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LIFE SCIENCES SOLUTIONS CONSULTANT  
CENTRAL-EASTERN EUROPE

**INTRODUCING  
REAXYS**



# WHAT'S IN A TYPICAL CHEMISTRY DOCUMENT (PUBLICATION OR PATENT)?

## Scientific topic, author

Can be searched in full text, but difficult to find the right search term

1. Introduction

Covalently linked porphyrin dimers have furnished important models to elucidate mechanisms of excitation energy transfer and photoinduced electron transfer in natural photosynthetic processes [1–8]. In addition, some of these models are potentially important materials for use in molecular-scale electronic devices [9–11]. Recently, a molecular optoelectronic gate consisting of an array of porphyrins has been reported [12]. Two basic photophysical properties have been exploited in the design of molecular devices, (i) singlet–singlet energy transfer and (ii) photoinduced electron transfer. We made use of the differential basicity of the inner imino nitrogens of the meso-fluoroarylporphyrin and meso-tetraarylporphyrin to construct simple dimeric porphyrins wherein absorption of a photon of visible light by a neutral porphyrin leads to an emission of a photon from diprotonated porphyrin with very high efficiency ( $\phi$  95%). The occurrence of such processes can be easily tuned by the acidity of the medium, fundamentals of which could be used in the construction of artificial photonic devices.

The substitution of pentafluoroaryl groups in the meso positions of the porphyrin confers unique inertness of the inner amino nitrogens towards protonation and metallation reactions. The fluoroarylporphyrins exhibit interesting optical and electrochemical properties [13]. We synthesised porphyrin dimers (Fig. 1) comprising of meso-fluoroarylporphyrin and meso-tetraarylporphyrin with an ethylenedioxy covalent bridge to accomplish selective protonation and demetallation of the meso-tetraarylporphyrin moiety in the dimer. We demonstrate here that the dicationic porphyrin dimer exhibits efficient intramolecular singlet excitation energy transfer (eet) from

Corresponding author. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India. E-mail: vkp@ipc.iisc.ernet.in

Chemical structure

Cannot be searched by text terms in full text

## Chemical reactions

Cannot be searched by text terms in full text

Fig. 2. Schematic representation of different processes of dimer porphyrins.

Chemical spectra

Cannot be searched by text terms in full text

Fig. 3. The fluorescence emission spectra ( $\lambda_{exc}$  at 280 nm) of (a) intermolecular mixture of  $ZnF_5OCH_3$  and  $ZnH_5OCH_3$  (1:1,  $CH_2Cl_2$ ; MeOH,  $\nu/\nu'$ ) (1)  $ZnF_5OCH_3$ , (2)  $ZnH_5OCH_3$ , (3) intermolecular mixture of  $ZnF_5OCH_3$  and  $ZnH_5OCH_3$  (1:1,  $CH_2Cl_2$ ; MeOH,  $\nu/\nu'$ ) and (4)  $ZnF_5-ZnH_5$  DM. Inset shows the comparison of the corrected excitation spectrum (solid line) and absorption spectrum (dotted line) of the (i) intermolecular mixture of  $ZnF_5OCH_3$  and  $ZnH_5OCH_3$ , and (ii)  $ZnF_5-ZnH_5$  DM.

## 2. Experimental

Covalently linked porphyrin dimer was synthesised by the method of Little [14]. We have used 5-(4-methoxyphenyl)-10,15,20-triphenylporphyrin ( $H_2H_5OCH_3$ ) and 5-(4-methoxyphenyl)-10,15,20-tri(pentafluorophenyl)porphyrin ( $H_2F_5OCH_3$ ) as reference compounds for comparison studies. Hereafter these two porphyrins are referred to as meso-tetraarylporphyrin and meso-fluoroarylporphyrin, respectively. The meso-tetraarylporphyrin dimer was demethylated by treatment with  $BF_3 \cdot OEt_2$  to give the meso-fluoroarylporphyrin dimer. The meso-fluoroarylporphyrin dimer was demethylated by treatment with  $BF_3 \cdot OEt_2$  to give the meso-tetraarylporphyrin dimer. The meso-tetraarylporphyrin dimer was demethylated by treatment with  $BF_3 \cdot OEt_2$  to give the meso-fluoroarylporphyrin dimer. The meso-fluoroarylporphyrin dimer was demethylated by treatment with  $BF_3 \cdot OEt_2$  to give the meso-tetraarylporphyrin dimer.

## Experimental procedures

Substances and their physicochemical properties

Cannot be searched by text terms in full text

Compound	$\lambda_{abs}$ (nm; log $\epsilon$ ) <sup>a</sup>	$\lambda_{em}$ (nm) <sup>b</sup>
$H_2F_5OCH_3$	415(5.45), 509(4.28), 543(3.60), 584(3.82), 640(3.23)	644, 707

Table 1  
Optical

Compound	$\lambda_{exc}$ (nm)	$\lambda_{em}$ (nm)	$\phi_{FET}$ (%)	$\phi_{EET}$ (%)	$\tau_{FET}$ (ns)	$\tau_{EET}$ (ns)
$H_2F_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$H_2H_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$H_2F_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$H_2H_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$ZnF_5-ZnH_5$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$ZnF_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$ZnH_5OCH_3$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15
$ZnF_5-ZnH_5$	415(4.5), 509(4.28), 543(3.6), 584(3.8), 644(3.0)	644, 707	96	100	1.15	1.15

<sup>a</sup> In 1:1 (MeOH/MeOH,  $\nu/\nu'$ )  
<sup>b</sup> In 1:1 (MeOH/MeOH,  $\nu/\nu'$ )  
<sup>c</sup> Electrochemical redox data of the porphyrins in  $CH_2Cl_2$  solution containing 0.1 M TBAPI. Potential values are referenced to saturated  $Fc^+/Fc$  couple. All the potentials observed involve one electron oxidation/reduction processes unless otherwise mentioned.  
<sup>d</sup> In presence of TPA acid.  
<sup>e</sup> Involves more than one electron process.

## Chemistry as the organizing principle



# REAXYS IS BUILT

With experimental data from journal articles and patents

**Diaryl-2-pyrrolidones: new insight into the effect of structural modifications**

**Physical Data**

**Spectra**

**Bioactivity Data**

**Natural Product**

**Abstract**—Catalytic enantioselective epoxidation of α,β-unsaturated ketones (T-BHP) is described. Stereoselectivities of the substituted catalysts, significantly reduced load...

**1. Introduction**

Enantiomerically enriched α,β-epoxy ketones are versatile intermediates in organic synthesis and important synthetic pharmaceuticals.<sup>1</sup> Efficient asymmetric epoxidation reactions of α,β-unsaturated ketones, mainly dialcones, have been reported using chiral metal alkyl hydroperoxide systems.<sup>2</sup> Moreover, polyaminocatalytic and chiral organocatalytic systems 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 organocatalysis 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 protine-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-pyrrolidones have been successfully employed as organocatalysts in different transformations such as C–C bond forming reactions,<sup>3</sup> functionalizations of carbonyl compounds<sup>4</sup> and epoxidation of α,β-unsaturated aldehydes.<sup>5</sup> On the other hand, the

**United States**  
Moriarty et al.

**US 6,900,191 B1**  
May 31, 2005

**United States**

**6,900,191 B1**  
May 31, 2005

**Physical Data**

**Spectra**

**Bioactivity Data**

**Natural Product**

**Abstract**

**1. Introduction**

The present invention relates to a process for the preparation of a substituted pyrrolidone derivative. The process involves the reaction of a substituted pyrrolidone derivative with a carbonyl compound.<sup>6</sup> Very recently, the asymmetric vinylogous Michael addition reaction has been promoted by diaryl-2-pyrrolidonesethanols through the formation of iminium intermediates.<sup>10</sup> We have recently discovered that commercially available (S)-diaryl-2-pyrrolidonesethanol 2a and T-BHP oxidize unsaturated α,β-ketones into the corresponding epoxides in good yield and enantioselectivity (up to 80% ee), using 30 mol % catalyst loading at room temperature (Scheme 1).<sup>11</sup>

**Scheme 1.**

In epoxidative activity, 10% loading of the substituted pyrrolidone and more is generally preferred. The reaction efficiency is generally high (80% ee) and the catalyst loading is generally low (10–20 mol %).

**1. Introduction**

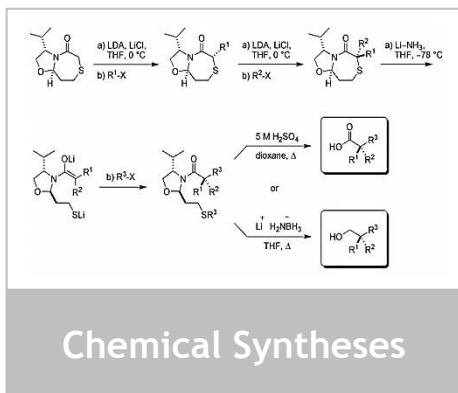
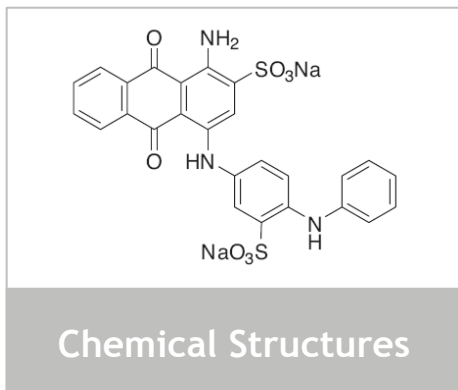
The present invention relates to a process for the preparation of a substituted pyrrolidone derivative. The process involves the reaction of a substituted pyrrolidone derivative with a carbonyl compound.<sup>6</sup> Very recently, the asymmetric vinylogous Michael addition reaction has been promoted by diaryl-2-pyrrolidonesethanols through the formation of iminium intermediates.<sup>10</sup> We have recently discovered that commercially available (S)-diaryl-2-pyrrolidonesethanol 2a and T-BHP oxidize unsaturated α,β-ketones into the corresponding epoxides in good yield and enantioselectivity (up to 80% ee), using 30 mol % catalyst loading at room temperature (Scheme 1).<sup>11</sup>

**Scheme 1.**

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# CHEMISTRY AS THE ORGANIZING PRINCIPLE



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

### High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet P2Y<sub>12</sub> Receptors

Younis Baqi,<sup>1</sup> Kerstin Atzler,<sup>1</sup> Merjem Köse,<sup>1</sup> Markus Glünzel,<sup>1,4</sup> and Christa E. Müller<sup>1,5\*</sup>

*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

Antraquinone derivatives related to the moderately potent, nonselective P2Y<sub>12</sub> receptor antagonist reactive blue 2 (6) have been synthesized and optimized with respect to P2Y<sub>12</sub> receptor affinity. A radioligand binding assay utilizing human blood platelet membranes and the P2Y<sub>12</sub> receptor-selective antagonist radioligand [<sup>3</sup>H]-propylthioadenosine-5'-adenylic acid (1-[1-dichloro-1-phosphonomethyl-1-phosphonyl] anhydride ([<sup>3</sup>H]PSB-0413)) was applied for compound testing. 1-Amino-2-sulfonanthraquinone derivatives bearing a *o*-phenylamino/lanino substitution in the 4-position and an additional acidic function in the *meta*-position of the aniline ring showed high P2Y<sub>12</sub> 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

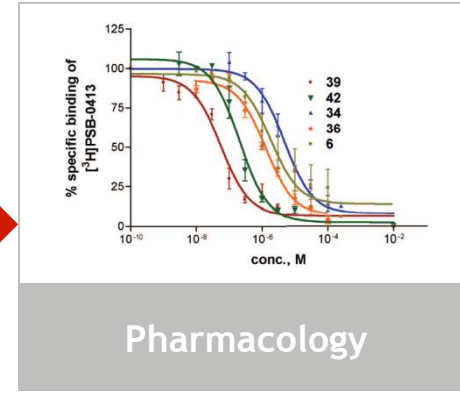
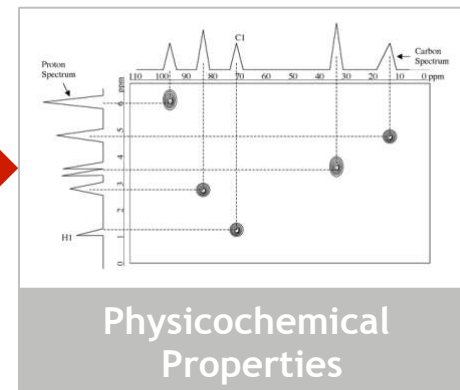
and sustained aggregation not preceded by shape changes. The latter receptor also plays an important role in the potentiation of platelet secretion induced by several agonists, and its congenital deficiency has been shown to result in a lifelong bleeding disorder.<sup>6</sup> Modulation of P2 receptors 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

*to the receptor, present serving a unique role and presumably act as covalent, possibly allosteric antagonists at P2Y<sub>12</sub> receptors<sup>9</sup> (see Supporting Information, Scheme 1). Major drawbacks of clopidogrel and related thienotetrahydropyridine derivatives are: (i) slow onset of action (up to several days) due to the required metabolism, (ii) long duration of action due to irreversible inhibition, (iii) "drug resistance" in a high percentage of patients (up to 30%), (iv) moderate potency (therefore high doses are required), and (v) difficulties in steering and controlling the effects.*

Therefore, it is highly desirable to develop P2Y<sub>12</sub> antagonists that are lacking the drawbacks associated with the standard P2Y<sub>12</sub> antagonists such as clopidogrel and other thienotetrahydropyridine derivatives. Several groups have recently been developing competitive, reversible P2Y<sub>12</sub> antagonists that may be superior to clopidogrel and related drugs. Most approaches started from the adenine nucleotides as lead structures, ADP,

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<sup>1</sup> PharmaCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn.  
<sup>2</sup> Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg.  
<sup>3</sup> 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

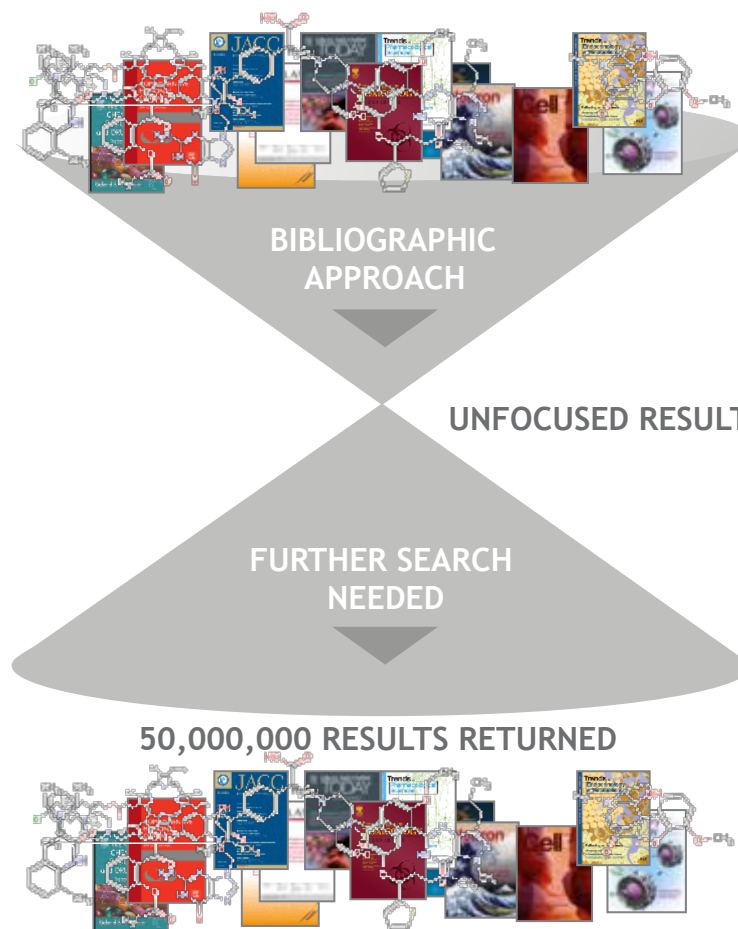


# STRUCTURED TO HELP YOU SEARCH

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



# KEYWORDS

A single bibliographic record in **Reaxys** contains index keywords from:

Authors, Compendex, Embase, Geobase, Medline and Reaxys.

