



PIOTR GOLKIEWICZ
LIFE SCIENCES SOLUTIONS CONSULTANT
CENTRAL-EASTERN EUROPE

**INTRODUCING
REAXYS**



SERVING THE LIFE SCIENCES SPACE

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN

Characterize targets & analyze disease pathways

 **PATHWAY STUDIO**

Characterize & discover molecules
Identify & confirm lead compounds

 **REAXYS**
Medicinal Chemistry
 **REAXYS**

Translate preclinical data in humans (Translational)

 **PHARMAPENDIUM**

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

 **EMBASE**

 **QUOSA**

Drug Candidate Selection

Go-No Go Decision

Preclinical Data Validation

Managing risk

Discovery

Pre-clinical

Clinical

Post-launch

Broader full-text indexing of biomedical content

 **LIFE SCIENCE SOLUTIONS**

Text Mining & Data Integration

Integrate the world of data & solutions

ScienceDirect

 **EMBASE**

Scopus

Search full-text, peer-reviewed journal articles

Largest database for access to abstract & citation data

 **REAXYS**
HOW YOU THINK HOW YOU WORK

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

Abstract
Dimers consisting differing porphyrin basicities undergo selective demetallation or protonation of one unit of the dimer. The efficiency of singlet excited energy transfer from neutral free-base/zinc(II) porphyrin to diprotonated porphyrin unit could be fine tuned by varying acidity in the covalently linked dimers. © 1998 Elsevier Science B.V. All rights reserved.

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-fluorophenylporphyrin and meso-tetraphenylporphyrin 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 pentafluorophenyl groups in the meso positions of the porphyrin confers unique inertness of the inner imino nitrogen towards protonation and metallation reactions. The fluorophenylporphyrins exhibit interesting optical and electrochemical properties [13]. We synthesised porphyrin dimers (Fig. 1) comprising of meso-fluorophenylporphyrin and meso-tetraphenylporphyrin with an ethylenedioxy covalent bridge to accomplish selective protonation and demetallation of the meso-tetraphenylporphyrin moiety in the dimer. We demonstrate here that the dicationic porphyrin dimer exhibits efficient intramolecular singlet excitation energy transfer (see) from

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

Cannot be searched by text terms in full text

Chemical structure

Chemical reactions

Cannot be searched by text terms in full text

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

Cannot be searched by text terms in full text

Chemical spectra

Fig. 3. The fluorescence emission spectra of (1) ZnF₅-ZnH₅ (1:1, CH₂Cl₂/MeOH, ν/ν'), (2) ZnF₅OCH₃, (3) ZnH₅OCH₃, (4) ZnF₅-ZnH₅ DM. Inset shows the comparison of the corrected excitation spectrum (solid line) and absorption spectrum (dotted line) of the (a) intermolecular mixture of ZnF₅OCH₃ and ZnH₅OCH₃, and (b) ZnF₅-ZnH₅ 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 (H₂H₅OCH₃) and 5-(4-methoxyphenyl)-10,15,20-tri(pentafluorophenyl)porphyrin (H₂F₅OCH₃) as reference compounds for comparison studies. Hereafter these two porphyrins are referred to as meso-tetraphenylporphyrin and meso-pentafluorophenylporphyrin, respectively. The absorption and fluorescence spectra of the porphyrins were characterised by UV–VIS, ¹H-NMR

Experimental procedures

Cannot be searched by text terms in full text

Substances and their physicochemical properties

| Compound | λ_{abs} (nm; log ϵ) ^a | λ_{em} (nm) ^b |
|--|---|----------------------------------|
| H ₂ F ₅ OCH ₃ | 415(5.45), 509(4.28), 543(3.60), 584(3.82), 640(3.23) | 644, 707 |

Chemistry as the organizing principle



REAXYS IS BUILT

With experimental data from journal articles and patents

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

Physical Data

Spectra

Bioactivity Data

Natural Product

Abstract—Cis-diacetone oxirane (T-BHP) is described. The steric and electronic effects of the substituents on the catalyst, significantly reduced the yield of the product.

1. Introduction

Enantioselectively enriched α,β -epoxy ketones are versatile intermediates in organic synthesis and important synthetic pharmaceuticals.¹ Efficient asymmetric epoxidation reactions of α,β -unsaturated ketones, mainly dialdehydes, have been reported using chiral metal allyl hydroperoxide systems.² Moreover, polyaminocatalyzed and chiral alcohol³ 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 organocatalysis⁴ 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 proton-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-pyrrolidines⁵ (1) have been successfully employed as organocatalysts in different transformations such as C–C bond forming reactions,⁶ functionalizations of carbonyl compounds⁷ and epoxidation of α,β -unsaturated aldehydes.⁸ On the other hand, the

United States Moriarty et al.

US 6,900,191 B1

May 31, 2005

Abstract

Subject to an disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 424(b)(1)-(2).

Physical Data

Spectra

Bioactivity Data

Natural Product

Related U.S. Application Data

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

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

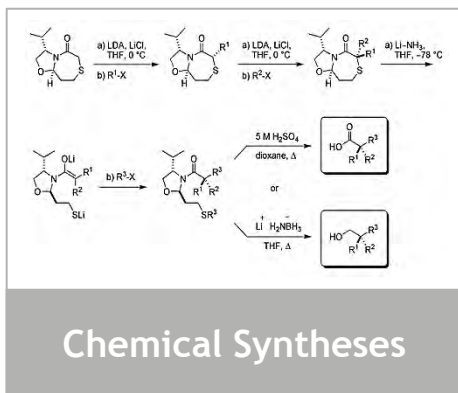
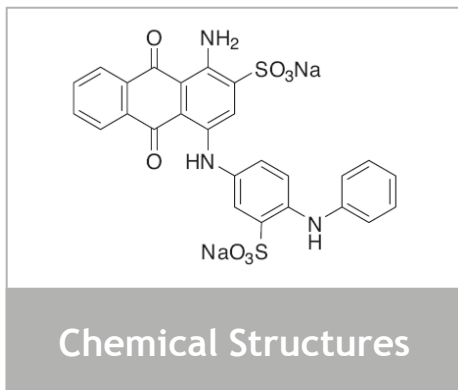
(52) **U.S. Cl.** 514/167; 552/653; 552/653; 514/167

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

1 Claim, 4 Drawing Sheets



CHEMISTRY AS THE ORGANIZING PRINCIPLE



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

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

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

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

Received March 16, 2009

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

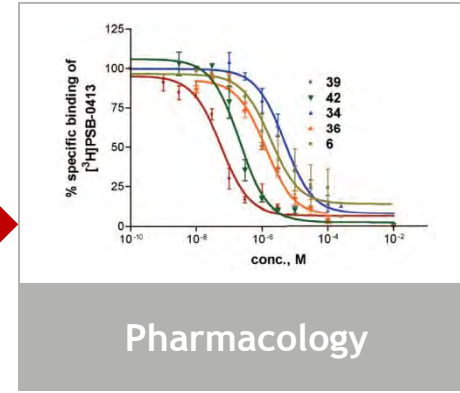
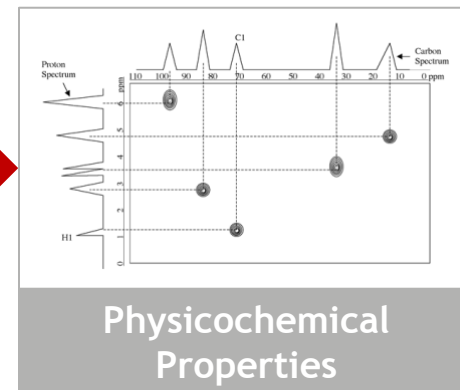
**Reaxys excerpts
all relevant data
even from
footnotes and text**

are shown to be competitive antagonists of the P2Y₁₂ receptor, presumably act as covalent, possibly allosteric antagonists at P2Y₁₂ receptors⁹ (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 P2Y₁₂ antagonists that are lacking the drawbacks associated with the standard P2Y₁₂ antagonists such as clopidogrel and other thienotetrahydropyridine derivatives. Several groups have recently been developing competitive, reversible P2Y₁₂ 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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¹ PharmaCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn.
² Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg.
³ Present address: Elsevier Pharma Biotech Group, Elsevier Information Systems, GmH, 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

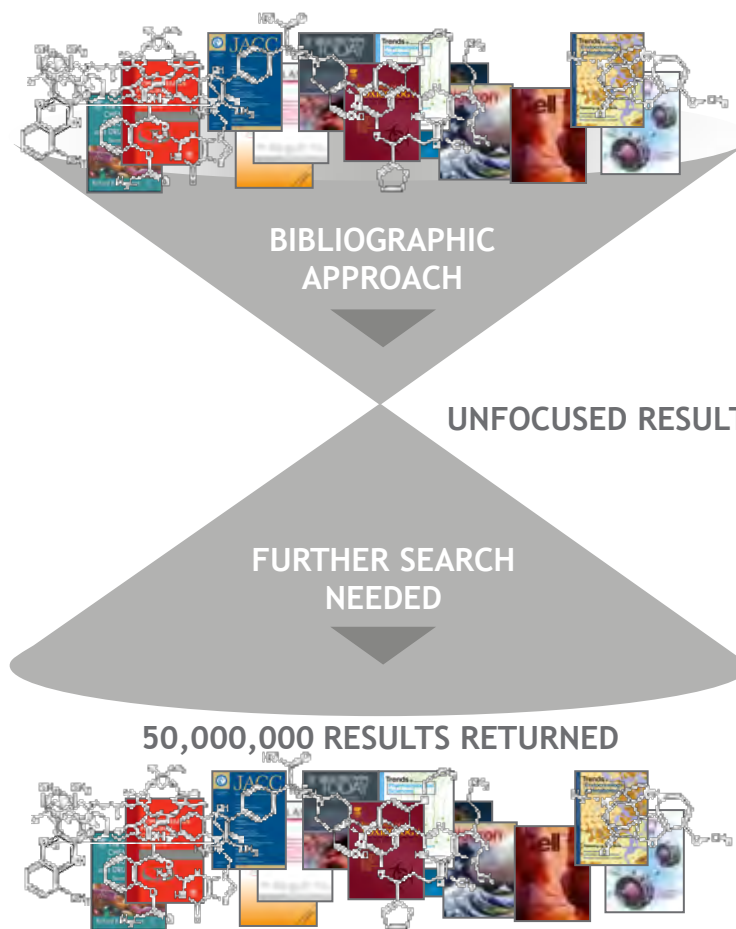


STRUCTURED TO HELP YOU SEARCH

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

We are adding Asian patents - expected completion 2016

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

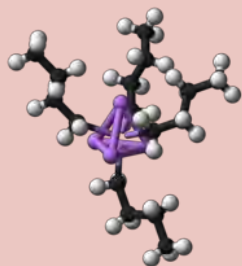
Searching for classes of substances in Reaxys

Found in REAXYS SUBSTANCE RECORDS
and ...

