



CAS

The World's Chemical Information Authority

Dr. Míriam Plana

Regional Marketing Manager Spain & Portugal

mplana@acsi.info



A division of the American Chemical Society

ACS Proprietary and Confidential

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®



A division of the American Chemical Society

ACS Proprietary and Confidential

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



A division of the American Chemical Society

ACS Proprietary and Confidential

CAS is a division of the American Chemical Society

ACS Vision

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



A division of the American Chemical Society

ACS Proprietary and Confidential

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.

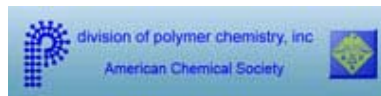


A division of the American Chemical Society

ACS Proprietary and Confidential

Building the highest quality chemistry databases

Patents,
journals, web,
catalogs, etc.



**U.S. Patent
Office**

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*TM
- 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



A division of the American Chemical Society

ACS Proprietary and Confidential

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.”

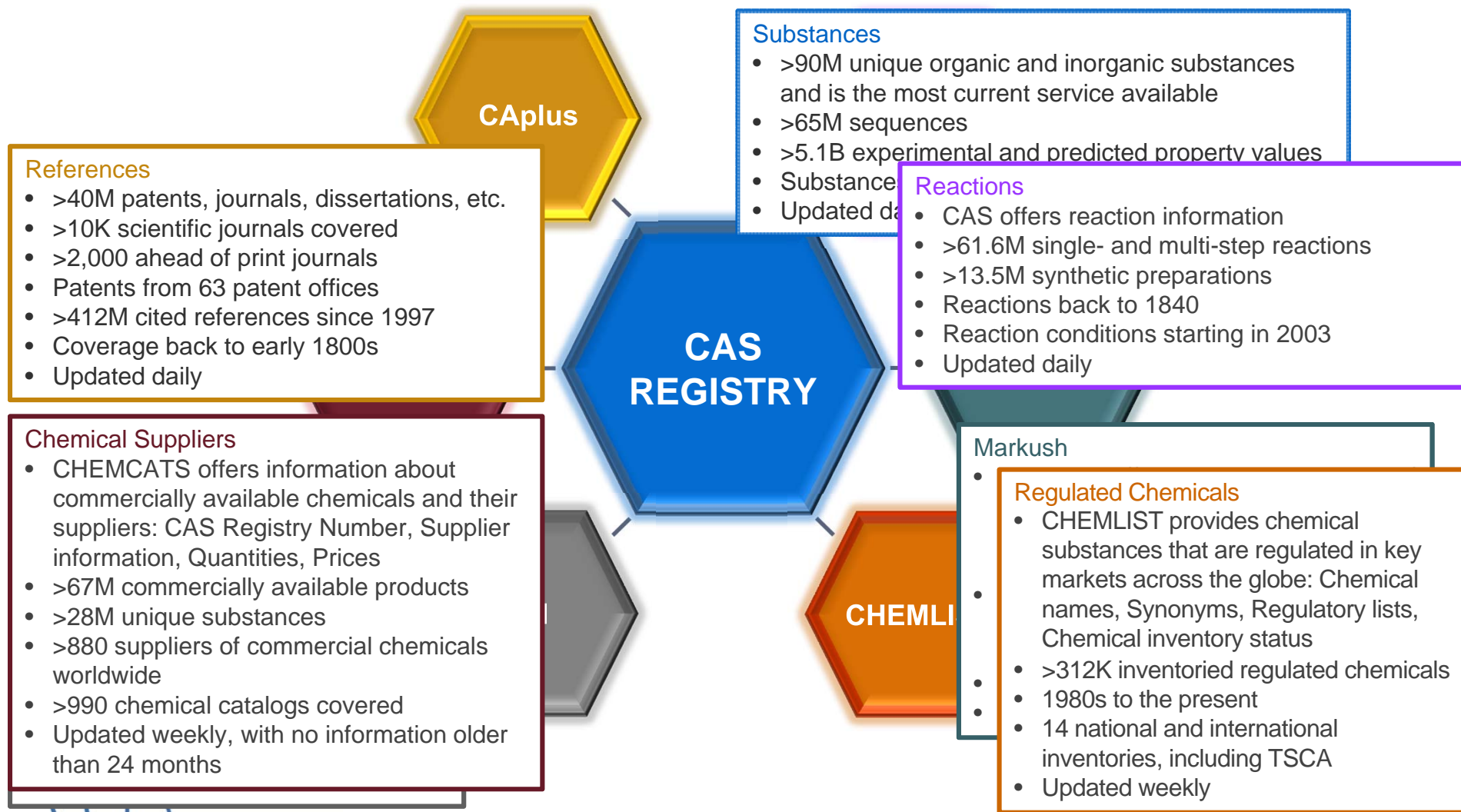
Dr. Robert H. Grubbs
Nobel Laureate
Victor and Elizabeth Atkins Professor of Chemistry
California Institute of Technology



