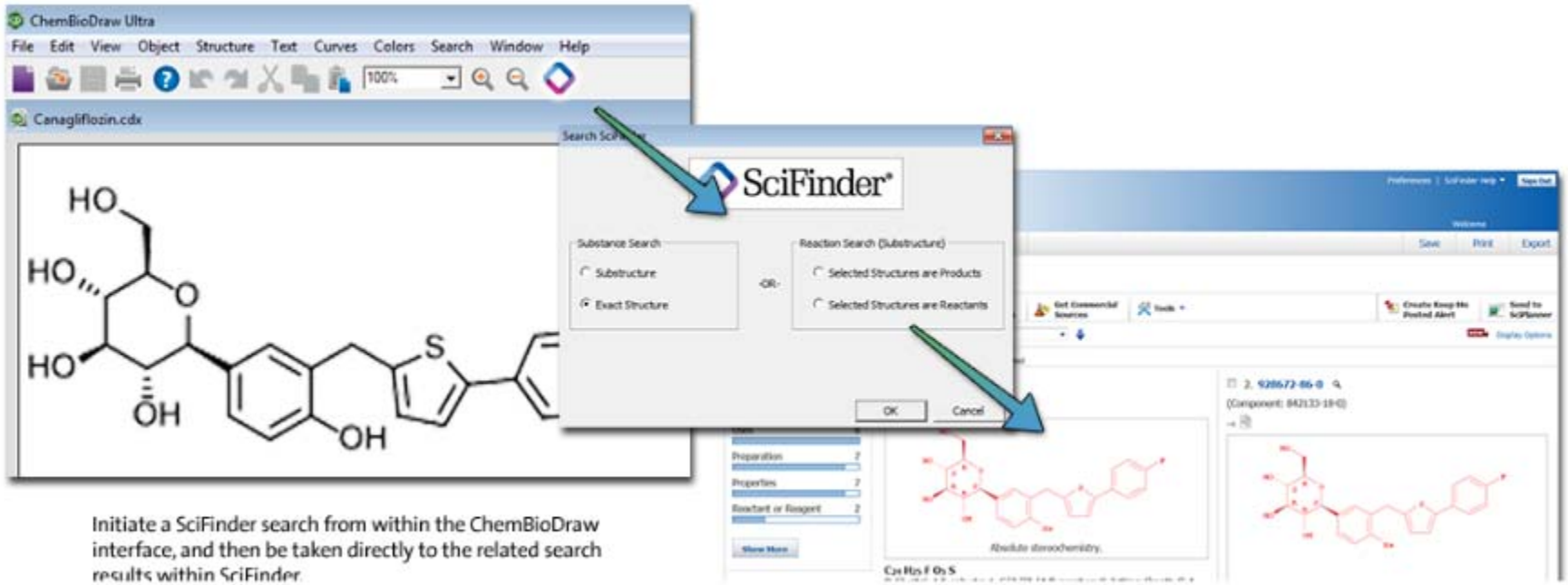
News in SciFinder

- SciFinder/ChemDraw® Collaboration

THE CHOICE FOR CHEMISTRY RESEARCH
MEETS THE CHOICE FOR CHEMISTRY DRAWING.
(The choice is clear.)