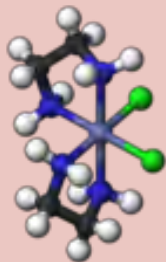
Found in KEYWORDS in REAXYS BIBLIOGRAPHIC
RECORDS



CLASSIC ORGANICS



ORGANOMETALLICS
COORDINATION
COMPOUNDS

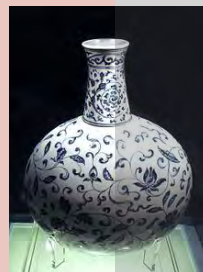


CLASSIC INORGANICS

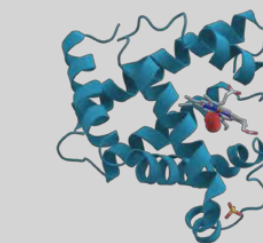
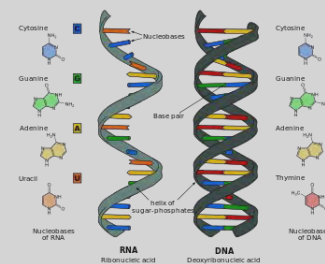
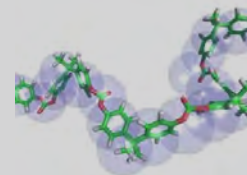


ALLOYS & METALS

CERAMICS



POLYMERS



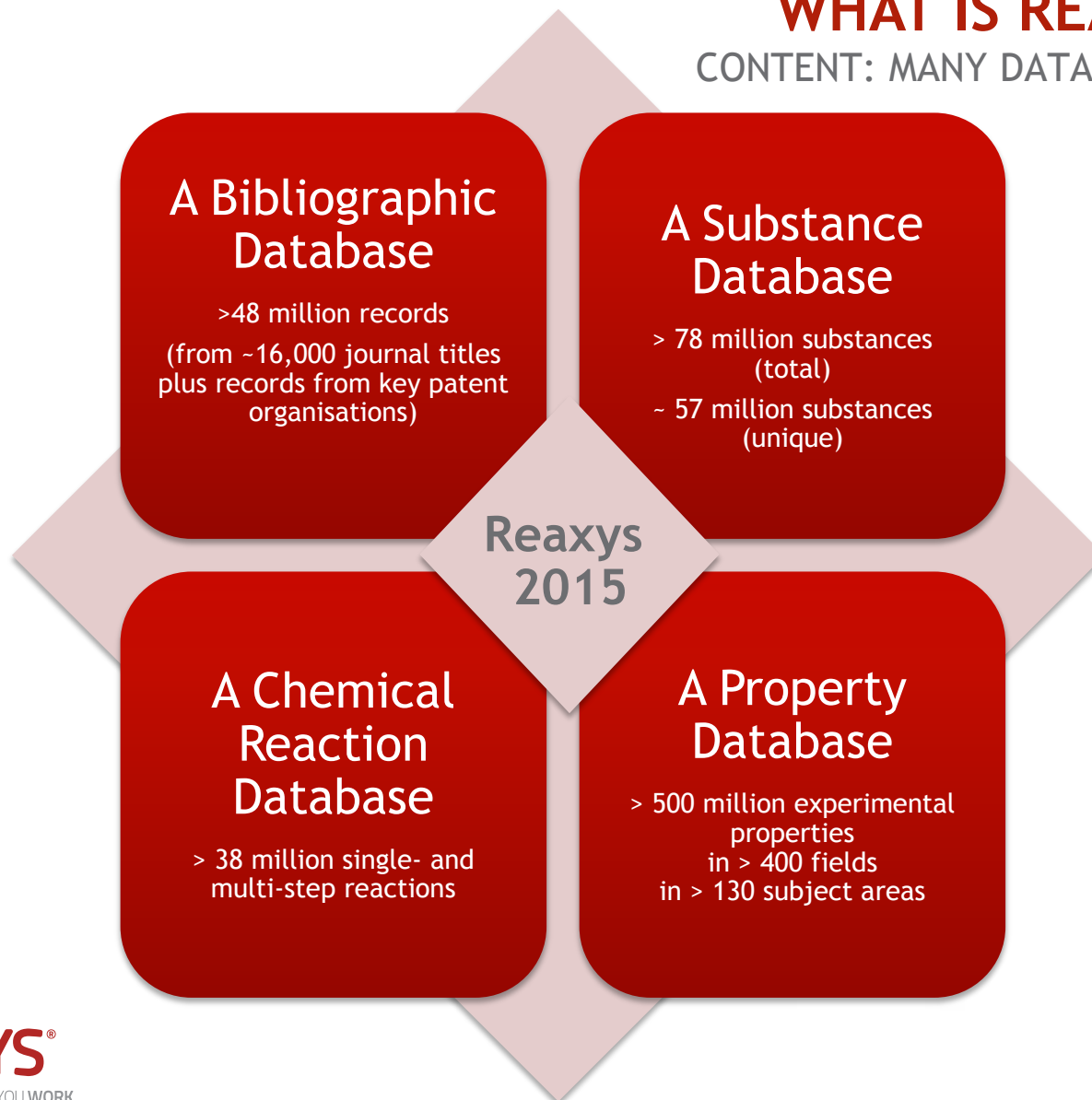
NUCLEIC ACIDS &
PROTEINS

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 interface. At the top, there is a navigation bar with links: Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, Help, Register, and Login. Below the navigation bar is a search bar with the text "Ask Reaxys" and a search icon. Below the search bar is a row of five main search categories: Reactions (with a flask icon), Substances, Names, Formulas (with a molecular model icon), Medicinal Chemistry (with a target icon), Literature (with a book icon), and ReaxysTree (with a tree icon). Below these categories is a section titled "You can also search directly by these common property groups:" with icons for Physical, Spectra, Natural Products, and Advanced. Callout boxes point to various features: "Ask Reaxys, a quick, easy topic 'concept search'" points to the search bar; "Perform a literature search" points to the Literature category; "Open Reaction search form" points to the Reactions category; "Data search form by 'property'" points to the "You can also search directly by these common property groups:" section; "Open a structure search form" points to the Substances, Names, Formulas category; "Search using chemical identifiers" points to the Substances, Names, Formulas category; "Access detailed Biodata, and MedChem specific features" points to the Medicinal Chemistry category; and "Browse database via taxonomies rather than search database" points to the ReaxysTree category.

SEARCH SUBSTANCES

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

File Edit View Insert Options Object Template Chemistry Calculation Help

Transfer Query Cancel & Return

Reaxys supports various structure editors. Please check "My Settings" for more.

As drawn

Substructure

Similar compounds, incl. stereo- and position- isomers

Include tautomers

Stereo

No mixtures

No isotopes

No charges

No radicals

No ring closures

Include results with query

SEARCH SUBSTANCES

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

Molecular Formula ×

Molecular Formula Lookup × Formula Builder

Identification

Reaxys Registry Number = ▼ Lookup ×

CAS Registry Number is ▼ Lookup ×

Chemical Name is ▼ Lookup ×

Molecular Formula is ▼ Lookup ×

Number of Components = ▼ Lookup ×

Molecular Weight > ▼ Lookup ×

LogP = ▼ Lookup ×

Show AND Buttons

Physical Data

Melting Point (°C) < ▼ Lookup ×

Boiling Point (°C) = ▼ Lookup ×

Density exists ×

Colour & Other Properties is ▼ Lookup ×

Show AND Buttons

Spectra

Mass Spectrometry exists ×

Description (Mass Spectrom...) is ▼ Lookup ×

Show AND Buttons

naproxene

naproxene ((+)-6-methoxy- α -methyl-2-naphthalen...)

naproxene [inn-french]

naproxene chloride

naproxen glucuronide

naproxen methylester

naproxeno

naproxeno [inn-spanish]

naproxenoyl isothiocyanate

naproxensodium

naproxenum

naproxenum [inn-latin]

naproxi 250

naproxol

naproxren-hydroxyprolinol

napryn

naps

naps-2-(d)-chg-gly-arg 3-chloro-4-hydroxyanilide

naps-2-gly-pro-arg 3-chloro-4-hydroxyanilide

nansulile-trn-cho

Search Substances

ADD OR REMOVE SEARCH FIELDS

Insert/Remove Properties
Define the "Substances" query layout

Find any property

- Reaxys
 - Physical Data
 - Solubility (MCS) *exists*
 - Solubility, g·l⁻¹ (SLB.SLB)
 - Saturation (SLB.SAT)
 - Temperature (Solubility (MCS)), °C (SLB.T)
 - Solvent (Solubility (MCS)) (SLB.SOL)
 - Ratio of Solvents (SLB.RAT)
 - Solubility Product (MCS) *exists*
 - Solubility Product (SLBP.SLBP)
 - Temperature (Solubility Product (MCS)), °C (SLBP.T)
 - Solvent (Solubility Product (MCS)) (SLBP.SOL)
 - Ratio of Solvents (SLBP.RAT)

Available to add Already selected Searches in multiple databases

- Reaxys Registry Number (in Reaxys)
- CAS Registry Number (in Reaxys)
- Chemical Name (in multiple)
- Molecular Formula (in multiple)
- Number of Components (in Reaxys)
- Molecular Weight (in multiple)
- LogP (in Reaxys)
- Melting Point (in Reaxys)
- Boiling Point (in Reaxys)
- Density (in Reaxys)
- Colour & Other Properties (in Reaxys)
- Mass Spectrometry (in Reaxys)
- Description (Mass Spectrometry) (in Reaxys)

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

Reaction Type 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 alkynylation (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

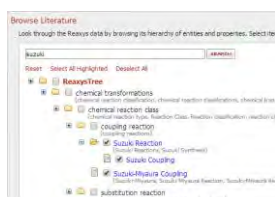
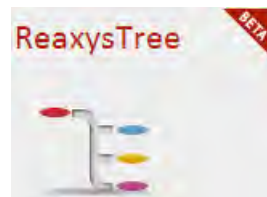
Enter a keyword, concept or author

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

Intelligent interpretation of topic query



Reaxys Tree

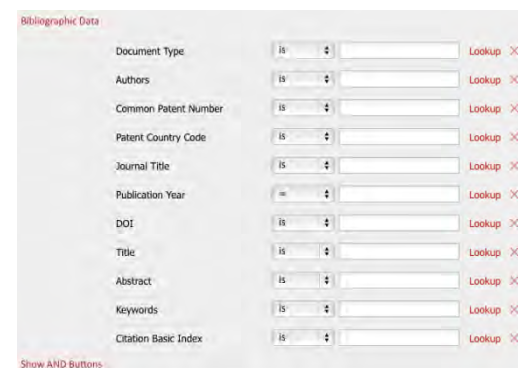


ReaxysTree lets users “browse” the database by taxonomies: helps with search precision and answer comprehension

Browse through taxonomies



You are in control



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

Use truncation/proximity if you like



Reactions (96) Substances (81) Citations (150) go to Page Page 1 of 11

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

Yield Conditions References

1

H2C=CH2 + H2C=CH2 >> H3C-CH=CH2 + H3C-CH2-CH=CH2 + H2C=CH-CH3

 Synthesize Find similar

Rx-ID: 38295231
Find similar reactions

C: 55% T=450°C; P=750.075 Torr; 10 h; AutoclaveInert atmosphere;
Show Experimental Procedure

Reagent/catalyst;
Show Experimental Procedure

Maksasithorn, Surasa; Praserthdam, Piyasan; Suriye, Kongkiat; Devillers, Michel; Debecker, Damien P.
Applied Catalysis A: General, **2014**, vol. 488, p. 200 - 207
Title/Abstract Full Text View citing articles Show Details

Maksasithorn, Surasa; Debecker, Damien P.; Praserthdam, Piyasan; Panpranot, Joongjai; Suriye, Kongkiat; Ayudhya, Sirachaya Kunjara Na
Chinese Journal of Catalysis, **2014**, vol. 35, # 2, p. 232 - 241
Title/Abstract Full Text Show Details

2

H2C=CH2 >> H3C-CH=CH2 + H3C-CH2-CH=CH2

 Synthesize Find similar

Rx-ID: 28699149
Find similar reactions

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;

Gao, Rong; Xiao, Liwei; Hao, Xiang; Sun, Wen-Hua; Wang, Fosong
Dalton Transactions, **2008**, # 41, p. 5645 - 5651
Title/Abstract Full Text View citing articles Show Details

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

Mogorosi, Mokgolela M.; Mahamo, Tebello; Moss, John R.; Mapolie, Selwyn F.; Slootweg, J. Chris; Lammertsma, Koop; Smith, Gregory S.
Journal of Organometallic Chemistry, **2011**, vol. 696, # 23, p. 3585 - 3592
Title/Abstract Full Text View citing articles Show Details

3

H2C=CH2 >> H3C-CH=CH2 + H3C-CH2-CH2-CH=CH2

 Synthesize Find similar

Rx-ID: 209127
Find similar reactions

A: 90% B: 6% With [Ph₂PC₆H₄C(OB(C₆F₅)₃)O-k²P(O)](η³-CH₂CMeCH₂) in toluene
T=0°C; oligomerization; P=2280.15 Torr; 1 h; Product distribution, Further Variations:TemperaturesPressures;

Konon, Zachary J.A.; Bu, Xianhui; Bazan, Guillermo C.
Journal of the American Chemical Society, **2000**, vol. 122, # 8, p. 1830 - 1831
Title/Abstract Full Text View citing articles Show Details

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

Saudi Basic Industries Corporation
Patent: US2012/29258 A1, **2012**,
Location in patent: Page/Page column 4-5 ;
Title/Abstract Full Text Show Details

A: 88% B: 9% With [6,6'-diphenyl-[2,2']-bipyridinyl]NiBr₂; triethyl aluminum sesquichloride in toluene
Inert atmosphereSchlenk technique; Catalytic behavior; Reagent/catalyst;
Show Experimental Procedure

Chandran, Deepak; Lee, Kyeong Mi; Chang, Hyuk Chul; Song, Ga Young; Kim, Il; Lee, Ji-Eun; Suh, Hongsuk
Journal of Organometallic Chemistry, **2012**, vol. 718, p. 8 - 13,6
Title/Abstract Full Text Show Details