A division of the American Chemical Society

ACS Proprietary and Confidential

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



CAS REGISTRYSM is the gold standard for chemical substance information

SciFinder[®]

Explore ▾ Saved Searches ▾ SciPlanner

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

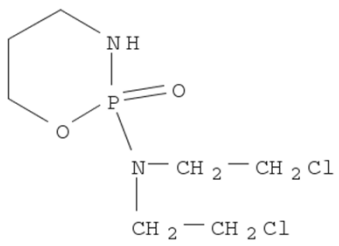
Analyze Refine

Sort by: CAS Registry Number ▾

0 of 1 Substance Selected

1. 50-18-0

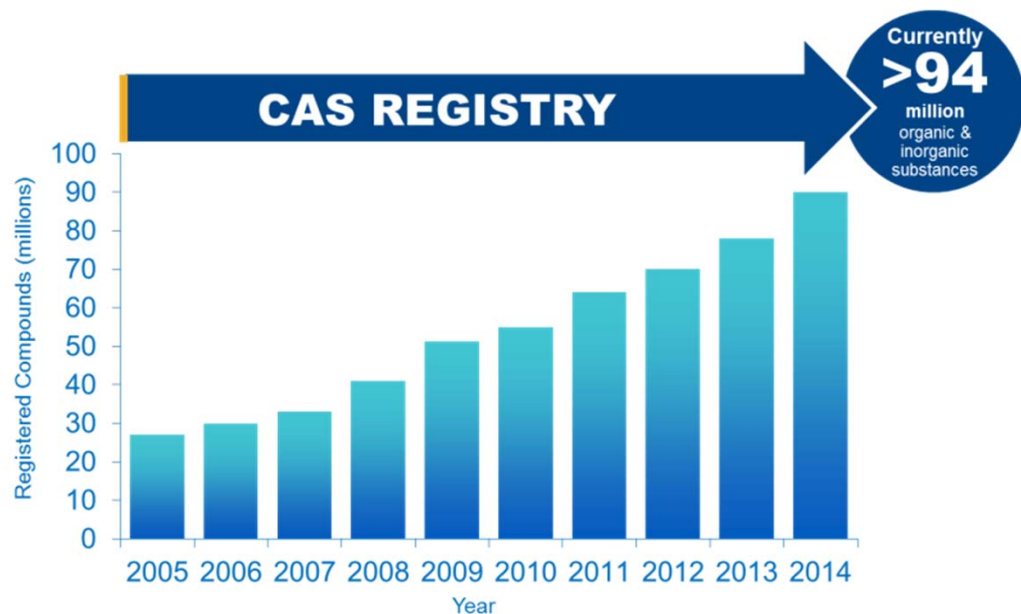
~26818 ~65



ClCCN(CCCl)P(=O)(N1CCOCC1)C2=CC=CC=C2

C₇ H₁₅ Cl₂ N₂ O₂ P
2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide

Regulatory Information
Spectra
Experimental Properties



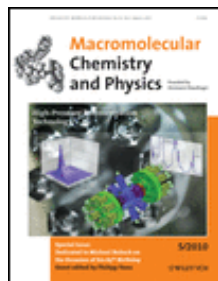
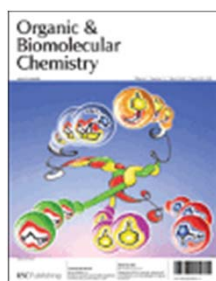
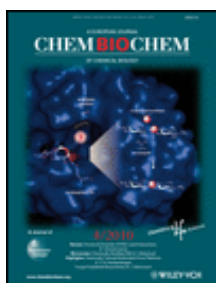
A division of the American Chemical Society

