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Miriam Plana (mplana@cas.org)



A division of the American Chemical Society

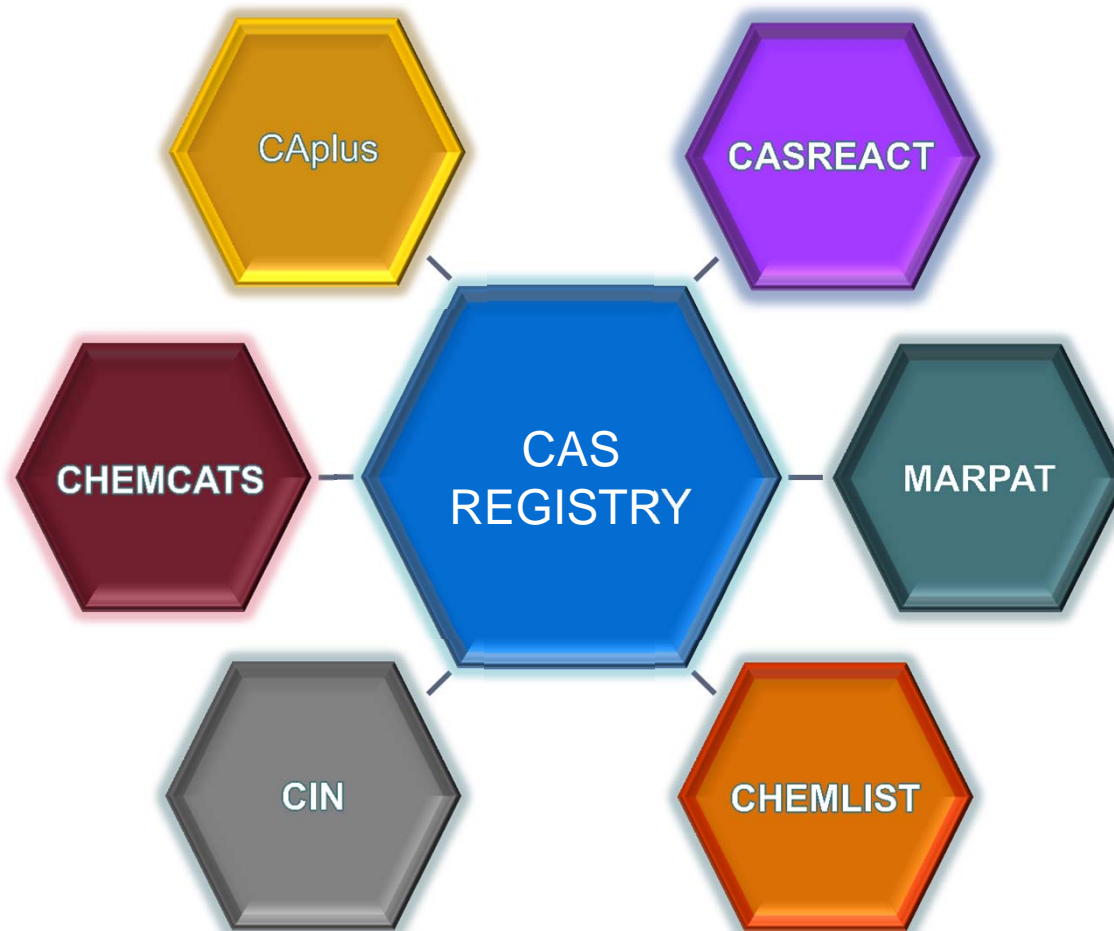
www.cas.org

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.”

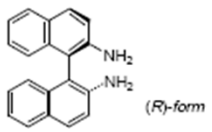
Dr. Robert H. Grubbs
Nobel Laureate
Victor and Elizabeth Atkins Professor of Chemistry
California Institute of Technology

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



CAS REGISTRYSM is the gold standard for chemical substance information

Entry name → **2,2'-Diamino-1,1'-binaphthyl**

Structural formula and stereochemical description →  (R)-form

Alternative names → [1,1'-Binaphthalene]-2,2'-diamine, SCI, 2,2'-Diamino-1,1'-dinaphthyl, 1,1'-Bi[2-naphthylamine]

CAS Registry Number → **FNCT6-Y [4488-22-6]**

Molecular Formula → **C₂₀H₁₆N₂** Molecular weight → **M 284.360** RTECS® Number → **U0300000**

Use → Intermediate for chiral auxiliaries.

Hazard alert symbol and description of hazards → **Exp. mutagen by skin contact. Dec. with emission of toxic fumes. DU3090000**

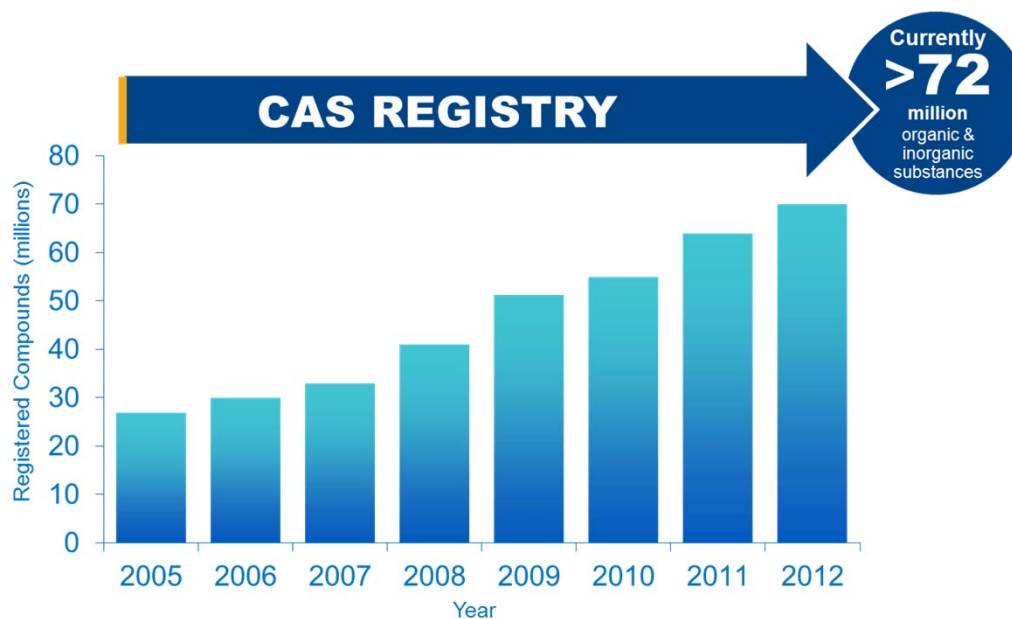
Supplier information → (R)-form: FNCT7-Z [18741-85-0] Mp 242.5-243°, [α]_D²⁵ + 155.5° (c. 1 in Py), [α]_D²⁵ + 46.8° (2M HCl). Supplier: Aldrich 38242-6; Fluka 32787.
N,N'-Di-Me: MNKXZ-E [93713-30-5] Cryst. (EtOH). Mp 143-144° [α]_D²⁵ + 182° (c. 1.09 in C₆H₆).
N,N,N',N'-Tetra-Me: MNKXZ-A [135029-77-5] Cryst. (EtOH/C₆H₆). Mp 216-218°.

Stereoisomer heading → (S)-form: FNCT8-A [18531-95-8] Cryst. Mp 243° (235-239°), [α]_D²⁵ - 149° (Py), [α]_D²⁵ - 46° (2M HCl). Supplier: Aldrich 38243-4; Fluka 32788.

Derivative Subheading → N,N'-Di-Ac: FNCT6-V C₂₂H₂₀N₂O₂ M 368.434. Prisms (C₆H₆). Mp 226-227°. [α]_D²⁵ + 10.8° (c. 1 in THF).
(±)-form: FNCT8-W [79082-81-8] Silvery plates (EtOH), Mp 193.2-194.5° (191°).
Picrate: FNCT8-Z Brownish-yellow plates (C₆H₆). Mp 185° (dec.).
N,N'-Di-Ac: FNCT6-X Cubes (EtOH), Mp 235-236°.
N,N'-Dibenzoyl: FNCT6-Y C₂₄H₁₈N₂O₂ M 492.576. Prisms (PhNO₂). Mp 235°.

Additional CAS Registry Numbers → [93621-61-5] [97644-73-0]