MAKE A COMPOUND

REAXYS[®]

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

Reaxys

Query
No structure
Create Alert

29 reactions

Open Analysis View

29 reactions out of 3 substances and 31 citations

Filter by:

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

Reactions Substances (Grid) Substances (Table) Citations

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

Yield Conditions References

6 H₂O + Cl₂Ni + [Catalyst] → [Product]

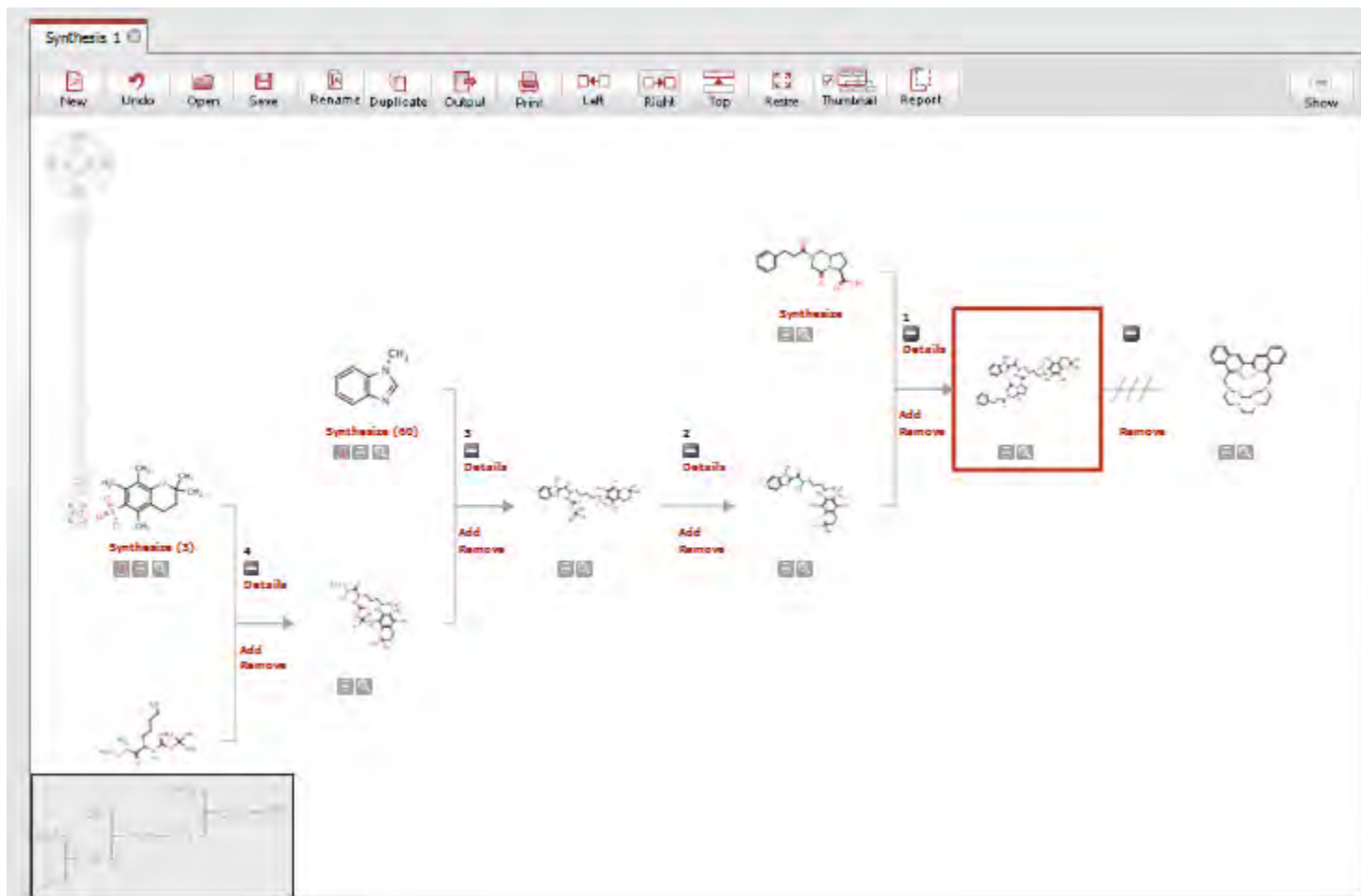
84% in water; acetic acid
washing with acetic acid, drying in vac. over concd. H₂SO₄ or KOH;

41% in water; acetic acid
T=100°C; 0.666667 h;
Show Experimental Procedure

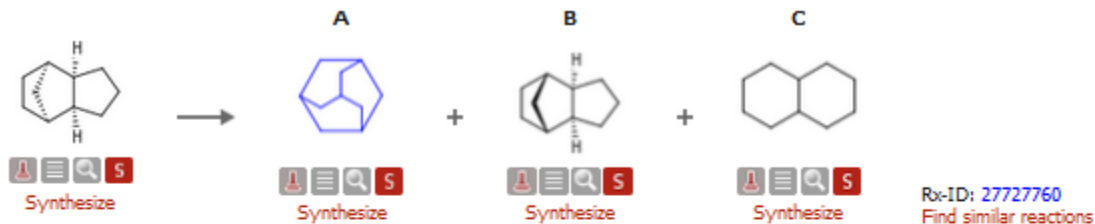
Venanzi, L. M.
Journal of the Chemical Society, 1958, p. 719 - 724
Full Text View citing articles Show Details
Gmelin Handbook: Ni; M/Vol.C2, 8.18.1, page 1041 - 1052
Full Text Show Details

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.

SYNTHESIS PLAN: AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES



SHOW EXPERIMENTAL PROCEDURE



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

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

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




5:

EXAMPLE 5 is the comparative example of EXAMPLE 4. 6.5 g of endo-THDCPD crystals from the same source of EXAMPLE 4 are placed in a 250 ml of glass bottle, followed by adding 40 g of dichloromethane thereto to dissolve the nitrogen and stirring in the ice bath. Subsequently, 10 g of AlCl_3 is added to the dichloromethane solution of endo-THDCPD, followed by stirring for 2 hours in the ice bath, and continuously stirring for 16 hours at room temperature. Subsequently, the mixture washed with the saturated KCl solution is washed with 100 ml of deionized water, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the lower layer in the separatory funnel. The above saturated KCl solution washing procedure is repeated for three times. Subsequently, the lower layer is distilled to remove dichloromethane and water. The bottoms is collected, and determined by chemical analysis. The chemical analysis is composed of 85.7 wt percent of exo-THDCPD, 0.5 wt percent of endo-THDCPD, 1.2 wt percent of Decalin, 5.8 wt percent of adamantane, 1.3 wt percent of exo-THMDCPD, and the other two-stage hydrotreated and saturated C_{10} and/or MCPD dimers. The bottoms has a volumetric heating value of 39.17 MJ/L, a density of 0.9339 at 15° C., and a viscosity of 3.52 cSt at 20° C. and more than 26.7 cSt at -20° C. In this example, the isomerization reaction is very slow so that portions of exo-THDCPD is further isomerized to adamantane which will increase the viscosity of the high energy fuel. Under such a violent reaction conditions, a small amount of THDCPD will be ring-opened to 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 high.

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 |
|--|--|---|--|--------------|-----------|
|    Synthesize Hide Details | Chemical Name: Titanium(IV) oxide Reaxys Registry Number: 4360545 Type of Substance: Glass or Ceramic materialCoordination compoundIsotope or isotope containing compoundSolid solution Molecular Formula: O ₂ Ti Linear Structure Formula: O ₂ Ti Molecular Weight: 79.8788 InChI Key: QWWIMOOOFEDJKFN-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 Title/Abstract |
| pigment in biocide coatings formulations containing hindered alkylamine polymers | Page/Page column 5 | ROHM AND HA Raymond; Man Patent: US2014 Title/Abstract |
| Cosmetics/dental/toilet | Page/Page column 33 | UNIVERSITY O Patent: WO2014 Title/Abstract |
| Polymers/polymer applications | Page/Page column 33 | UNIVERSITY O Patent: WO2014 Title/Abstract |
| antibacterial component of resins useful in dental composites | Page/Page column 33 | UNIVERSITY O Patent: WO2014 Title/Abstract |
| Pharmaceuticals | Paragraph 34 | SHOWA DENK Masahiro; LI D Patent: WO2013 Title/Abstract |
| photocatalytic material in antimicrobial composition | Paragraph 34 | SHOWA DENK Masahiro; LI D Patent: WO2013 Title/Abstract |
| photocatalytic material in antiviral composition | Paragraph 34 | SHOWA DENK Masahiro; LI D Patent: WO2013 Title/Abstract |
| Pharmaceuticals | Page/Page column 5; 6 | OLD DOMINIO Patent: US2013 Title/Abstract |
| increasing absorbency of the first material in a wound care system upon exposure to light | Page/Page column 5; 6 | OLD DOMINIO Patent: US2013 Title/Abstract |
| inhibiting growth of bacteria in a wound care system upon exposure to light | Page/Page column 5; 6 | OLD DOMINIO Patent: US2013 Title/Abstract |
| second material in a wound care system | Page/Page column 5; 6 | OLD DOMINIO Patent: US2013 Title/Abstract |
| Coating/paints/lacquers | Page/Page column 22 | AT PROMOTIC Title/Abstract |

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 Title/Abstract Full Text View Article Online |
| Density of states | Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock) | | Feng, Ningdong; Wang, Qian Journal of the American Chemical Title/Abstract Full Text View Article Online |
| 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; Feng Journal of Physical Chemistry A, Title/Abstract Full Text View Article Online |
| 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 Title/Abstract Full Text View Article Online |
| Electronic energy levels | Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock) | | Lu, Xiaoping; Wei, Shuxian; Journal of Organometallic Chemis Title/Abstract Full Text View Article Online |
| Density of states Band structure | Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock) | | Munnix, S.; Schmeits, M. Physical Review B: Condensed Matter Full Text View citing articles Sarkar, Ghosh; Haldin; Chattop Physica B: Condensed Matter, 2 Title/Abstract Full Text View Article Online |
| 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 Title/Abstract Full Text View Article Online |
| 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 Title/Abstract Full Text View Article Online |
| 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, Title/Abstract Full Text View Article Online |
| 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 Title/Abstract Full Text View Article Online |
| 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 Title/Abstract Full Text View Article Online |
| Atomization energy | Ab initio calcs. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock) | | Shinzato, Yoshifumi; Yukawa; Journal of Alloys and Compounds Title/Abstract Full Text View Article Online West, Richard Hu; Baran, G. Journal of Physical Chemistry A, Title/Abstract Full Text View Article Online Hirate; Morinaga; Yukawa; Journal of Alloys and Compounds Title/Abstract Full Text View Article Online |

Physical Data

Chromatographic Data

 exists

Solvent (Solubility (MCS))

is

Lookup



Show AND Buttons

Add to Query:

Structure

Molecular Formula

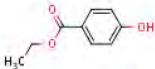
Alloy

Add/Remove Fields...