Our competition has keywords only from two sources:  
CAplus and Medline

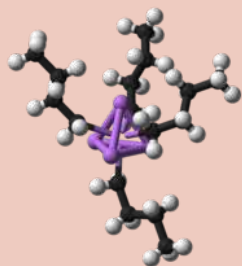
# Searching for classes of substances in Reaxys

Found in REAXYS SUBSTANCE RECORDS  
and ...

Found in KEYWORDS in REAXYS BIBLIOGRAPHIC  
RECORDS



CLASSIC ORGANICS



ORGANOMETALLICS  
COORDINATION  
COMPOUNDS



CLASSIC INORGANICS

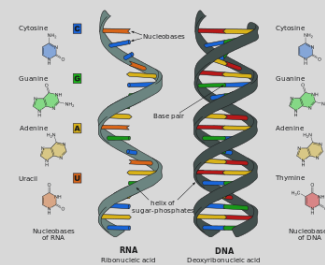
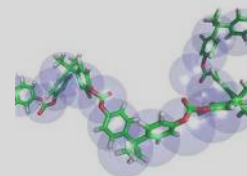


ALLOYS & METALS

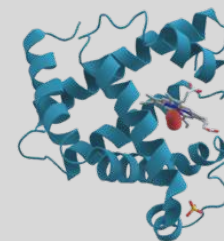
CERAMICS



POLYMERS



NUCLEIC ACIDS &  
PROTEINS

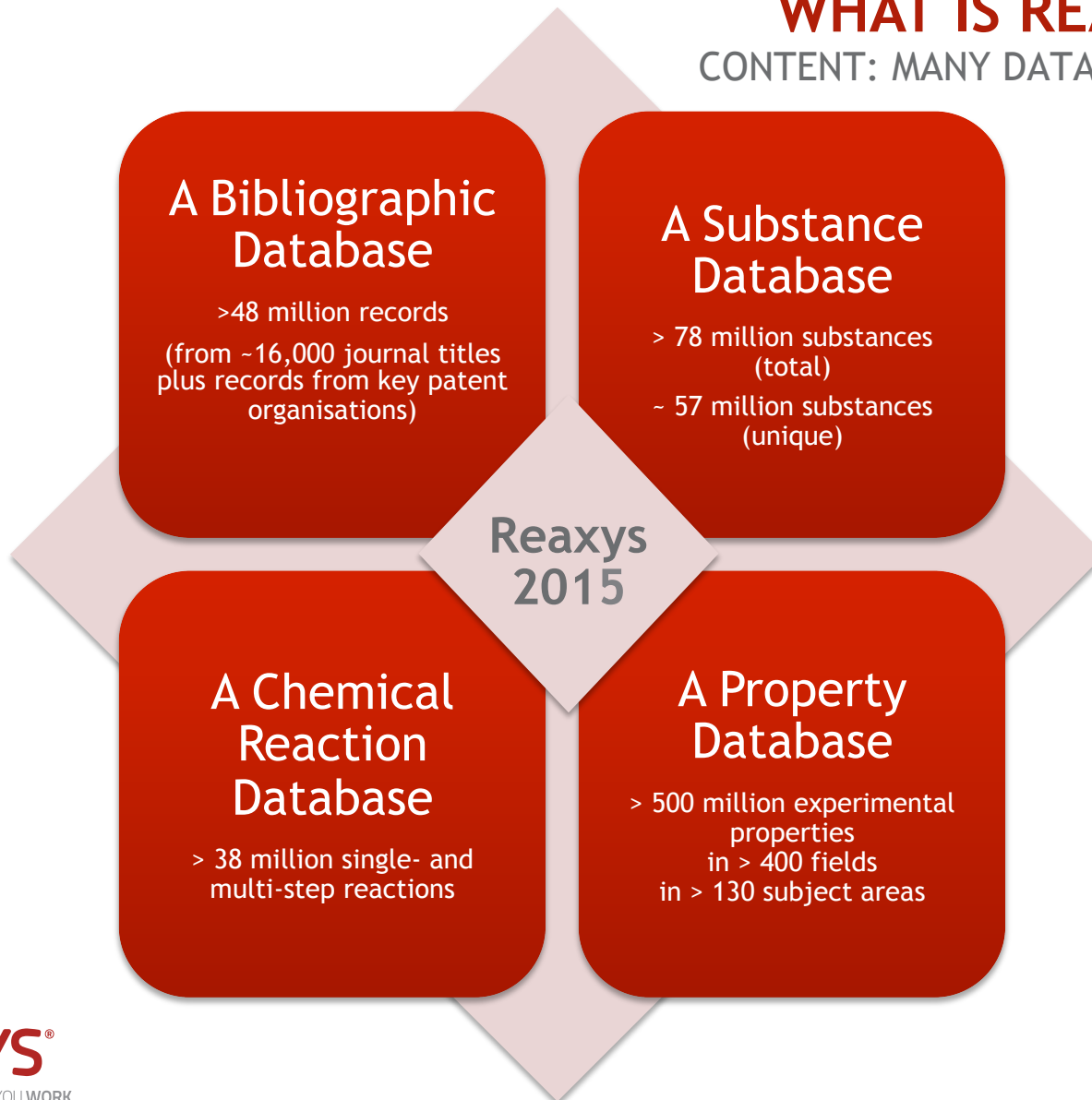


Search Substances Context

Search Literature Context

# WHAT IS REAXYS 2015?

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 website search interface. At the top left is the Reaxys logo. A navigation bar contains links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. On the right of the navigation bar, it says 'Anonymous user (145.35.235.1)' and has 'Register' and 'Login' links. Below the navigation bar is a search bar with the placeholder text 'Enter a keyword, concept or author'. Below the search bar is a row of five 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 is a row of search options: 'You can also search directly by these common property groups:' followed by icons for 'Physical', 'Spectra', 'Natural Product', and 'Advanced'. Several callout boxes with red borders and lines pointing to specific features are overlaid on the screenshot:

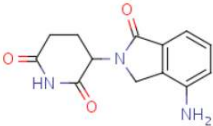
- Ask Reaxys, a quick, easy topic 'concept search'**: Points to the search bar.
- Perform a literature search**: Points to the Literature category button.
- Open Reaction search form**: Points to the Reactions category button.
- Data search form by "property"**: Points to the 'Advanced' search option.
- Open a structure search form**: Points to the Substances, Names, Formulas category button.
- Search using chemical identifiers**: Points to the Substances, Names, Formulas category button.
- Access detailed Biodata, and MedChem specific features**: Points to the Medicinal Chemistry category button.
- Browse database via taxonomies rather than search database**: Points to the ReaxysTree category button.

# 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

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

Chemical Name Segment

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)
- taxuseone (1)

Chemical Name ✓

Part of Chemical Name ✓

Reaxys helps on the way ✓✓

## FORMULA

Molecular Formula

Search MF Range

Element Counts

Element Symbols

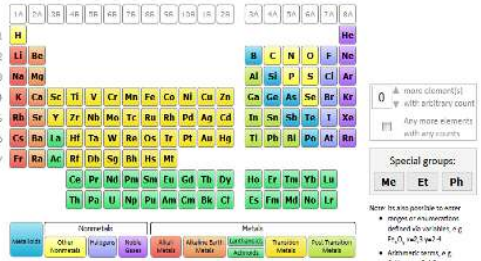
Number of Atoms

Number of Elements

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 elemental

Special groups:

Note: It is also possible to search for a group or substructure defined with an asterisk, e.g. FeO\* or \*nH2O  
\* Acyclic name, e.g. C12H22O11

Formula ✓

Part of Formula ✓

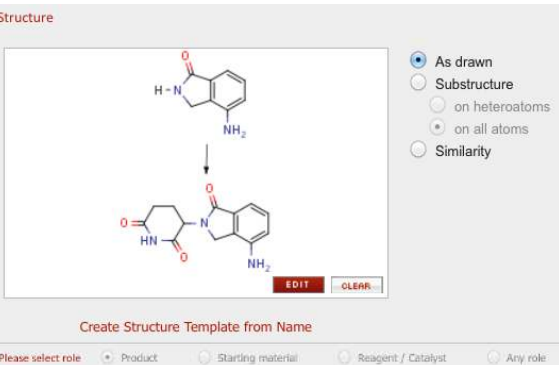
Reaxys helps on the way ✓✓

# 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)	=		Lookup X
Solvent	is		Lookup X
Reagent/Catalyst	is		Lookup X
Time (h)	=		Lookup X
Temperature (°C)	=		Lookup X
Pressure (Torr)	=		Lookup X
Reaction Type	is		Lookup X
Reaction Basic Index	is		Lookup X

Search reactions by reaction conditions



## TYPE

Reaction Data

is starts with ends with 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



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		Lookup	X
Authors	IS		Lookup	X
Common Patent Number	IS		Lookup	X
Patent Country Code	IS		Lookup	X
Journal Title	IS		Lookup	X
Publication Year	=		Lookup	X
DOI	IS		Lookup	X
Title	IS		Lookup	X
Abstract	IS		Lookup	X
Keywords	IS		Lookup	X
Citation Basic Index	IS		Lookup	X

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

Physical Spectra Natural Product

Substances MedChemistry Literature ReaxysTree Physical Spectra Natural Product

NMR Spectroscopy  exists

Nuclear

IR Spectroscopy  exists

Description

Mass Spectrometry  exists

Description

UV/VIS Spectroscopy  exists

Description

ESR Spectroscopy  exists

Description

Structure Molecular Formula Alloy Add/Remove Fields...

PROPERTIES



easy to set up

## BUILD YOUR OWN

Find any property

Ecological Data

Exposure Assessment exists

Concentration in the Environment exists

Transport and Distribution exists

Biodegradation exists

Biodegradation, Biomagnification and Biomonitoring exists

Abiotic Degradation, Hydrolysis exists

Abiotic Degradation, Photolysis exists

Stability in Soil exists

Oxygen Demand exists

Use/Application

Available to add Already selected Searches in multiple databases

Ecological Data

Exposure Assessment  exists

Biodegradation, 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

Bioassay Category

Putative action on target

Effect

Cells/Cell lines

Organs/Tissues

Target Name

Target Subunit Name

Target Nature

Species

pK

Show AND Buttons

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

Select index items and click 'Transfer'

Reaxys

Search for: STREP

streptococcus hindustanus (12)

streptococcus (40)

streptococcus (556)

streptococcus 72 (5)

streptococcus acidominimus (4)

streptococcus agalactiae (315)

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)

FIELDS





Reactions (96)	Substances (81)	Citations (190)	go to Page <input type="text"/> Page 1 of 11
<div style="display: flex; justify-content: space-between; align-items: center;"> <div> <p>Limit to  Exclude  Export  Print  Zoom in  Zoom out  Hide </p> <p>Sort by Reaxys-Ranking </p> </div> <div> <p>Yield</p> <p>Conditions</p> <p>References</p> </div> </div>			
<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>A</b></p> <p></p> <p>Synthesize Find similar</p> </div> <div style="text-align: center;"> <p><b>B</b></p> <p></p> <p>Synthesize Find similar</p> </div> <div style="text-align: center;"> <p><b>C</b></p> <p></p> <p>Synthesize Find similar</p> </div> </div> <p>Rx-ID: 38295231 Find similar reactions</p>			
C: 55%	T=450°C; P=750.075 Torr; 10 h; AutoclaveInert atmosphere; Show Experimental Procedure	<p><b>Maksasithorn, Surasa; Praserttham, Piyasan; Suriye, Kongkiat; Devillers, Michel; Debecker, Damien P.</b> Applied Catalysis A: General, <b>2014</b>, vol. 488, p. 200 - 207 Title/Abstract Full Text View citing articles Show Details</p>	
	Reagent/catalyst; Show Experimental Procedure	<p><b>Maksasithorn, Surasa; Debecker, Damien P.; Praserttham, Piyasan; Panpranot, Joongjai; Suriye, Kongkiat; Ayudhya, Sirachaya Kunjara Na</b> Chinese Journal of Catalysis, <b>2014</b>, vol. 35, # 2 p. 232 - 241 Title/Abstract Full Text Show Details</p>	
<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>A</b></p> <p></p> <p>Synthesize Find similar</p> </div> <div style="text-align: center;"> <p><b>B</b></p> <p></p> <p>Synthesize Find similar</p> </div> </div> <p>Rx-ID: 28699149 Find similar reactions</p>			
A: 84.9 %Chromat.	With [2-(5-tert-butyl-2-benzoxazolyl)-6-methylpyridine]dichloronickel; diethylaluminium chloride in toluene T=20°C; Inert atmosphere; regioselective reaction;	<p><b>Gao, Rong; Xiao, Liwei; Hao, Xiang; Sun, Wen-Hua; Wang, Fosong</b> Dalton Transactions, <b>2008</b>, # 41 p. 5645 - 5651 Title/Abstract Full Text View citing articles Show Details</p>	
	With [PdCl((2-diphenylphosphino-benzylidene)-furan-3-ylmethyl-amine-N,P)]; diethylaluminium chloride in toluene T=20°C; P=7500.75 Torr; 0.25 h; AutoclaveInert atmosphere; Show Experimental Procedure	<p><b>Mogorosi, Mokgolela M.; Mahamo, Tebello; Moss, John R.; Mapolie, Selwyn F.; Slootweg, J. Chris; Lammertsma, Koop; Smith, Gregory S.</b> Journal of Organometallic Chemistry, <b>2011</b>, vol. 696, # 23 p. 3585 - 3592 Title/Abstract Full Text View citing articles Show Details</p>	
<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p><b>A</b></p> <p></p> <p>Synthesize Find similar</p> </div> <div style="text-align: center;"> <p><b>B</b></p> <p></p> <p>Synthesize Find similar</p> </div> </div> <p>Rx-ID: 209127 Find similar reactions</p>			
A: 90% B: 6%	With [Ph <sub>2</sub> PC <sub>6</sub> H <sub>4</sub> C(OB(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> )O-k <sup>2</sup> P(O)](η <sup>3</sup> -CH <sub>2</sub> CMeCH <sub>2</sub> ) in toluene T=0°C; oligomerization; P=2280.15 Torr; 1 h; Product distribution; Further Variations:TemperaturesPressures;	<p><b>Komon, Zachary J.A.; Bu, Xianhui; Bazan, Guillermo C.</b> Journal of the American Chemical Society, <b>2000</b>, vol. 122, # 8 p. 1830 - 1831 Title/Abstract Full Text View citing articles Show Details</p>	
A: 7.5% B: 88.3%	With tetraphenyl-phosphonium chloride; chromium T=80°C; P=37503.8 Torr; 1 h; Product distribution / selectivity; Show Experimental Procedure	<p><b>Saudi Basic Industries Corporation</b> Patent: US2012/29258 A1, <b>2012</b>; Location in patent: Page/Page column 4-5 ; Title/Abstract Full Text Show Details</p>	
A: 88% B: 9%	With [6,6'-diphenyl-[2,2']-bipyridinyl]NiBr <sub>2</sub> ; triethyl aluminum sesquichloride in toluene Inert atmosphereSchlenk technique; Catalytic behavior; Reagent/catalyst; Show Experimental Procedure	<p><b>Chandran, Deepak; Lee, Kyeong Mi; Chang, Hyuk Chul; Song, Ga Young; Kim, Il; Lee, Ji-Eun; Suh, Hongsuk</b> Journal of Organometallic Chemistry, <b>2012</b>, vol. 718, p. 8 - 13,6 Title/Abstract Full Text Show Details</p>	