ACS Proprietary and Confidential

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

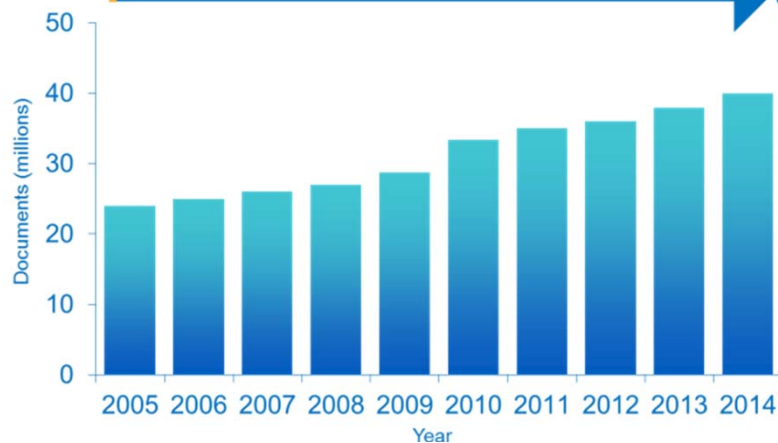


CAplusSM is your single source for chemistry and related scientific information



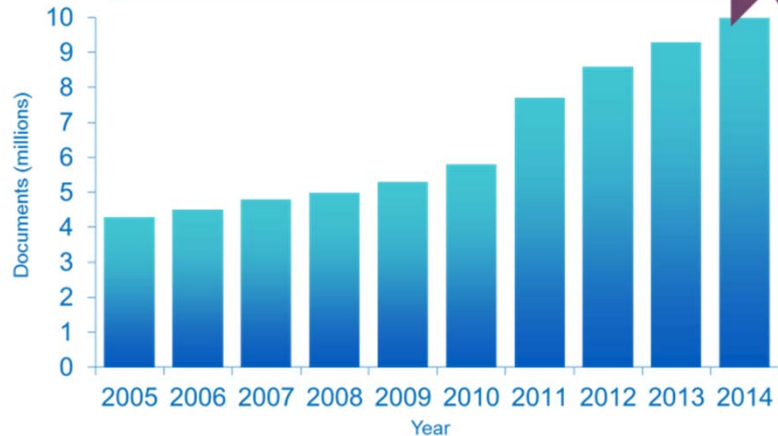
CAplus INDEXED PUBLICATIONS

Currently
>41