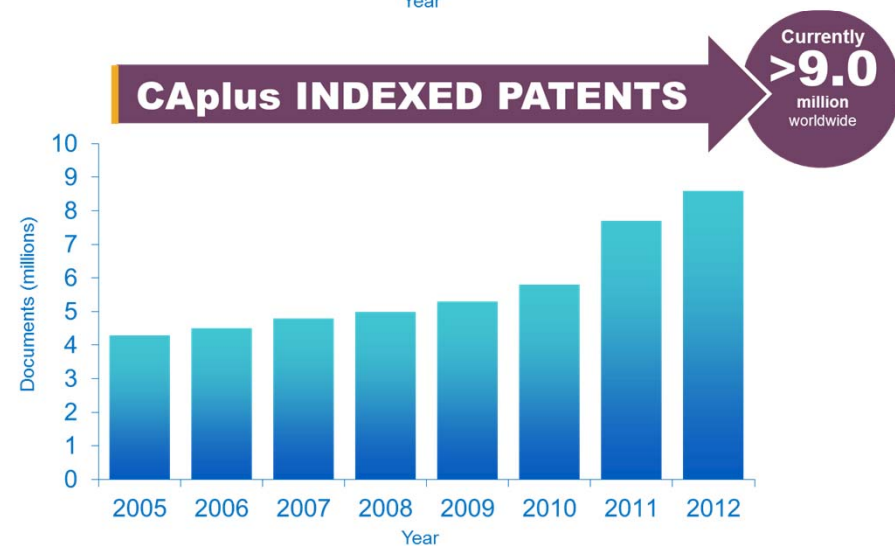
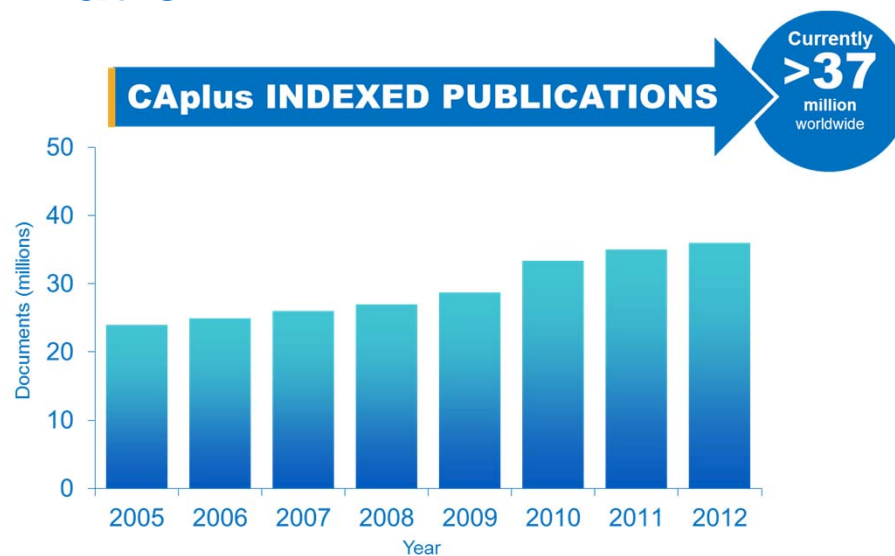
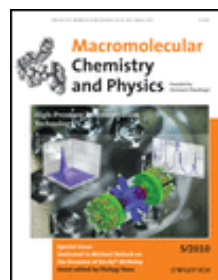
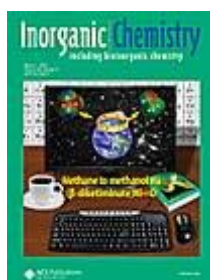
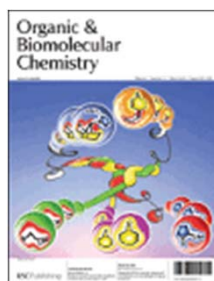
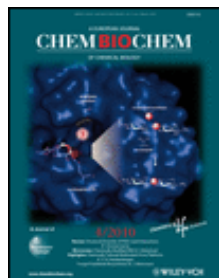
Bibliographic references → Kuhn, R. et al., *Annalen*, 1929, 470, 183 (*synth, resoln*)
Cumming, WM et al., *J.C.S.*, 1932, 528 (*synth*)
Clemo, GR. et al., *J.C.S.*, 1939, 1114 (*synth*)
Mislow, K. et al., *J.A.C.S.*, 1962, 84, 1455 (*rev, ord*)
Akimoto, H. et al., *Tetrahedron*, 1971, 27, 5999 (*resoln, abs config*)
Miyano, S. et al., *Bull. Chem. Soc. Jpn.*, 1984, 57, 2171 (*pmr, ir, deriv*)
Brown, KJ et al., *J.O.C.*, 1985, 50, 4345 (*synth, resoln*)
Benson, SC et al., *J.O.C.*, 1988, 53, 5335 (*synth, N-tetramethyl*)
Fieser and Fieser's *Reagents for Organic Synthesis*, Wiley, 1989, 14, 32 (*use*)
Fransini, L. et al., *Acta Cryst. C*, 1991, 47, 1259 (*cryst struct, N-tetra-Me*)
Suzcins, M. et al., *J.O.C.*, 1992, 57, 1917 (*synth, resoln, hbh*)
Lewis, RJ et al., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BGB750



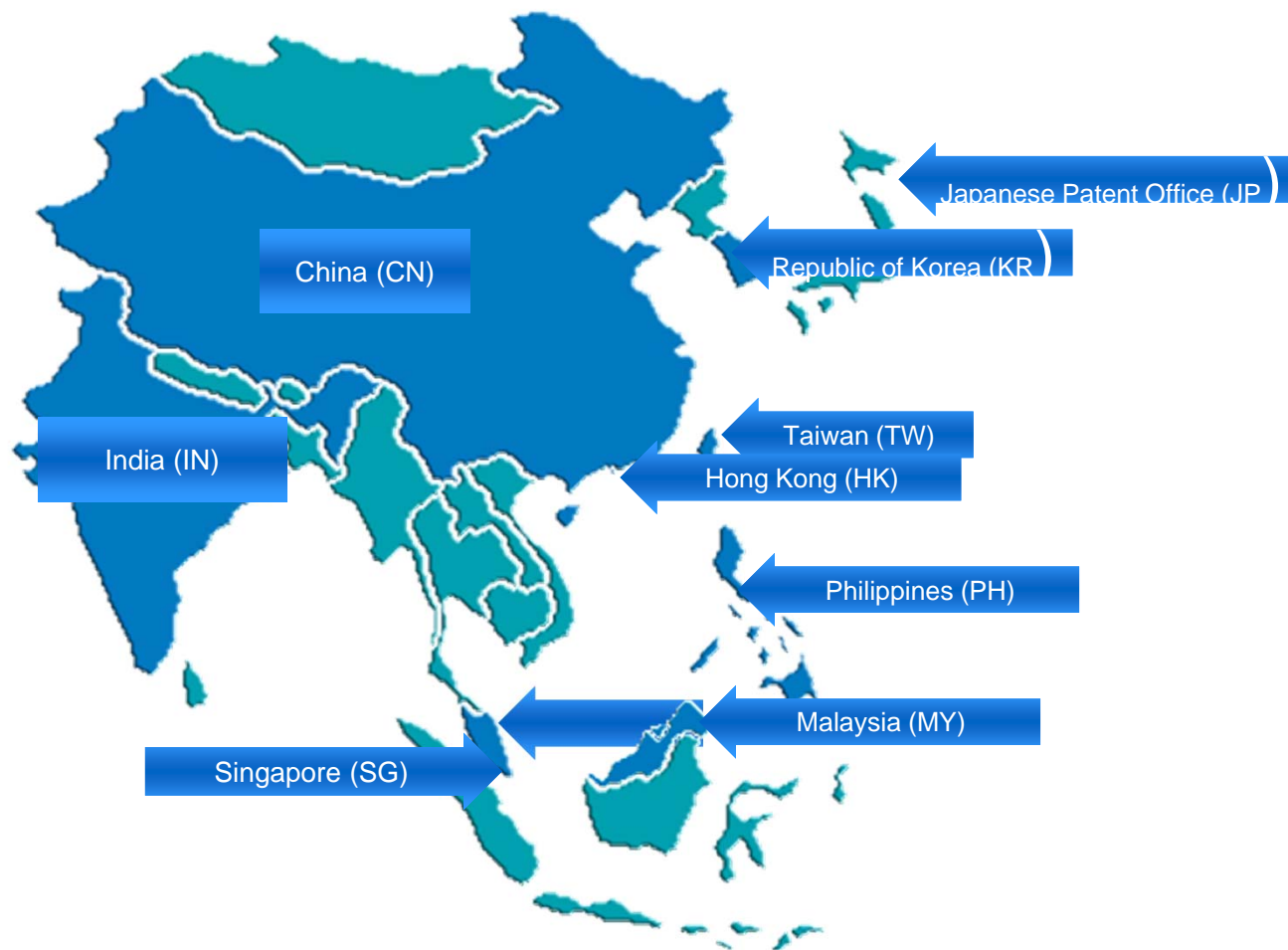
CAS REGISTRY is the only integrated, complete source of chemical information



CPlusSM is your single source for chemistry and related scientific information



CPlus coverage of patents from Asia is unmatched



CASREACT[®] is the authoritative source for chemical reactions

The screenshot displays the CASREACT web interface. At the top, there are navigation options: 'Reactions', 'Get References', 'Tools', and 'Send to SciPlanner'. Below this, a search bar shows '3 Reactions' and '0 Selected'. The main content area features a chemical reaction scheme for a Suzuki coupling. The reactants are a polytriazole chain with a terminal alkyne and a phenylboronic acid derivative. The reaction arrow is labeled '[Step 2.1]'. The product is the coupled polytriazole chain. Below the reaction, there is an 'Overview' section with 'Steps/Stages' and 'References'.

Steps/Stages

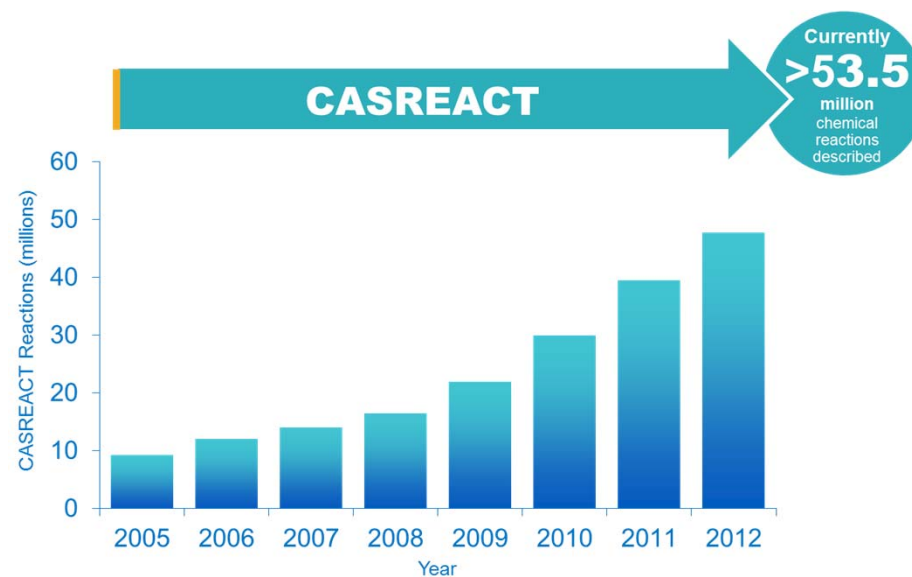
- 1.1 C:862678-56-6, C:CuI, S:CH₂Cl₂, 15 min, rt
- 1.2 S:CH₂Cl₂, 3 h, rt
- 2.1 R:K₂CO₃, C:Pd, C:Pd(OAc)₂, S:DMF, overnight, 80°C

Notes

- 1) in-situ generated catalyst, 2) Suzuki coupling, Reactants: 2, Reagents: 1, Catalysts: 4, Solvents: 2, Steps: 2, Stages: 3, Most stages in any one step: 2

References

Synthesis and Postpolymerization Functionalization of Poly(5-iodo-1,2,3-triazole)s
 By Schwartz, Erik et al
 From Macromolecules (Washington, DC, United States), 44(12), 4735-4741; 2011



CASREACT answers your chemical reaction questions quickly, precisely, comprehensively



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

Commercial Source Detail

Link | Print | Export

[Return](#) ◀ Previous | Next ▶

6. Aaron Chemistry GmbH Product List

Catalog Information

Catalog Publication Date: 6 Jul 2011
Order Number: 90626
Purity: ≥97%
Quantity: 5g, **Price:** 14.98 EUR
Quantity: 10g, **Price:** 24.61 EUR
Quantity: 25g, **Price:** 48.15 EUR

Substance Information

CAS Registry Number: 98-80-6
CAS Index Name: Boronic acid, B-phenyl-
Chemical Name: Phenylboronic acid

$$\begin{array}{c} \text{Ph} \\ | \\ \text{HO} - \text{B} - \text{OH} \end{array}$$

Catalog Suppliers
Below are the contributing supplier(s) to this catalog.