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29 reactions

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29 reactions out of 3 substances and 31 citations

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- Reactant Availability
- Availability in other DBs
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data

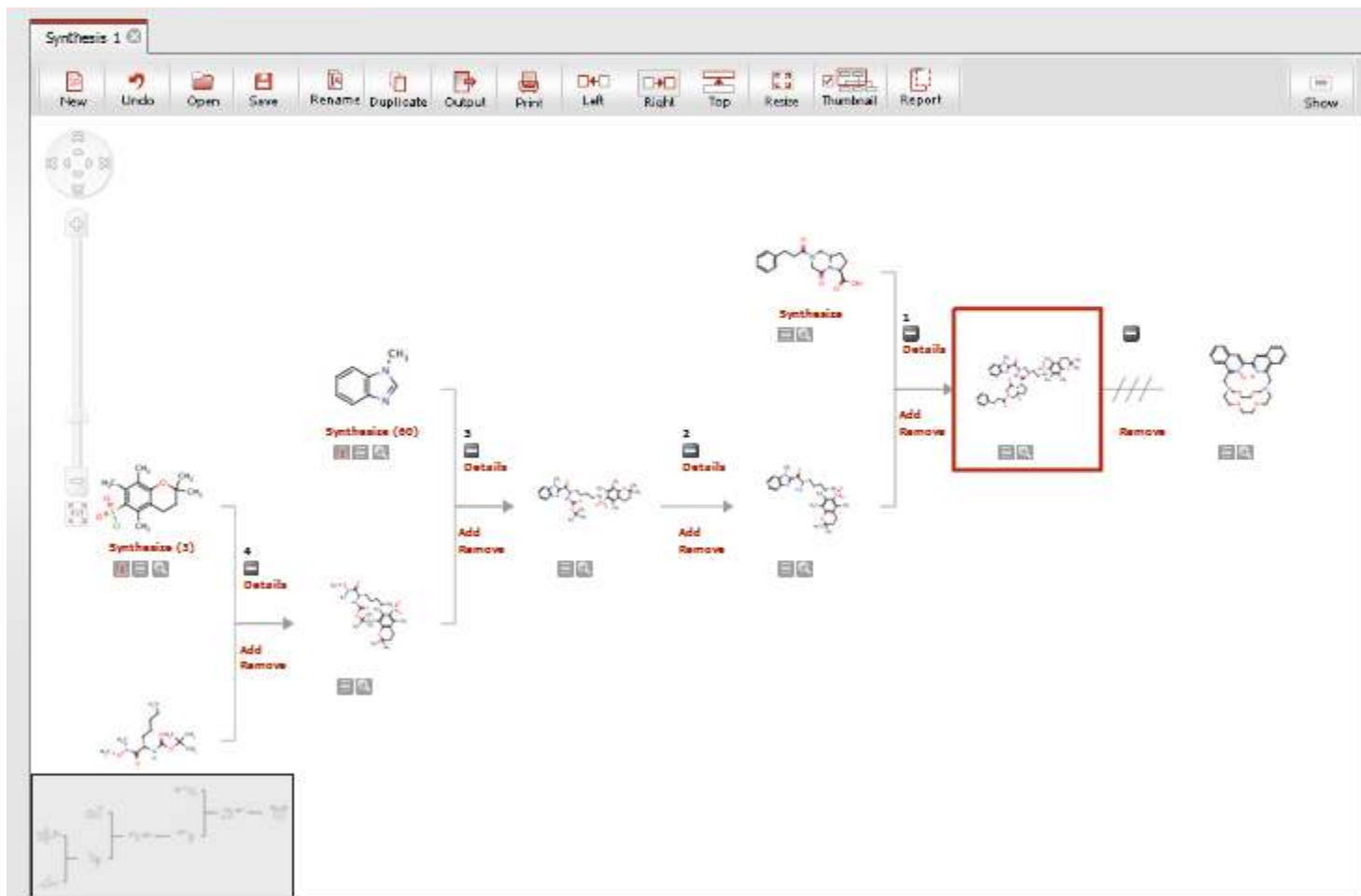
Reactions Substances (Grid) Substances (Table) Citations

go to Page 1 of 4

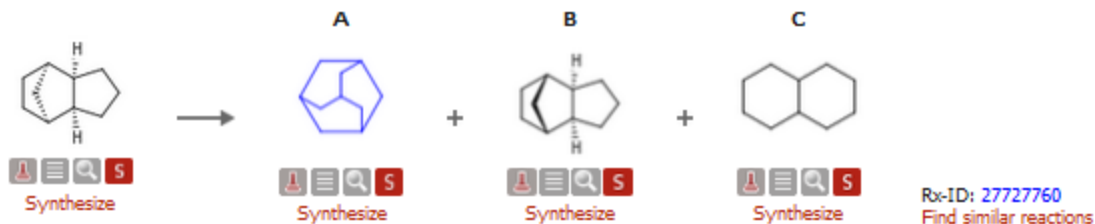
Limit to Exclude Output Print Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
84%	<p>in water; acetic acid washing with acetic acid, drying in vac. over concd. H2SO4 or KOH;</p>	<b>Venanzi, L. M.</b> Journal of the Chemical Society, <b>1958</b> , p. 719 - 724 <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Ni; MVol.C2, 8.18.1, page 1041 - 1052 <a href="#">Full Text</a> <a href="#">Show Details</a>
41%	<p>in water; acetic acid T=100°C; 0.666667 h; <a href="#">Show Experimental Procedure</a></p>	<b>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.</b>

# SYNTHESIS PLAN: AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES



# SHOW EXPERIMENTAL PROCEDURE



With  $\text{AlCl}_3$ , 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  $\text{AlCl}_3$  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 is washed with 100 ml of saturated KCl solution, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the upper layer in the separatory funnel. The above saturated KCl solution washing procedure is repeated for three times. Subsequently, the lower layer 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 deionized water 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  $\text{C}_{10}$  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 form 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 low.

# TiO2 - PROPERTIES

## Physical Data

- ▼ Melting Point (8)
- ▼ Refractive Index (48)
- ▼ Density (33)
- ▼ Adsorption (MCS) (994)
- ▼ Conformation (1)
- ▼ Crystal Phase (24)
- ▼ Crystal Property Description (30)
- ▼ Crystal System (5)
- ▼ Decomposition (1)
- ▼ Dielectric Constant (20)
- ▼ Dissociation Energy (1)
- ▼ Dynamic Viscosity (3)
- ▼ Electrical Data (56)
- ▼ Electrical Moment (1)
- ▼ Electrochemical Behaviour (1)
- ▼ Electrochemical Characteristics (17)
- ▼ Electrochemistry Data (54)
- ▼ Electron Binding (2)
- ▼ Enthalpy of Formation (3)
- ▼ Enthalpy of Vaporization (1)
- ▼ Further Information (1742)
- ▼ Heat Capacity Cp (90)
- ▼ Interatomic Distances and Angles (3)
- ▼ Ionization Potential (2)
- ▼ Liquid/Liquid Systems (MCS) (5)
- ▼ Magnetic Data (7)
- ▼ Magnetic Susceptibility (9)
- ▼ Mechanical Properties (15)
- ▼ Molecular Deformation (1)
- ▼ Optics (3)
- ▼ Other Thermochemical Data (10)
- ▼ Solubility (MCS) (12)
- ▼ Space Group (78)
- ▼ Thermal Expansion (3)
- ▼ Transition Point(s) of Crystalline Modification(s) (129)
- ▼ Transport Data (9)
- ▼ Transport Phenomena (MCS) (15)

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	Target	N° of ref
  <a href="#">Synthesize</a>   <a href="#">Hide Details</a>	<b>Chemical Name:</b> Titanium(IV) oxide  <b>Reaxys Registry Number:</b> 4360545 <b>Type of Substance:</b> Glass or Ceramic materialCoordination compoundIsotope or isotope containing compoundSolid solution <b>Molecular Formula:</b> O <sub>2</sub> Ti <b>Linear Structure Formula:</b> O <sub>2</sub> Ti <b>Molecular Weight:</b> 79.8788 <b>InChI Key:</b> QWWIMOOFFDJKFN-UHFFFAOYSA-N	542 prep out of 14302 reactions.	Druglikeness Bioactivity Identification Physical Data (3437) Spectra (621) Use/Application (1555) Quantum Chemical Data (61)	Show Targets	11082

## Spectra

- ▼ NMR Spectroscopy (2)
- ▼ IR Spectroscopy (259)
- ▼ Mass Spectrometry (1)
- ▼ UV/VIS Spectroscopy (304)
- ▼ ESR Spectroscopy (30)
- ▼ Raman Spectroscopy (6)
- ▼ Luminescence Spectroscopy (8)
- ▼ Fluorescence Spectroscopy (6)
- ▼ Other Spectroscopic Methods (5)

## Use (1555)

Use/Patent	Location	Reference
Coating/paints/lacquers	Page/Page column 5	ROHM AND HA Raymond; Man Patent: US2014 <a href="#">Title/Abstract</a>
pigment in biocide coatings formulations containing hindered alkylamine polymers	Page/Page column 5	ROHM AND HA Raymond; Man Patent: US2014 <a href="#">Title/Abstract</a>
Cosmetics/dental/toilet	Page/Page column 33	UNIVERSITY O Patent: WO2014 <a href="#">Title/Abstract</a>
Polymers/polymer applications	Page/Page column 33	UNIVERSITY O Patent: WO2014 <a href="#">Title/Abstract</a>
antibacterial component of resins useful in dental composites	Page/Page column 33	UNIVERSITY O Patent: WO2014 <a href="#">Title/Abstract</a>
Pharmaceuticals	Paragraph 34	SHOWA DENK Masahiro; LI D Patent: WO2013 <a href="#">Title/Abstract</a>
photocatalytic material in antimicrobial composition	Paragraph 34	SHOWA DENK Masahiro; LI D Patent: WO2013 <a href="#">Title/Abstract</a>
photocatalytic material in antiviral composition	Paragraph 34	SHOWA DENK Masahiro; LI D Patent: WO2013 <a href="#">Title/Abstract</a>
Pharmaceuticals	Page/Page column 5; 6	OLD DOMINIO Patent: US2013 <a href="#">Title/Abstract</a>
increasing absorbency of the first material in a wound care system upon exposure to light	Page/Page column 5; 6	OLD DOMINIO Patent: US2013 <a href="#">Title/Abstract</a>
inhibiting growth of bacteria in a wound care system upon exposure to light	Page/Page column 5; 6	OLD DOMINIO Patent: US2013 <a href="#">Title/Abstract</a>
second material in a wound care system	Page/Page column 5; 6	OLD DOMINIO Patent: US2013 <a href="#">Title/Abstract</a>
Coating/paints/lacquers	Page/Page column 22	AT PROMOTIC <a href="#">Title/Abstract</a>

## Quantum Chemical Calculations (61)

Calculated Properties	Method	Location	Reference
Atom distances, angles	DFT - density functional methods	supporting information	Andreev, Yuri G.; Panchmat Journal of the American Chemical <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Density of states	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Feng, Ningdong; Wang, Qian Journal of the American Chemical <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Atom distances, angles Potential energy function, potential curve Vibrational constants	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhuang, Jia; Li, Zhen Hua; F Journal of Physical Chemistry A, <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Molecular orbitals Electronic energy levels	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		El-Shafei, Ahmed; Hussain, Journal of Materials Chemistry, 2 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Electronic energy levels	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Lu, Xiaoping; Wei, Shuxian; Journal of Organometallic Chemis <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Density of states Band structure	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Munnich, S.; Schmeits, M. Physical Review B: Condensed M <a href="#">Full Text</a> <a href="#">View citing articles</a> Sarkar, Ghosh; Haldin; Chattop Physica B: Condensed Matter, 2 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Band structure Density of states UV/VIS wave lengths	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Guo; Zhang; Liang Physica B: Condensed Matter, 2 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Density of states Molecular orbitals Electronic energy levels Band structure	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhao, Dongqiu; Huang, Xiaop Applied Physics Letters, 2011, 1 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Population analysis, charge distribution Density of states Band structure	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Shi, Weimei; Chen, Qifeng; Journal of Solid State Chemistry, <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Band structure Effective masses Population analysis, charge distribution UV/VIS wave lengths	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhang, Rui-Shuo; Liu, Yong; Journal of Alloys and Compounds <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Density of states UV/VIS wave lengths	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhang, Zhi-Kun; Bai, Mei-Lin; Chemical Communications, 2011, 1 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>
Atomization energy	Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Shinzato, Yoshifumi; Yukawa; Journal of Alloys and Compounds <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a> West, Richard Hu Baran, G Journal of Physical Chemistry A, <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a> Hirate; Morinaga; Yukawa; Journal of Alloys and Compounds <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View Article</a>

## Physical Data

Chromatographic Data  exists ✕

Solvent (Solubility (MCS))   Lookup ✕

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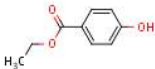
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Substances (549779)
Citations (1746232)
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Structure	Structure/Compound Data	N° of preparations <small>All Preps   All Reactions</small>	Available Data	N° of ref.
<div style="text-align: center;">  <p>892</p> <p style="font-size: 8px;">Synthesize   Hide Details Find similar</p> </div>	<p><b>Chemical Name:</b> Ethyl-4-hydroxy-benzoate</p> <p><b>Reaxys Registry Number:</b> 1101972 <b>CAS Registry Number:</b> 120-47-8 <b>Type of Substance:</b> isocyclic <b>Molecular Formula:</b> C<sub>9</sub>H<sub>10</sub>O<sub>3</sub> <b>Linear Structure Formula:</b> HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>C<sub>2</sub>H<sub>5</sub> <b>Molecular Weight:</b> 166.177 <b>InChI Key:</b> NUVBSKCKDOMJSU-UHFFFAOYSA-N</p>	<p>70 prep out of 2652 reactions.</p>	<p>Hit Data (4) Identification Physical Data (276) Spectra (106) Bioactivity (105) Ecological Data (7) Use/Application (149) Natural Product (13) Quantum Chemical Data (1)</p>	1166

