

PIOTR GOŁKIEWICZ
SOLUTION SALES MANAGER
LIFE SCIENCES
CENTRAL-EASTERN EUROPE
AND RUSSIA



focused

**INTRODUCING
REAXYS**

SERVING THE LIFE SCIENCES SPACE

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN

Characterize targets & analyze disease pathways

 **PATHWAY STUDIO™**

Characterize & discover molecules
Identify & confirm lead compounds

 **REAXYS®**
Medicinal Chemistry

 **REAXYS®**

Translate preclinical data in humans (Translational)

 **PHARMAPENDIUM®**

Monitor drug adverse events & real-world evidence data in literature

 **EMBASE™**

 **QUOSA**

Drug Candidate Selection

Go-No Go Decision

Preclinical Data Validation

Managing risk

Discovery

Pre-clinical

Clinical

Post-launch

Broader full-text indexing of biomedical content

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ScienceDirect

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 **REAXYS®**
HOW YOU THINK HOW YOU WORK

Chemistry as the organizing principle



REAXYS IS BUILT

With experimental data from journal articles and patents

Diaryl-2-pyrrolidines: new insight into the effect of structural modification on the enantioselective epoxidation of α,β -unsaturated ketones

Physical Data

Spectra

Bioactivity Data

Natural Product

Abstract—Catalytic enantioselective epoxidation of α,β -unsaturated ketones with TBHP is described. Stereoelectronics of the substituents on the catalyst, significantly reduced load © 2006 Elsevier Ltd. All rights reserved.

1. Introduction

Enantioselectively enriched α,β -epoxy ketones are versatile intermediates in organic synthesis and important synthetic pharmaceuticals.¹ Efficient asymmetric epoxidation reactions of α,β -unsaturated ketones, mainly dialcones, have been reported using chiral metal-allyl hydroperoxide systems.² Moreover, polyammoniacs³ and cinchona alkaloids⁴ have been used in the presence of hydrogen peroxide as an oxygen source under basic conditions. The development of simple, catalytic and environmentally benign methodologies to access optically pure compounds is a fundamental goal of current organic synthesis. Asymmetric organocatalysis⁵ satisfies most of these requirements, low cost and easily accessible chiral organic molecules are able to catalyze an ever-increasing number of reactions under operational simplicity and mild conditions. In order to achieve good yields of products and satisfactory level of enantioselectivity, in most of the reactions, e.g., those promoted by proline-based compounds, 20–30 mol % of catalyst loading is generally employed. Thus, one of the most challenging goals in organocatalysis is to reduce catalyst loading to the level used in metal-catalyzed asymmetric synthesis (<10 mol %).

Chiral diaryl-2-pyrrolidines⁶ have been successfully employed as organocatalysts in different transformations such as C–C bond forming reactions,⁶ functionalizations of carbonyl compounds⁷ and epoxidation of α,β -unsaturated aldehydes.⁸ On the other hand, the

Scheme 1.

In epoxidation activity, less phenyl moieties and more loading action efficiency, pyrrolidines loading, and/or (up)tion using (ent degree) suggesting catalyst in

Keywords: Epoxidation; α,β -Unsaturated; Asymmetric organocatalysis; Pyrrolidines.

* Corresponding author. Tel.: +39 089 969563; e-mail: lantini@unisa.it

0950-4230/\$ - see front matter © 2006 Elsevier Ltd. All rights reserved. doi:10.1016/j.tet.2006.10.085

United States Moriarty et al.

US 6,900,191 B1

May 31, 2005

(12) Unit Moriarty et al.

(54) Title AND U

(75) Inventor

(73) Assignor

(*) Notice:

(21) Appl. No. 09/900,307

(22) Filed: Jan. 20, 1998

Related U.S. Application Data

(60) Provisional application No. 60/039,106, filed on Feb. 25, 1997.

(51) Int. Cl. A61K 31/59; C07C 401/00

(52) U.S. Cl. 514/167; 552/653; 552/653; 514/167

Physical Data

Spectra

Bioactivity Data

Natural Product

Abstract

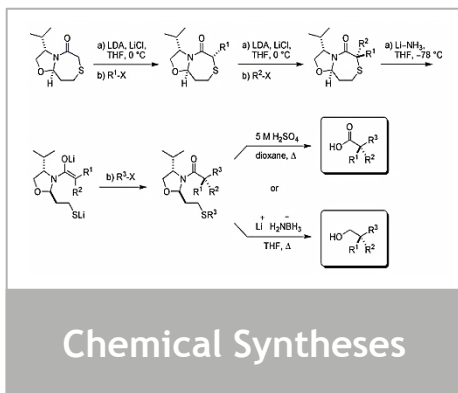
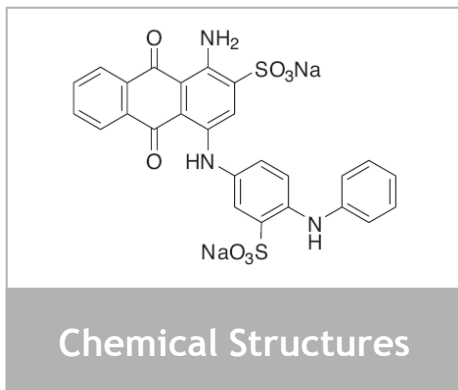
Chemical Structure:

wherein R1 is hydrogen, R2 is —CH₃, R3 is —CH₃, and R4 is hydrogen, useful in cancer prevention and therapy.