Supplier Name	Address	Contact Information	Status
Aaron Chemistry GmbH	Am Fischweiher 41 - 43 Mittenwald, 82481 Germany	Contact: Dr. Alexander v. Zychlinski Phone: +49(0)8823- 917521 Fax: +49(0)8823-917523 Email: sales@aaron-chemistry.de Web: http://www.aaron-chemistry.de	Unclassified ▼

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CHEMCATS provides fast access to chemical suppliers

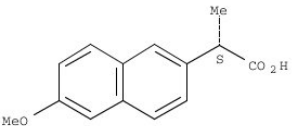


CHEMLIST[®] is the comprehensive source for information on regulated chemicals

Regulatory Information Detail Print Export

CAS Registry Number: 22204-53-1

2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, (aS)- (DSL, ASIA-PAC, NZIoC)
naproxen (English, German) (EINECS)
naproxene (French) (EINECS)
naproxeno (Spanish) (EINECS)
2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, (S)- (AICS)
(S)-6-Methoxy- α -methyl-2-naphthaleneacetic acid (ECL)
(+)-(S)-Naproxen
(+)-2-(6-Methoxy-2-naphthyl)propionic acid
(+)-6-Methoxy- α -methyl-2-naphthaleneacetic acid
(+)-Naproxen
(S)-(+)-2-(6-Methoxy-2-naphthyl)propionic acid
(S)-(+)-Naproxen
(S)-(+)-Naproxene
(S)- α -Methyl-6-methoxynaphthalene-2-acetic acid
(S)-2-(6-Methoxy-2-naphthyl)propanoic acid
(S)-2-(6-Methoxy-2-naphthyl)propionic acid
(S)-2-(6-Methoxynaphthalen-2-yl)propanoic acid
(S)-2-(6-Methoxynaphthalen-2-yl)propionic acid
(S)-Naproxen
2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, (+)-
224: PIN: US20050107325 PAGE: 180 claimed sequence
Apo-Naproxen
Aproxen
Bonyl
CG 3117
d-2-(6-Methoxy-2-naphthyl)propionic acid
d-Naproxen
Diocodal
Dysmenalgit
Equiproxen
Floginax
Laraflex
Laser
MNPA
Naixan
Napren
Naprium
Naprius
Naprosyn
Naprosyne
Napruux
Naxen
Nycopren

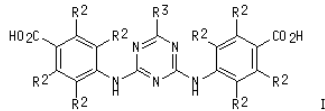
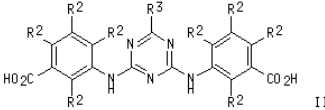


Absolute stereochemistry. Rotation (+).

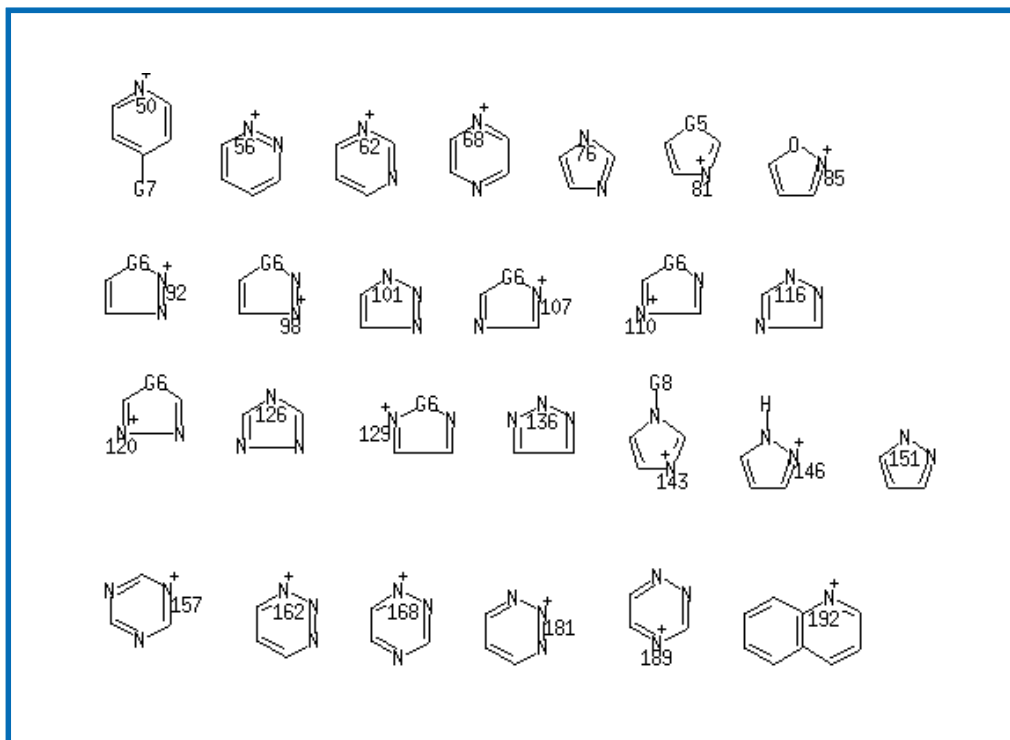
CHEMLIST enables you to discover how and where substances are regulated



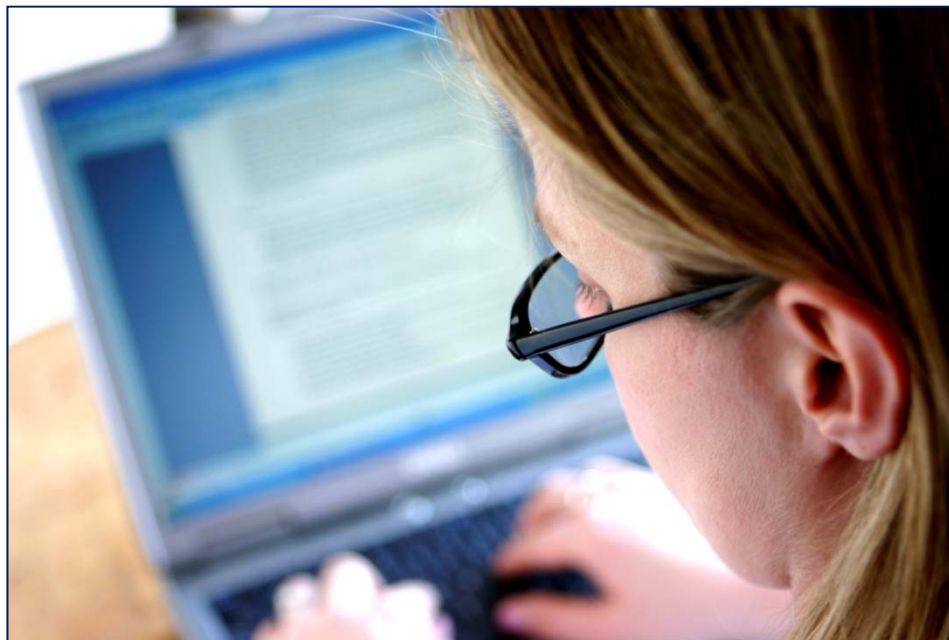
MARPAT[®] is the leading collection of Markush structures from the world's patent literature

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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 Sahuani, Hassan; Scherrer, Robert A.; Jumaas, 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
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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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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

What's new on SciFinder

Sign In

Username

Password

NEW 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.



What's new on SciFinder

1.- New Non-Java CAS Structure Editor

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, there are navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. On the left, a sidebar menu lists various search categories: REFERENCES (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (Reaction Structure). The 'Chemical Structure' option is currently selected. The main area features a 'Structure Editor' section with two tabs: 'Java' and 'Non-Java'. The 'Non-Java' tab is highlighted with a red box and contains a 'Click to Edit' button. To the right of the editor, there are search options: 'Search Type' with radio buttons for 'Exact Structure', 'Substructure' (selected), and 'Similarity', and a checkbox for 'Show precision analysis'. Below the editor, there is an 'Import CXF' link and a blue 'Search' button. At the bottom, there is a link for 'Advanced Search'.

What's new on SciFinder

2.- Analyze by reagents

SciFinder®

Preferences | SciFinder Help | Sign Out

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

Reaction Structure substructure > reactions (3407) > reactions with transformation "Reduction of Nitro Compounds t..." (407)

REACTIONS ⓘ

Analyze | Refine

Analyze by: ⓘ

Reagent (New) ▼

H ₂	123
Fe	57
HCl	56
SnCl ₂	51
NH ₄ Cl	30
AcOH	21
NaHCO ₃	21
Zn	20
NaOH	17
N ₂ H ₄ ·H ₂ O	12

Show More

Get References | Tools ▼

Group by: No Grouping | Sort by: Relevance ▼


Answers per Page [15] Display: []

0 of 407 Reactions Selected

Page: 1 of 28

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 R:H₂, C:Pt, C:Mo, C:Carbon, C:O=Ph₂OH, C:H₂O, S:PhMe, 60°C → 100°C, 5 atm; 38 min, 100°C, 5 atm

Notes

autoclave used, catalyst prepared and used, chemoselective, full conversion, Haber type reduction, alternative reaction condition shown, solid-supported catalyst (activated carbon, Mo promotor), Reactants: 1, Reagents: 1, Catalysts: 5, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Chemoselective hydrogenation of functionalized nitroarenes using supported Mo promoted Pt nanoparticles 🔍 Full Text

What's new on SciFinder

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

SciFinder®

Preferences | SciFinder Help | Sign Out

Explore | Saved Searches | SciPlanner | Print | Export

COMMERCIAL SOURCES

Analyze

Sort by: Supplier Preference | Answers per Page [20]

0 of 111 Commercial Sources Selected | Page: 1 of 6

Analyze by: Preferred Suppliers

- 3B SCIENTIFIC CORPORATION, LIBERTYVILLE, USA 1
- AMERICAN CUSTOM CHEMICALS CORP., SAN DIEGO, USA 1
- SIGMA-ALDRICH, ST. LOUIS, USA 8
- Others 101

Show More

1. **3B Scientific Corporation Product List** ✓ Catalog is associated with a preferred supplier(s)
Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 15 Jul 2013
Order Number: 383-005474
Quantity: 1000g
3658-77-3 4-Hydroxy-2,5-dimethyl-3(2H)-furanone

2. **ACC Corp. Catalog** ✓ Catalog is associated with a preferred supplier(s)
Supplier Name: American Custom Chemicals Corp., Catalog Publication Date: 15 Jul 2013
Order Number: CHM0025781
Quantity: N/A
3658-77-3 4-HYDROXY-2,5-DIMETHYL-3(2H)-FURANONE

3. **ALDRICH** ✓ Catalog is associated with a preferred supplier(s)
Supplier Name: Sigma-Aldrich, Catalog Publication Date: 15 Jul 2013
Order Number: 322482
Quantity: N/A
3658-77-3 4-Hydroxy-2,5-dimethyl-3(2H)-furanone 95%