**Chemical Names and Synonyms**

Ethyl-4-hydroxy-benzoate, ethyl 4-hydroxy-benzoate, para-hydroxybenzoic acid ethyl ester, 4-hydroxybenzoic acid ethylester, 4-hydroxybenzoic acid ethyl ester, 4-hydroxybenzoic ethyl ester, ethyl para-hydroxybenzoate

**Hit Data**

**Chromatographic Data ( 4 Hits out of 4 view all )**

Chromatographic data	Location	Reference
GC (Gas chromatography)		<b>Zhang, Yi; Ni, Yan-Peng; He, Ming-Xin; Wang, Xiu-Li; Chen, Li; Wang, Yu-Zhong</b> Polymer (United Kingdom), <b>2015</b> , vol. 60, p. 50 - 61 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>
HPLC (High performance liquid chromatography)		<b>Lee, Seung-You; Son, Eunjung; Kang, Jin-Young; Lee, Hee-Seok; Shin, Min-Ki; Nam, Hye-Seon; Kim, Sang-Yub; Jang, Young-Mi; Rhee, Gyu-Seok</b> Bulletin of the Korean Chemical Society, <b>2013</b> , vol. 34, # 4 p. 1131 - 1136 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> <b>Zabrzewska, Beata; Chyla, Anna; Bogdan, Anna</b> Acta Poloniae Pharmaceutica - Drug Research, <b>2014</b> , vol. 71, # 4 p. 563 - 573 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>
UPLC (Ultra performance liquid chromatography)		<b>Zhang, Jun-Xian; Miao, Ming-Ming; Niu, Xue-Mei; Li, Jin-Zhu; Han, Yi; Zhang, Ke-Qin; Zhang, Cheng-Ming</b> Asian Journal of Chemistry, <b>2014</b> , vol. 26, # 16 p. 5082 - 5086 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>
TLC (Thin layer chromatography)	supporting information	<b>Carta, Fabrizio; Vullo, Daniela; Maresca, Alfonso; Scozzafava, Andrea; Supuran, Claudiu T.</b> Bioorganic and Medicinal Chemistry, <b>2013</b> , vol. 21, # 6 p. 1564 - 1569 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>



Comb polymer

The various shapes of polymer backbones may easily be searched by words:

Citation Basic Index

231 citations out of 259 reactions and 229 substances

Reactions Substances (Grid) Substances (Report) **Citations** go to Page  Page 1 of 26

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Title of the Document	Authors	Year	Source	Times cited
Inhibition of bacterial adhesion on well ordered comb-like polymer surfaces	Sohn, Eun-Ho; Kim, Jaeeun; Kim, Byoung Gak; Kang, Jun Il; Chung, Jae-Seung; Ahn, Jooyeon; Yoon, Jeyong; Lee, Jong-Chan	2010	Colloids and Surfaces B: Biointerfaces, <b>2010</b> , vol. 77, # 2 p. 191 - 199 Full Text <a href="#">View citing articles</a>	15

**Title/Abstract**  
**Inhibition of bacterial adhesion on well ordered comb-like polymer surfaces**  
 The surfaces of comb-like poly(oxyethylene) derivatives with n-alkylsulfonyl side groups were more effective at reducing Pseudomonas aeruginosa adhesion than the surfaces of common materials such as polystyrene, poly(methyl methacrylate), poly(dimethylsiloxane), fluorinated polyacrylate, and glass. When the comb-like poly(oxyethylene) was mixed with polystyrene and poly(methyl methacrylate), the topology and roughness of the surfaces varied according to the mixture compositions. However the surface energies of the mixtures were close to that of the comb-like poly(oxyethylene) in the range of 21-23. mN/m and bacterial adhesion resistances of the mixture surfaces were also comparable to that of the pure comb-like poly(oxyethylene) surface.

**Keywords:**  
**Author:** Bacterial adhesion; Blend; Comb-like polymer; Surface energy  
**Compendex Free Language:** Bacterial adhesion; Comb-like; Comblike polymers; Common materials; Fluorinated polyacrylate; Mixture compositions; Poly(oxyethylene); Pseudomonas aeruginosa; Surface energies  
**Compendex Descriptor:** Adhesion; Bacteriology; Esters; Interfacial energy; Mixtures; Polyacrylates; Polyethylene glycols; Polymers; Polystyrenes; Surface chemistry; Surface tension  
**Compendex Mainhead:** Surfaces  
**EMTREE drug term:** dimeticone; glass; poly(methyl methacrylate); poly(oxyethylene); polyacrylic acid; polymer; polystyrene; unclassified drug  
**EMTREE medical term:** article; bacterium adherence; chemical composition; controlled study; energy; nonhuman; priority journal; Pseudomonas aeruginosa; surface property  
**Medline descriptor:** Apoptosis; Bacterial Adhesion; Hydrocarbons; Microscopy, Atomic Force; Models, Biological; Molecular Weight; Polyethylene Glycols; Polymers; Polystyrenes; Pseudomonas aeruginosa; Silicon; Surface Properties; Water  
**Species index:** Bacteria (microorganisms); Pseudomonas aeruginosa  
**Reaxys Terms:** poly(dimethylsiloxane); poly(methyl methacrylate); poly(oxyethylene); polyacrylate - roughness

## FIND: Polymer Blends

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blends with linear low density polyethylenes

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	Title of the Document	Authors	Year	Source	Times cited
1	Phenomenon of double yielding under tension in low-density polyethylene, linear low-density polyethylene and their blends	Balsamo; Mueller	1993	Journal of Materials Science Letters, <b>1993</b> , vol. 12, # 18 p. 1457 - 1459 <a href="#">Full Text</a> <a href="#">View citing articles</a>	30
<b>Title/Abstract</b> <b>Phenomenon of double yielding under tension in low-density polyethylene, linear low-density polyethylene and their blends</b> We studied the rate dependence of double yielding under tension in low density polyethylene (LDPE), linear low density polyethylene (LLDPE) and their blends. The phenomenon was found to be sensitive to the crystallization conditions of the samples. The blends prepared were found to be mechanically compatible in all of the composition range. <b>Keywords:</b> <b>Compindex Free Language:</b> Double yielding; Partial miscibility; Polyethylene blends <b>Compindex Descriptor:</b> Crystallization; Linear low density polyethylenes; Mechanical properties; Polymer blends <b>Compindex Mainhead:</b> Low density polyethylenes <b>Reaxys Terms:</b> low density polyethylene; low-density polyethylene - crystallization					
2	Application of chemiluminescence to probe miscibility in metallocene-catalyzed polyethylene blends	Cran, Marlene J.; Fearon, Peter K.; Billingham, Norman C.; Bigger, Stephen W.	2003	Journal of Applied Polymer Science, <b>2003</b> , vol. 89, # 11 p. 3006 - 3015 <a href="#">Full Text</a> <a href="#">View citing articles</a>	1
<b>Title/Abstract</b> <b>Application of chemiluminescence to probe miscibility in metallocene-catalyzed polyethylene blends</b> Chemiluminescence (CL) monitoring has successfully been applied to the study of the oxidative degradation of two-component polyethylene blends made with commercially available low-density polyethylene, linear low-density polyethylene, high-density polyethylene, and metallocene-catalyzed linear low-density polyethylene (mLLDPE) formulations. The emphasis in the analysis of the results is placed on blends containing mLLDPE to address the lack of CL information on these blends. The CL data are consistent with the thermal and physicomechanical properties of the blends, with a decreased blend miscibility being reflected in the CL data as a departure from the idealized behavior observed for more miscible blends. Furthermore, the results suggest that immiscibility in the solid state is reflected to some extent in the behavior of the melt. Preliminary experiments conducted to determine the level of consistency of CL results with respect to both variability between instruments and variability between techniques indicate a high degree of correlation in each case. <b>Keywords:</b> <b>GEObase Subject Index for World Textile Abstracts:</b> luminescence; polyethylene; polymer blend <b>Author:</b> Blends; Luminescence; Metallocene catalysts; Polyethylene (PE); Stabilization <b>Compindex Free Language:</b> Metallocene catalysts; Metallocene catalyzed polyethylene blends; Oxidative degradation <b>Compindex Descriptor:</b> Catalysts; Chemiluminescence; Degradation; High density polyethylenes; Linear low density polyethylenes; Low density polyethylenes; Mechanical properties; Organometallics; Solubility; Thermodynamic properties <b>Compindex Mainhead:</b> Polymer blends <b>Reaxys Terms:</b> high-density polyethylene; low-density polyethylene - miscibility					

Go to Next Slide

24



General Mechanical Properties, or specific Mechanical Properties (such as Young's modulus) may easily be found through searches in the CITATION BASIC INDEX QUERYLET. Simply type in the entry field, take note of the auto-suggest terms (and perhaps use them as a guide to application of truncation)

The screenshot shows the 'Citation Basic Index' search interface. The search query 'mech\* prop\* polytetrafluor' is entered in the search box. A dropdown menu displays several suggestions: 'polytetrafluor', 'polytetrafluoroethylen', 'polytetrafluoroethylen dispersionen', 'polytetrafluoroethylene', 'polytetrafluoroethylene (ptfe)', and 'polytetrafluoroethylene'. A red arrow points from the suggestions to the search box in the second part of the screenshot, which shows the query 'mech\* prop\* polytetrafluor\*' with a 'Lookup' button.

1744 citations out of 23 reactions and 57 substances

Reactions Substances (Grid) Substances (Report) Citations go to Page Page 1 of 194

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Relevance

Title of the Document	Authors	Year	Source	Times cited
Mechanical and electrical properties of laminated polytetrafluoroethylene films	Wang, Xuewen; Lou, Kexing; Zhang, Xiaoqing; Sun, Zhuanlan; Cao, Gongxun; Xia, Zhongfu	2011	IEEE Transactions on Dielectrics and Electrical Insulation, 2011, vol. 18, # 1 art. no. 5704493, p. 57 - 63 Full Text View citing articles	

**Title/Abstract**  
**Mechanical and electrical properties of laminated polytetrafluoroethylene films**  
 Laminated polytetrafluoroethylene (PTFE) films, which are made of compact and porous PTFE layers, are prepared through the process of sintering. The corona charging technique is utilized to make the laminated PTFE films piezoelectric, thus transforming them into piezoelectrets. The crystallinity, Young's modulus in compression mode, stress-strain behavior, charge dynamics, and thermal stability of the fabricated films are investigated by particular techniques, such as differential scanning calorimetry (DSC), dielectric resonance spectra, dynamic mechanical analysis (DMA), thermally stimulated discharge (TSD) spectra, and isothermal annealing, respectively. The results reveal that the crystallinity of the fabricated PTFE films with three and five-layer systems are 79.5 and 59.8 percent, respectively. The compressive and tensile moduli at room temperature are 7.4 and 167 MPa for the three-layer system samples. The resulting temperature peak increases by 20 C as the heating rate increases from 2 to 4 C in TSD measurement. Two charge drift mechanisms exist in the films when the samples are thermally stimulated and discharged. With the increase of corona charging voltage from -10 to -25 kV, more and more detrapped charges from the deeper traps in the laminated PTFE films are released, corresponding to the current peaks identified in the temperature range from 130 to 140 °C, which prefer to drift through the solid PTFE layers. However, charges also escaped from the relevant shallow traps, corresponding to the current peaks identified in the temperature that range from 80 to 95 °C. The charge drift along the surface of the PTFE fibers is always a dominant mechanism, showing resistance of the corona charging voltage under the experimental-study conditions. The sample shows a stable piezoelectric d33 coefficient of 50 pC/N at 120 C after one day annealing at the same temperature.

**Keywords:**  
**Author:** electric property; mechanical property; piezoelectret; Polytetrafluoroethylene; thermal stability  
**Compendex Free Language:** Charge drift; Charge dynamics; Compression mode; Corona charging; Crystallinities; Current peak; Dielectric resonances; Dominant mechanism; Mechanical and electrical properties; piezoelectret; Polytetrafluoroethylene films; PTFE films; Rate increase; Room temperature; Shallow traps; Stress-strain behaviors; Temperature peaks; Temperature range; Tensile moduli; thermal stability; Three-layer systems; Young's Modulus  
**Compendex Descriptor:** Differential scanning calorimetry; Dynamic analysis; Dynamic mechanical analysis; Dynamics; Elastic moduli; Electric discharges; Isothermal annealing; Laminating; Mechanical properties; Mechanisms; Piezoelectricity; Polytetrafluoroethylenes; Sintering; Stresses; Thermodynamic stability  
**Compendex Mainhead:** Electric properties  
**Reaxys Terms:** PTFE; polytetrafluoroethylene - ambient reaction temperature; crystallinity; dielectric constant; differential scanning calorimetry; electrical property; mechanical property; piezoelectricity; sintering

# MOLECULAR FORMULA

## MOLECULAR FORMULA BUILDER

Formula:  Lookup

Classification of catalysis:  is  Lookup

### Formula Builder

Molecular Formula:

1A	2A	3B	4B	5B	6B	7B	8B	9B	10B	1B	2B	3A	4A	5A	6A	7A	8A	
1	H																He	
2	Li	Be										B	C	N	O	F	Ne	
3	Na	Mg										Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy		Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf		Es	Fm	Md	No	Lr	

more element(s)  
 with arbitrary count

Any more elements  
with any counts

Special groups:

Note: its also possible to enter

- ranges or enumerations defined via variables, e.g.  $Fe_xO_y$   $x=2,3$   $y=2-4$
- Arithmetic terms, e.g.  $C_nH_{2n+2}$   $n=3,4,5$

Classification:

Nonmetals:

Metals:

# Chrome compounds

Formula Builder

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

0  more element(s) with arbitrary count  
 Any more elements with any counts

Special groups:  
 Me  Et  Ph

Note: its also possible to enter  
 • ranges or enumerations defined via variables, e.g.  $Fe_xO_y$  x=2,3 y=2-4  
 • Arithmetic terms, e.g.  $C_nH_{2n+2}$  n=3,4,5

Formula Builder

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

Selected Element definition:  
 Cr  
 Charge(s): [ ]  
 Count(s): 1 - 10  
 Add

0  more element(s) with arbitrary count  
 Any more elements with any counts

Special groups:  
 Me  Et  Ph

Note: its also possible to enter  
 • ranges or enumerations defined via variables, e.g.  $Fe_xO_y$  x=2,3 y=2-4  
 • Arithmetic terms, e.g.  $C_nH_{2n+2}$  n=3,4,5

Query Results Synthesis Plans History Report My Alerts My Settings Help

Start Over

Ask Reaxys e.g. Ask Reaxys about reaction type 'phosphorylation' reactions  
 Smart searching with Ask Reaxys. See examples >

Reactions Substances Literature ReaxysTree Physical Spectra Natural Product Advanced

Molecular Formula  
 Lookup  Formula Builder

Identification  
 Reaxys Registry Number =  Lookup   
 CAS Registry Number is  Lookup   
 Chemical Name is  Lookup   
 Element Symbols is  Lookup

Show AND Buttons

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

Formula Builder

Molecular Formula:   Use this Formula

0  more element(s) with arbitrary count  
 Any more elements with any counts









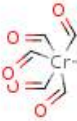



Special groups:  
 Me  Et  Ph

Note: its also possible to enter  
 • ranges or enumerations defined via variables, e.g.  $Fe_xO_y$  x=2,3 y=2-4  
 • Arithmetic terms, e.g.  $C_nH_{2n+2}$  n=3,4,5