Search Substances

Reaction Substances (549779) Citations (1746232) go to Page 100 Page 100 of 61087

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. |
|--|--|---|--|------------|
|  <p>892</p> <p>Synthesize Hide Details Find similar</p> | <p>Chemical Name: Ethyl-4-hydroxy-benzoate</p> <p>Reaxys Registry Number: 1101972 CAS Registry Number: 120-47-8 Type of Substance: isocyclic Molecular Formula: C₉H₁₀O₃ Linear Structure Formula: HOC₆H₄CO₂C₂H₅ Molecular Weight: 166.177 InChI Key: NUVBSKCKDOMJSU-UHFFFAOYSA-N</p> | 70 prep out of 2652 reactions. | Hit Data (4) Identification Physical Data (276) Spectra (106) Bioactivity (105) Ecological Data (7) Use/Application (149) Natural Product (13) Quantum Chemical Data (1) | 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) | | Zhang, Yi; Ni, Yan-Peng; He, Ming-Xin; Wang, Xiu-Li; Chen, Li; Wang, Yu-Zhong Polymer (United Kingdom), 2015 , vol. 60, p. 50 - 61 Title/Abstract Full Text View citing articles Show Details |
| HPLC (High performance liquid chromatography) | | 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 Bulletin of the Korean Chemical Society, 2013 , vol. 34, # 4 p. 1131 - 1136 Title/Abstract Full Text View citing articles Show Details Zabrzewska, Beata; Chyla, Anna; Bogdan, Anna Acta Poloniae Pharmaceutica - Drug Research, 2014 , vol. 71, # 4 p. 563 - 573 Title/Abstract Full Text View citing articles Show Details |
| UPLC (Ultra performance liquid chromatography) | | Zhang, Jun-Xian; Miao, Ming-Ming; Niu, Xue-Mei; Li, Jin-Zhu; Han, Yi; Zhang, Ke-Qin; Zhang, Cheng-Ming Asian Journal of Chemistry, 2014 , vol. 26, # 16 p. 5082 - 5086 Title/Abstract Full Text View citing articles Show Details |
| TLC (Thin layer chromatography) | supporting information | Carta, Fabrizio; Vullo, Daniela; Maresca, Alfonso; Scozzafava, Andrea; Supuran, Claudiu T. Bioorganic and Medicinal Chemistry, 2013 , vol. 21, # 6 p. 1564 - 1569 Title/Abstract Full Text View citing articles Show Details |



Comb polymer

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

Citation Basic Index is comb polyacryl* Lookup **Search Literature**

231 citations out of 259 reactions and 229 substances

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

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

| 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, 2010 , vol. 77, # 2 p. 191–199 Full Text View citing articles | 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

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)

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, Zhanlan; 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: 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:

Pressure (Torr):

Solvent:

Electrochemical Cell:

Description:

Nucleus:

Description:

Pressure (Torr):

Structure:

Legend:

| | | | | | | | | | | |
|------------|-----------------|----------|-------------|---------------|-----------------------|-------------|-------------------|------------------------|-----------|--|
| Metalloids | Nonmetals | | | | Metals | | | | | |
| | Other Nonmetals | Halogens | Noble Gases | Alkali Metals | Alkaline Earth Metals | Lanthanoids | Transition Metals | Post Transition Metals | Actinoids | |

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: it's 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)
Add

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

Special groups:
Me Et Ph

Note: it's 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

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Reactions Substances Literature ReaxysTree Physical Spectra Natural Product Advanced

Molecular Formula

Molecular Formula Lookup Formula Builder

Identification

Reaxys Registry Number Lookup

CAS Registry Number Lookup

Chemical Name Lookup

Element Symbols Lookup

Show AND Buttons

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

Formula Builder

Molecular Formula:

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

Special groups:
Me Et Ph

Note: it's 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 | Chemical Name: chromium Reaxys Registry Number: 3587157 CAS Registry Number: 7440-47-3 Molecular Formula: Cr Linear Structure Formula: Cr Molecular Weight: 51.996 InChI Key: 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 | Chemical Name: Catalyst M-Chromium oxide Reaxys Registry Number: 11323461 Type of Substance: Glass or Ceramic material/Isotope or isotope containing compound Molecular Formula: Cr ₂ O ₃ Linear Structure Formula: (Cr ₂ O ₂)O Molecular Weight: 151.99 InChI Key: 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 Pla is **History** Report My Alerts My Settings Help

Reaxys PubChem eMolecules

Select how you want to combine the hitsets



All "inorganic" chromium-containing substances

Cancel

Combine hitsets

Select at least two hitsets for combining

| Query | Temporary result description |
|---|--|
| <input checked="" type="checkbox"/> 6 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"/> 1 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)

The screenshot displays the Reaxys search interface with the following components:

- Navigation Bar:** Includes icons and labels for Reactions, **Substances** (highlighted), Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced.
- Molecular Formula Section:** Contains a text input field for the molecular formula, a 'Lookup' button, and a 'Formula Builder' button.
- Identification Section:** Features four search criteria, each with a dropdown menu, an input field, and a 'Lookup' button:
 - Reaxys Registry Number: dropdown set to '=', input field empty.
 - CAS Registry Number: dropdown set to 'is', input field empty.
 - Chemical Name: dropdown set to 'is', input field empty.
 - Element Symbols: dropdown set to 'is', input field empty.
- Physical Data Section:** Features one search criterion: 'Colour & Other Properties' with a dropdown set to 'is' and an input field containing the text 'yellow'.
- Footer:** Includes 'Add to Query:' with buttons for 'Structure', 'Molecular Formula', and 'Alloy'; an 'Add/Remove Fields...' button; and a prominent 'Search Substances' button.



> 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


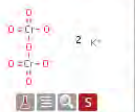
Select at least two hitsets for combining

| 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 <input checked="" type="checkbox"/> 9 <input type="checkbox"/> 8 <input type="checkbox"/> 7 | <p>Edit Create Alert</p> <p>Substances: Colour & Other Properties = 'yellow'</p> <p>909053 substances Substances: Colour & Other Properties = 'yellow'</p> <p>9935155 reactions</p> <p>1793757 citations</p> <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> |

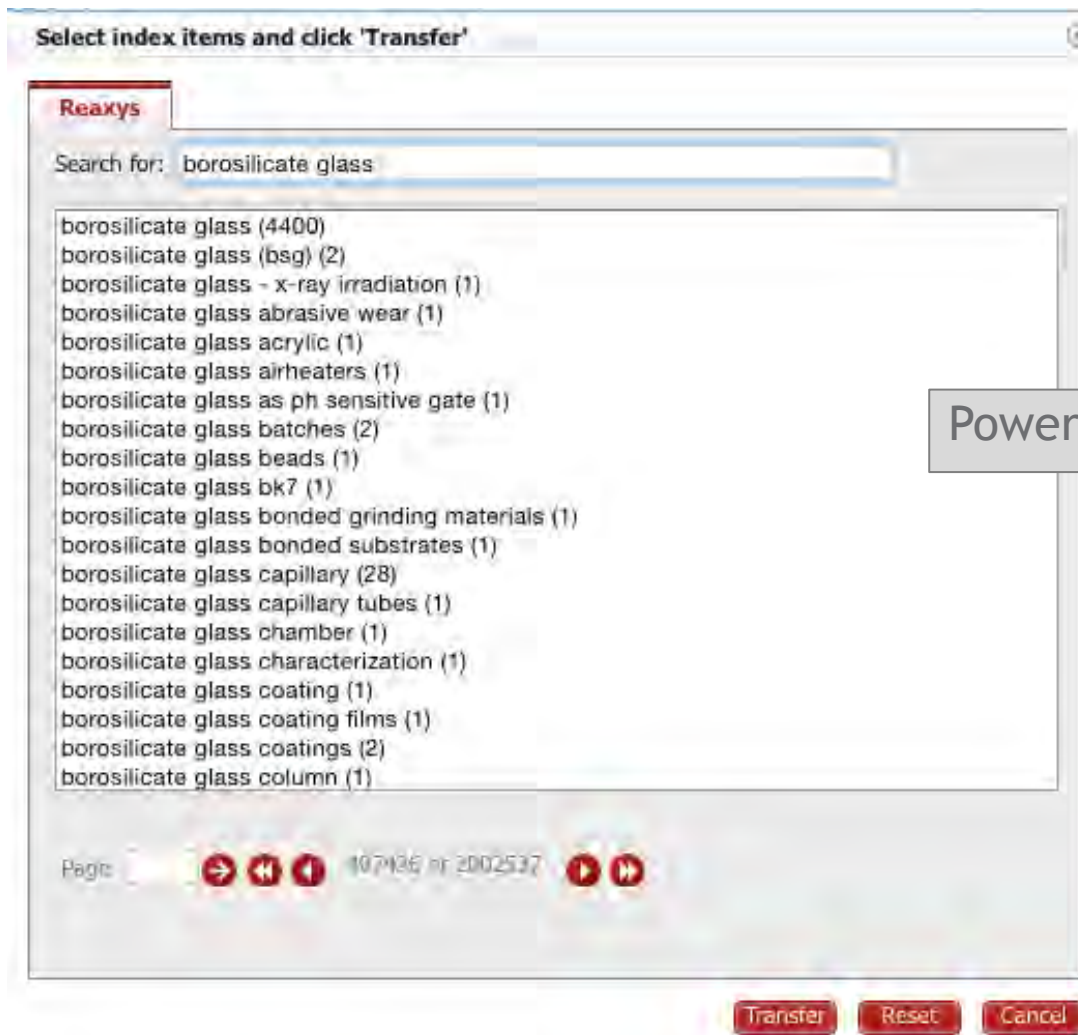
CHROME COMPOUNDS (Yellow Inorganics)

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 | Nº of preparations All Preps All Reactions | Available Data | Nº of ref | | | | | | |
|--|--|--|---|-----------|---------------------------|---------|-----------|--------|----------------------|--|
|  Synthesize Hide Details Find similar | Chemical Name: chromium(VI) oxide Reaxys Registry Number: 10773376 Type of Substance: Glass or Ceramic material/Isotope or isotope containing compound Molecular Formula: CrO ₃ Linear Structure Formula: CrO ₃ Molecular Weight: 99.9942 InChI Key: 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 | | | | | | |
| Chemical Names and Synonyms chromium(VI) oxide, chromium(IV) trioxide, chromic anhydride, chromium trioxide, chromium oxide, CrO ₃ , ruthenium(IV) oxide | | | | | | | | | | |
| ± Hit Data ± Crystal Property Description (1 Hits out of 15 view all) | | | | | | | | | | |
| <table border="1"> <thead> <tr> <th>Colour & Other Properties</th> <th>Comment</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>yellow</td> <td>water</td> <td> Oeholm, L. W. Suomen Kemistiseuran Tiedonantoja, 1940, vol. 49, p. 9 - 13 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 66, page 132 - 134 Full Text Show Details </td> </tr> </tbody> </table> | | | | | Colour & Other Properties | Comment | Reference | yellow | water | Oeholm, L. W. Suomen Kemistiseuran Tiedonantoja, 1940 , vol. 49, p. 9 - 13 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 66, page 132 - 134 Full Text Show Details |
| Colour & Other Properties | Comment | Reference | | | | | | | | |
| yellow | water | Oeholm, L. W. Suomen Kemistiseuran Tiedonantoja, 1940 , vol. 49, p. 9 - 13 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 66, page 132 - 134 Full Text Show Details | | | | | | | | |
| Identification Physical Data Spectra Bioactivity Use/Application Quantum Chemical Data | | | | | | | | | | |
|  Synthesize Hide Details Find similar | Chemical Name: potassium dichromate Reaxys Registry Number: 11322242 Type of Substance: Coordination compound Molecular Formula: Cr ₂ O ₇ *2K Linear Structure Formula: 2K ¹⁺ *Cr ₂ O ₇ (2-) Molecular Weight: 294.184 InChI Key: IMNUAUFMVCNBHR-UHFFFAOYSA-N | 69 prep out of 774 reactions. | Hit Data (3) Identification Physical Data (330) Spectra (73) Bioactivity (3) Use/Application (11) | 1472 | | | | | | |
| Chemical Names and Synonyms potassium dichromate, K ₂ Cr ₂ O ₇ , PDC, potassium bichromate, Potassium dichromate, bichromate potassium, potassium chromate | | | | | | | | | | |
| ± Hit Data ± Crystal Property Description (3 Hits out of 11 view all) | | | | | | | | | | |
| <table border="1"> <thead> <tr> <th>Colour & Other Properties</th> <th>Comment</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>yellow</td> <td>liq. SO₂</td> <td> Shatenshtein, A. I.; Viktorov, M. M. Acta physicochim. URSS, 1937, vol. 7, p. 883 - 898 Full Text Show Details Shatenshtein, A. I.; Viktorov, M. M. Zhurnal Fizicheskoi Khimii, 1938, vol. 11, p. 18 - 27 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 261, page 578 - 580 Full Text Show Details Cady, H. P.; Taft, R. Journal of Physical Chemistry, 1925, vol. 29, p. 1075 - 1084 Full Text Show Details </td> </tr> </tbody> </table> | | | | | Colour & Other Properties | Comment | Reference | yellow | liq. SO ₂ | Shatenshtein, A. I.; Viktorov, M. M. Acta physicochim. URSS, 1937 , vol. 7, p. 883 - 898 Full Text Show Details Shatenshtein, A. I.; Viktorov, M. M. Zhurnal Fizicheskoi Khimii, 1938 , vol. 11, p. 18 - 27 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 261, page 578 - 580 Full Text Show Details Cady, H. P.; Taft, R. Journal of Physical Chemistry, 1925 , vol. 29, p. 1075 - 1084 Full Text Show Details |
| Colour & Other Properties | Comment | Reference | | | | | | | | |
| yellow | liq. SO ₂ | Shatenshtein, A. I.; Viktorov, M. M. Acta physicochim. URSS, 1937 , vol. 7, p. 883 - 898 Full Text Show Details Shatenshtein, A. I.; Viktorov, M. M. Zhurnal Fizicheskoi Khimii, 1938 , vol. 11, p. 18 - 27 Full Text Show Details Gmelin Handbook: Cr: MVol.B, 261, page 578 - 580 Full Text Show Details Cady, H. P.; Taft, R. Journal of Physical Chemistry, 1925 , vol. 29, p. 1075 - 1084 Full Text Show Details | | | | | | | | |

borosilicate glass



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Identification

Alloy Composition exists

Formula

Show AND buttons

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

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BETA

Enter a keyword, concept or author

Go

Component Formula

Ti

Al

V

Percentage

Number on range: 20 on 20-40

Percentage Type:

Additional Components:

| Structure | Structure and compound data | Prep. out of 1 reactions | Available Data |
|---|--|----------------------------------|---|
| <p>mixture (composition completely given):</p> <p>titanium</p> <p>aluminum</p> <p>vanadium</p> <p><input type="button" value="Show Details"/></p> | <p>Chemical Name:</p> <p>Ti 6Al4V</p> <p>Reaxys Registry Number: 16552591</p> <p>Type of Substance: mixture (composition completely given)Alloy</p> | <p>0 prep out of 1 reactions</p> | <p>Physical Data (55)</p> <p>Toxicology (1)</p> <p>User Application (1)</p> |
| <p>mixture (composition completely given):</p> <p>titanium</p> <p>aluminum</p> <p>vanadium</p> <p><input type="button" value="Show Details"/></p> | <p>Chemical Name:</p> <p>TA6V</p> <p>Reaxys Registry Number: 16911805</p> <p>Type of Substance: mixture (composition completely given)Alloy</p> | <p>0 prep out of 1 reactions</p> | <p>Physical Data (13)</p> <p>Spectra (1)</p> |

This Article On

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Ti6Al4V

Go

A study of the α solubility during mechanical abrasion and the repassivation rate of titanium and Ti6Al4V in inorganic buffer solutions and bovine serum

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 (preventing corrosion). To study this effect, open-circuit potential (ocp) measurements before, during and after mechanical disruption of the passive film in a three-electrode cell on commercial pure titanium and Ti6Al4V alloy in inorganic buffer solutions in the pH range from 2.0 to 11.0 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 dissolution of Ti6Al4V are the same as those characterizing pure titanium, which indicates that the corrosion current of both materials is not active stable 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 reduction reaction observed on the pure metal in comparison with the alloy. Proteolytic 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 cp titanium significantly decreases both at pH 4.0 and 7.0.

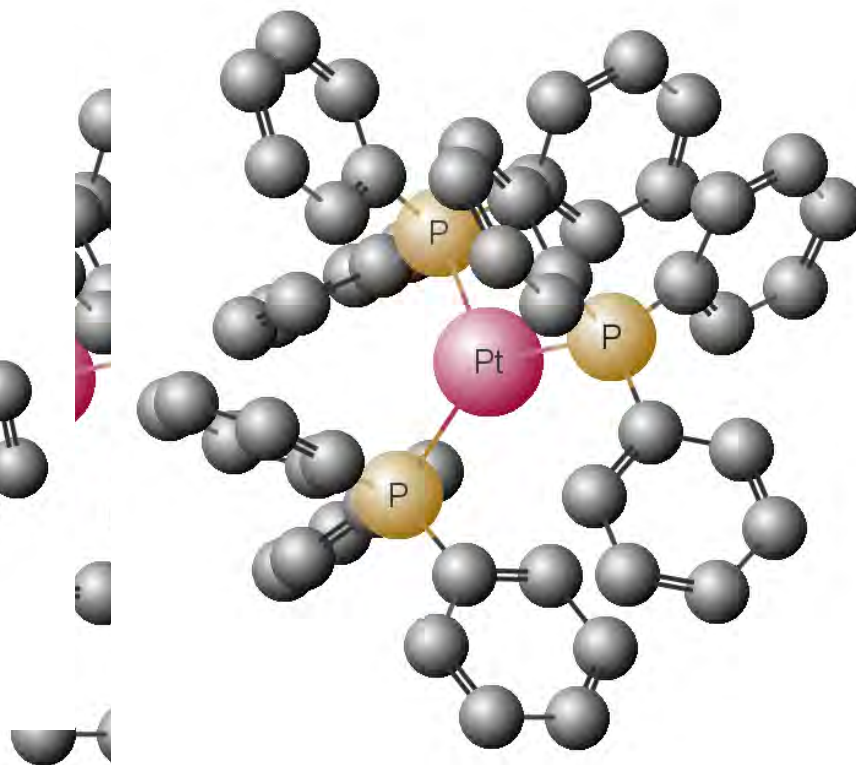
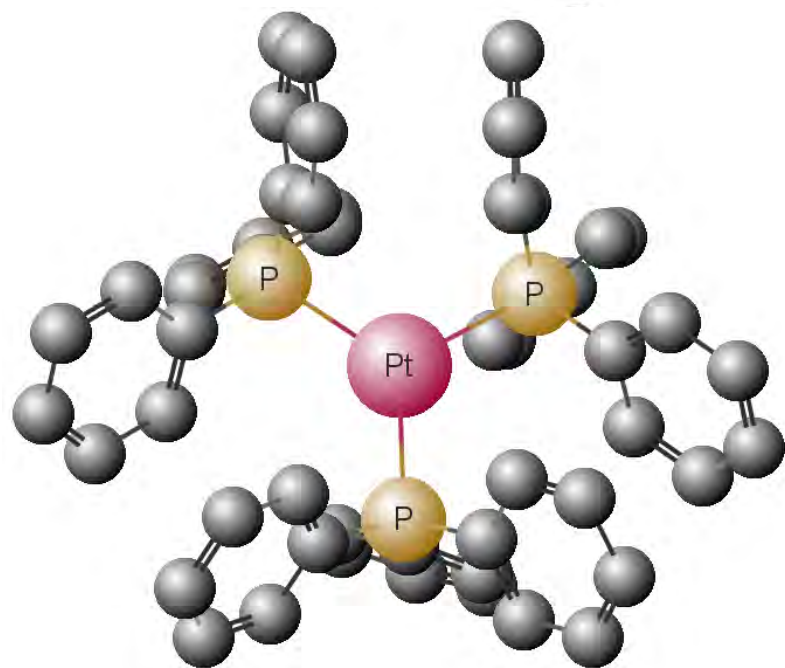
Keywords: Anodic reaction; Bovine serum; Cathodic reaction; Repassivation rate; Ti6Al4V; Titanium

Compound Free Language: Anodic reaction; Bovine serum; Cathodic reaction; Repassivation rate; Ti6Al4V

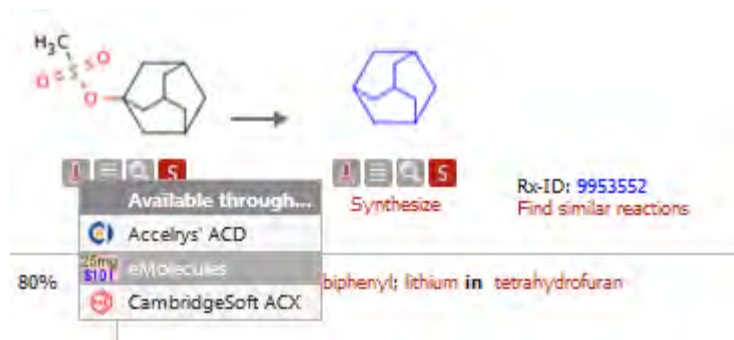
Compound Descriptor: Body Fluid; Corrosion resistance; Current density; Electrochemistry; Implants (surgical); Oxidation; Reaction kinetics

Compound Matchhead: 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

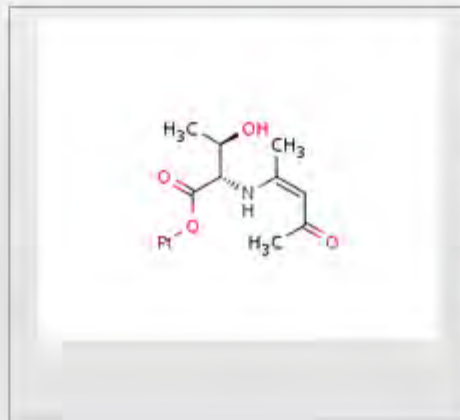
The following editors can only be used, if the **Reaxys Structure Editor PlugIn** is installed:

- 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

The screenshot displays the REAXYS web interface. At the top, the REAXYS logo is on the left, and the user is identified as 'Anonymous user (198.105.10.72)'. A navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'Report', 'My Alerts', 'My Settings', and 'Help'. On the right of the navigation bar are 'Live Chat', 'Register', and 'Logout'. Below the navigation bar is a toolbar with icons for Print, Upload, Open, Save, Repeat, Send, Send to Desktop, and Clear All.

The main content area shows a report titled 'Report ID#: Spillover Peak Synthesis 4' with a creation date of 2013-05-01 10:23 and a modified date of 2013-05-01 10:23. Below this, another report entry is shown: 'Report ID#: IDE-XDR-67944' with a creation date of 2013-05-01 10:26 and a modified date of 2013-05-01 10:26.

The report content is divided into sections. The first section is 'Disassociation', which includes a table with the following data:

| Disassociation | Location | Reference |
|----------------|------------------------|--|
| 210 - 221 °C | supplement information | Ohsawa, Ken; Yam, Takahiro; Suzuki, Kenjiro. <i>Organic and Biomolecular Chemistry</i> , 2012, vol. 8, p. 2603 - 2606. Title/Abstract - Full Text - View single article - Show Details |

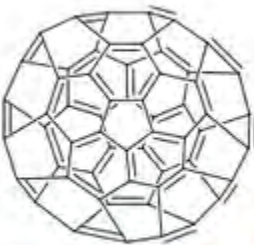
The second section is 'Dissociation Exponent', which includes a table with the following data:

| Dissociation Exponent (kJ) | Dissociation Group | Method | Type | Comments | Reference |
|----------------------------|--------------------|-----------------|------------|--------------------------|---|
| 7.68 | OH | spectrochemical | allopentyl | DE | Pluta, Filip; Szymanski, Henryk; Gluczyńska-Swięta, Anna; Tytkowska, Beata; Bortys, Joanna. <i>J. Agric. Food Chem.</i> , 2008, vol. 56, # 1, p. 818 - 822. <i>Journal of Agricultural and Food Chemistry</i> , 2008, vol. 56, # 1, p. 818 - 822. Title/Abstract - Full Text - View single article - Show Details |
| -0.8812°C - 0.82063 | OH | | allopentyl | in the presence of salts | Kamamoto, Hiroyuki; Senda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Hirotaki. <i>Bioscience, Biotechnology, and Biochemistry</i> , 2001, vol. 45, # 1, p. 126 - 132. Title/Abstract - Full Text - View single article - Show Details |
| -1.02938 | OH | | allopentyl | | Kamamoto, Hiroyuki; Senda, Tamiyoshi; Nagayama, Kinuyo; Tabata, Hirotaki. <i>Bioscience, Biotechnology, and Biochemistry</i> , 2001, vol. 45, # 1, p. 126 - 132. Title/Abstract - Full Text - View single article - Show Details |

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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.; Eyley, John
R.; Bach, Stephan B.H.; McElvany,
Stephen W.

1991

Journal of Chemical Physics, 1991, vol. 94, # 5 p. 3556 - 3562
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"Magic number" carbon clusters: ionization potentials and selective reactivity

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

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

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- 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 |
| Full Text View at Publisher | | | |
| <input type="checkbox"/> On the dynamics of photo-electrons in C∞ 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 |
| Full Text View at Publisher | | | |
| <input type="checkbox"/> First-principles photoemission spectroscopy and orbital tomography in molecules from koopmans- 3 compliant functionals | Nguyen, N.L., Borghi, G., Ferretti, A., Dabo, I., Marzari, N. | 2015 Physical Review Letters | 1 |
| Full Text 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**

WHY IS IT SO DIFFICULT TO MAKE DRUGS?

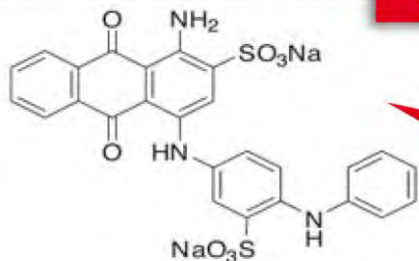
Estimates of the number of possible drug molecules average 10^{40} . In contrast, the number of seconds since the Big Bang is only 10^{17} .