1 Claim, 4 Drawing Sheets



CHEMISTRY AS THE ORGANIZING PRINCIPLE



3784 *J. Med. Chem.* 2009, 52, 3784-3793

High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet P2Y₁₂ Receptors

Younis Baqi,¹ Kerstin Atzler,¹ Merjem Köse,¹ Markus Glünzel,^{1,4} and Christa E. Müller^{1,4}

PharmaCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn, An der Innenburg 4, D-53121 Bonn, Germany, Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg, Albertstraße 25, D-79104 Freiburg, Germany

Received March 16, 2009

Anthraquinone derivatives related to the moderately potent, nonselective P2Y₁₂ receptor antagonist reactive blue 2 (6) have been synthesized and optimized with respect to P2Y₁₂ receptor affinity. A radioligand binding assay utilizing human blood platelet membranes and the P2Y₁₂ receptor-selective antagonist radioligand [³H]-propylthioadenosine-5'-adenylic acid (1-[1-dichloro-1-phosphonomethyl-1-phosphonyl] anhydride ([³H]PSB-0413)) was applied for compound testing. 1-Amino-2-sulfonanthraquinone derivatives bearing a *p*-phenylamino/anilino substitution in the 4-position and an additional acidic function in the *meta*-position of the aniline ring showed high P2Y₁₂ receptor affinity. These new anthraquinone derivatives became accessible by a recently developed copper(0)-catalyzed Ullmann coupling reaction of 1-amino-4-bromanthraquinone derivatives with anilines in absolute buffer under microwave irradiation. The most potent compounds

**Reaxys excerpts
all relevant data
even from
footnotes and text**

antagonize the platelet P2Y₁₂ receptor and mediate a progressive and sustained aggregation not preceded by shape changes. The latter receptor also plays an important role in the potentiation of platelet secretion induced by several agonists, and its congenital deficiency has been shown to result in a lifelong bleeding disorder.⁵ Modulation of P2 receptors in platelets appears to be of paramount importance in regulating platelet function and, as a consequence, in controlling thrombotic diseases, which are the most common cause of morbidity and mortality.

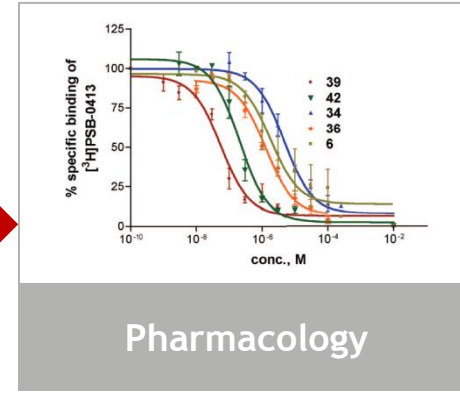
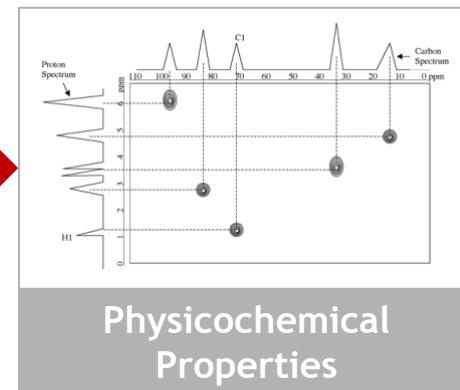
* To whom correspondence should be addressed. Phone: +49-228-73-2301. Fax: +49-228-73-2567. E-mail: christa.mueller@uni-bonn.de

¹ PharmaCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn.

² Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg.

³ Present address: Elsevier Pharma Biotech Group, Elsevier Information Systems, GmBH, Theodor-Heuss-Allee 108, D-60486 Frankfurt (Main), Germany.

10.1021/jm9003297 CCC: \$40.75 © 2009 American Chemical Society
Published on Web 05/22/2009