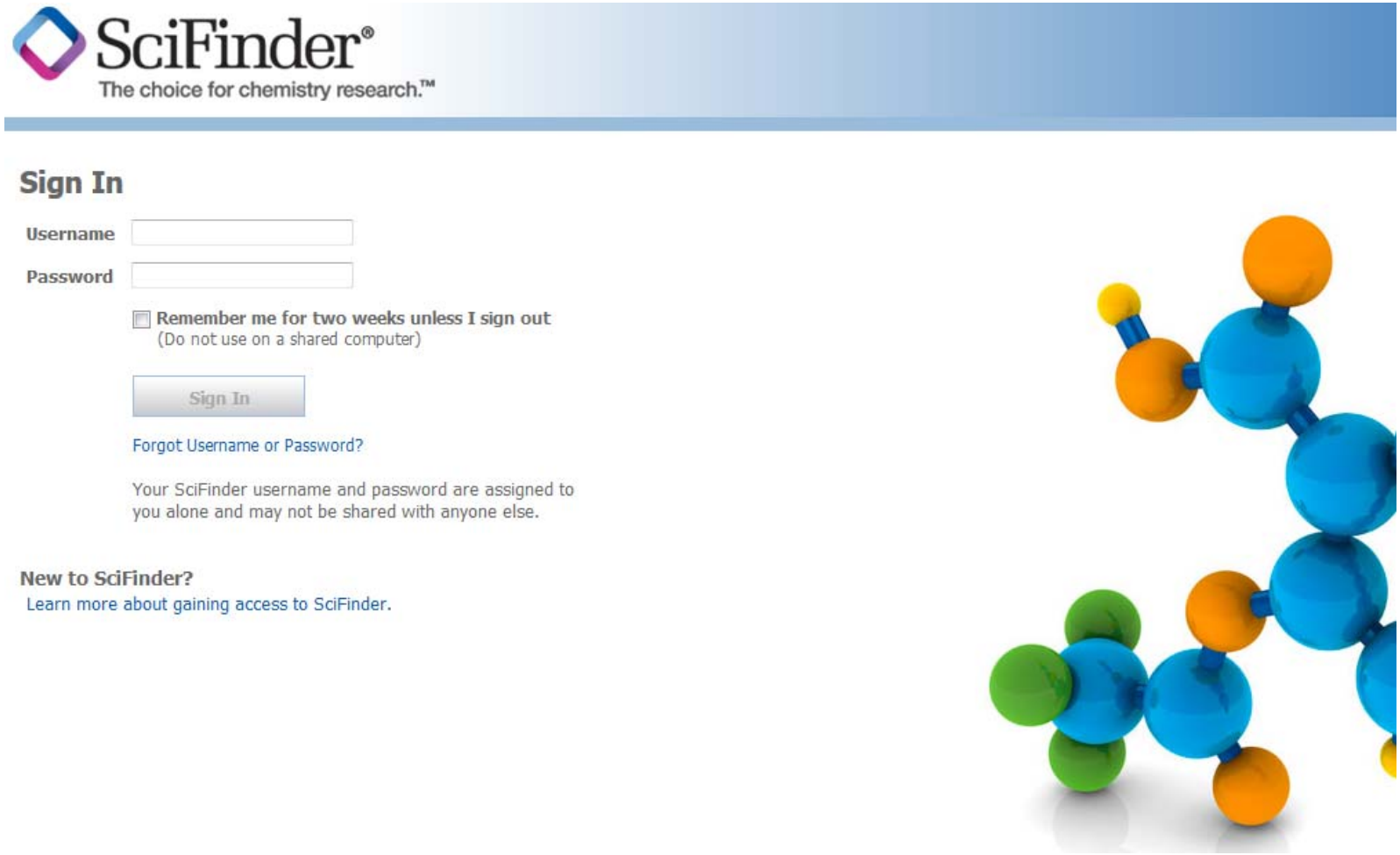
News in SciFinder

- SciFinder/ChemDraw® Collaboration



Initiate a SciFinder search from within the ChemBioDraw interface, and then be taken directly to the related search results within SciFinder

Example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The choice for chemistry research.™
Sign In
Username
Password
Remember me for two weeks unless I sign out
(Do not use on a shared computer)
Sign In
Forgot Username or Password?
Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.
New to SciFinder?
Learn more about gaining access to SciFinder.

Example

- Somos un laboratorio farmacéutico y la competencia ha sacado al mercado un nuevo producto llamado CC 4047…

  – ¿Qué es?
  – Buscar derivados de este compuesto. ¿Para qué se utilizan?
  – ¿Hay alguno que ayude a cicatrizar heridas?
  – Buscar toda la bibliografía que mencione este tipo de compuestos
  – ¿Hay alguna técnica analítica que permita la detección de CC 4047 en sangre? ¿Qué técnica utilizan?
  – Buscar bibliografía sobre cicatrización de heridas.
  – Buscar métodos de síntesis para preparar CC 4047.

CAS Customer Center

Ask us! We can help.

- Account information
- How to
- IT support

"I need to change something on my account."

"Can I speak with someone in IT?"

"I need help with my search strategy."

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