If 10,000 chemists were to prepare 1 compound each per second, it would take 10,000,000,000,000,000,000,000,000,000 years to finish the job.

ESSENTIAL INFORMATION: 100+ EXPERIMENTAL FIELDS

Chemical Structures



398
J. Med. Chem. 2006, 49, 398-399

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

Yoonsi Baek,¹ Kristin Anten,¹ Myoung Kwon,¹ Martin Ohmst,^{1,2} and Christa E. Miller^{1*}

¹Pharmaceutical Biotech Pharmaceutical Division, Pharmaceutical Sciences Area (P2B), University of Pittsburgh Medical Center (UPMC), University of Pittsburgh School of Medicine, Department of Experimental and Clinical Pharmacology and Toxicology, University of Pittsburgh, Pittsburgh, PA 15261, USA; ²Department of Pharmacy, University of Freiburg, Albertstrasse 23, D-70529 Freiburg, Germany

Received March 26, 2006

Abstract: Antagonists related to the nucleotide guanosine, nonfluorinated P2Y₁₂ receptor antagonists inactive Mar 2 06 have been synthesized and optimized with respect to P2Y₁₂ receptor affinity. A sulfonamide binding motif, which binds to the extracellular domain of the P2Y₁₂ receptor-selective antagonist cilostazol [(7S)-6-(4-chlorophenyl)-5,7-dihydro-2H-tetrazolo[5,4-b]pyridine-2-thione] (Cilostazol, (M1)) was applied for compound testing. 1-Amino-2-oxo-1,2,3,4-tetrahydropyridine derivatives bearing a p-phenylenesulfonamide substitution in the 4-position and an additional acidic function in the meta-position of the sulfonamide showed high P2Y₁₂ receptor affinity. These new antagonism derivatives became accessible by a recently developed copper-catalyzed Ullmann coupling reaction of 1-oxo-4-(4-aminophenyl)pyridine derivatives with sulfonamide phenols under microwave irradiation. The most potent compound exhibited K_d values of 24.9 nM (1-oxo-4-(4-phenylamino-3-sulfophenylamino)-1H-imidazo[5,1-b]imidazole-2-thione, P2B-0739, 39), and 2.10 nM (1-oxo-4-(4-phenylamino-3-carboxylphenylamino)-1H-imidazo[5,1-b]imidazole-2-thione, P2B-0741, 39) respectively. 1-Amino-2-oxo-1,2,3,4-tetrahydropyridine

Reaxys Medical Chemistry Excerpt

identified. Blood platelets express two P2Y receptor subtypes, P2Y₁ and P2Y₁₂, both of which are activated by the nucleotide ADP, which induces platelet aggregation.¹ The activated action of both P2Y receptor subtypes on thromboxane is regulated by a heterotrimeric G-protein-coupled receptor (GPCR) system. P2Y₁ is coupled to G_i and activates phospholipase C β , which is responsible for the mobilization of calcium from internal stores, modulating platelet shape change and onset of rapidly reversible platelet aggregation induced by ADP. On the other hand, it is coupled to inhibition of adenylate cyclase through G_s protein and mediates a proaggregatory and sustained aggregation not provided by shape change. The latter receptor also plays an important role in the generation of platelet activation induced by several agonists, and its coupled deficiency has been shown to result in a bleeding bleeding disorder.² Modulation of P2Y receptors to platelets appears to be of paramount importance in regulating platelet function and, as a consequence, in controlling thrombotic disorders, which are the most common cause of morbidity and mortality.

* To whom correspondence should be addressed. Phone: +49 761 203-7510; Fax: +49 761 203-7519; E-mail: christa.miller@upmc.edu

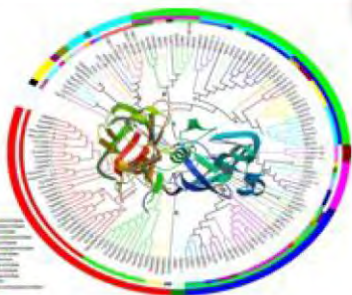
¹Pharmaceutical Biotech Pharmaceutical Division, Pharmaceutical Sciences Area (P2B), University of Pittsburgh Medical Center (UPMC), University of Pittsburgh School of Medicine, Department of Experimental and Clinical Pharmacology and Toxicology, University of Pittsburgh, Pittsburgh, PA 15261, USA; ²Department of Pharmacy, University of Freiburg, Albertstrasse 23, D-70529 Freiburg, Germany.

10.1021/jm060200c CCC: \$40.00 © 2006 American Chemical Society
Published on Web 03/23/2006

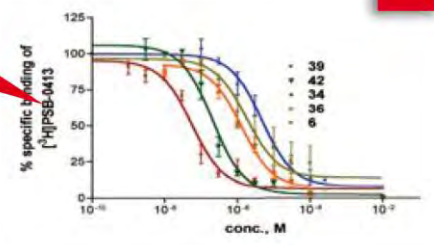
Bioassays: Cell lines, Species



Druggable Proteins

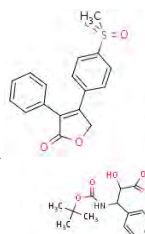


Quantitative Results

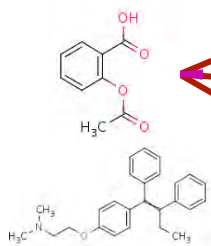
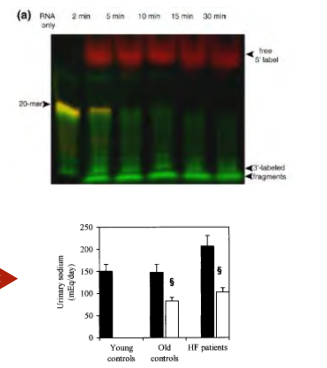
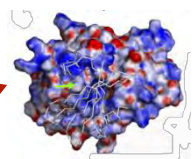


Reaxys Medical Chemistry excerpts all the relevant Quantitative data

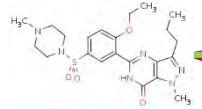
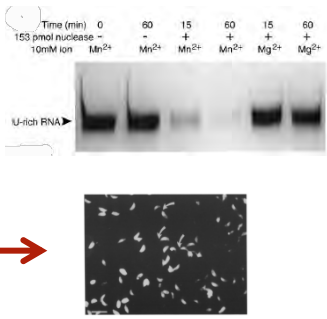
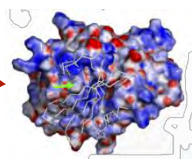
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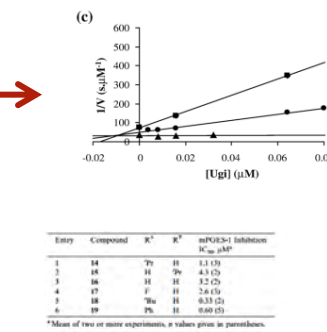
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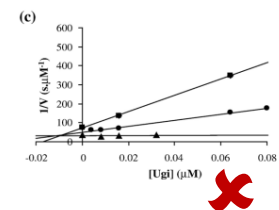
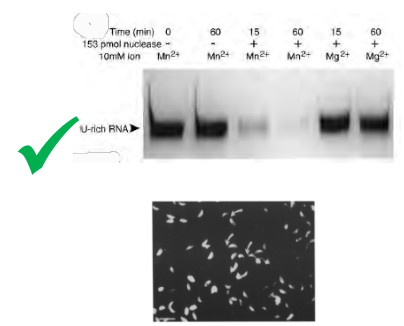
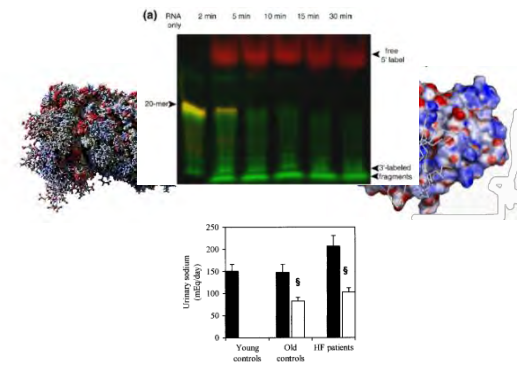
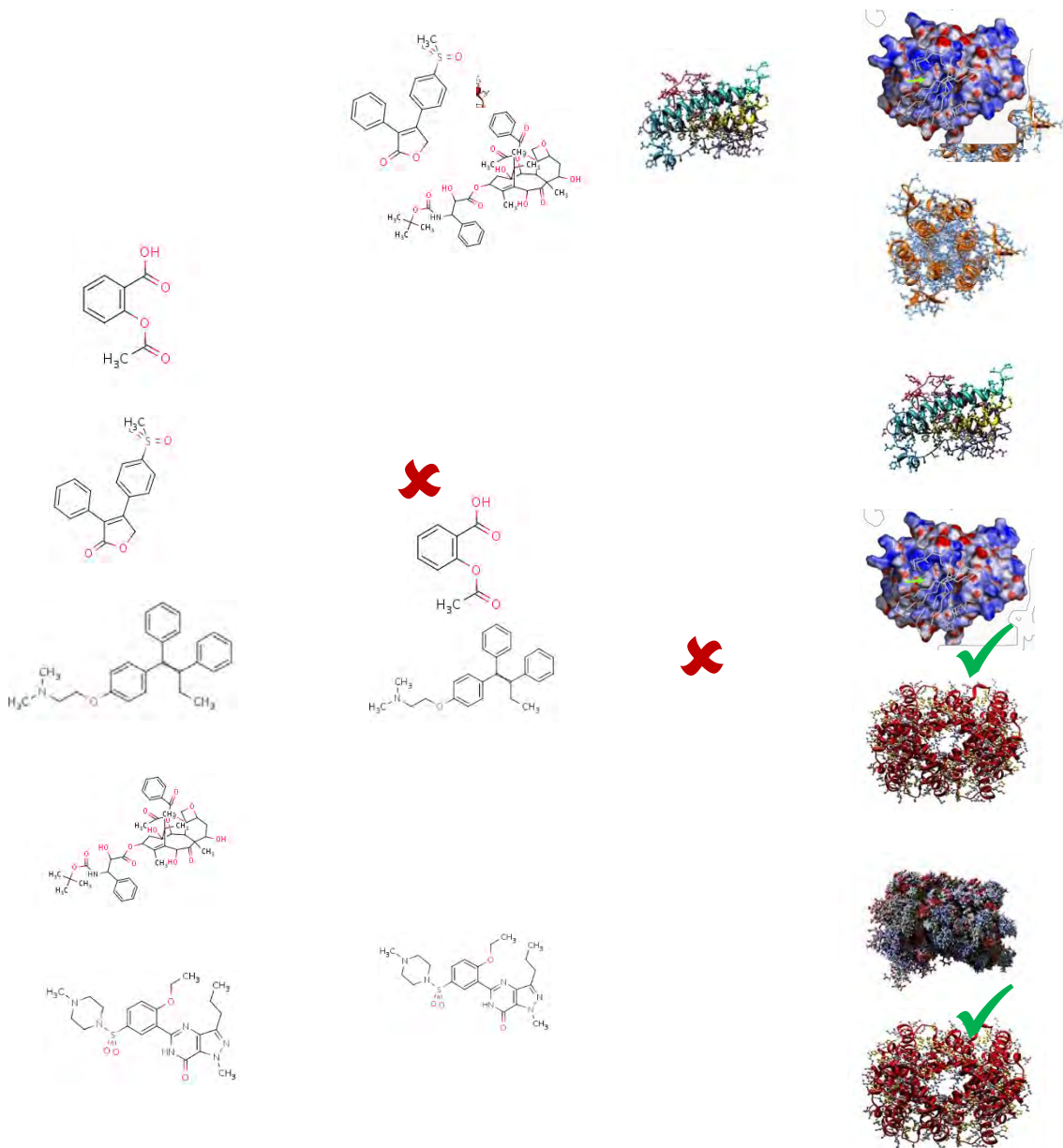
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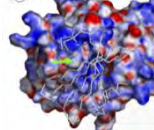
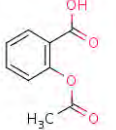
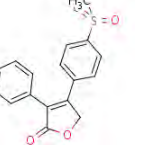
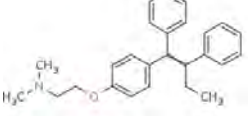
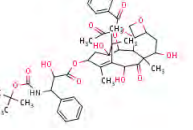
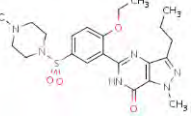
| Entry | Compound | R ² | R ³ | miPGES-1 inhibition K ₅₀ μM ^a |
|-------|----------|----------------|----------------|---|
| 1 | 14 | 79 | H | 3.1 (3) |
| 2 | 18 | H | 76 | 4.1 (2) |
| 3 | 16 | H | H | 3.2 (2) |
| 4 | 17 | F | H | 2.6 (3) |
| 5 | 18 | 76 | H | 0.33 (2) |
| 6 | 19 | 76 | H | 0.60 (2) |