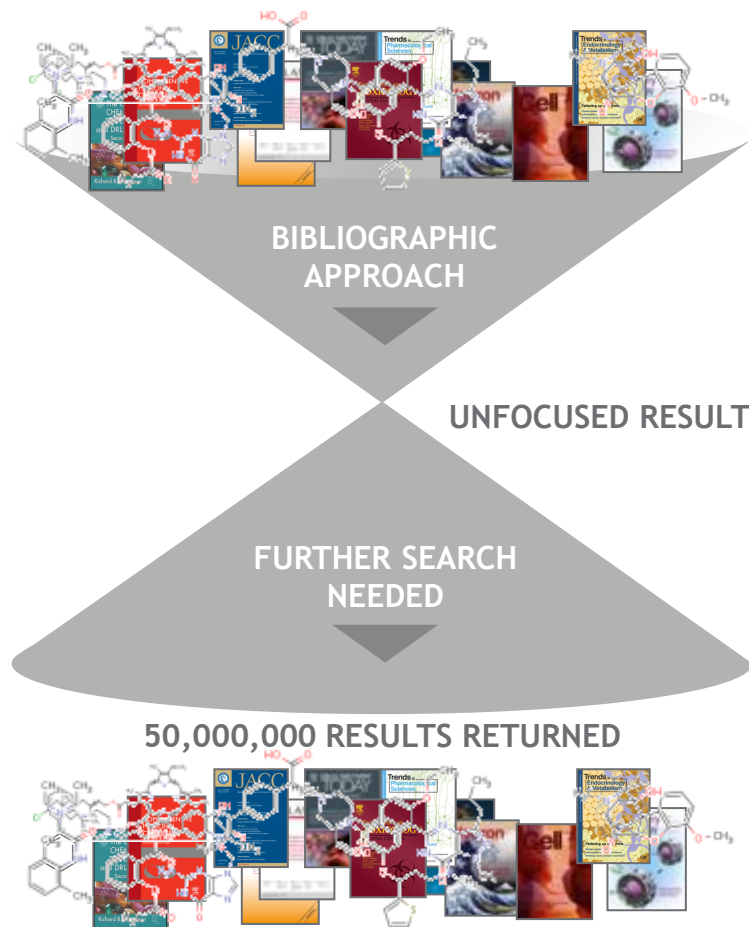


STRUCTURED TO HELP YOU SEARCH

OTHER DATABASES

REAXYS

CATALOGUED AND TAXONMISED BY CHEMISTS FOR CHEMISTS



REAXYS INCLUDES

Patent Content: English language only patents from the major chemistry patent classes of the US, European, and World Patent Offices

REAXYS INCLUDES

Over 500 million facts

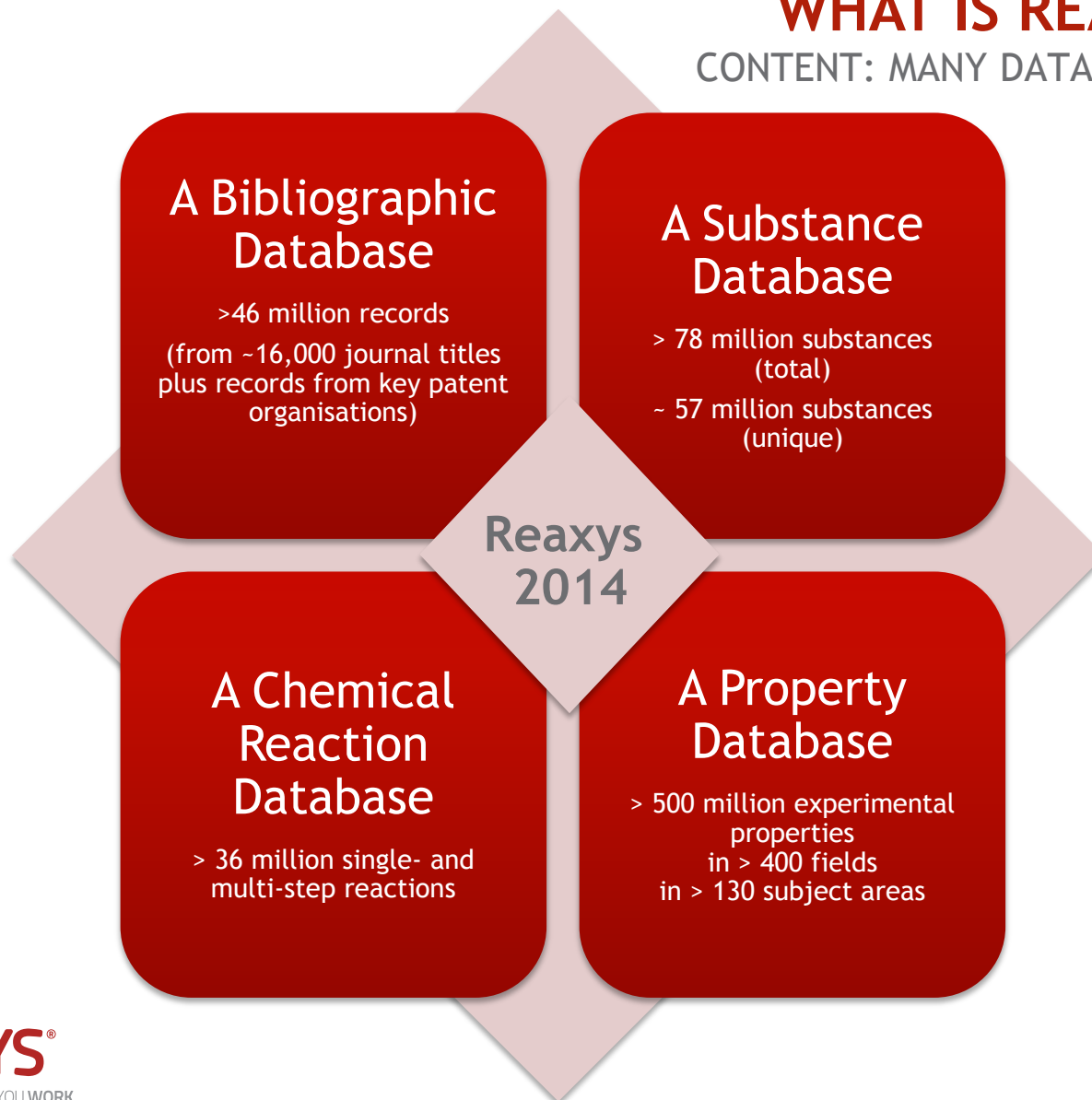
Over 400+ searchable data fields

HIGH QUALITY experimental results



WHAT IS REAXYS 2014?