million
worldwide



CAplus INDEXED PATENTS

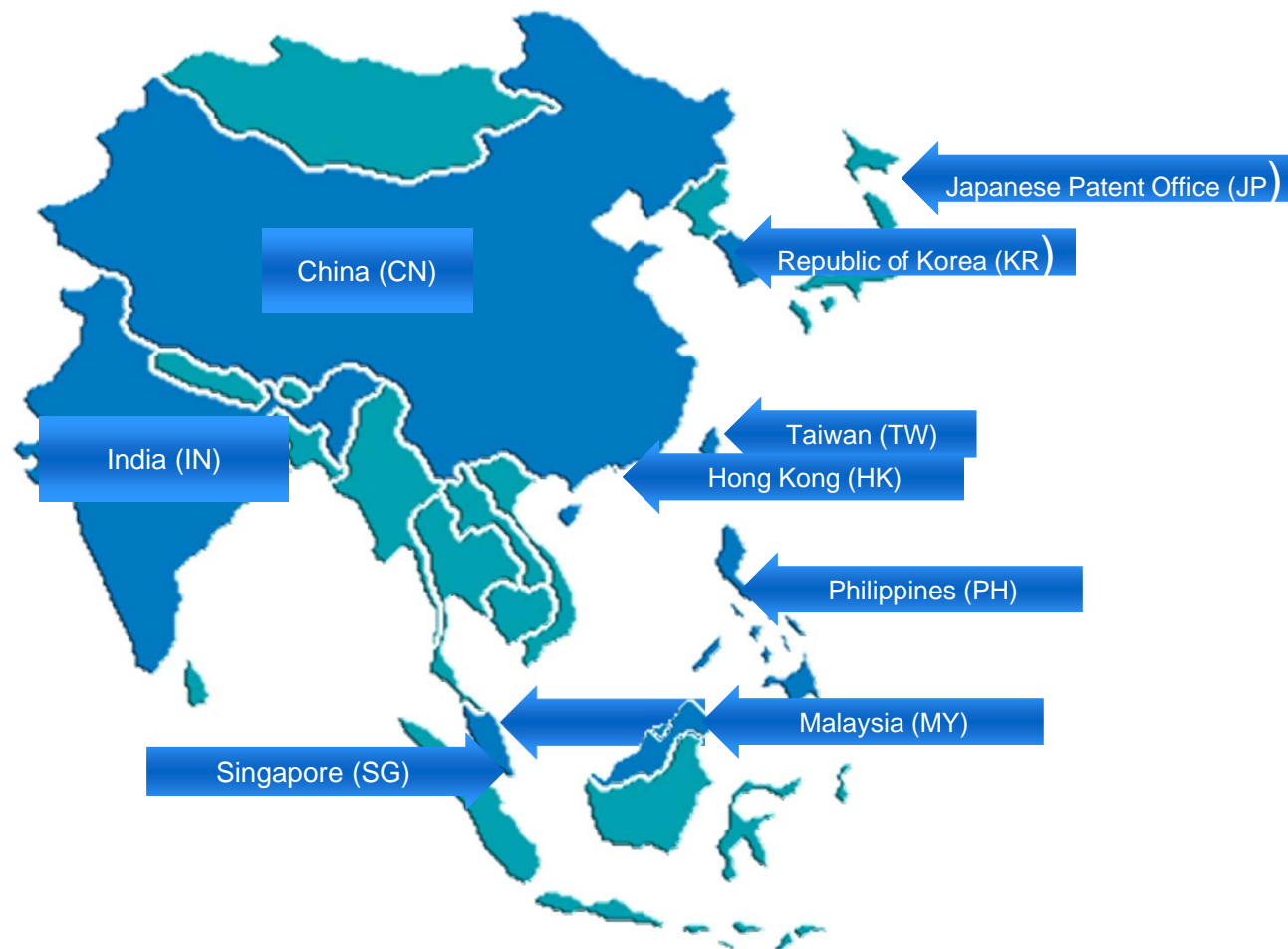
Currently
>10.2
million
worldwide



A division of the American Chemical Society

ACS Proprietary and Confidential

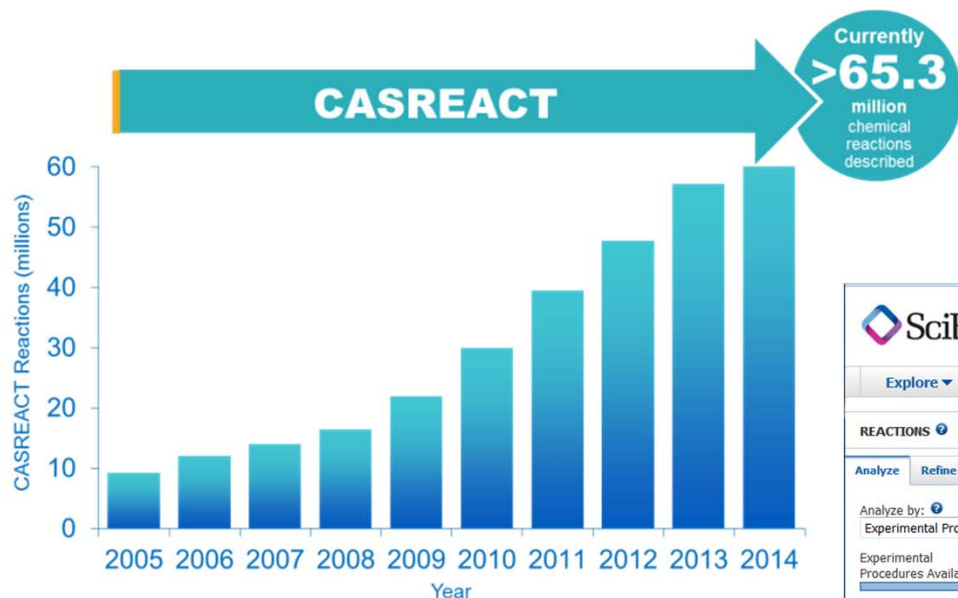
CAplus coverage of patents from Asia is unmatched