^aMean 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

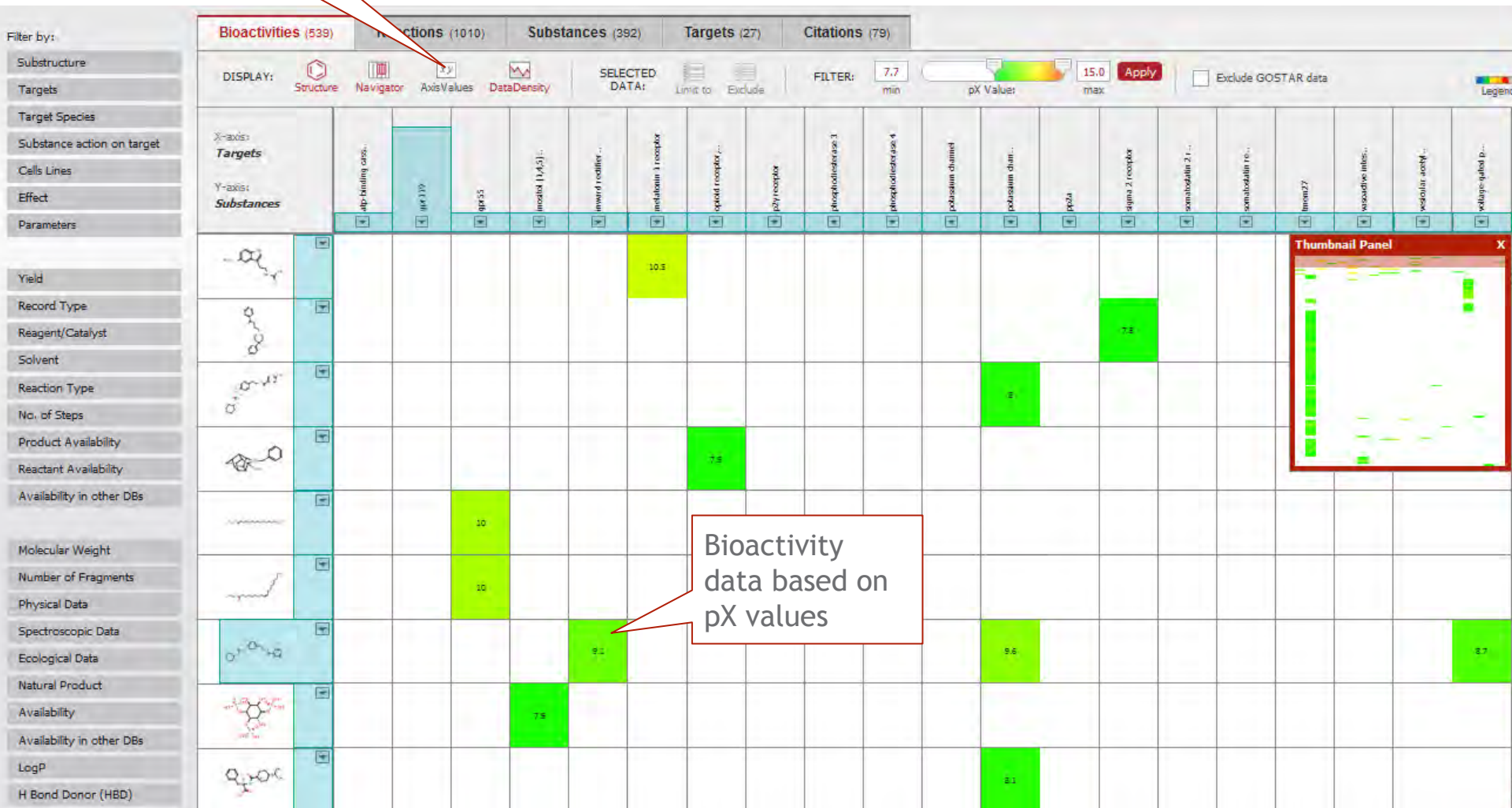
| Enzyme or cell assay | Inhibition potency IC ₅₀ μM ^a | |
|---|---|-----------|
| | 23 | 30 |
| Human miPGES-1 | 0.007 (9) | 0.003 (8) |
| Human miPGES-2 | >1 (3) | >1 (3) |
| Thromboxane synthase | 1.4 (3) | 0.95 (3) |
| FLAP binding | >1 (3) | >1 (3) |
| Human eosinophiles (PGE ₂) (2% FBS) | 0.61 (4) | 0.25 (3) |
| A549 cells (PGE ₂) (2% FBS) | 0.49 (49) | 0.27 (3) |
| A549 cells (PGE ₂) (50% FBS) | 8.0 (49) | 5.8 (3) |
| A549 cells (PGE ₂) (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

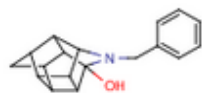
X-axis: Targets

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:** C₁₈H₁₉NO**Linear Structure Formula:** C₁₈H₁₉NO**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 |
|-----------|--------------|---------------|------|-----------------------|--------------------------|----------------|----------------|--------------|------|----------|----------|------------------|-------------------------------|
| Ki | = | 12 | nM | Radioligand (/ligand) | Opioid Receptor, Sigma 2 | | Rat | | PC12 | | = 100 μM | binding activity | Bioorganic and Title/Abstract |



H

EXAMPLE: SUBSTANCES ACTIVE ON COX-2

Select index items and click 'Transfer'

Reaxys

Enter search term:

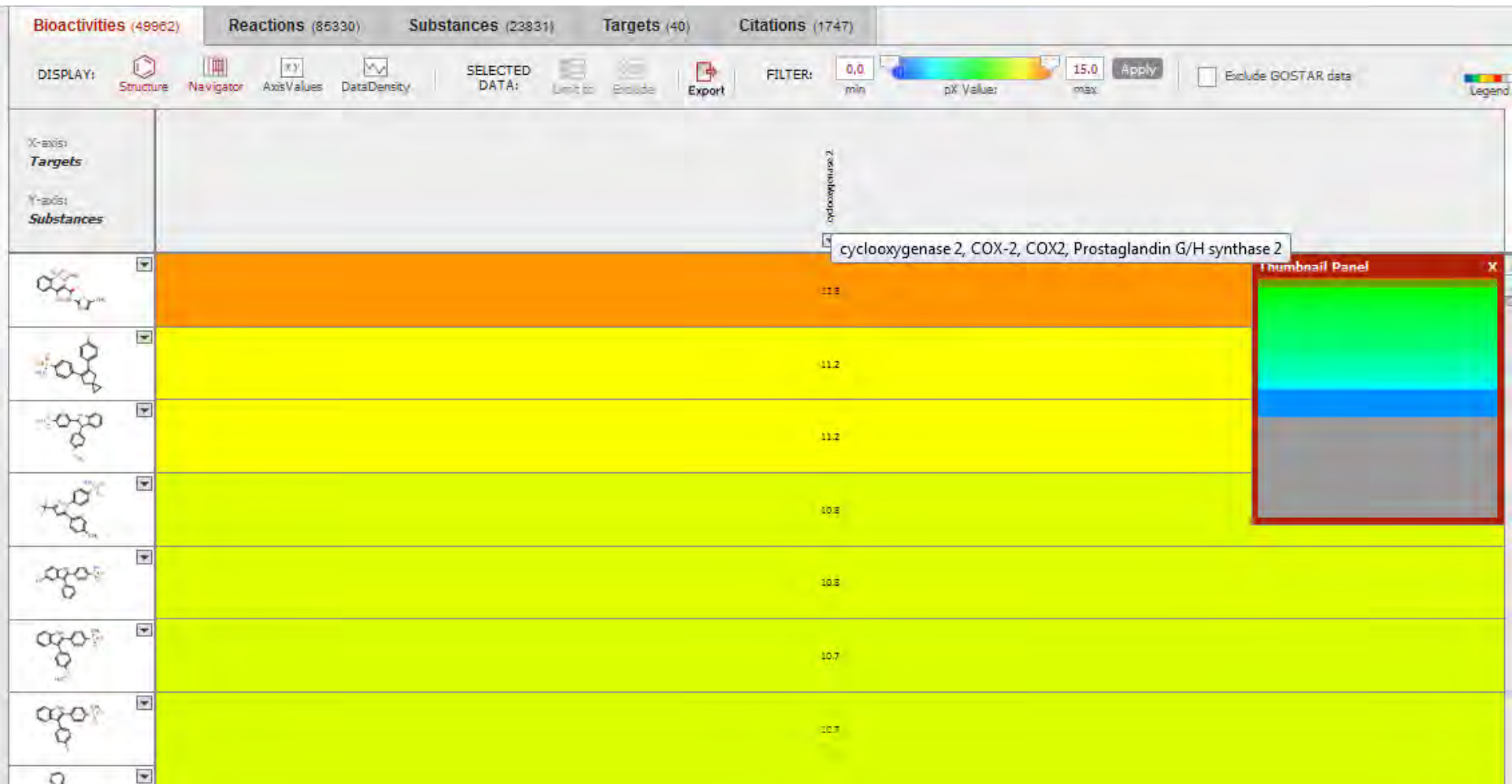
Bioactivities

| | | | |
|----------------------------|----|---|----------|
| Target Name | is | <input type="text" value="'Cyclooxygenase 2'"/> | Lookup X |
| Target PDB ID | is | <input type="text"/> | Lookup X |
| Substance Route of Adm. | is | <input type="text"/> | Lookup X |
| Substance Dosing Regimen | is | <input type="text"/> | Lookup X |
| Substance Action on Target | is | <input type="text"/> | Lookup X |
| Substance Effect | is | <input type="text"/> | Lookup X |
| Bioassay Category | is | <input type="text"/> | Lookup X |
| Biological Species | is | <input type="text"/> | Lookup X |
| Organs/Tissues | is | <input type="text"/> | Lookup X |
| Cells/Cell Lines | is | <input type="text"/> | Lookup X |
| Measurement pX | > | <input type="text" value="8"/> | Lookup X |