CONTENT: MANY DATABASES ALL IN ONE



SEARCH

- What are the search options?
- Substances
- Reactions
- Literature
- Properties
- Is there “search intelligence”?
- Truncation
- Proximity
- Algorithmic interpretation of natural language query

SEARCH

REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION

The screenshot shows the REAXYS search interface. At the top, there is a navigation bar with links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. A search bar is prominently displayed with the text "Ask Reaxys" and "Enter a keyword, concept or author". Below the search bar, there are five main search categories: Reactions (with a flask icon), Substances, Names, Formulas (with a molecular model icon), Medicinal Chemistry (with a target icon), Literature (with a book icon), and ReaxysTree (with a tree icon). Below these categories, there are search options for "You can also search directly by these common property groups:" including Physical, Spectra, Natural Products, and Advanced. Callout boxes provide detailed explanations for each of these search paths.

Ask Reaxys, a quick, easy topic 'concept search'

Perform a literature search

Open Reaction search form

Browse database via taxonomies rather than search database

Data search form by "property"

Open a structure search form

Search using chemical identifiers

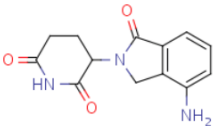
Access detailed Biodata, and MedChem specific features

SEARCH SUBSTANCES

SEARCH STRUCTURE, NAME, OR FORMULA - IN FULL, OR IN PART

STRUCTURE

Structure



As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

By name translation EDIT CLEAR

Create Structure Template from Name

- Include tautomers
 - Ignore stereo
 - No salts
 - No mixtures
 - No isotopes
 - No charges
 - No radicals
 - No ring closures
 - Align results with query
- More options
- Include related Markush
 - Keep fragments
 - separate
 - together
- (type values in fields e.g. 3-5)
- # of Atoms
 - # of Fragments
 - # of Ring Closures

As Drawn ✓

Substructure ✓

Similarity ✓

CHEMICAL NAME

Chemical Name Lookup ✕

Chemical Name Segment Lookup ✕

Reaxys PubChem eMolecules

Search for: TAXOL

- taxol (1203)
- taxol174 (1)
- taxoleic (2)
- taxolformate (1)
- taxoprexin (1)
- taxoquinon (1)
- taxotere (94)
- taxoterereg (1)
- taxpropellane (1)
- taxtgcacatgc (2)
- taxuchin (2)
- taxucustin (1)
- taxumaiglucoside (3)
- taxumain (2)
- taxumairin (1)
- taxumairol (31)
- taxumairone (1)
- taxus (56)
- taxusabietane (3)
- taxusecone (1)

Transfer
Reset
Cancel

Chemical Name ✓

Part of Chemical Name ✓

Reaxys helps on the way ✓✓

FORMULA

Molecular Formula Lookup ✕

Search MF Range Lookup ✕

Element Counts Lookup ✕

Element Symbols Lookup ✕

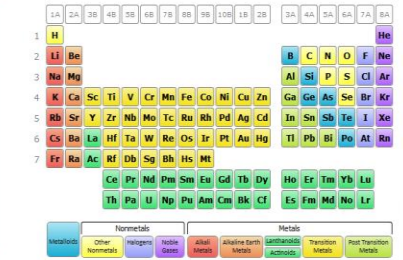
Number of Atoms Lookup ✕

Number of Elements Lookup ✕

Formula Builder: easy way to find substances right across the Periodic Table

Formula Builder

Click any element, group, or series to start building your query:



More elements (1) with arbitrary count
 Any more elements with any counts

Special groups: Me Et Ph

Note: It is also possible to enter ranges or enumerations defined via variables, e.g. Fe₀₋₂, n=2-4
* Acyclic terms, e.g. C₂₋₃, n=3,5

Formula ✓

Part of Formula ✓

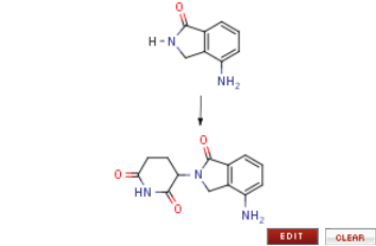
Reaxys helps on the way ✓✓

SEARCH REACTIONS

SEARCH BY STRUCTURE, DATA, OR TYPE

STRUCTURE

Structure



As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

Create Structure Template from Name

Please select role Product Starting material Reagent / Catalyst Any role

Atom mapping
Bond forming/breaking

Search reactions by structure



DATA

Reaction Data

Yield (numerical)	=	<input type="text"/>	Lookup X
Solvent	is	<input type="text"/>	Lookup X
Reagent/Catalyst	is	<input type="text"/>	Lookup X
Time (h)	=	<input type="text"/>	Lookup X
Temperature (°C)	=	<input type="text"/>	Lookup X
Pressure (Torr)	=	<input type="text"/>	Lookup X
Reaction Type	is	<input type="text"/>	Lookup X
Reaction Basic Index	is	<input type="text"/>	Lookup X