A division of the American Chemical Society

ACS Proprietary and Confidential

CASREACT® is the authoritative source for chemical reactions



SciFinder®

Explore | Saved Searches | SciPlanner | Save | Print | Export

REACTIONS | Get References | Tools | Send to SciPlanner

Analyze | Refine | Group by: No Grouping | Sort by: Accession Number | 0 of 58 Reactions Selected | Page: 1 of 4

Analyze by: Experimental Procedure | Experimental Procedures Available: 58 | Show More

1. View Reaction Detail | Link | Similar Reactions

Single Step | Hover over any structure for more options.

OCC(O)CO >> OCCCO

Overview

Steps/Stages

1.1 C:9077-68-3, S:H₂O, 48 h, rt

Notes

regioselective, fermentation, enzymic, biotransformation, whole cells of *Lactobacillus* sp. cultured from thin stillage expressing glycerol dehydratase used, 90% conversion, Reactants: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

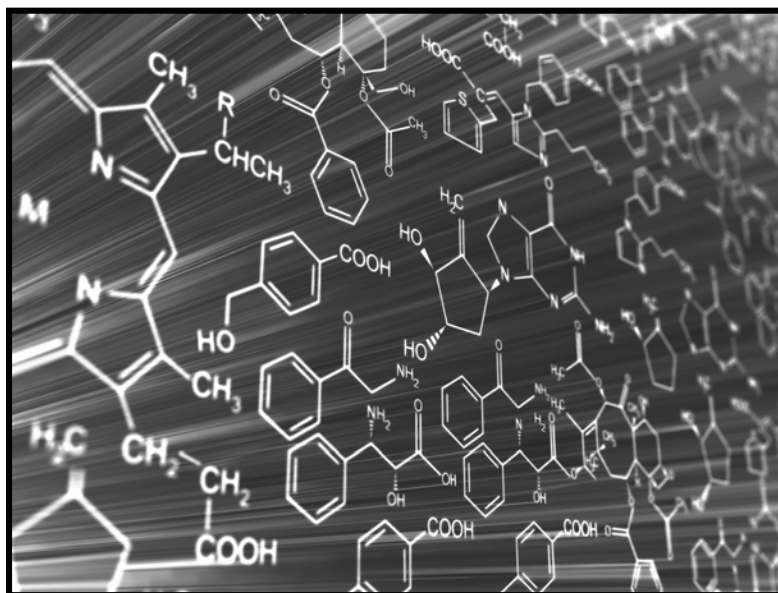
Process for the conversion of glycerol to 1,3-propanediol by novel *Lactobacillus* strains isolated from stillage | Full Text | By Reaney, Martin J. T. et al | From PCT Int. Appl., 2012045179, 12 Apr 2012



A division of the American Chemical Society

ACS Proprietary and Confidential

CASREACT answers your chemical reaction questions quickly, precisely and comprehensively



A division of the American Chemical Society

ACS Proprietary and Confidential

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

SciFinder® Preferences | SciFinder Help | Sign Out

Explore ▾ Saved Searches ▾ SciPlanner Print Export

Substance Identifier "acetone d6" > substances (1) > commercial sources (146)

COMMERCIAL SOURCES ⓘ

Analyze Sort by: Purity ↑ Display Options

0 of 146 Commercial Sources Selected Page: 1 of 8

Commercial Source	Substance	Purity	Quantity	Purchasing Details	Stock Status	Ships Within
1. The Index of Laboratory Chemicals - General Catalog of Kanto Reagents, Chemicals & Biologicals Japan Set Preference	666-52-4 Acetone-d6, 99.9 atom % D	>=99%		50mL, 25000 YEN 10mL, 6000 YEN 0.75mL x 10, 5000 YEN	Maintained in stock	
2. The Index of Laboratory Chemicals - General Catalog of Kanto Reagents, Chemicals & Biologicals Japan Set Preference	666-52-4 Acetone-d6, 99.9 atom % D with 0.03vol% TMS	>=99%		50mL, 25000 YEN 10mL, 7000 YEN	Maintained in stock	
3. Alfa Aesar United States Set Preference	666-52-4 Acetone-d6	>=99%		Order from Source 10g, \$36 5x10g, \$149 Bulk Screening	Typically in stock	1 week