Quick View

CAS Registry Number: 3658-77-3
Formula: C₈H₁₀O₂
CA Index Name: 3(2H)-Furanone, 4-hydroxy-2,5-dimethyl-

Other Names
2,5-Dimethyl-3-hydroxy-4-oxo-4,5-dihydrofuran; 2,5-Dimethyl-4,5-dihydrofuran-3-ol-4-one; 2,5-Dimethyl-4-hydroxy-2,3-dihydrofuran-3-one; 2,5-Dimethyl-4-hydroxy-3(2H)-furanone; 4-Hydroxy-2,5-Dimethyl-3-oxo-2,3-dihydrofuran; 4-Hydroxy-2,5-Dimethyl-2,3-dihydrofuran-3-one; 4-Hydroxy-2,5-dimethyl-2H-furan-3-one; 4-Hydroxy-2,5-dimethyl-3(2H)-furanone; 4-Hydroxy-2,5-dimethyl-3-furanone; Alletone; Furanol; Pineapple ketone

Number of References
~1,450

Document Types
Conference, Dissertation, Journal, Patent

Properties
Experimental
Spectra
Predicted

Commercial Sources
Available

CC1=C(C)OC(O)C1=O

What's new on SciFinder

4.- Commercial Supplier Email Hyperlinks

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "acetaldehyde" > substances (1) > 75-07-0 > commercial sources (133) > ACC Corp. Catalog

SOURCE DETAIL ⓘ

Return Previous | Next

1. ACC Corp. Catalog

<p>Catalog Information</p> <p>Catalog Publication Date: 19 Dec 2012</p> <p>Order Number: CHM0028256</p> <p>Quantity: N/A, Price: contact supplier</p>	<p>Substance Information</p> <p>CAS Registry Number: 75-07-0 🔍</p> <p>CAS Index Name: Acetaldehyde</p> <p>Chemical Name: ACETALDEHYDE</p>
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CC=O

Catalog Suppliers

Below are the contributing supplier(s) to this catalog.

Supplier Name	Address	Contact Information	Status
American Custom Chemicals Corp.	P O Box 262527 San Diego, CA 92196-2527 USA	Phone: 858-201-6118 Fax: 858-451-8607 Email: sales@accorporation.com Web: http://www.acccorporation.com Other Contact Information: accorporation (Skype)	✔ Preferred ▾

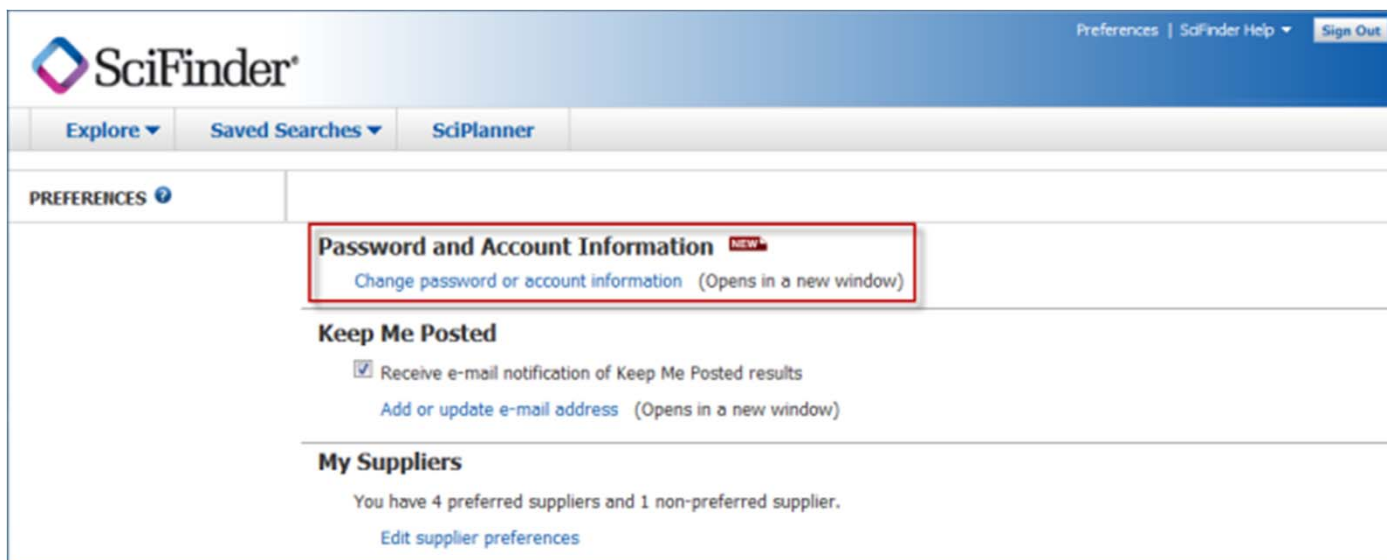
What's new on SciFinder

5.- Increased Availability of SciPlanner Tutorials

The screenshot displays the SciPlanner software interface. The main window is titled "Lisinopril Syntheses" and shows a chemical reaction scheme. A "SciPlanner Introduction" dialog box is overlaid on the workspace, providing information about the software and offering three interactive options: "Send data to SciPlanner (1 min.)", "Manipulate workspace objects (1 min.)", and "Share a project (1 min.)". A checkbox labeled "Do not show this screen when SciPlanner starts." is checked and highlighted with a red rectangle. A "Close" button is located at the bottom of the dialog box. The background workspace shows a chemical reaction scheme for the synthesis of Lisinopril, with various chemical structures and reagents visible.

What's new on SciFinder

6.- Enhanced Account Management



The screenshot displays the SciFinder user interface. At the top, the SciFinder logo is on the left, and navigation links for "Preferences", "SciFinder Help", and "Sign Out" are on the right. Below the logo, there are tabs for "Explore", "Saved Searches", and "SciPlanner". The main content area is titled "PREFERENCES" and contains three sections: "Password and Account Information" (highlighted with a red box and a "NEW" badge), "Keep Me Posted", and "My Suppliers".

SciFinder Preferences | SciFinder Help Sign Out

Explore Saved Searches SciPlanner

PREFERENCES

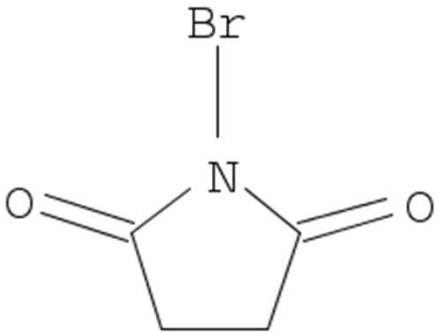
Password and Account Information NEW
[Change password or account information](#) (Opens in a new window)

Keep Me Posted
 Receive e-mail notification of Keep Me Posted results
[Add or update e-mail address](#) (Opens in a new window)

My Suppliers
You have 4 preferred suppliers and 1 non-preferred supplier.
[Edit supplier preferences](#)

What's new on SciFinder

7.- Content Addition

<p>CAS Registry Number:128-08-5</p> <p>2,5-Pyrrolidinedione, 1-bromo- (TSCA, IECSC, DSL, ENCS, AICS, SWISS, PICCS, NZIoC)</p> <p>N-Bromosuccinimide (English, French) (DSL, REACH, EINECS)</p> <p>N-Bromsuccinimid (German) (EINECS, SWISS)</p> <p>N-bromosuccinimida (Spanish) (EINECS)</p> <p>1-Bromo-2,5-pyrrolidinedione (ECL)</p> <p>SUCCINIMIDE, N-BROMO- (PICCS)</p> <p>Bromosuccinimide</p> <p>NBS</p> <p>NSC 16</p>	
<p>Regulatory List Number</p> <p>EC No.: 204-877-2</p> <p>EINECS No.: 204-877-2</p> <p>ENCS No.: 5-121X</p> <p>ECL Serial No.: KE-03714</p> <p>SWISS No.: G-8195</p>	
<p>Harmonized Tariff Code NEW</p> <p>Harmonized Tariff Code: 292519</p> <p>EU Customs Code CN: 29251995</p>	

What's new on SciFinder

8.- New SciFinder Design

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out' are on the right. Below the logo, a navigation bar contains 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field with a 'Search' button and an 'Advanced Search' link. Below the search field, there are examples of search terms: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A play button is centered at the bottom of the main content area. On the left side, there is a sidebar with categories: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). On the right side, there are two panels: 'SAVED ANSWER SETS' with items like 'km_sss', 'Lipitor_frame3_sss_patents', and 'rxn_center_mechanism'; and 'KEEP ME POSTED' with items like 'carbon nanotubes' and dates.



CAS Customer Center

Ask us! We can help.

- Account information
 - How to
 - IT support

“I need to change something on my account.”

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help@cas.org

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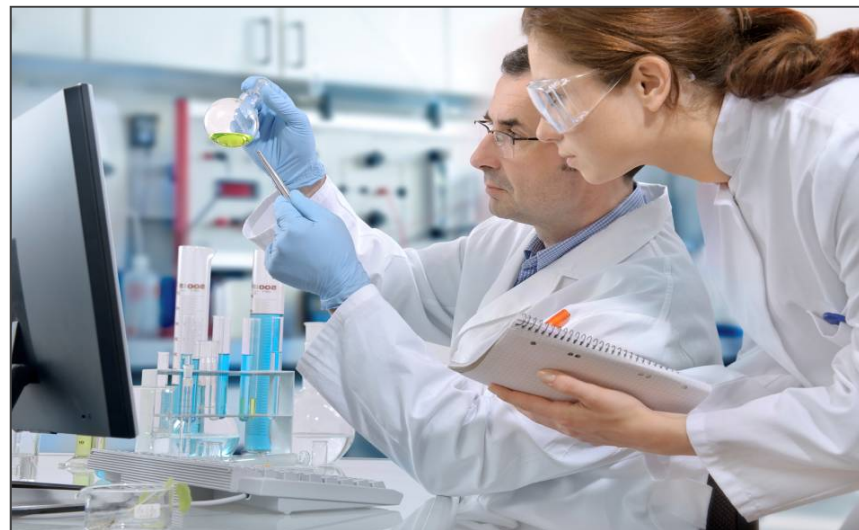
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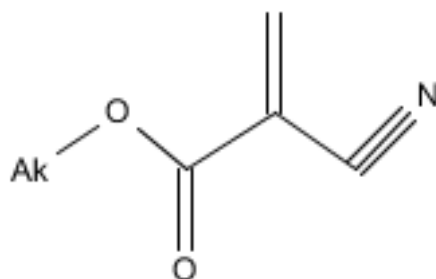
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SciFinder options
Searches: topic, structure, reaction
Analysis tools