Search reactions by reaction conditions



TYPE

Reaction Data

Reaction Type is starts with ends with contains contains SONOGASHIRA Lookup X

Reaxys

Search for: SONOGASHIRA

- sonogashira (13)
- sonogashira coupling (1)
- sonogashira cross-coupling reaction (5)
- sonogashira reaction (1)
- sonogashira -hagihara coupling (5)
- sonogashira alkylation (1)
- sonogashira alkylation (49)
- sonogashira and castro reaction (1)
- sonogashira carbonylation (1)
- sonogashira condensation (4)
- sonogashira conditions (1)
- sonogashira contions (1)
- sonogashira couplig reaction (6)
- sonogashira coupling (18540)
- sonogashira coupling - wittig reaction (3)
- sonogashira coupling reaction (1152)
- sonogashira coupling-benzannulation reaction (13)
- sonogashira coupling-cyclization (29)
- sonogashira coupling-isomerization reaction (28)
- sonogashira coupling-michael addition-cyclocondensation-sulfur extrusion

Transfer
Reset
Cancel

Search reactions by type or name



SEARCH LITERATURE

OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

Ask Reaxys

Ask Reaxys

BETA

Enter a keyword, concept or author

Ask Reaxys provides new user experience for text searching: content better discoverable, answers more immediately available

Intelligent interpretation of topic query



Reaxys Tree

ReaxysTree

BETA



Browse Literature
Look through the Reaxys data by browsing its hierarchy of entities and properties. Select the

ReaxysTree

- chemical transformations
 - chemical reaction class
 - chemical reaction class
 - coupling reaction
 - Suzuki Reaction
 - Suzuki Coupling
 - Suzuki-Miyaura Coupling
 - substitution reaction

ReaxysTree lets users “browse” the database by taxonomies: helps with search precision and answer comprehension

Browse through taxonomies



You are in control

Bibliographic Data

Document Type	is	<input type="text"/>	Lookup ×
Authors	is	<input type="text"/>	Lookup ×
Common Patent Number	is	<input type="text"/>	Lookup ×
Patent Country Code	is	<input type="text"/>	Lookup ×
Journal Title	is	<input type="text"/>	Lookup ×
Publication Year	=	<input type="text"/>	Lookup ×
DOI	is	<input type="text"/>	Lookup ×
Title	is	<input type="text"/>	Lookup ×
Abstract	is	<input type="text"/>	Lookup ×
Keywords	is	<input type="text"/>	Lookup ×
Citation Basic Index	is	<input type="text"/>	Lookup ×

Show AND Buttons

You can also search with truncation/proximity - like you do through other interfaces

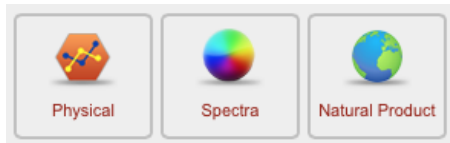
Use truncation/proximity if you like



SEARCH PROPERTIES

>500 MILLION EXPERIMENTAL PROPERTIES, >400 FIELDS, >130 SUBJECT AREAS

PRE-PROGRAMMED



Substances **MedChemistry** Literature **ReaxysTree** Physical **Spectra** Natural Product

NMR Spectroscopy exists ×
Nucleus Lookup ×
IR Spectroscopy exists ×
Description Lookup ×
Mass Spectrometry exists ×
Description Lookup ×
UV/VIS Spectroscopy exists ×
Description Lookup ×
ESR Spectroscopy exists ×
Description Lookup ×

Structure Molecular Formula **Alloy** Add/Remove Fields...

PROPERTIES



easy to set up

BUILD YOUR OWN

Find any property Reset

Ecological Data exists
 Exposure Assessment exists
 Concentration in the Environment exists
 Transport and Distribution exists
 Bioaccumulation, Biomagnification and Biomonitoring exists
 Biodegradation exists
 Abiotic Degradation, Hydrolysis exists
 Abiotic Degradation, Photolysis exists
 Stability in Soil exists
 Oxygen Demand exists
 Use/Application

Exposure Assessment (in Reaxys)
 Bioaccumulation, Biomagnification and Biomonitoring (in Reaxys)
 Biodegradation (in Reaxys)
 Stability in Soil (in Reaxys)
 Oxygen Demand (in Reaxys)

Add >>
Remove
Remove all
Add Default

Already selected Searches in multiple databases Save

Ecological Data

Exposure Assessment exists ×
Bioaccumulation, Biomagnification and Biomonitoring exists ×
Biodegradation exists ×
Stability in Soil exists ×
Oxygen Demand exists ×

Show AND Buttons

Add to Query: Structure Molecular Formula **Alloy** Add/Remove Fields...

CONTENT



easy to search

MedChem

Bioactivities

Substance Route Lookup ×
Bioassay Category Lookup ×
Putative action on target Lookup ×
Effect Lookup ×
Cells/Cell lines Lookup ×
Organs/Tissues Lookup ×
Target Name Lookup ×
Target Subunit Name Lookup ×
Target Nature Lookup ×
Species Lookup ×
pK Lookup ×

Show AND Buttons

Add to Query: Structure Molecular Formula **Alloy** Add/Remove Fields...