# CHROME COMPOUNDS

Reactions (73206) Substances (75389) Citations (40652) go to Page  Page 1 of 8377

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as:

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	N° of ref.
 1    Synthesize   Show Details Find similar	<b>Chemical Name:</b> chromium <b>Reaxys Registry Number:</b> 3587157 <b>CAS Registry Number:</b> 7440-47-3 <b>Molecular Formula:</b> Cr <b>Linear Structure Formula:</b> Cr <b>Molecular Weight:</b> 51.996 <b>InChI Key:</b> VYZAMTAEIAYCRO-UHFFFAOYSA-N	241 prep out of 5933 reactions.	Identification Physical Data (2290) Spectra (28) Bioactivity (3) Use/Application (387) Quantum Chemical Data (172)	5685
 2    Synthesize   Show Details Find similar	<b>Chemical Name:</b> Catalyst M-Chromium oxide <b>Reaxys Registry Number:</b> 11323461 <b>Type of Substance:</b> Glass or Ceramic material/Isotope or isotope containing compound <b>Molecular Formula:</b> Cr <sub>2</sub> O <sub>3</sub> <b>Linear Structure Formula:</b> (Cr <sub>2</sub> O <sub>2</sub> )O <b>Molecular Weight:</b> 151.99 <b>InChI Key:</b> OWYUGDPRPMNASD-UHFFFAOYSA-N	739 prep out of 4138 reactions.	Identification Physical Data (799) Spectra (101) Bioactivity (2) Use/Application (51) Quantum Chemical Data (23)	3509
 3    Synthesize   Show Details Find similar				

Find substances that contain Cr and C

Reactions Substances Literature ReaxysTree Physical Spectra Natural Product

Molecular Formula

Molecular Formula  Lookup

# CHROME COMPOUNDS

Reactions (52445) Substances (53819) Citations (18602)

Limit to Exclude Export Print Zoom in Zoom out Hide

All carbon + chromium-containing substances

Query Results Synthesis Plans **History** Report My Alerts My Settings Help

Reaxys PubChem eMolecules

Select how you want to combine the hitsets

Merge 3 with 6 Overlap 3 with 6 Exclude 3 from 6 **Exclude 6 from 3**

Cancel

All "inorganic" chromium-containing substances

Combine hitsets

Select at least two hitsets for combining

	Query	Temporary result description
<input checked="" type="checkbox"/>	<a href="#">Edit</a> <a href="#">Create Alert</a> Substances: Molecular Formula = 'Cr[1-10]C[1-100]*'	53819 substances Substances: Molecular Formula = 'Cr[1-10]C[1-100]*' 52445 reactions 18602 citations
<input checked="" type="checkbox"/>	<a href="#">Edit</a> <a href="#">Create Alert</a> Substances: Molecular Formula = 'Cr[1-10]*'	75389 substances Substances: Molecular Formula = 'Cr[1-10]*' 73206 reactions 40652 citations

All carbon + chromium-containing substances

All chromium-containing substances

# CHROME COMPOUNDS (Yellow Inorganics)

Reactions **Substances** Literature ReaxysTree Physical Spectra Natural Product Advanced

Molecular Formula  Lookup

Identification

Reaxys Registry Number =  Lookup

CAS Registry Number is  Lookup

Chemical Name is  Lookup

Element Symbols is  Lookup

Show AND Buttons

Physical Data

Colour & Other Properties is  Lookup

Show AND Buttons

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



> 900,000  
YELLOW SUBSTANCES

# CHROME COMPOUNDS (Yellow Inorganics)

Query Results Synthesis Plans **History** Report My Alerts My Settings Help

Reaxys PubChem eMolecules

Select how you want to combine the hitsets

Merge 9 with 15  
Overlap 9 with 15  
Exclude 9 from 15  
Exclude 15 from 9

Cancel

---

Combine hitsets



Select at least two hitsets for combining

Query	Temporary result description
<input checked="" type="checkbox"/> 15 <input type="checkbox"/> 14 <input type="checkbox"/> 13 <input type="checkbox"/> 12 <input type="checkbox"/> 11 <input type="checkbox"/> 10	<p><a href="#">Edit</a> <a href="#">Create Alert</a></p> <p>Substances: Colour &amp; Other Properties = 'yellow'</p> <p>909053 substances Substances: Colour &amp; Other Properties = 'yellow'</p> <p>9935155 reactions</p> <p>1793757 citations</p>
<input checked="" type="checkbox"/> 9 <input type="checkbox"/> 8 <input type="checkbox"/> 7	<p>7 substances filtered by Molecular Weight</p> <p>5 reactions</p> <p>4 citations</p> <p>21570 substances Subtract 2 items from History</p> <p>28383 reactions</p> <p>26732 citations</p>

# CHROME COMPOUNDS (Yellow Inorganics)

Reactions (5407) Substances (250) Citations (6884) go to Page  Page 1 of 28

Link to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as:

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	N° of ref						
 Synthesize   Hide Details Find similar	<b>Chemical Name:</b> chromium(VI) oxide <b>Reaxys Registry Number:</b> 10773376 <b>Type of Substance:</b> Glass or Ceramic material/Isotope or isotope containing compound <b>Molecular Formula:</b> CrO <sub>3</sub> <b>Linear Structure Formula:</b> CrO <sub>3</sub> <b>Molecular Weight:</b> 99.9942 <b>InChI Key:</b> LXMQZGGLHVSEBA-UHFFFAOYSA-N	102 prep out of 1355 reactions.	Hit Data (1) Identification Physical Data (291) Spectra (33) Bioactivity (3) Use/Application (22) Quantum Chemical Data (8)	1968						
<b>Chemical Names and Synonyms</b> chromium(VI) oxide, chromium(IV) trioxide, chromic anhydride, chromium trioxide, chromium oxide, CrO <sub>3</sub> , ruthenium(IV) oxide										
<b>Hit Data</b> <b>Crystal Property Description ( 1 Hits out of 15 view all )</b>										
<table border="1"> <thead> <tr> <th>Colour &amp; Other Properties</th> <th>Comment</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>yellow</td> <td>water</td> <td> <b>Oehlm, L. W.</b>            Suomen Kemistiseuran Tiedonantoja, <b>1940</b>, vol. 49, p. 9 - 13  <a href="#">Full Text</a> <a href="#">Show Details</a>  <b>Gmelin Handbook:</b> Cr: MVol.B, 66, page 132 - 134  <a href="#">Full Text</a> <a href="#">Show Details</a> </td> </tr> </tbody> </table>		Colour & Other Properties	Comment	Reference	yellow	water	<b>Oehlm, L. W.</b> Suomen Kemistiseuran Tiedonantoja, <b>1940</b> , vol. 49, p. 9 - 13 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Cr: MVol.B, 66, page 132 - 134 <a href="#">Full Text</a> <a href="#">Show Details</a>			
Colour & Other Properties	Comment	Reference								
yellow	water	<b>Oehlm, L. W.</b> Suomen Kemistiseuran Tiedonantoja, <b>1940</b> , vol. 49, p. 9 - 13 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Cr: MVol.B, 66, page 132 - 134 <a href="#">Full Text</a> <a href="#">Show Details</a>								
Identification Physical Data Spectra Bioactivity Use/Application Quantum Chemical Data										
 Synthesize   Hide Details Find similar	<b>Chemical Name:</b> potassium dichromate <b>Reaxys Registry Number:</b> 11322242 <b>Type of Substance:</b> Coordination compound <b>Molecular Formula:</b> Cr <sub>2</sub> O <sub>7</sub> *2K <b>Linear Structure Formula:</b> 2K(1+)*Cr <sub>2</sub> O <sub>7</sub> (2-) <b>Molecular Weight:</b> 294.184 <b>InChI Key:</b> IMNUAUFMVCNBHR-UHFFFAOYSA-N	69 prep out of 774 reactions.	Hit Data (3) Identification Physical Data (330) Spectra (73) Bioactivity (3) Use/Application (11)	1472						
<b>Chemical Names and Synonyms</b> potassium dichromate, K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> , PDC, potassium bichromate, Potassium dichromate, bichromate potassium, potassium chromate										
<b>Hit Data</b> <b>Crystal Property Description ( 3 Hits out of 11 view all )</b>										
<table border="1"> <thead> <tr> <th>Colour &amp; Other Properties</th> <th>Comment</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>yellow</td> <td>liq. SO<sub>2</sub></td> <td> <b>Shatenshtein, A. I.; Viktorov, M. M.</b>            Acta physicochim. URSS, <b>1937</b>, vol. 7, p. 883 - 898  <a href="#">Full Text</a> <a href="#">Show Details</a>  <b>Shatenshtein, A. I.; Viktorov, M. M.</b>            Zhurnal Fizicheskoi Khimii, <b>1938</b>, vol. 11, p. 18 - 27  <a href="#">Full Text</a> <a href="#">Show Details</a>  <b>Gmelin Handbook:</b> Cr: MVol.B, 261, page 578 - 580  <a href="#">Full Text</a> <a href="#">Show Details</a>  <b>Cady, H. P.; Taft, R.</b>            Journal of Physical Chemistry, <b>1925</b>, vol. 29, p. 1075 - 1084  <a href="#">Full Text</a> <a href="#">Show Details</a> </td> </tr> </tbody> </table>		Colour & Other Properties	Comment	Reference	yellow	liq. SO <sub>2</sub>	<b>Shatenshtein, A. I.; Viktorov, M. M.</b> Acta physicochim. URSS, <b>1937</b> , vol. 7, p. 883 - 898 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Shatenshtein, A. I.; Viktorov, M. M.</b> Zhurnal Fizicheskoi Khimii, <b>1938</b> , vol. 11, p. 18 - 27 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Cr: MVol.B, 261, page 578 - 580 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Cady, H. P.; Taft, R.</b> Journal of Physical Chemistry, <b>1925</b> , vol. 29, p. 1075 - 1084 <a href="#">Full Text</a> <a href="#">Show Details</a>			
Colour & Other Properties	Comment	Reference								
yellow	liq. SO <sub>2</sub>	<b>Shatenshtein, A. I.; Viktorov, M. M.</b> Acta physicochim. URSS, <b>1937</b> , vol. 7, p. 883 - 898 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Shatenshtein, A. I.; Viktorov, M. M.</b> Zhurnal Fizicheskoi Khimii, <b>1938</b> , vol. 11, p. 18 - 27 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Cr: MVol.B, 261, page 578 - 580 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Cady, H. P.; Taft, R.</b> Journal of Physical Chemistry, <b>1925</b> , vol. 29, p. 1075 - 1084 <a href="#">Full Text</a> <a href="#">Show Details</a>								



# borosilicate glass

Select index items and click 'Transfer'

**Reaxys**

Search for: borosilicate glass

- borosilicate glass (4400)
- borosilicate glass (bsg) (2)
- borosilicate glass - x-ray irradiation (1)
- borosilicate glass abrasive wear (1)
- borosilicate glass acrylic (1)
- borosilicate glass airheaters (1)
- borosilicate glass as ph sensitive gate (1)
- borosilicate glass batches (2)
- borosilicate glass beads (1)
- borosilicate glass bk7 (1)
- borosilicate glass bonded grinding materials (1)
- borosilicate glass bonded substrates (1)
- borosilicate glass capillary (28)
- borosilicate glass capillary tubes (1)
- borosilicate glass chamber (1)
- borosilicate glass characterization (1)
- borosilicate glass coating (1)
- borosilicate glass coating films (1)
- borosilicate glass coatings (2)
- borosilicate glass column (1)

Page  407436 of 2002537

Transfer Reset Cancel

Power of lookup

### INITIAL ALLOY SEARCH OPTIONS

Identification

Alloy Composition  exists ✕

Formula   ✕

Show AND Buttons

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

Ask Reaxys **BETA**

Enter a keyword, concept or author

Go

#### Component Formula

#### Percentage

Number or range: 20 or 20-40

Percentage Type:

Additional Components:

Structure	Structure/Compound Data	Nº of preparations All Props.   All Reactions	Available Data
mixture (composition completely given): titanium aluminum vanadium  	<b>Chemical Name:</b> Ti-6Al-4V  <b>Reaxys Registry Number:</b> 16552591 <b>Type of Substance:</b> mixture (composition completely given)Alloy	0 prep out of 1 reactions.	Physical Data (55) Bioactivity (1) Use/Application (1)
mixture (composition completely given): titanium aluminum vanadium  	<b>Chemical Name:</b> Ti6V  <b>Reaxys Registry Number:</b> 16011805 <b>Type of Substance:</b> mixture (composition completely given)Alloy	0 prep out of 1 reactions.	Physical Data (15) Spectra (1)