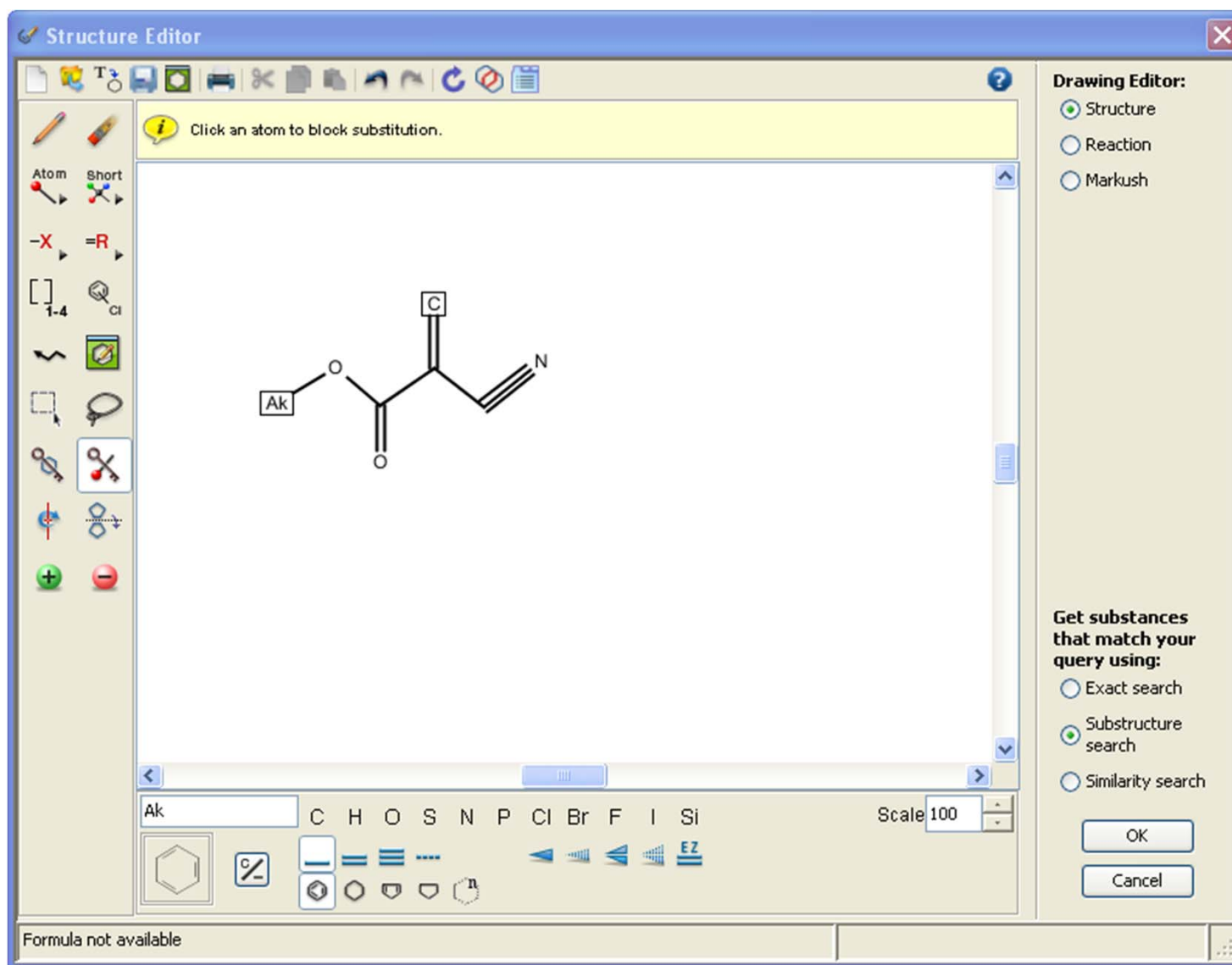
EJERCICIO

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



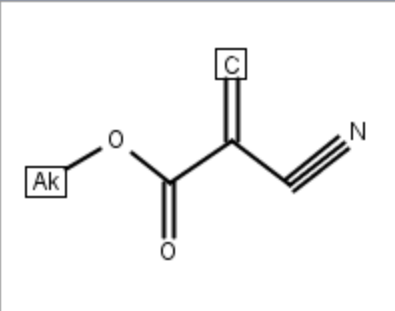
Substructure search limited to polymers only

Explore Substances [?](#)

Chemical Structure [?](#)

Markush
Molecular Formula
Property
Substance Identifier

Search



Click image to change structure or view detail

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

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Substances Get References Get Reactions Tools Send to SciPlanner

Sort by: Number of References ↓

Answers per Page [50] View: [Icons]

0 of 677 Substances Selected Page: 1 of 14

1. Substance Detail
25154-80-7 ~816

6606-65-1
C₈ H₁₁ N O₂

$$n\text{-BuO}-\overset{\text{O}}{\parallel}{\text{C}}-\overset{\text{CH}_2}{\parallel}{\text{C}}-\text{CN}$$

(C₈ H₁₁ N O₂)_n
2-Propenoic acid, 2-cyano-, butyl ester, homopolymer

2. Substance Detail
25067-30-5 ~610

7085-85-0
C₆ H₇ N O₂

$$\text{NC}-\overset{\text{H}_2\text{C}}{\parallel}{\text{C}}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OEt}$$

(C₆ H₇ N O₂)_n
2-Propenoic acid, 2-cyano-, ethyl ester, homopolymer

3. Substance Detail
26809-38-1 ~382

4. Substance Detail
25067-29-2 ~272

Analysis Refine

Analyze by: Substance Role

Click bar to view only those substances within the current answer set

Uses	573
Preparation	322
Properties	236
Biological Study	105
Process	35
Reactant or Reagent	25
Analytical Study	9
Formation, Nonpreparative	8
Miscellaneous	2

Refine 2376 references to Nanotechnology including other nano-synonyms

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References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

Sort by: Accession Number | Save | Print | Export | Answers per Page [50] | Display: [Icons]

0 of 2376 References Selected | Page: 1 of 48

- 1. Stent covering film having hemostatic and antimicrobial functions**

By Han, Zhichao; Xu, Shanshan
From Faming Zhuanli Shenqing (2013), CN 102908673 A 20130206. | Language: Chinese, Database: CAPLUS

The title stent covering film consists of composite fiber material. The composite fiber material is manufd. through prepg. a mixed soln. org. polymers, drug mol., and microspheres contg. antimicrobial agent, and carrying out electrostatic spinning. The stent covering film contg. hemostatic and antimicrobial agent, and has the advantages of high drug embedding amt. and rate, controlled release of hemostatic and antimicrobial agent, simple manuf. process, easy operation, and low cost.
- 2. Method for manufacturing stent covering film having hemostatic and antimicrobial functions**

By Han, Zhichao; Xu, Shanshan
From Faming Zhuanli Shenqing (2013), CN 102908674 A 20130206. | Language: Chinese, Database: CAPLUS

The title method comprises the steps of: dissolving drug mol. in cosolvent to obtain drug soln., ultrasonically treating, stirring, dissolving antimicrobial agent mol. in solvent, adding microspheres, prepg. microspheres contg. antimicrobial agent, dissolving org. polymers in the drug soln. and microsphere soln., injecting the soln. of drug and org. polymer and the soln. of org. polymer and microsphere contg. antimicrobial agent to injectors, carrying out electrostatic spinning to obtain composite fibers, vacuum-drying, and storing at 4°C. The stent covering film contg. hemostatic and antimicrobial agent, and has the advantages of high drug embedding amt. and rate, controlled release of hemostatic and antimicrobial agent, simple manuf. process, easy operation, and low cost.
- 3. Methods for preventing or treating memory impairment using pharmaceutical compositions targeting miRNAs or any precursors thereof**

By Fischer, Andre; Zovoilis, Athanasios; Agbemenyah, Hope
From PCT Int. Appl. (2013), WO 2013017542 A1 20130207. | Language: English, Database: CAPLUS

Analysis | **Refine**

Refine by:

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine 1158 reference to magnetic applications

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References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

Sort by: Accession Number | Save | Print | Export | Answers per Page [50] | Display: [] [] []

0 of 1158 References Selected | Page: 1 of 24

1. **Methods for preventing or treating memory impairment using pharmaceutical compositions targeting miRNAs or any precursors thereof**

By Fischer, Andre; Zovoilis, Athanasios; Agbemeyah, Hope
From PCT Int. Appl. (2013), WO 2013017542 A1 20130207. | Language: English, Database: CAPLUS

In a first aspect, the invention relates to a method for prevention or treating memory impairment and/or a neurodegenerative condition, disorder or disease in a subject in need thereof, comprising administering to the subject a therapeutically effective amt. of a compd. targeting a miRNA or any precursor, or targeting the activity of said miRNA or any precursor thereof. In particular, the invention relates to a method wherein the targeted miRNA is miR-34. Moreover, the invention relates to a method for improving memory functionality in a subject suffering from memory loss, said method comprises the redn. or reducing the level of miR-34 levels or precursor mol. levels in brain tissue of said subject administering to the subject a therapeutically effective amt. of a compd. targeting miR-34 or any precursor thereof. Moreover, the invention relates to a method of inducing memory loss in an individual comprising administering to said individual an effective amt. of one or more compds. having the functionality of miR-34, in particular of miR-34c or any precursor thereof. In addn., a method for diagnosing or predicting memory impairment and/or neurodegenerative condition, disorder or disease is provided. Pharmaceutical compns. comprising miR-34 targeting compds. are selected from oligonucleotides, oligopeptides etc.

2. **Methods for preventing or treating memory impairment using pharmaceutical compositions targeting miRNAs or any precursors thereof**

By Fischer, Andre; Zovoilis, Athanasios; Agbemeyah, Hope
From U.S. Pat. Appl. Publ. (2013), US 20130028956 A1 20130131. | Language: English, Database: CAPLUS

In a first aspect, the invention relates to a method for prevention or treating memory impairment and/or a neurodegenerative condition, disorder or disease in a subject in need thereof, comprising administering to the subject a therapeutically effective amt. of a compd. targeting a miRNA or any precursor, or targeting the activity of said miRNA or any precursor thereof. In particular, the invention relates to a method wherein the targeted miRNA is miR-34. Moreover, the invention relates to a method for improving memory functionality in

Analysis | **Refine**

Refine by: ?