Select index items and click "Transfer"

Reaxys

Search for: **STREP**

- streptothricus hindustanus (12)
- streptobacillus (40)
- streptococcus (856)
- streptococcus 72 (5)
- streptococcus acidominimus (4)
- streptococcus agalactiae (3015)
- streptococcus alactolyticus (12)
- streptococcus albus (11)
- streptococcus alvarez (5)
- streptococcus anginosus (71)
- streptococcus aranson (2)
- streptococcus aureus (33)
- streptococcus bovis (97)
- streptococcus capitis (20)
- streptococcus constellatus (57)
- streptococcus cristatus (2)
- streptococcus defectivus (2)
- streptococcus durans (27)
- streptococcus dysgalactiae (296)
- streptococcus entericus (56)

Transfer
Reset
Cancel

FIELDS



MAIN NEW FEATURES & FUNCTIONALITIES

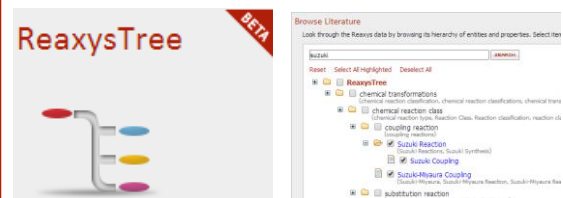
OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

Ask Reaxys



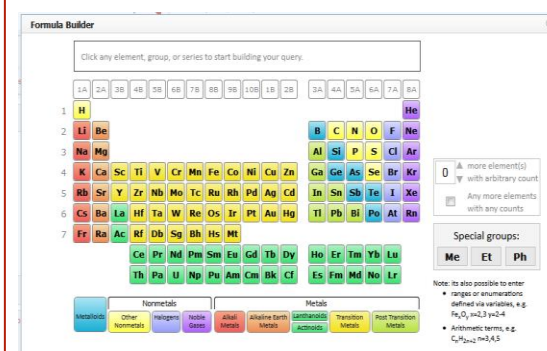
Ask Reaxys provides new user experience for text searching: content better discoverable, answers more immediately available

Reaxys Tree



ReaxysTree lets users “browse” the database by taxonomies: helps with search precision and answer comprehension

Formula Builder



Formula Builder improves the searchability of substances through molecular formulas: easy way to find substances right across the Periodic Table

REAXYS 2014

MAKE A COMPOUND



Query Results Synthesis Plans History Report My Alerts My Settings Help Register Login

Reaxys

Query
No structure
Create Alert

29 reactions

Open Analysis View

29 reactions out of 3 substances and 31 citations

Filter by:

- Sub-structure
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data

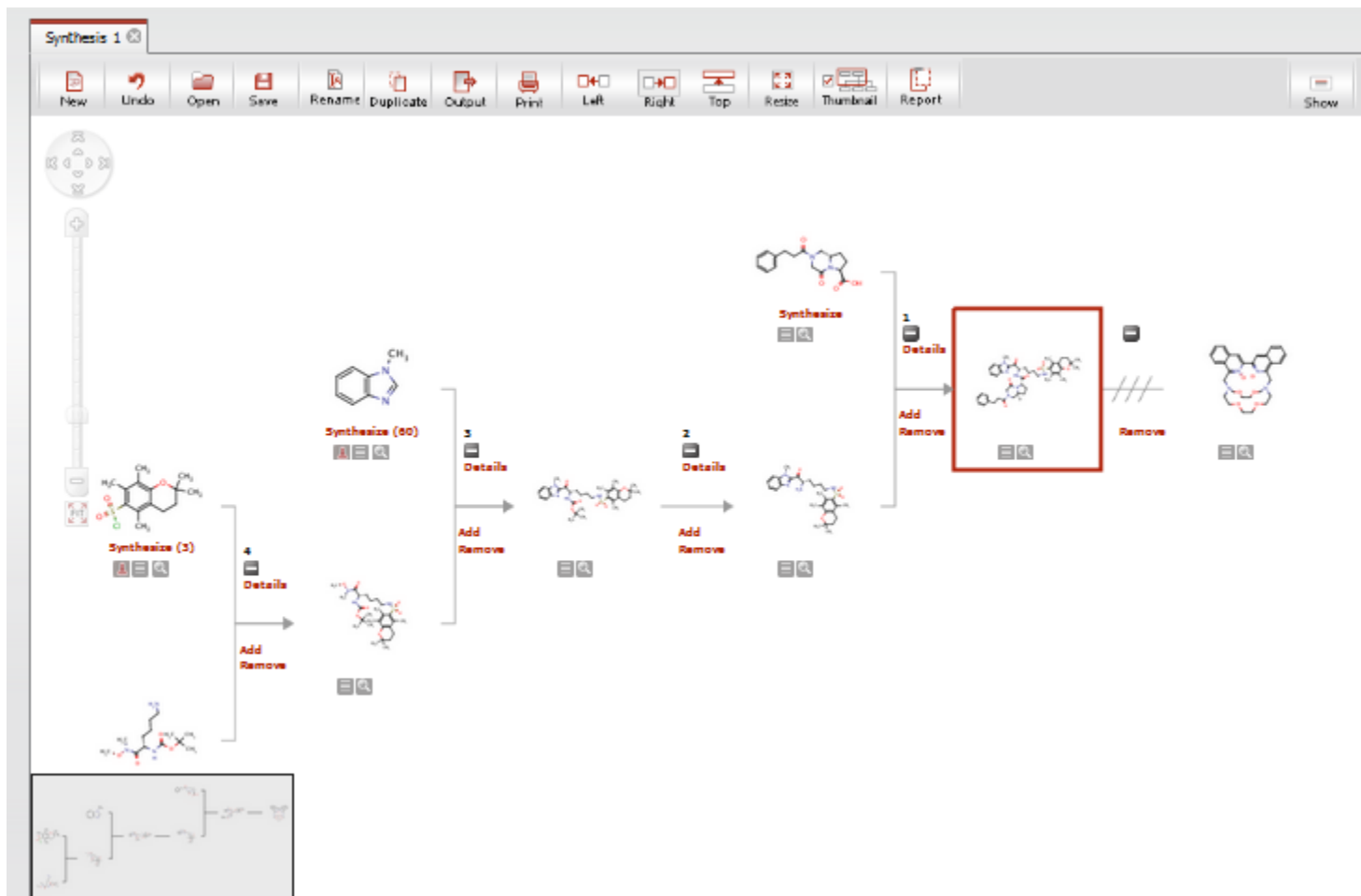
Reactions Substances (Grid) Substances (Table) Citations