Analyze by: ⓘ
Preferred Sources ▾
ABCR Product List 13
No Preference 133
[Show More](#)



A division of the American Chemical Society

ACS Proprietary and Confidential

CHEMCATS provides fast access to chemical suppliers



A division of the American Chemical Society

ACS Proprietary and Confidential

CHEMLIST® is the comprehensive source for information on regulated chemicals

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner Link Save Print Export

SUBSTANCE DETAIL ⓘ Get References Get Reactions Get Commercial Sources Send to SciPlanner

CAS Registry Number 23726-93-4

~2,688 ~18

C₁₃H₁₈O

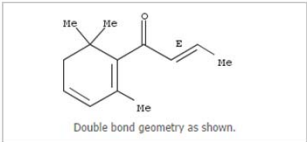
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)-

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)- (BCI)
(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-crotonyl-1,3-cyclohexadiene
[View more...](#)



Double bond geometry as shown.

[Expand All](#) | [Collapse All](#)

- ▶ EXPERIMENTAL PROPERTIES
- ▶ EXPERIMENTAL SPECTRA
- ▶ PREDICTED PROPERTIES
- ▶ PREDICTED SPECTRA
- ▼ REGULATORY INFORMATION
 - ▶ Regulatory Synonyms
 - ▼ Regulatory Overview by Country
 - Confidentiality Status**
Public
 - ▶ Canada
 - ▼ China
 - Inventory Status**
On IECSC Inventory of Existing Chemical Substances in China, 2013
 - ▶ European Union
 - ▶ Japan
 - ▶ Korea
 - ▶ Philippines
 - ▶ United States
 - ▶ File Segment



A division of the American Chemical Society

ACS Proprietary and Confidential

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_{4,7}]
 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

...

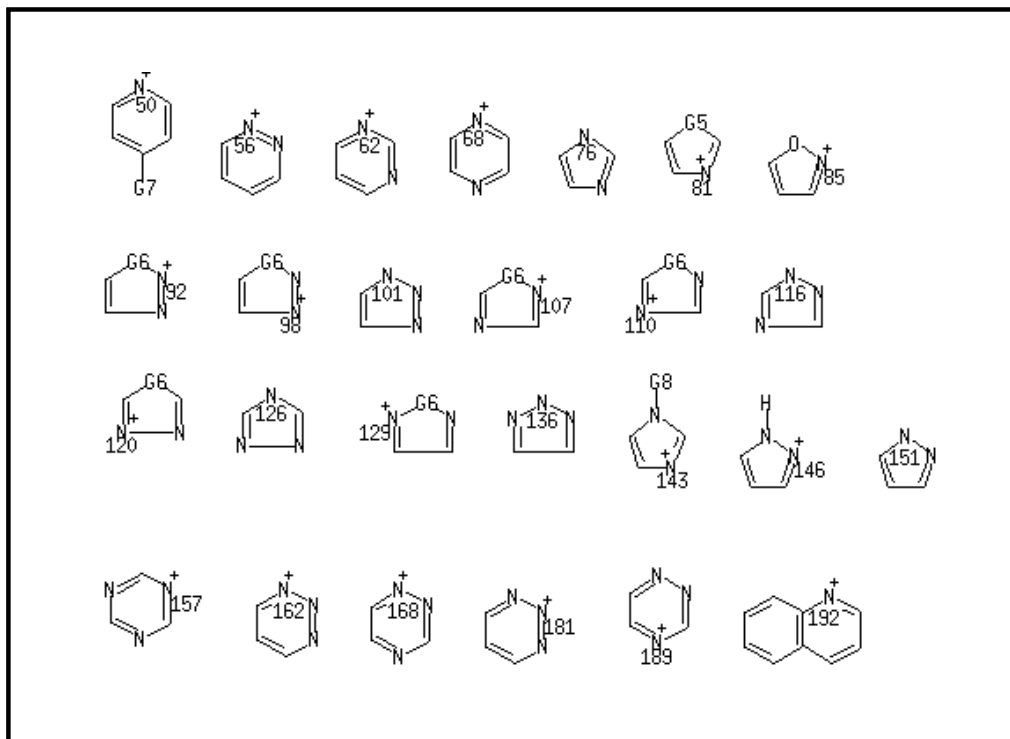
I

II

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



MARPAT supports maximum recall of patented information



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



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

PatentPak™ now available



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



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



Trust NCI Global for the regulatory information you need whether you manufacture, import, export or transport chemicals.