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

magnet

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

54 references with University of Granada at the top

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References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

Sort by: Accession Number | Save | Print | Export | Answers per Page [50] | Display: [List Icon]

0 of 54 References Selected | Page: 1 of 2

- 1. Rendering waterproof and multifunctional fibrous sheets of cellulose: from packaging and anticounterfeit to construction applications**

By Fragouli, Despina; Bayer, Ilker S.; Attanasio, Agnese; Cingolani, Roberto; Athanassiou, Athanassia
From Annual Technical Conference - Society of Plastics Engineers (2012), 70th(Vol 1), 607-612. | Language: English, Database: CAPLUS

The authors present a scalable, inexpensive and green process to render cellulosic sheets waterproof with addnl. functional properties (**magnetic**, photoluminescent, antibacterial, etc.). The fibrous cellulose-based sheets are treated in their final, dry phase, with a huge potential economic impact in the manufg. industry. This method is based on the impregnation of cellulose sheets with acrylate monomers and micro or **nano**-scale functional fillers solns., which polymerize as soon as they come in contact with the fibers. The formed polymeric **nanocomposite** creates a cladding around each individual fiber and not an overall coating onto the cellulose sheets. The treated cellulose fibers can be still recycled due to biodegradability of the used polymer.
- 2. Functionalized magnetic nanoparticles and use in imaging amyloid deposits and neurofibrillary tangles**

By Akhtari, Massoud
From PCT Int. Appl. (2012), WO 2012145169 A2 20121026. | Language: English, Database: CAPLUS

The present disclosure provides functionalized **magnetic nanoparticles** (MNPs) comprising a functional group that binds to β -amyloid deposits and/or neurofibrillary tangles. The present disclosure provides compns. comprising the functionalized MNPs, and methods of using the functionalized MNPs in imaging β -amyloid deposits and neurofibrillary tangles. HODNP (2-(1-{6-[(2-hydroxyethyl)(methyl)amino]-2-naphthyl}ethylidene)malononitrile)-conjugated **magnetic nanoparticles** were used for for imaging imaging of hippocampus, cortex, and midbrain of rats.
- 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. Adolfin

Analysis | **Refine**

Analyze by: Company-Organization

Click bar to view only those references within the current answer set

University of Granada, Spain	6
Wuhan University, Peop Rep China	3
Bioalliance Pharma, Fr	2
Central South University, Peop Rep China	2
Fudan University, Peop Rep China	2
Peop Rep China	2
RWTH Aachen University, Germany	2
Yonsei University, S Korea	2
Bulgarian Academy of	

Pubmed (Medline) has only 5 references out of 54

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0 of 54 References Selected Page: 1 of 2

1. **Rendering waterproof and multifunctional fibrous sheets of cellulose: from packaging and anticounterfeit to construction applications** Full Text
 By Fragouli, Despina; Bayer, Ilker S.; Attanasio, Agnese; Cingolani, Roberto; Athanassiou, Athanassia
 From Annual Technical Conference - Society of Plastics Engineers (2012), 70th(Vol 1), 607-612. | Language: English, Database: CAPLUS

The authors present a scalable, inexpensive and green process to render cellulosic sheets waterproof with addnl. functional properties (**magnetic**, photoluminescent, antibacterial, etc.). The fibrous cellulose-based sheets are treated in their final, dry phase, with a huge potential economic impact in the manufg. industry. This method is based on the impregnation of cellulose sheets with acrylate monomers and micro or **nano**-scale functional fillers solns., which polymerize as soon as they come in contact with the fibers. The formed polymeric **nanocomposite** creates a cladding around each individual fiber and not an overall coating onto the cellulose sheets. The treated cellulose fibers can be still recycled due to biodegradability of the used polymer.

2. **Functionalized magnetic nanoparticles and use in imaging amyloid deposits and neurofibrillary tangles** Full Text
 By Akhtari, Massoud
 From PCT Int. Appl. (2012), WO 2012145169 A2 20121026. | Language: English, Database: CAPLUS

The present disclosure provides functionalized **magnetic nanoparticles** (MNPs) comprising a functional group that binds to β -amyloid deposits and/or neurofibrillary tangles. The present disclosure provides compns. comprising the functionalized MNPs, and methods of using the functionalized MNPs in imaging β -amyloid deposits and neurofibrillary tangles. HODDNP (2-(1-{6-[(2-hydroxyethyl)(methyl)amino]-2-naphthyl}ethylidene)malononitrile)-conjugated **magnetic nanoparticles** were used for for imaging imaging of hippocampus, cortex, and midbrain of rats.

3. **Synthesis of a biodegradable magnetic nanomedicine based on the antitumor molecule tegafur** Full Text
 By Aziz, Jazal; Saad, Esmaeel; Ezz, Leman; Ustun, Merve; Baki, Birol; Ozturk, Dilek; A. D. Ruiz, M. Adelfina

Analysis Refine

Analyze by: Database

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CAPLUS	49
MEDLINE	5

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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. Adolfin

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) nanoplatfoms were synthesized by an emulsion/polymn. procedure. An exhaustive physicochem. characterization (including IR spectrometry, electrophoresis, and thermodyn. 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

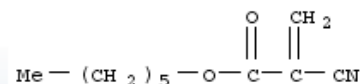
Substances

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

Categorize ?

1. Select a heading and category. 2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in medicine (237)	Select All Deselect All	
Biotechnology	Medicine (41)	<input type="checkbox"/> Drug delivery systems 24	
General chemistry		<input type="checkbox"/> Drug delivery systems, nanoparticles 14	
Polymer chemistry	Substances in adverse effects (13)	<input type="checkbox"/> Antitumor agents 13	
Technology	Agriculture (7)	<input type="checkbox"/> Drug delivery systems, carriers 7	
Physical chemistry	Food (6)	<input type="checkbox"/> Drug delivery systems, controlled-release 6	
Biology	Toxicology & forensics (5)	<input type="checkbox"/> Imaging agents 6	
Genetics & protein chemistry	Substances in biological uses (2)	<input type="checkbox"/> Antibiotics 3	
Synthetic chemistry		<input type="checkbox"/> Diagnosis, agents 3	
Analytical chemistry		<input type="checkbox"/> Drug delivery systems, nanocapsules 3	
Environmental chemistry		<input type="checkbox"/> Medical goods 3	
		<input type="checkbox"/> Pharmacokinetics 3	
		<input type="checkbox"/> Cephalosporin 2	

Biotechnology > Medicine

OK Cancel

..or by type of polymers indexed

Categorize ?

1. Select a heading and category. 2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Polymers (72)	Select All Deselect All	
Biotechnology	Modifiers & additives (20)	<input type="checkbox"/> Polybutylcyanoacrylate 30	
General chemistry	Applications & phenomena (7)	<input type="checkbox"/> Poly(ethyl-2-cyanoacrylate) 12	
Polymer chemistry	Processes & apparatus (6)	<input type="checkbox"/> Dextran 9	
Technology	Miscellaneous substances (2)	<input type="checkbox"/> Poly(isobutyl cyanoacrylate) 9	
Physical chemistry		<input type="checkbox"/> Polymers 8	
Biology		<input type="checkbox"/> Polyoxyethylene sorbitan monooleate 8	
Genetics & protein chemistry		<input type="checkbox"/> Chitosan 6	
Synthetic chemistry		<input type="checkbox"/> Polyoxyalkylenes 6	
Analytical chemistry		<input checked="" type="checkbox"/> Cyanoacrylates 5	
Environmental chemistry		<input type="checkbox"/> Poloxamer 188 5	
		<input type="checkbox"/> Poly(ethylene glycol) 5	
		<input type="checkbox"/> Poly(hexylcyanoacrylate) 5	
		<input type="checkbox"/> Polyhexadecylcyanoac 4	

Polymer chemistry > Polymers

OK **Cancel**

Míriam Plana

CAS Regional Marketing Manager, Spain & Portugal

mplana@cas.org

Example 2: Check novelty and design your synthesis



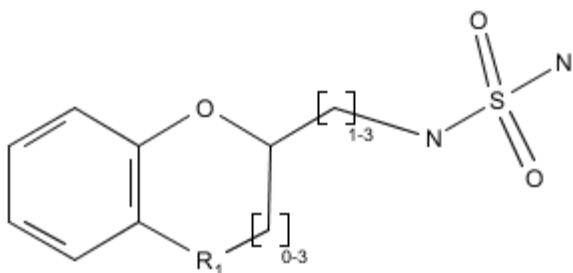
Explore
References

Explore
Substances

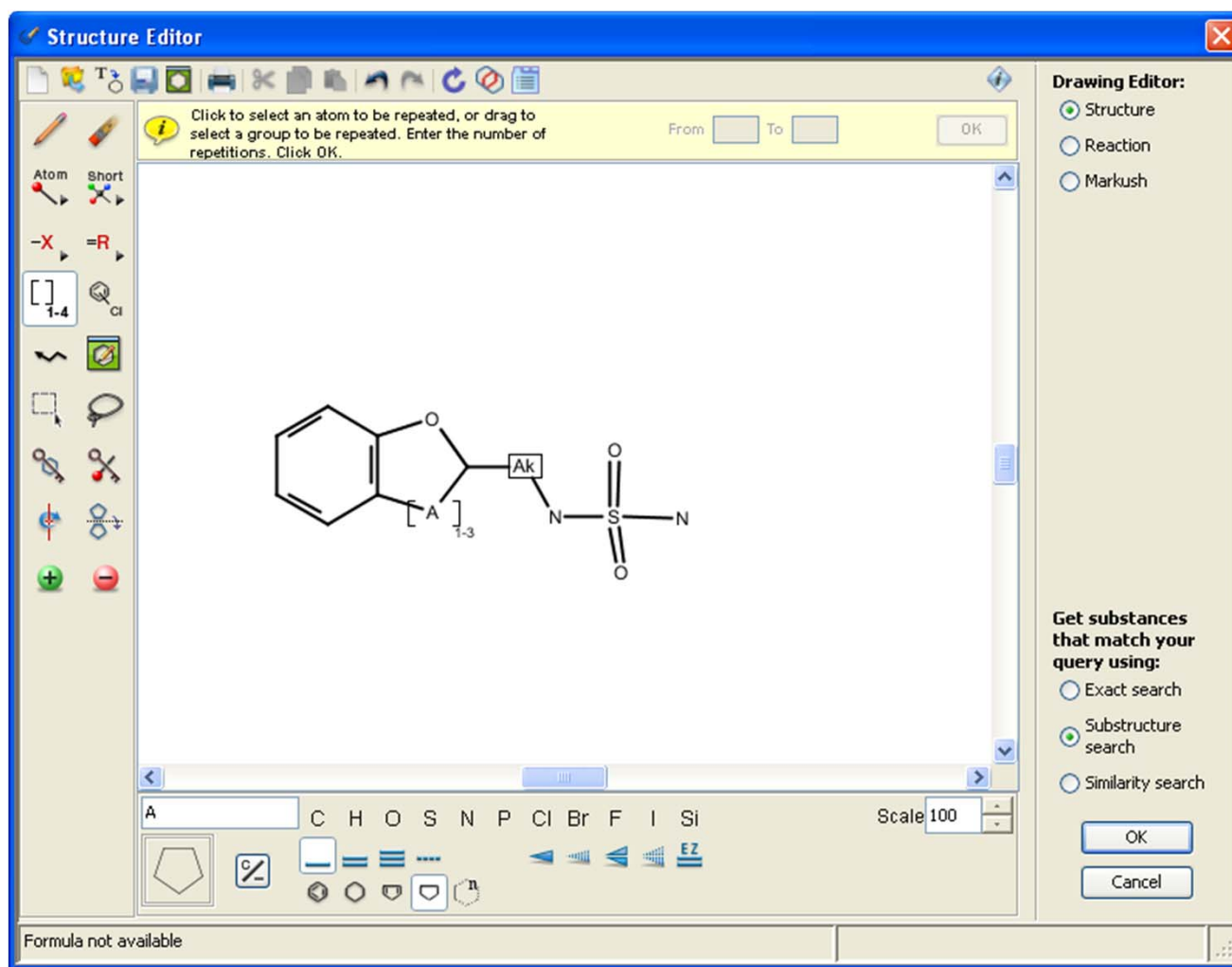
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Reactions