go to Page: Page 1 of 4

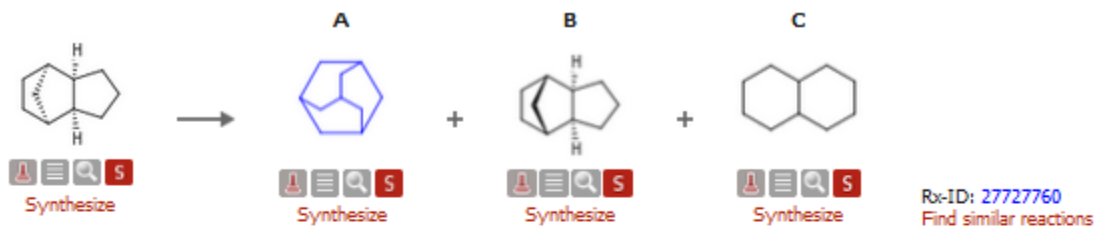
Limit to Exclude Output Print Zoom in Zoom out Hide Sort by: Reaxys-Ranking

Yield	Conditions	References
84%	<p>6 H₂O</p> <p>Cl₂Ni</p> <p>in water; acetic acid washing with acetic acid, drying in vac. over concd. H₂SO₄ or KOH;</p>	<p>Venanzi, L. M. Journal of the Chemical Society, 1958, p. 719 - 724 Full Text View citing articles Show Details Gmelin Handbook: Ni; MVol.C2, 8.18.1, page 1041 - 1052 Full Text Show Details</p>
41%	<p>in water; acetic acid T=100°C; 0.666667 h; Show Experimental Procedure</p>	<p>Gaillard, Sylvain; Mabaye, Mbaye D.; Mboyi, Cleve D.; Pannetier, Nicolas; Renaud, Jean-Luc; Gaillard, Sylvain; Mabaye, Mbaye D.; Mboyi, Cleve D.; Pannetier, Nicolas; Renaud, Jean-Luc; Gaillard, Sylvain; Mabaye, Mbaye D.</p>

AUTOPLAN: AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES



SHOW EXPERIMENTAL PROCEDURE



With AlCl_3 , aluminium chloride in dichloromethane
T=0 - 20°C; 18 h;
[Hide Experimental Procedure](#)

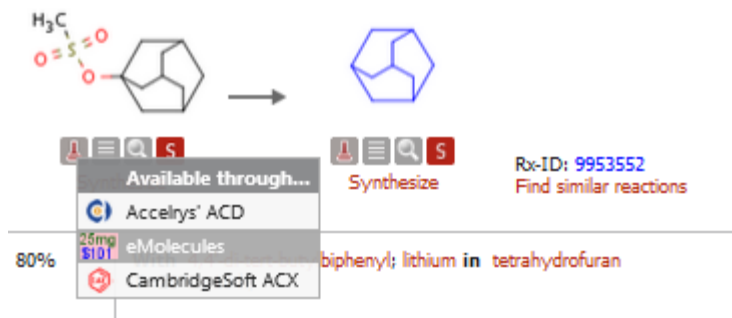
Tsao, Ying-Yen; Liao, Chyuan-Neng; Chen, Chi-Yu; Lin, Chin-Ming; Wei, Kuo-M
Patent: US2008/249341 A1, 2008 ;
Location in patent: Page/Page column 8 ;

[Title/Abstract](#) [Full Text](#) [Show Details](#)

5:

EXAMPLE 5 is the comparative example of EXAMPLE 4. 6.5 g of endo-THDCPD crystals from the same source of EXAMPLE 4 are placed in a 250 ml of glass bottle, followed by adding 40 g of dichloromethane thereto to dissolve the nitrogen and stirring in the ice bath. Subsequently, 10 g of AlCl_3 is added to the dichloromethane solution of endo-THDCPD, followed by stirring for 2 hours in the ice bath, and continuously stirring for 16 hours at room temperature. Subsequently, the mixture washed with the saturated KCl solution is washed with 100 ml of deionized water, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the lower layer in the separatory funnel. The above saturated KCl solution washing procedure is repeated for three times. Subsequently, the lower layer is distilled to remove dichloromethane and water. The bottoms is collected, and determined by chemical analysis. The chemical analysis is composed of 85.7 wt percent of exo-THDCPD, 0.5 wt percent of endo-THDCPD, 1.2 wt percent of Decalin, 5.8 wt percent of adamantane, 1.3 wt percent of exo-THMDCPD, and the other two-stage hydrotreated and saturated C_{10} and/or MCPD dimers. The bottoms has a volumetric heating value of 39.17 MJ/L, a density of 0.9339 at 15° C., and a viscosity of 3.52 cSt at 20° C. and more than 26.7 cSt at -20° C. In this example, the isomerization reaction is very slow so that portions of exo-THDCPD is further isomerized to adamantane which will increase the viscosity of the high energy fuel. Under such a violent reaction conditions, a small amount of THDCPD will be ring-opened to decalin (the side product) with relatively less volumetric heating value as well as density. Therefore, the isomerization reaction of this example is not suitable for preparing the high energy fuels because the freezing point of the isomerized product is too high.

CHECK COMMERCIAL AVAILABILITY



SUPPORTS DIFFERENT STRUCTURE EDITORS



Query Results Synthesis Plans History Report My Alerts My Settings Help

Modify application settings

Structure editor

Editors that do not require a plugin to be installed:

- Dotmatics Elemental
- ChemAxon MarvinSketch *(Note: requires Java to be installed)*
- GGA Ketcher

Reaxys uses Dotmatics's Elemental as default structure and reaction query editor, if no other editor is selected

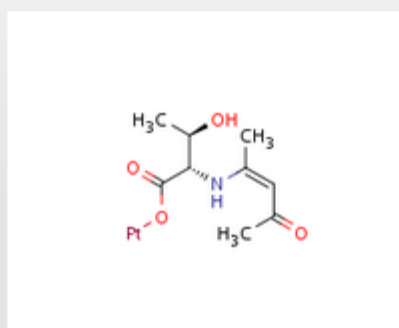
The following editors can only be used, if the **Reaxys Structure Editor PlugIn** is installed:

- Crossfire Structure Editor
- Accelrys Draw
- Accelrys ISIS/Draw
- CambridgeSoft ChemDraw
- ICEdit

Please check this with your administrator or click the hyperlink and download the installer.

Reaxys will present a warning message, if these editors are selected, but the **structure editor plugin** is not installed.

Structure display options



Carbon Labels

- Always
- Never
- At straight angles and H atoms

Implicit Hydrogens

- On All
- On Hetero
- On Hetero and Terminal
- Off

Display atom numbers

- On
- Off

R/S Labels

- On All
- Absolute Stereo
- None

E/Z Labels

- On
- Off

Display Atom Valence

- On
- Off



REPORTING: GATHER AND PREPARE THE INFORMATION

REAXYS Anonymous user (136.105.10.72)

Query Results Synthesis Plans History Report My Alerts My Settings Help Live Chat Register Login

Print Undo Open Save Refresh Send Send to Bookmarks Clear All

Report ID: **Synthesis Plan: Synthesis 4** Created: 2013-09-03 10:23 | Modified: 2013-09-03 10:23 Move Down Remove Annotation

Report ID: **IDE-XDR: 67944** Created: 2013-09-03 10:09 | Modified: 2013-09-03 10:09 Show Substance Move Up Move Down Remove Annotation

Decomposition

Decomposition	Location	Reference
210 - 221 °C	supporting information	Ohman, Ken; Yano, Takahiro; Suzuki, Keisuke Organic and Biomolecular Chemistry, 2013 , vol. 8, p. 2003 - 2006 Title/Abstract Full Text View citing articles Show Details

Report ID: **IDE-XDR: 67944** Created: 2013-09-03 10:09 | Modified: 2013-09-03 10:09 Show Substance Move Up Remove Annotation

Dissociation Exponent

Dissociation Exponent (pK)	Dissociation Group	Method	Type	Comment	Reference
7.68	OH	spectrophotometric	alloprenant	DE	Phuzell, Halgoronta; Szymusiak, Henryk; Gluszczyska-Swiglo, Anna; Tyrakowska, Beata; Bietjes, Joonne M. C. H. Journal of Agricultural and Food Chemistry, 2008 , vol. 56, # 3, p. 818 - 822 Title/Abstract Full Text View citing articles Show Details
-0.89242 - -0.18203	OH		alloprenant	in the presence of salts	Kamamoto, Hiroyuki; Sonda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Masaaki Bioscience, Biotechnology, and Biochemistry, 2001 , vol. 45, # 1, p. 125 - 132 Title/Abstract Full Text View citing articles Show Details
-1.02938	OH		alloprenant		Kamamoto, Hiroyuki; Sonda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Masaaki Bioscience, Biotechnology, and Biochemistry, 2001 , vol. 45, # 1, p. 125 - 132 Title/Abstract Full Text View citing articles Show Details

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PIOTR GOLKIEWICZ

SOLUTION SALES MANAGER LIFE SCIENCES

CENTRAL AND EASTERN EUROPE

P.GOLKIEWICZ@ELSEVIER.COM

MOBILE: +48 695 30 60 17