Title of the Doc

Ask Reaxys **BETA**

Ti6Al4V

Go

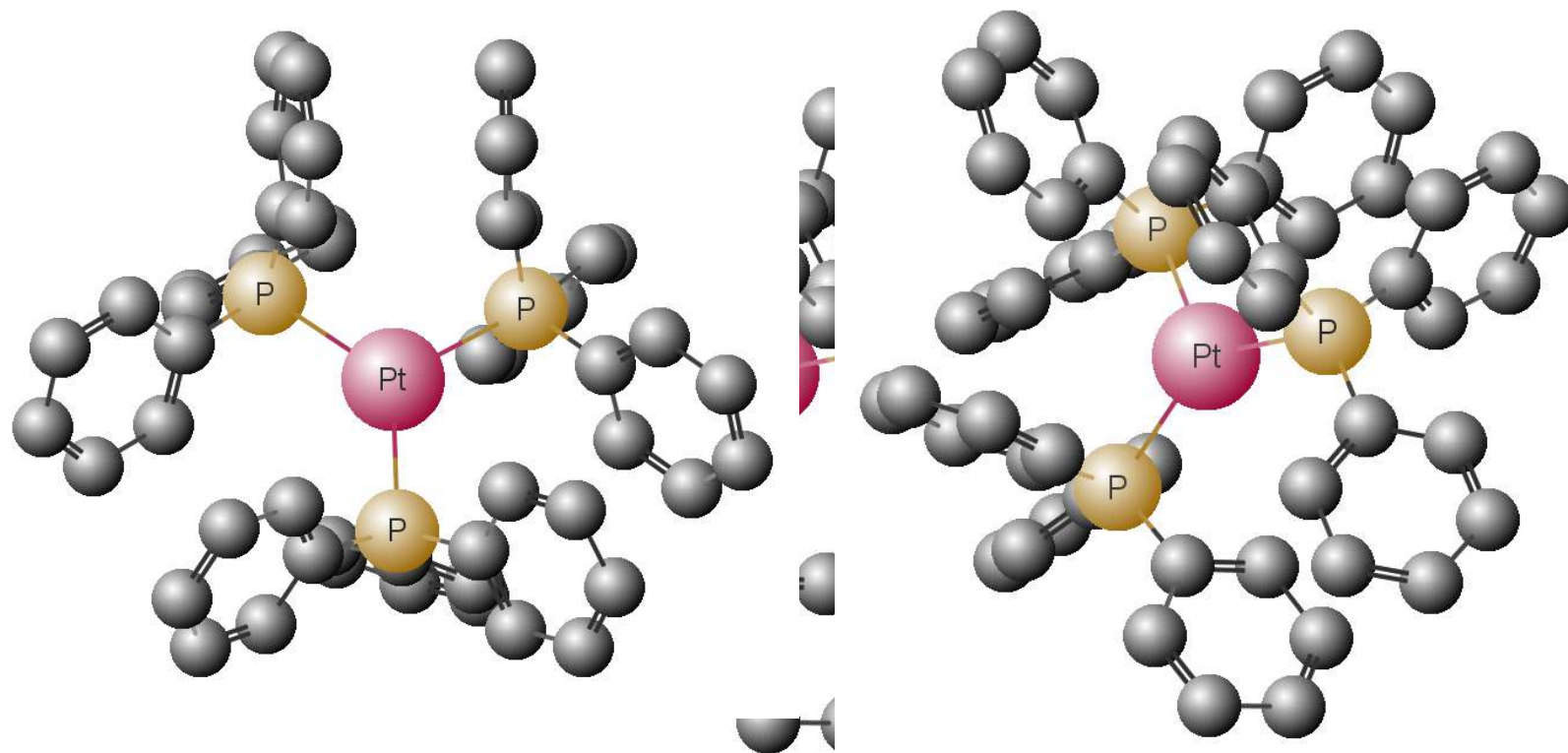
Items cited

SEARCHED	FOUND	ITEMS CITED
		32

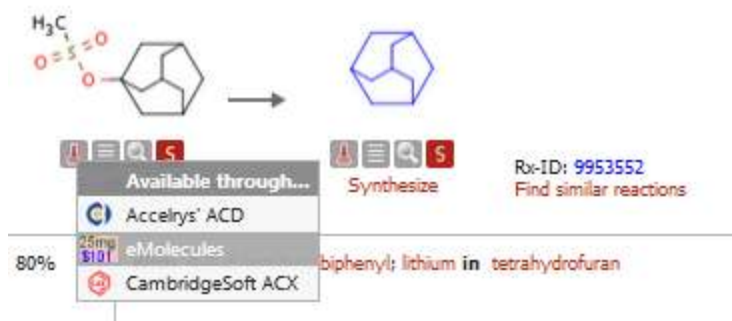
**Abstract**  
A study of the potentials achieved during mechanical abrasion and the repassivation rate of titanium and Ti6Al4V in inorganic buffer solutions and bovine serum. Titanium alloys in orthopedic implants are susceptible to mechanical disruption of the passive film (treating corrosion). To study this effect, open-circuit potential (ocp) measurements before, during and after mechanical disruption of the passive film in a half-cell electrochemical cell on commercial pure titanium and Ti6Al4V alloy in inorganic buffer solutions in the pH range from 2.0 to 12.0 and calf bovine serum at pH 4.0 and 7.0 are reported. Additionally, the effect of pH, electrolyte and sample composition on the repassivation rate has been investigated. The potentials achieved during the abrasion of Ti6Al4V are the same as those observed during pure titanium, which indicates that the corrosion current of both materials in the active state is due to the oxidation of titanium. However, commercial pure titanium displays a tendency to repassivate faster than Ti6Al4V in inorganic buffer solutions thanks to the lower critical current density and the higher cathodic activity towards the hydrogen evolution reaction observed on the pure metal in comparison with the alloy. Proteinaeous solutions like bovine serum, significantly slow down the anodic dissolution and the cathodic reactions both on titanium and the alloy. However, the repassivation rate of the Ti6Al4V is not affected by serum, while that of pure titanium significantly decreases both at pH 4.0 and 7.0.

**Keywords:**  
**Author:** Anodic reaction; Bovine serum; Cathodic reaction; Repassivation rate; Ti6Al4V; Titanium  
**Compound Free Language:** Anodic reaction; Bovine serum; Cathodic reaction; Repassivation rate; Ti6Al4V  
**Compound Descriptor:** Body fluid; Cobalt; Corrosion resistance; Current density; Electrochemistry; Implants (surgical); Oxidation; Reaction kinetics  
**Compound Meshhead:** Titanium alloy.

# ROTATE 3D VIEW



# 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 Dotmatic'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 (156.105.0.72)

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Report Date: Synthesis Plan: Synthesis 4 Created: 2013-09-03 18:23 Modified: 2013-09-03 18:23 [View Details](#) [Remove](#) [Annotation](#)

Report Date: IDE-XDR: 67944 Created: 2013-09-03 18:29 Modified: 2013-09-03 18:30 [Show Substances](#) [Mark Up](#) [Move Down](#) [Remove](#) [Annotation](#)

**Decomposition**

Decomposition	Location	Reference
210 - 221 °C	supporting information	Ohsumi, Ken; Yamu, Takahiro; Suzuki, Kenzoku. Organic and Biomolecular Chemistry, 2013, vol. 11, p. 2003 - 2006 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>

Report Date: IDE-XDR: 67944 Created: 2013-09-03 18:29 Modified: 2013-09-03 18:30 [Show Substances](#) [Mark Up](#) [Remove](#) [Annotation](#)

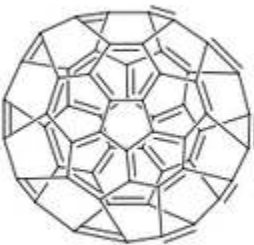
**Dissociation Exponent**

Dissociation Exponent (pK)	Dissociation Group	Method	Type	Comment	Reference
7.68	OH	spectrophotometric	dissociant	DE	Hladnik, Haljarmut; Szymanski, Henryk; Gluszczynska-Swiglo, Anna; Tyrolkowska, Sozena; Bietjes, Joenne M. C. H. Journal of Agricultural and Food Chemistry, 2008, vol. 56, # 3, p. 818 - 822 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>
0.89242 - 0.18203	OH		dissociant	in the presence of salts	Kamamoto, Hiroyuki; Sonda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Hisaaki. Bioscience, Biotechnology, and Biochemistry, 2001, vol. 45, # 1, p. 125 - 132 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>
-1.02938	OH		dissociant		Kamamoto, Hiroyuki; Sonda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Hisaaki. Bioscience, Biotechnology, and Biochemistry, 2001, vol. 45, # 4, p. 125 - 132 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>

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# INTEROPERABILITY

Structure



As drawn  
Substructure  
on heteroatoms  
on all atoms  
Similarity

Include tautomers  
Ignore stereo  
No salts  
No mixtures  
No isotopes  
No charges  
No radicals  
No ring closures  
Align results with query

By name search in Reaxys

Create Structure Template from

"Magic number" carbon clusters:  
ionization potentials and selective  
reactivity

Zimmerman, Jeffrey A.; Eyler, John  
R.; Bach, Stephan B.H.; McElvany,  
Stephen W.

1991

Journal of Chemical Physics, 1991, vol. 94, # 5 p. 3556 - 3562  
Full Text [View citing articles](#)

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"Magic number" carbon clusters: Ionization potentials and selective reactivity

Zimmerman J.A., Eyler J.R., Bach S.B.H., McElvany S.W.

(1991) The Journal of Chemical Physics, 94 (5) , pp. 3556-3562.

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145 documents [Analyze search results](#)

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Refine

Limit to Exclude

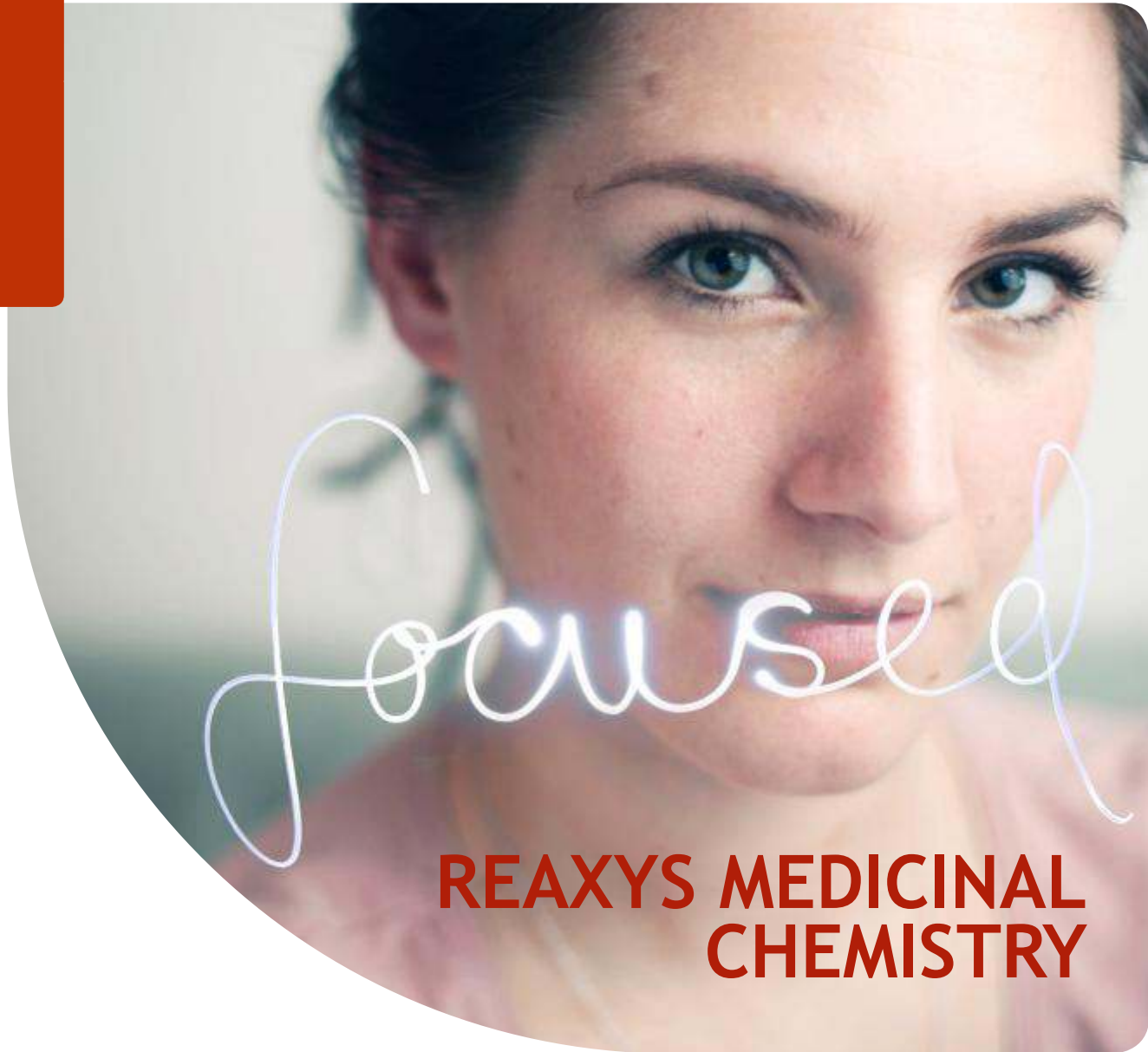
Year

- 2015 (3)
- 2014 (4)
- 2013 (2)
- 2012 (1)
- 2011 (4)

Author Name

- Bohme, D.K. (9)
- Echt, O. (7)
- Petrie, S. (6)

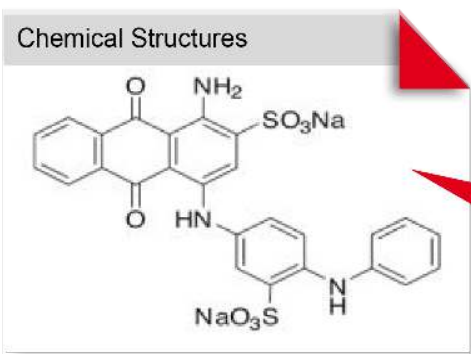
<input type="checkbox"/> Fragment approach to constrained density functional theory calculations using Daubechies wavelets 1	Ratcliff, L.E., Genovese, L., Mohr, S., Deutsch, T.	2015	Journal of Chemical Physics	0
<a href="#">Full Text</a> View at Publisher				
<input type="checkbox"/> On the dynamics of photo-electrons in C<math>_{60}</math> 2	Gao, C.-Z., Wopperer, P., Dinh, P.M., Suraud, E., Reinhard, P.-G.	2015	Journal of Physics B: Atomic, Molecular and Optical Physics	0
<a href="#">Full Text</a> View at Publisher				
<input type="checkbox"/> First-principles photoemission spectroscopy and orbital tomography in molecules from koopmans-compliant functionals 3	Nguyen, N.L., Borghi, G., Ferretti, A., Dabo, I., Marzari, N.	2015	Physical Review Letters	1
<a href="#">Full Text</a> View at Publisher				
<input type="checkbox"/> Laboratory formation of fullerenes from PAHS: Top-down interstellar chemistry 4	Zhen, J., Castellanos, P., Paardekooper, D.M., Linnartz, H., Tielens, A.G.G.M.	2014	Astrophysical Journal Letters	3



**REAXYS MEDICINAL  
CHEMISTRY**



# ESSENTIAL INFORMATION: 100+ EXPERIMENTAL FIELDS



**High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet P2Y<sub>12</sub> Receptors**

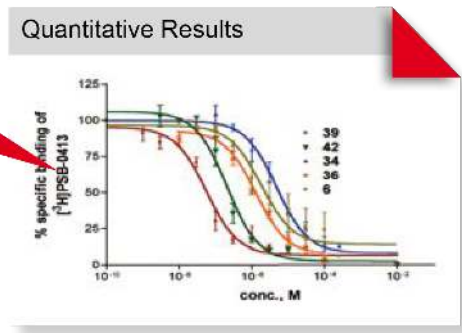
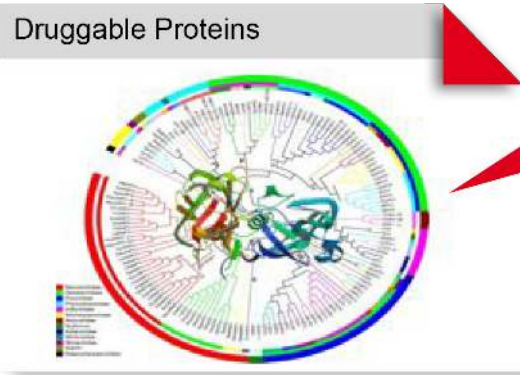
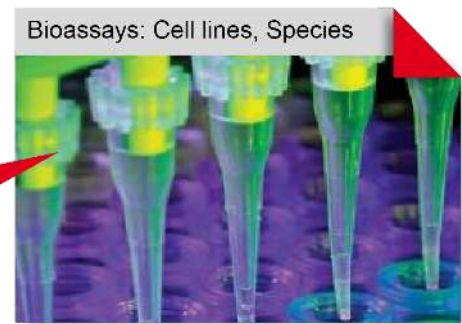
Younis Bag,<sup>1</sup> Kerim Arslan,<sup>1</sup> Meyren Khat,<sup>1</sup> Martin Glöckl,<sup>1,2</sup> and Christa E. Miller<sup>1\*</sup>

*Pharmazentrum Bonn Pharmaceutical Institute, Pharmaceutical Sciences Area (PSB), University of Bonn, An der Leyboldstr. 4, D-53123 Bonn, Germany; Department of Experimental and Clinical Pharmacology and Toxicology, Albert-Ludwigs 25, D-78104 Freiburg, Germany*

Received March 26, 2009

Adenine- and pyrimidine-derivatives related to the moderately potent, nonselective P2Y<sub>12</sub> receptor antagonist reactive Mar 2 (6) have been synthesized and optimized with respect to P2Y<sub>12</sub> receptor affinity. A sulfonamide binding moiety utilizing human blood platelet membranes and the P2Y<sub>12</sub> receptor-selective antagonist radioligand [<sup>3</sup>H]propylthioinosinic-5'-adenylic acid (1,1-dichloro-1-phenylmethylethyl-1-phenylthio) imide ([<sup>3</sup>H]PSB-0413) was applied for compound testing. 1-Amino-2-sulfonamide-quinoline derivatives bearing a 2-phenylamino-ethoxy substitution in the 4-position and an additional acidic function in the meta-position of the sulfonamide ring showed high P2Y<sub>12</sub> receptor affinity. These new adenine-derivatives became accessible by a recently developed copper(II)-catalyzed Ullmann coupling reaction of 1-amino-4-bromo-2-quinolinecarboxylic acid derivatives with sulfonamide phosphonic acid derivatives. The most potent compounds exhibited K<sub>d</sub> values of 24.9 nM (1-amino-4-[4-phenylamino-5-carboxyphenylamino]-6,10-dioxo-9,10-dihydro-2H-benzothiazine-2-one), PSB-0739, 39, and 2.10 nM (1-amino-4-[4-phenylamino-3-carboxyphenylamino]-6,10-dioxo-9,10-dihydro-2H-benzothiazine-2-one), PSB-0742, 41, respectively. 1-Amino-7-oxido-4-sulfonamide-2-quinolinecarboxylic acid derivatives were also tested and found to be inactive.