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

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99 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Number of References Answers per Page [15] 1 2 3 4 5 6 7 View: [Icons]

<input type="checkbox"/> 1. Substance Detail 871824-55-4 ~22 Absolute stereochemistry., Rotation (-). C ₉ H ₁₁ Cl N ₂ O ₄ S	<input type="checkbox"/> 2. Substance Detail 835894-65-0 ~17 C ₁₀ H ₁₄ N ₂ O ₃ S Experimental Properties	<input type="checkbox"/> 3. Substance Detail 871824-60-1 ~16 Absolute stereochemistry., Rotation (-). C ₉ H ₁₁ Cl N ₂ O ₄ S
<input type="checkbox"/> 4. Substance Detail 835894-69-4 ~15 C ₈ H ₁₀ N ₂ O ₄ S	<input type="checkbox"/> 5. Substance Detail 871824-49-6 ~14 C ₉ H ₁₂ N ₂ O ₄ S	<input type="checkbox"/> 6. Substance Detail 871824-50-9 ~14 Absolute stereochemistry., Rotation (-). C ₉ H ₁₂ N ₂ O ₄ S

Analysis | Refine

Analyze by: Commercial Availability

Click bar to view only those substances within the current answer set

Not Commercially Available 51

Commercially Available 48

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

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References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

31 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2

Display: [icon]

1. **Preparation of an acetylated sulfamide derivative** [Full Text]
 By McComsey, David F.; Parker, Michael H.
 From PCT Int. Appl. (2010), WO 2010011548 A1 20100128. | Language: English, Database: CAPLUS
 The present invention is directed to novel substituted sulfamide derivs., pharmaceutical compns. contg. said derivs. and the use of said derivs. form in the treatment of anxiety and related disorders; bipolar depression and mania; depression; epilepsy and related disorders; epileptogenesis; glucose related disorders; lipid related disorders; migraine; obesity; pain; substance abuse and as neuroprotective agents. I is prepd. by acetylation and formulated in capsules. The anticonvulsant activity of I is also detd. in the maximal electroshock test in mice.

2. **Crystalline form of (2S)-(-)-N-(6-chloro-2,3-dihydro-benzo[1,4]dioxin-2-ylmethyl)-sulfamide** [Full Text]
 By Mehrman, Steven J.; Wu, Wenju
 From U.S. Pat. Appl. Publ. (2009), US 20090318544 A1 20091224. | Language: English, Database: CAPLUS
 The present invention is directed to a novel cryst. form of (2S)-(-)-N-(6-chloro-2,3-dihydro-benzo[1,4]dioxin-2-ylmethyl)-sulfamide (I), pharmaceutical compns. contg. said cryst. form and the use of said cryst. form in the treatment of anxiety and related disorders; bipolar depression and mania; depression; epilepsy and related disorders; epileptogenesis; glucose related disorders; lipid related disorders; migraine; obesity; pain; substance abuse; or for neuroprotection. The present invention is further directed to a process for the prepn. of the novel cryst. form. Thus, as a specific embodi...

Analysis | Refine

Analyze by: Company-Organization

Click bar to view only those references within the current answer set

Janssen Pharmaceutica N V, Belg	14
Janssen Pharmaceutica NV, Belg	5
Chugai Pharmaceutical Co Ltd, Japan	2
USA	2
C and C Research Laboratories, S Korea	1
Haneishi Tsuyoshi	1

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

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.


Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in medicine (1279)	Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Medicine (32)	<input checked="" type="checkbox"/> Anticonvulsants 11	<input checked="" type="checkbox"/> Biotechnology > Medicine (5 Terms)
Synthetic chemistry	Toxicology & forensics (5)	<input type="checkbox"/> Chemotherapy 6	
Biotechnology	Substances in adverse effects (4)	<input type="checkbox"/> Drug delivery systems 4	
Biology		<input type="checkbox"/> Drugs 3	
Physical chemistry		<input type="checkbox"/> Therapy 3	
Genetics & protein chemistry		<input type="checkbox"/> Adrenoceptor antagonists, α 2- 2	
Technology		<input type="checkbox"/> Anticoagulants 2	
Analytical chemistry		<input checked="" type="checkbox"/> Antidepressants 2	
Polymer chemistry		<input type="checkbox"/> Antiobesity agents 2	
		<input checked="" type="checkbox"/> Anxiolytics 2	
		<input type="checkbox"/> Cytoprotective agents, neuroprotectants 2	
		<input type="checkbox"/> Dopamine antagonists 2	
		<input type="checkbox"/> Drug delivery systems, capsules 2	
		<input type="checkbox"/> Drug delivery systems, oral 2	

Biotechnology > Medicine > 5 Index Term(s) Selected

OK **Cancel**

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

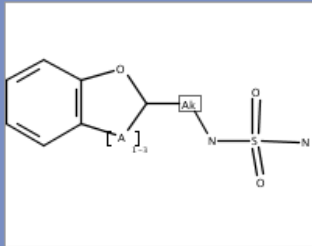
Explore Substances

Chemical Structure **Markush** 

Markush

Molecular Formula

Substance Identifier



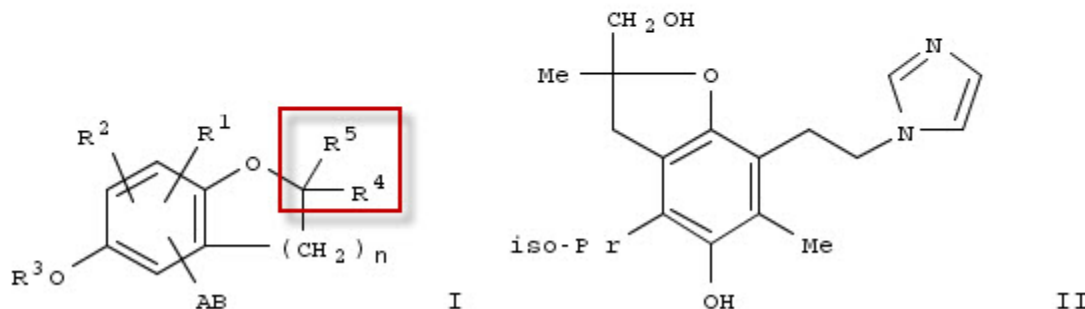
Click image to change structure or view detail

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.



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

The screenshot displays the SciFinder interface with the following elements:

- Navigation:** Explore References, Explore Substances, Explore Reactions.
- User Area:** Welcome | Sign Out, Add KMP Alert, Chemical Structure substructure > substances (99).
- Substances List:** 99 Substances, 0 Selected. Sort by: Number of References. Answers per Page [15].
- Substance 1 (CAS 871824-55-4):**
 - Chemical structure: Clc1ccc2c(c1)OC(C2)COP(=O)(O)O
 - Properties: Absolute stereochemistry, Rotation (-).
 - Formula: C₉ H₁₁ Cl N₂ O₄ S
 - References: ~22
- Substance 3 (CAS 871824-60-1):**
 - Chemical structure: Clc1ccc2c(c1)OC(C2)COP(=O)(O)O
 - Properties: Absolute stereochemistry, Rotation (-).
 - Formula: C₉ H₁₁ Cl N₂ O₄ S
 - References: ~16
- Substance 4 (CAS 835894-69-4):**
 - Chemical structure: c1ccc2c(c1)OC(C2)COP(=O)(O)O
 - Properties: Absolute stereochemistry, Rotation (-).
 - Formula: C₉ H₁₀ N₂ O₄ S
 - References: ~15
- Substance 6 (CAS 871824-50-9):**
 - Chemical structure: c1ccc2c(c1)OC(C2)COP(=O)(O)O
 - Properties: Absolute stereochemistry, Rotation (-).
 - Formula: C₉ H₁₀ N₂ O₄ S
 - References: ~14
- Context Menu (over Substance 1):**
 - View Substance Detail
 - Explore by Structure
 - Synthesize this...
 - Get Reactions where Substance is a
 - Get Commercial Sources
 - Get Regulatory Information
 - Get References
 - Export as Image
 - Export as molfile
 - Send to SciPlanner
- Bioactivity Analysis Sidebar:**
 - Analyze by: Bioactivity Indicators (New)
 - Nervous system agents (all): 12
 - Antitumor agents (all): 6
 - Hematologic agents: 4
 - Cardiovascular agents (all): 2
 - Show More

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

Reactions Get References Tools Send to SciPlanner
Save Print Export

56 Reactions 0 Selected
Answers per Page [15] 1 2 3 4

Select All Deselect All
Sort by: Number of Steps
Display:

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

► Overview

▼ Experimental Procedure

(S)-N-(6-Chloro-2,3-dihydro-benzo[1,4]dioxin-2-ylmethyl)-sulfamide A 12-L four necked flask (equipped with mechanical stirrer, water condenser topped with a nitrogen inlet, and two stoppers) was charged with (S)-(6-chloro-2,3-dihydro-benzo[1,4]dioxin-2-yl)-methylamine (5, 214 g, 1.07 mol), sulfamide (412 g, 4.29 mol), and *iso*-propyl acetate (4 L). The reaction mixture was then heated to reflux for a total of 15 h over 3 days and then cooled to room temperature. The reaction mixture was chilled in an ice-bath and the residues were collected by filtration and washed with *iso*-propyl acetate. The filtrate was washed with 1 M hydrochloric acid (3 L), dried (MgSO₄), and concentrated to yield crude product. The entire portion of crude product was dissolved in ethyl acetate and absorbed onto silica gel (600 g) and loaded into a Biotage sample induction module, then eluted onto a Biotage 150M (2.5 g silica gel) using heptane (2 L), 1:9 ethyl acetate-heptane (4 L), 3:7 ethyl acetate-heptane (12 L), and 1:1 ethyl acetate-heptane (16 L) to yield the product along with mixed fractions. The mixed fractions were rechromatographed on a Biotage 75L (800 g silica) using heptane (1 L), 1:9 ethyl acetate-heptane (2 L), 3:7 ethyl acetate-heptane (6 L), and 1:1 ethyl acetate-heptane (8 L) to yield additional product. The two lots of product were combined to yield the title compound as an off-white solid. The title compound prepared according to the procedure as described in this Example yielded form (I-SA). **(S)-N-(6-Chloro-2,3-dihydro-benzo[1,4]dioxin-2-ylmethyl)-sulfamide** ¹H NMR (DMSO-*d*₆) δ ppm: 6.98 (d, J= 1.9 Hz, 1H), 6.89 (m, 3H), 6.67 (bs, 2H), 4.36 (dd, J= 11.7, 1.6, 1H), 4.28 (m, 1H), 4.00 (dd, J= 11.5, 6.8 Hz, 1H), 3.19 (m, 1H), 3.11 (m, 1H). Melting Point: 99-100°C. Optical rotation: [α]_D²⁰ = -57.6° (c 2.14, MeOH, 23°C). Chiral HPLC: Chiralpak AD-H, Hex(0.1 % TEA)/IPA (80:20), R_t = 11.407 min, >99% ee. Elemental Analysis for C₁₁H₁₁ClN₂O₄S: Calculated: %C 38.78, %H 3.98, %Cl 12.72, %N 10.05, %S 11.51. Measured: %C 38.81, %H 3.74, %Cl 12.83, %N 9.93, %S 11.53.