A division of the American Chemical Society

ACS Proprietary and Confidential

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 

C₁₃ H₁₈ O

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

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)

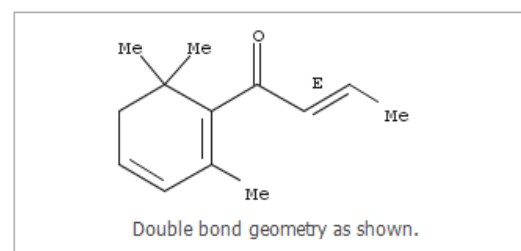
(E)-1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one

(E)-Damascenone

(E)-β-Damascenone

2,6,6-Trimethyl-1-*trans*-crotonoyl-1,3-cyclohexadiene

[View more...](#)



▶ EXPERIMENTAL PROPERTIES

▶ EXPERIMENTAL SPECTRA

▶ PREDICTED PROPERTIES

▶ PREDICTED SPECTRA



A division of the American Chemical Society

ACS Proprietary and Confidential

News in SciFinder

■ New Substance Detail View Improves Readability and User Experience

▼ EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR IR Mass UV and Visible

¹ H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See full text		(4)CAS
Proton NMR Spectrum	See full text		(7)IC
Proton NMR Spectrum	See full text		(8)IC
Proton NMR Spectrum	See full text		(3)CAS

Notes

(3) Campagnole, M.; Synthetic Communications 2007, V37(7), P1077-1090 CAPLUS 🔍

(4) Boulin, Bertrand; Synthetic Communications 2007, V37(15), P2579-2591 CAPLUS 🔍

(7) Snowden, Roger L.; Helvetica Chimica Acta 1987, V70(7), P1858-78 CAPLUS 🔍

(8) Azzari, Elisabetta; Journal of Organic Chemistry 1990, V55(3), P1106-8 CAPLUS 🔍



News in SciFinder

■ New Substance Detail View Improves Readability and User Experience

▼ REGULATORY INFORMATION

▶ Regulatory Synonyms

▼ Regulatory Overview by Country

Confidentiality Status

Public

▶ Canada

▶ China

▼ European Union

Inventory Status

On REACH List of Pre-Registered Substances, March 2009 Registration Date: 31-MAY-2013.