**Reaxys Medical Chemistry Excerpt**

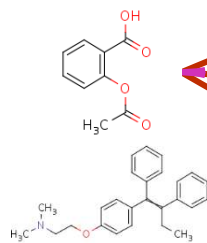


**Reaxys Medical Chemistry excerpts all the relevant Quantitative data**

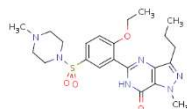
# ... BUT IT'S NOT THAT SIMPLE, MEDICINAL CHEMISTS FOR INSTANCE NEED TO COLLECT, ORGANIZE AND COMPARE INFORMATION FROM DIFFERENT SOURCES... THIS IS TIME CONSUMING AND ERROR PRONE



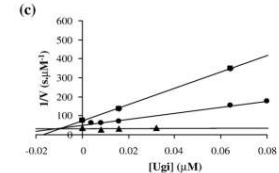
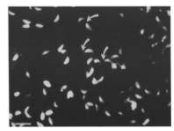
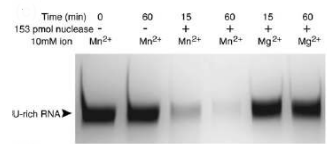
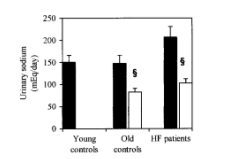
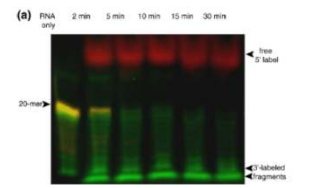
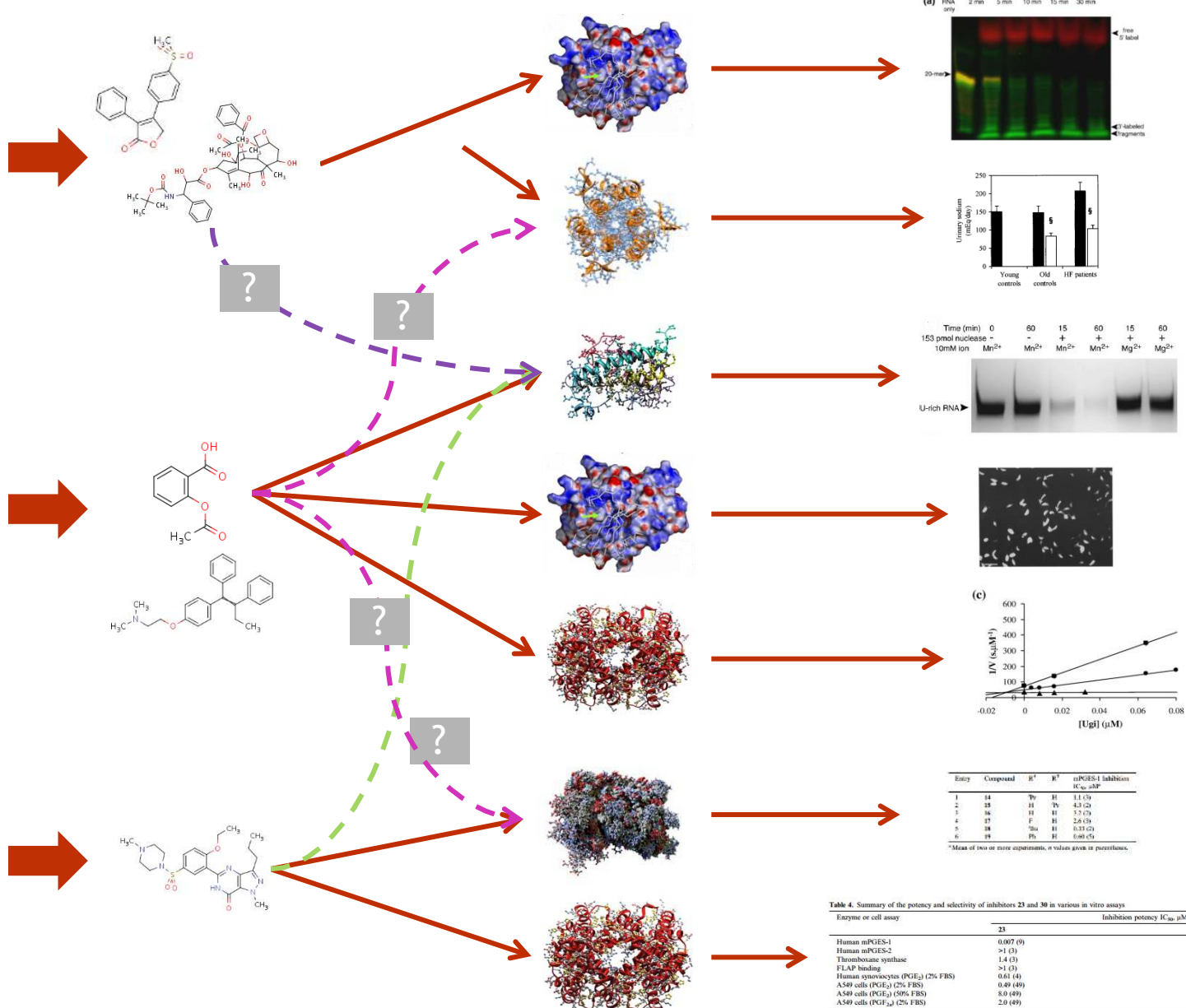
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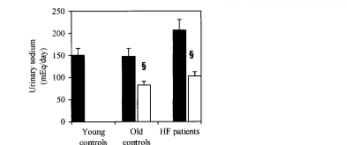
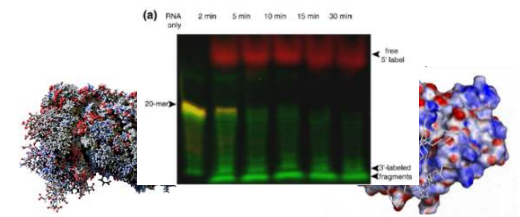
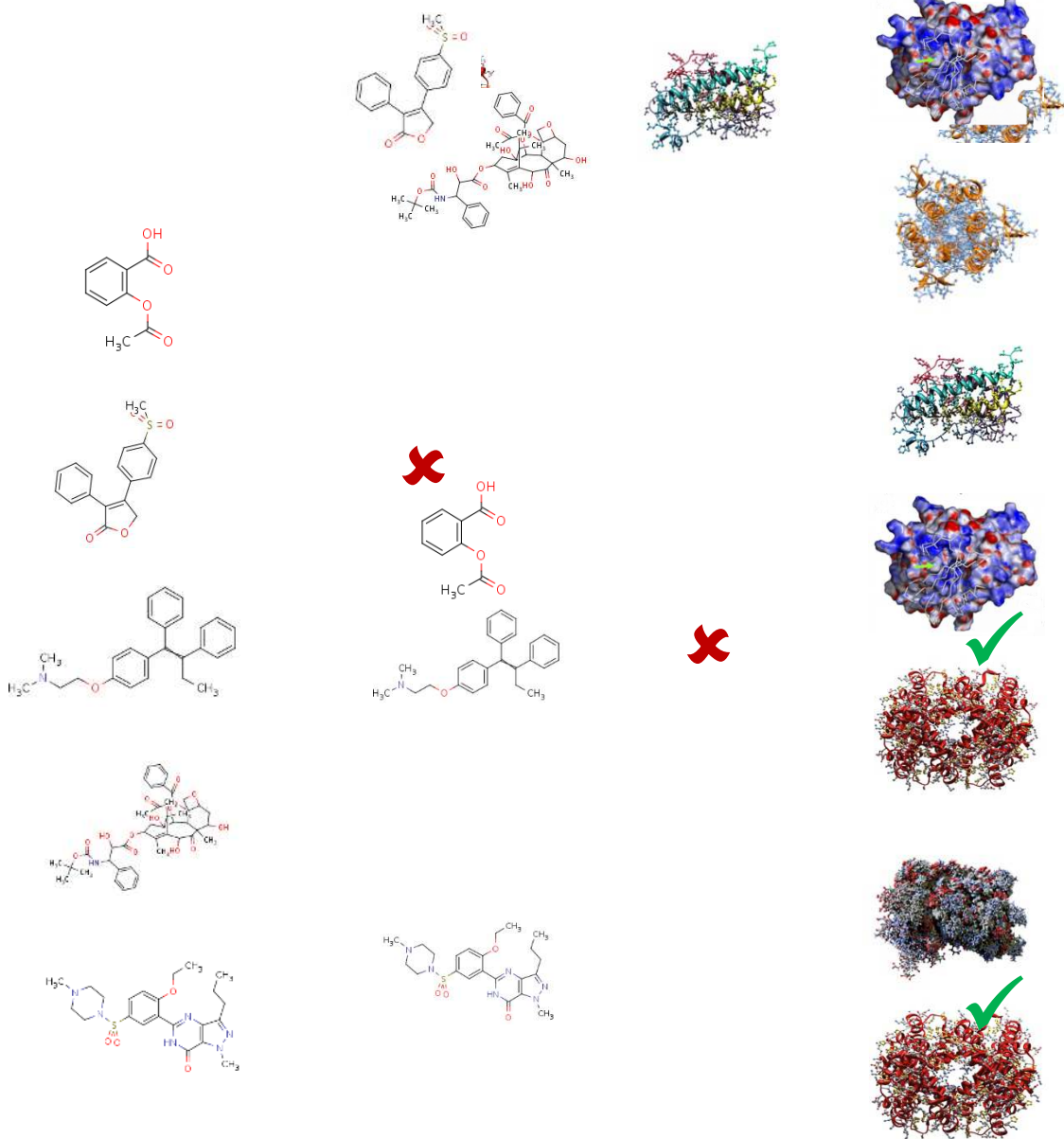
Entry	Compound	R <sup>2</sup>	R <sup>1</sup>	αPGES-1 inhibition IC <sub>50</sub> μM <sup>a</sup>
1	14	0.79	H	1.1 (3)
2	18	0.71	H	4.1 (3)
3	16	0.71	H	3.7 (3)
4	17	0.65	F	2.8 (3)
5	14	0.50	H	0.33 (2)
6	18	0.69	H	0.69 (3)

<sup>a</sup>Mean of two or more experiments, n values given in parentheses.

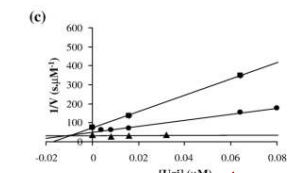
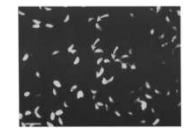
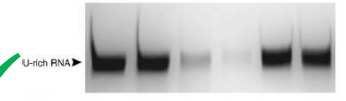
**Table 4.** Summary of the potency and selectivity of inhibitors 23 and 30 in various in vitro assays

Enzyme or cell assay	Inhibition potency IC <sub>50</sub> μM <sup>a</sup>	
	23	30
Human mPGES-1	0.007 (9)	0.003 (8)
Human mPGES-2	>1 (3)	>1 (3)
Thromboxane synthase	1.4 (3)	0.95 (3)
FLAP binding	>1 (3)	>1 (3)
Human xenopuscytus (PGE <sub>2</sub> ) (2% FBS)	0.65 (4)	0.25 (3)
A549 cells (PGE <sub>2</sub> ) (2% FBS)	0.49 (49)	0.27 (3)
A549 cells (PGE <sub>2</sub> ) (50% FBS)	8.0 (49)	5.8 (3)
A549 cells (PGE <sub>2</sub> ) (2% FBS)	2.0 (49)	2.4 (3)

# ... BUT IT'S NOT THAT SIMPLE, MEDICINAL CHEMISTS FOR INSTANCE NEED TO COLLECT, ORGANIZE AND COMPARE INFORMATION FROM DIFFERENT SOURCES... THIS IS TIME CONSUMING AND ERROR PRONE



Time (min) 0 60 15 60 15 60  
 153 pmol nuclease - - + + +  
 Mn<sup>2+</sup> Mn<sup>2+</sup> Mn<sup>2+</sup> Mn<sup>2+</sup> Mg<sup>2+</sup> Mg<sup>2+</sup>



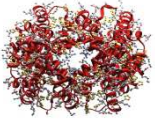
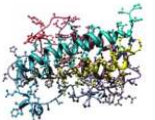
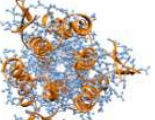

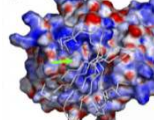
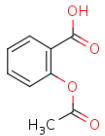
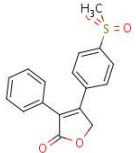
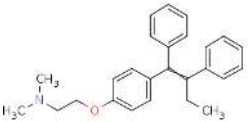
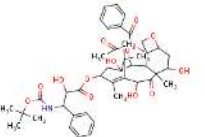
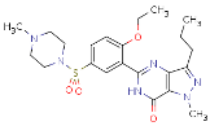
Entry	Compound	R <sup>2</sup>	R <sup>1</sup>	siPGES-1 inhibition IC <sub>50</sub> μM*
1	14	0.79	H	3.1 (3)
2	18	0.11	H	4.1 (3)
3	16	0.11	H	3.3 (3)
4	17	0.61	F	2.8 (3)
5	14	0.91	H	0.33 (2)
6	18	0.79	H	0.69 (3)

\*Mean of two or more experiments, a value given in parentheses.