Analysis Refine

Analyze by: Experimental Procedure

Click bar to view only those reactions within the current answer set

Experimental Procedures Available	53
Experimental Procedures Not Available	3

[Show More](#)

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

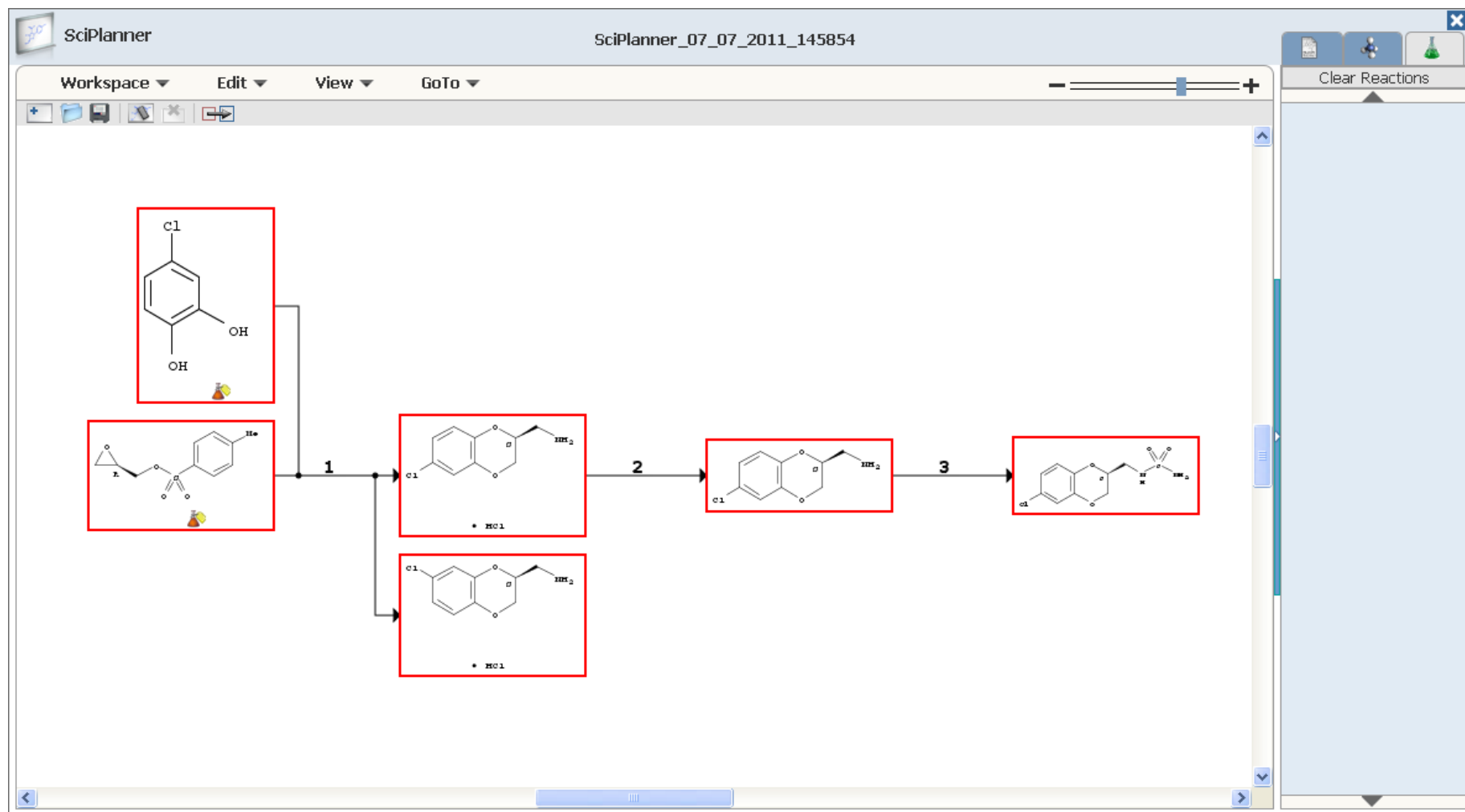
The screenshot displays the SciFinder interface for a search of reactions. The top navigation bar includes 'Explore References', 'Explore Substances', and 'Explore Reactions'. The search results show 56 reactions, with 0 selected. The 'Sort by' dropdown is set to 'Number of Steps'. The 'Display' dropdown shows '(13 Reactions)'. The 'Send to SciPlanner' button is highlighted with a red box. The 'Analysis' sidebar is open, showing 'Analyze by: Catalyst' and a table of catalysts.

Catalyst	Count
4-DMAP	10
Pd	5

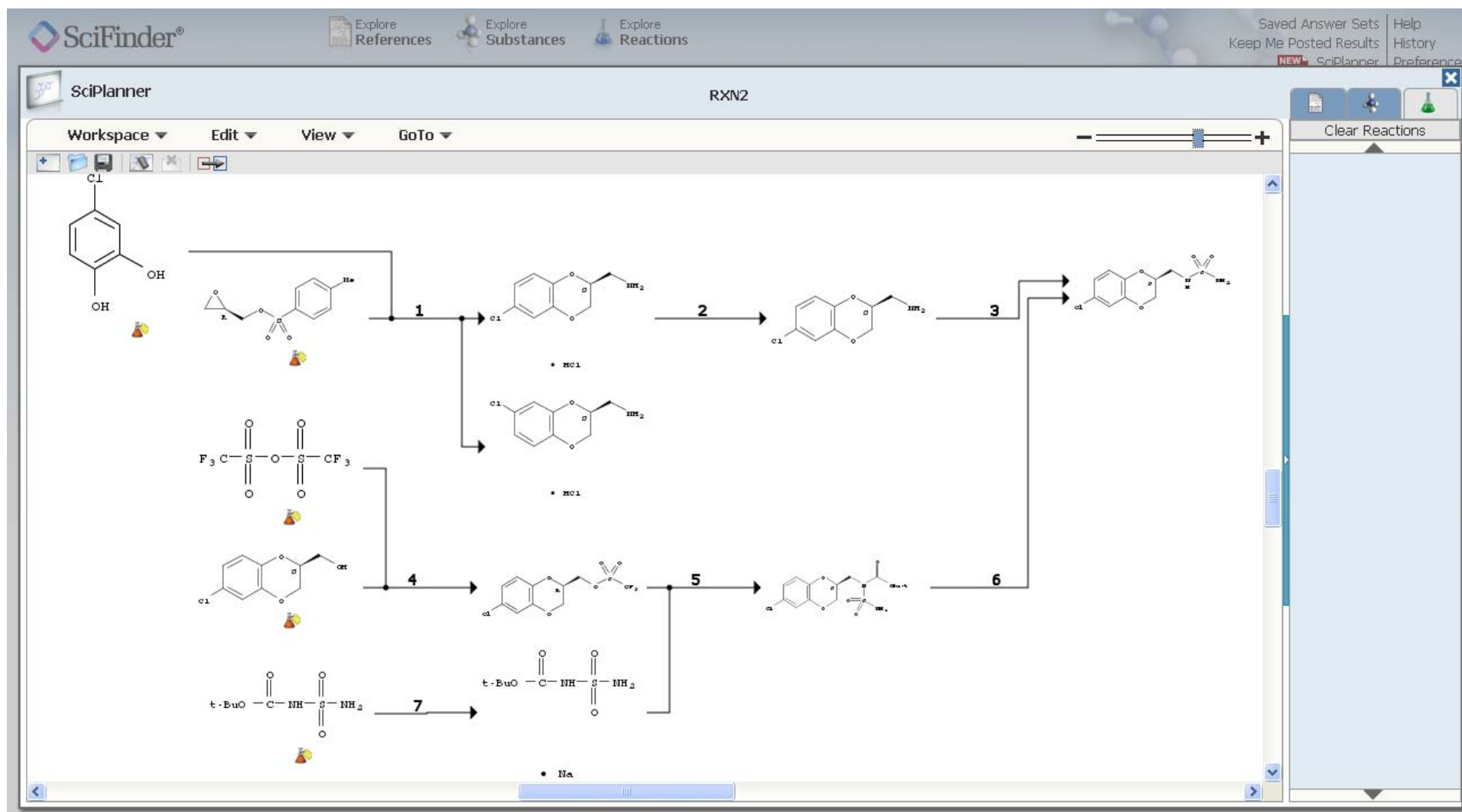
Chemical reaction 19: CC1=CC=C(C=C1)COP(=O)(O)O + ClC1=CC=C(O)C=C1 >> CC1=CC=C(C=C1)COP(=O)(O)O.C1=CC=C(O)C=C1

Chemical reaction 23: CC1=CC=C(C=C1)COP(=O)(O)O + ClC1=CC=C(O)C=C1 >> CC1=CC=C(C=C1)COP(=O)(O)O.C1=CC=C(O)C=C1

Relevant reactions can be moved to SciPlanner



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

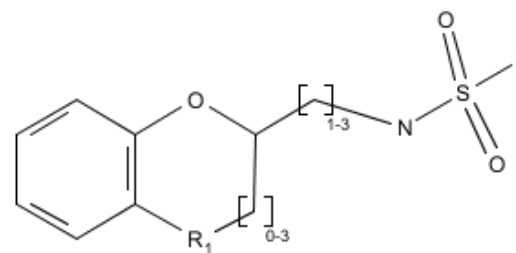


Example: Check novelty and design your synthesis



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
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¿Dudas?

¿Ideas?

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¡Muchísimas gracias por vuestra atención!



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