On EINECS Annex to Official Journal of the European Communities, 15 June 1990

Regulatory List Number

EC No.: 245-844-2

EINECS No.: 245-844-2

▶ Japan

▶ Korea

▶ Philippines

▶ United States

▶ File Segment



A division of the American Chemical Society

ACS Proprietary and Confidential

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

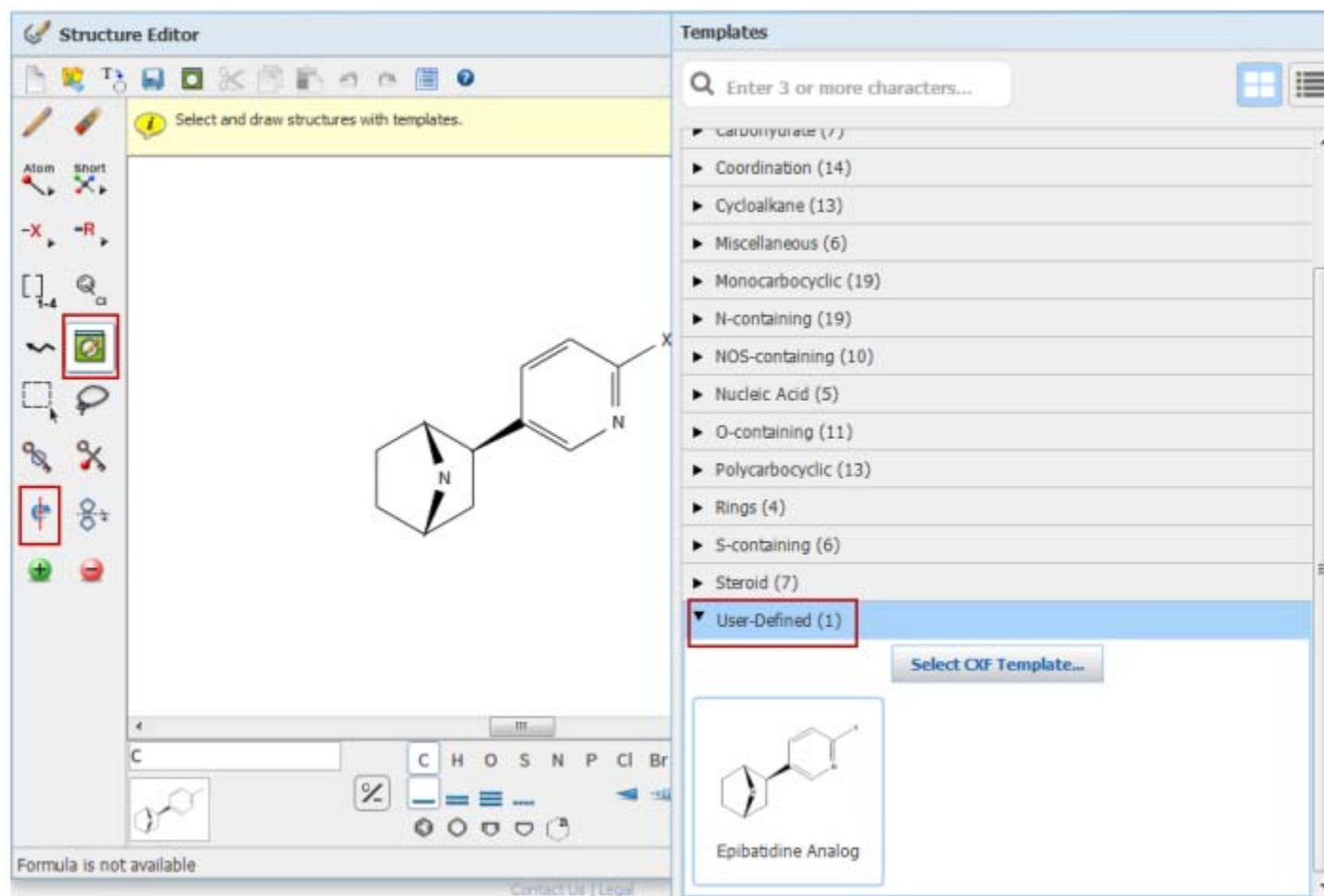


A division of the American Chemical Society

ACS Proprietary and Confidential

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.)



A division of the American Chemical Society

ACS Proprietary and Confidential

News in SciFinder

■ SciFinder/ChemDraw® Collaboration

The screenshot displays the ChemBioDraw Ultra software interface. The main window shows the chemical structure of Canagliflozin (Canagliflozin.cdx). Overlaid on this is the SciFinder search dialog box. The dialog box has two tabs: 'Substance Search' and 'Reaction Search (Substructure)'. The 'Substance Search' tab is active, showing options for 'Substructure' and 'Exact Structure'. The 'Reaction Search (Substructure)' tab is also visible, showing options for 'Selected Structures are Products' and 'Selected Structures are Reactants'. A green arrow points from the 'Exact Structure' option to the SciFinder logo. Another green arrow points from the 'OK' button to the SciFinder search results window. The search results window shows a list of results, with the first result highlighted. The chemical structure of Canagliflozin is shown in the background.

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



A division of the American Chemical Society

ACS Proprietary and Confidential

Example



Sign In

Username

Password

☐ Remember me for two weeks unless I sign out
(Do not use on a shared computer)

[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.](#)



A division of the American Chemical Society

ACS Proprietary and Confidential

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.”

Phone:

1-800-753-4227
(North America)

1-614-447-3700
(outside North America)

Email:

help@cas.org

Web:

www.cas.org



A division of the American Chemical Society

www.cas.org

Thank You!

www.cas.org