**Table 4.** Summary of the potency and selectivity of inhibitors 23 and 30 in various in vitro assays

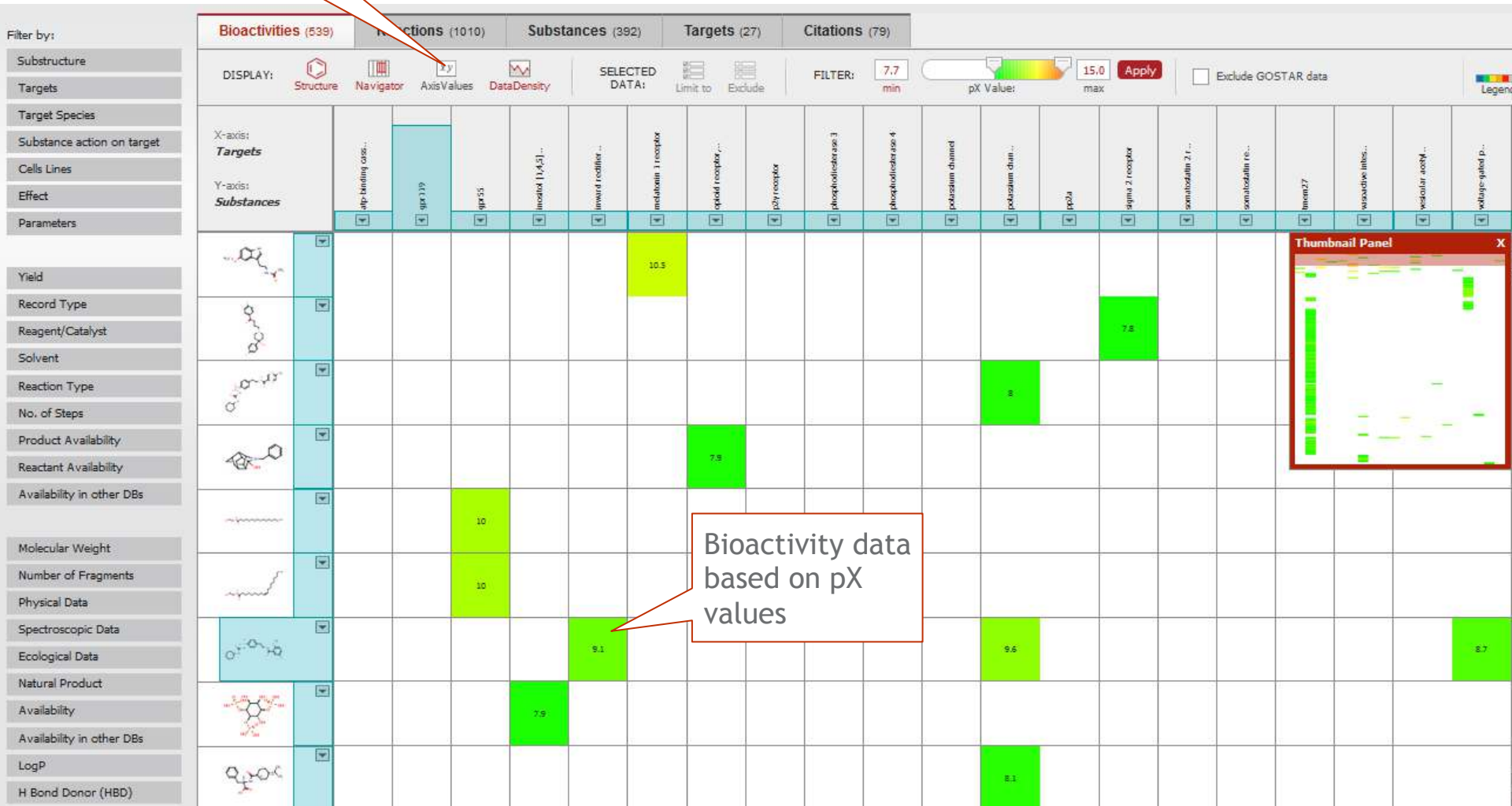
Enzyme or cell assay	Inhibition potency IC <sub>50</sub> μM*	
	23	30
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Human mPGES-2	>1 (3)	>1 (3)
Thromboxane synthase	1.4 (3)	0.95 (3)
FLAP binding	>1 (3)	>1 (3)
Human synovocytes (PGE <sub>2</sub> ) (2% FBS)	0.61 (4)	0.25 (3)
A549 cells (PGE <sub>2</sub> ) (2% FBS)	0.49 (49)	0.27 (3)
A549 cells (PGE <sub>2</sub> ) (50% FBS)	8.0 (49)	5.8 (3)
A549 cells (PGE <sub>2</sub> ) (2% FBS)	2.0 (49)	2.4 (3)

AND TO MAKE A DECISION ON WHICH EXPERIMENT TO DO, YOU WANT TO ORGANIZE YOUR CONTENT, NORMALIZE AND COMPARE, TO UNDERSTAND WHICH COMPOUND INTERACTS WITH WHICH TARGET AND TRIGGER WHICH BIOLOGICAL EFFECT—THAT'S A LOT OF MANUAL WORK!

					
	✓	✓	✓	✗	✓
	✗	✗	✗	✓	✗
	✓	✗	✓	✗	✓
	✗	✗	✗	✗	✗
	✓	✓	✓	✓	✓

# RESULTS VIEW - HEATMAP

Manage X and Y axis



Bioactivity data based on pX values

7.9

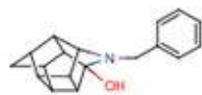
X-axis: Targets

Y-axis: Substances

Select value type: MAX

1 substances and 1  
bioactivities

Structure



Hide Details

Structure/Compound Data

**Chemical Name:**

N-benzyl-4-azaheptacyclo[5.4.1.0.2,6.0.0.5,9,08,11]dodecan-3-ol

**Reaxys Registry Number:** 1476838**CAS Registry Number:** 33226-57-2**Type of Substance:** heterocyclic**Molecular Formula:** C<sub>18</sub>H<sub>19</sub>NO**Linear Structure Formula:** C<sub>18</sub>H<sub>19</sub>NO**Molecular Weight:** 265.355**InChI Key:** YSEXVIPNIGQQMN-UHFFFAOYSA-N**Highest Clinical Phase:** Preclinical**Chemical Names and Synonyms**

N-benzyl-4-azaheptacyclo[5.4.1.0.2,6.0.0.5,9,08,11]dodecan-3-ol

**Druglikeness**

Lipinski rules component	
Molecular Weight	265.355
logP	2.434
HBA	2
HBD	1
Matching Lipinski Rules	4
Veber rules component	
Polar surface Area (PSA)	23.47
Rotatable bond count	2
Matching Veber rules	2

**Bioactivity****In vitro: Efficacy (1)****Quantitative Results**

Parameter	Value (qual)	Value (quant)	Unit	Action on Target	Target	Target subunit	Target Species	Tissue/Organ	Cell	Bioassay	Dose	Effect	Reference (ex
K <sub>i</sub>	=	12	nM	Radioligand (/ligand)	Opioid Receptor, Sigma 2		Rat		PC12		= 100 μM	binding activity	Bioorganic and Title/Abstract



H

# RMC 2 CONTENT

## Patents Origin and starting date

>90 000 Patents

- US : 1971-present
- EP : 1979-present
- WO : 1978-present (English only)
- Patents are coming from the A61K class mainly but not only.

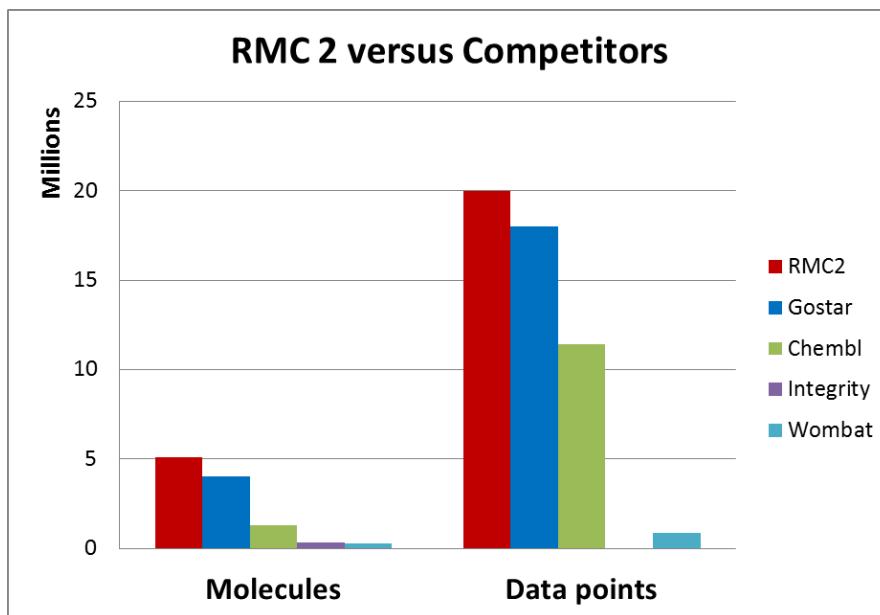
## Articles and Journals

- >5000 Journals Covered
- >230 000 Articles
- From 1980 to Present

## Drugable Targets

- >9000 Drugable Targets

« The most comprehensive medicinal chemistry solution on the market »



# EXPORT CAPABILITIES



# RMC2 EXPORT AND OUTPUT CAPABILITIES



## Reaxys: Output Substance Results

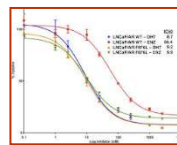
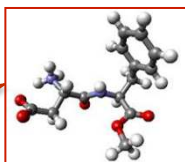
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<input type="radio"/> PDF/Print	<input type="radio"/> XML	<input type="radio"/> Literature Management Systems (e.g. ReferenceManager, EndNote etc.)	<input type="radio"/> RD File
	<input type="radio"/> Microsoft Word	<input type="radio"/> Electronic Lab Notebook	<input checked="" type="radio"/> SD/Molfile
	<input checked="" type="radio"/> Microsoft Excel		<input type="radio"/> Smiles



RMC2 Export format includes :  
- XML, Excel, SD file

RMC2 Export includes :  
- Substances and Physchem properties  
- Bioactivities and Bioassays  
- Targets  
- Bibliographic references



RMC2 Export is compatible with :  
- Pipeline pilot  
- Spotfire Etc...

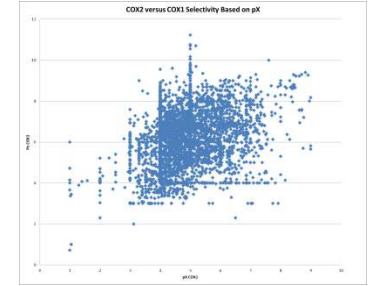
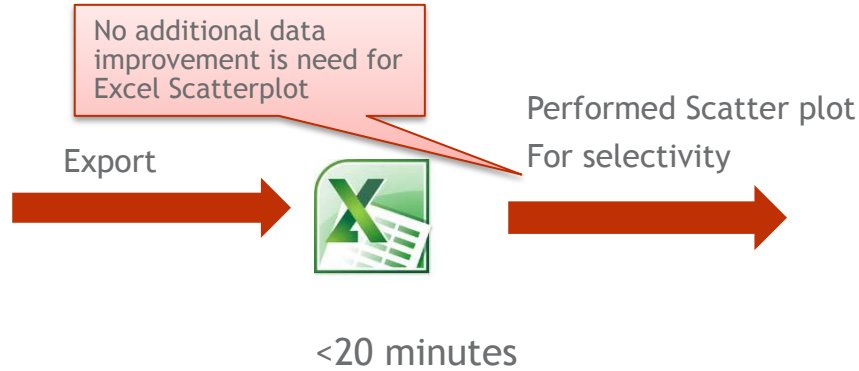


# RMC2 EXCEL EXPORT AND SCATTER PLOT GENERATION

TARGET SELECTIVITY



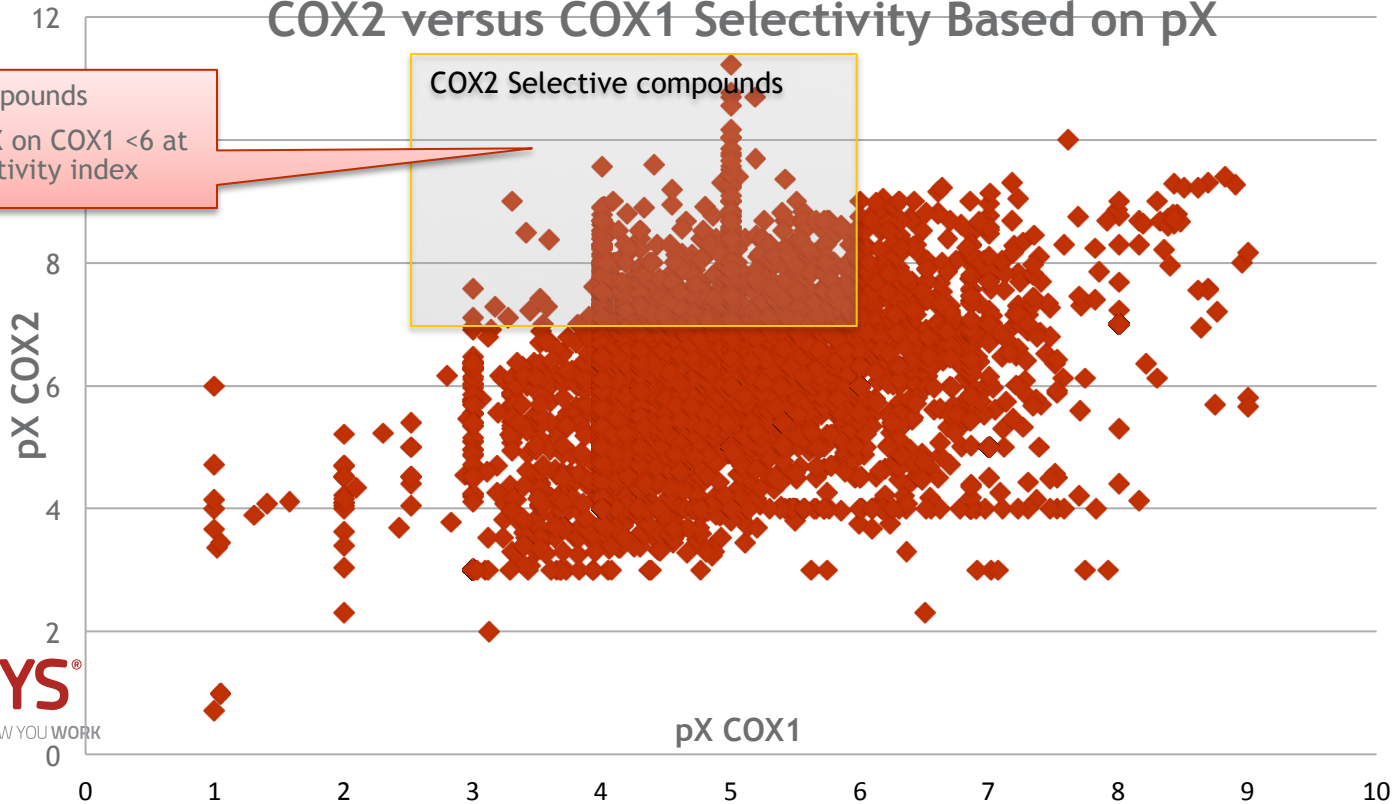
- Search for Substances tested on COX-1 and Cox-2



## COX2 versus COX1 Selectivity Based on pX

COX 2 Selective compounds  
pX on COX >7 and pX on COX1 <6 at  
least a 10 fold Selectivity index

COX2 Selective compounds



and...  
what is  
your  
reaction?

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P.GOLKIEWICZ@ELSEVIER.COM

MOBILE: +48 695 30 60 17