Show AND Buttons

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

EXAMPLE: SUBSTANCES ACTIVE ON COX-2



EXAMPLE: AND NOT ACTIVE ON COX-1

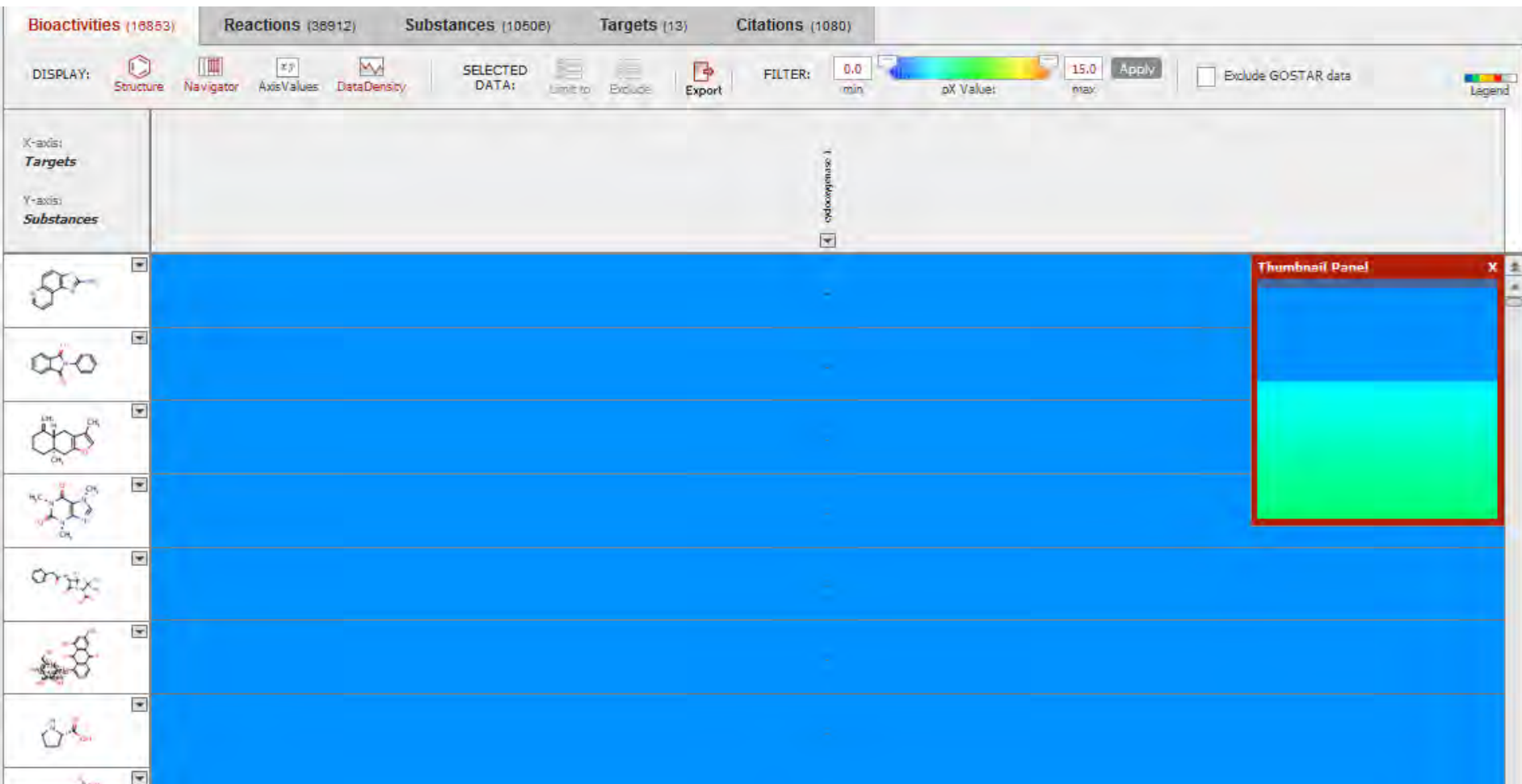
Bioactivities

| | | | | |
|----------------------------|----|-------------------|--------|---|
| Target Name | is | Cyclooxygenase 1' | Lookup | × |
| Target PDB ID | is | | Lookup | × |
| Substance Route of Adm. | is | | Lookup | × |
| Substance Dosing Regimen | is | | Lookup | × |
| Substance Action on Target | is | | Lookup | × |
| Substance Effect | is | | Lookup | × |
| Bioassay Category | is | | Lookup | × |
| Biological Species | is | | Lookup | × |
| Organs/Tissues | is | | Lookup | × |
| Cells/Cell Lines | is | | Lookup | × |
| Measurement pX | < | 6 | Lookup | × |

Show AND Buttons

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

EXAMPLE: AND NOT ACTIVE ON COX-1



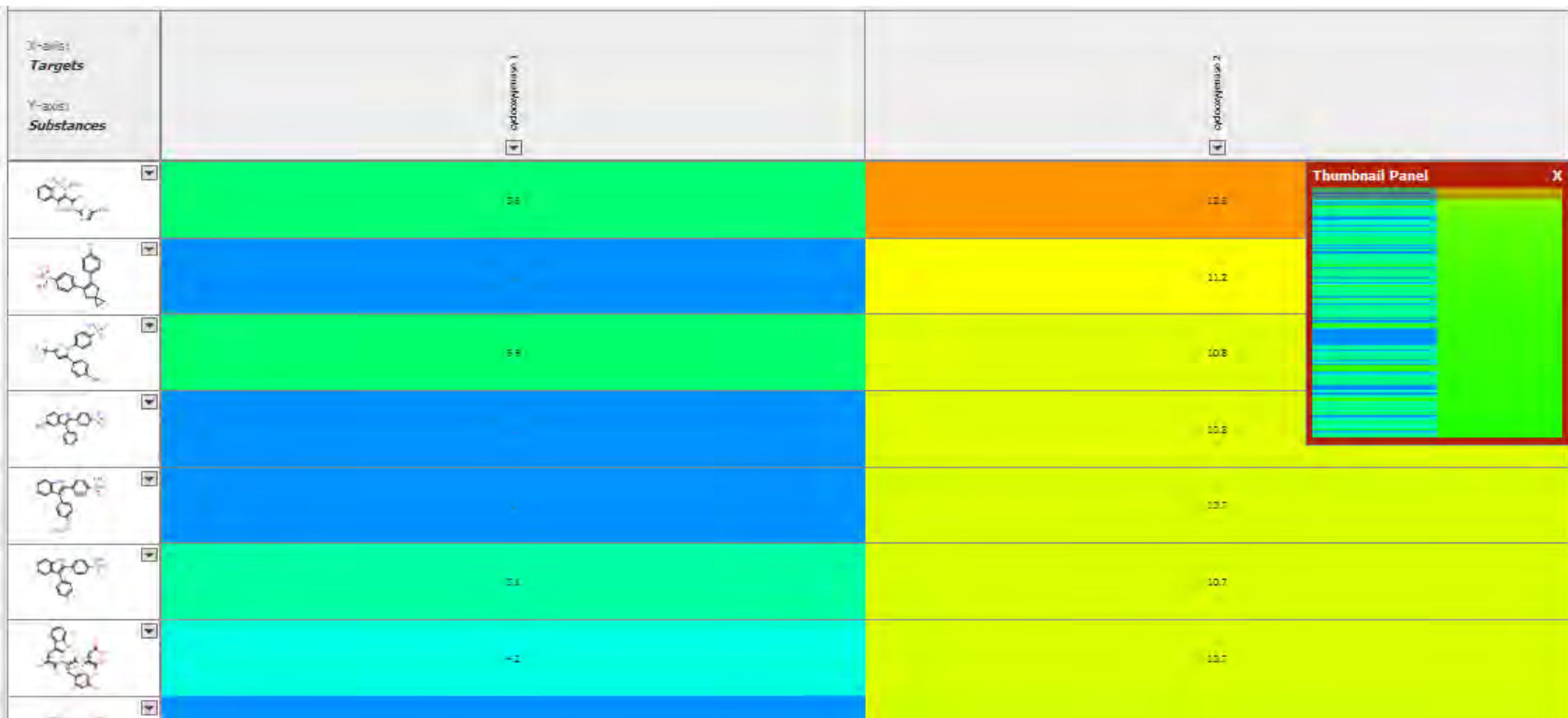
EXAMPLE: AND NOT ACTIVE ON COX-1

Select how you want to combine the hitsets

| Operation | Filter | Statistics |
|----------------------------|---|---|
| Merge 74 with 79 | Bioactivities: target name = Cyclooxygenase 1 AND Measurement pX < 6 | |
| Overlap 74 with 79 | | |
| Exclude 74 from 79 | | |
| Exclude 79 from 74 | | |
| Heatmap Overlay 74 with 79 | Bioactivities: target name = Cyclooxygenase 1 AND measurement pX < 6 | 36912 reactions 10506 substances 13 targets 1080 citations |
| | Edit Create Alert Bioactivities: Target Name = "Cyclooxygenase 2" AND Measurement pX > 8 | 1325 bioactivities 2080 reactions 581 substances |

79
78
77
76
75
 74
73
72

EXAMPLE: SUBSTANCES ACTIVE SELECTIVELY ON COX-1 AND COX-2



ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR

Bioactivities

| | | | | |
|----------------------------|----|--|--------|---|
| Target Name | is | 5-hydroxytryptamine 2 receptor [Human] | Lookup | X |
| Target PDB ID | is | | Lookup | X |
| Substance Route of Adm. | is | | Lookup | X |
| Substance Dosing Regimen | is | | Lookup | X |
| Substance Action on Target | is | antagonist | Lookup | X |
| Substance Effect | is | antagonist | Lookup | X |
| Bioassay Category | is | blocker | Lookup | X |
| Biological Species | is | inactivator | Lookup | X |
| Organs/Tissues | is | inhibitor | Lookup | X |
| Cells/Cell Lines | is | inverse agonist | Lookup | X |
| Measurement pX | < | irreversible antagonist | Lookup | X |
| | | irreversible inhibitor | Lookup | X |
| | | modulator | Lookup | X |
| | | opener | Lookup | X |
| | | partial agonist | | |
| | | radioligand (/ligand) | | |
| | | radioligand/ligand | | |
| | | stimulator | | |
| | | stimulator/protector | | |
| | | substrate | | |

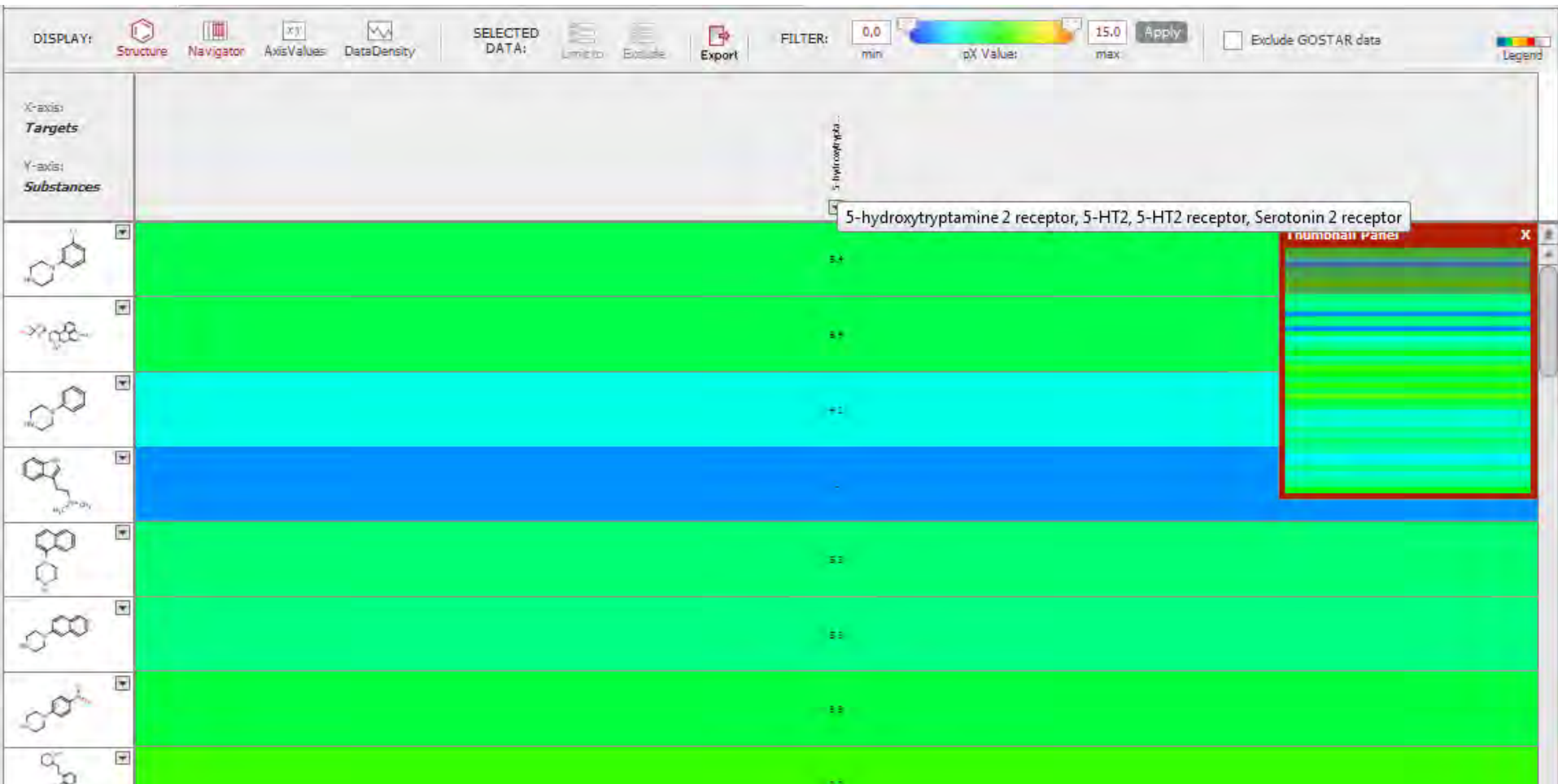
Show AND Buttons

Add to Query: Structure Molecule Alloy Add/Remove Fields...

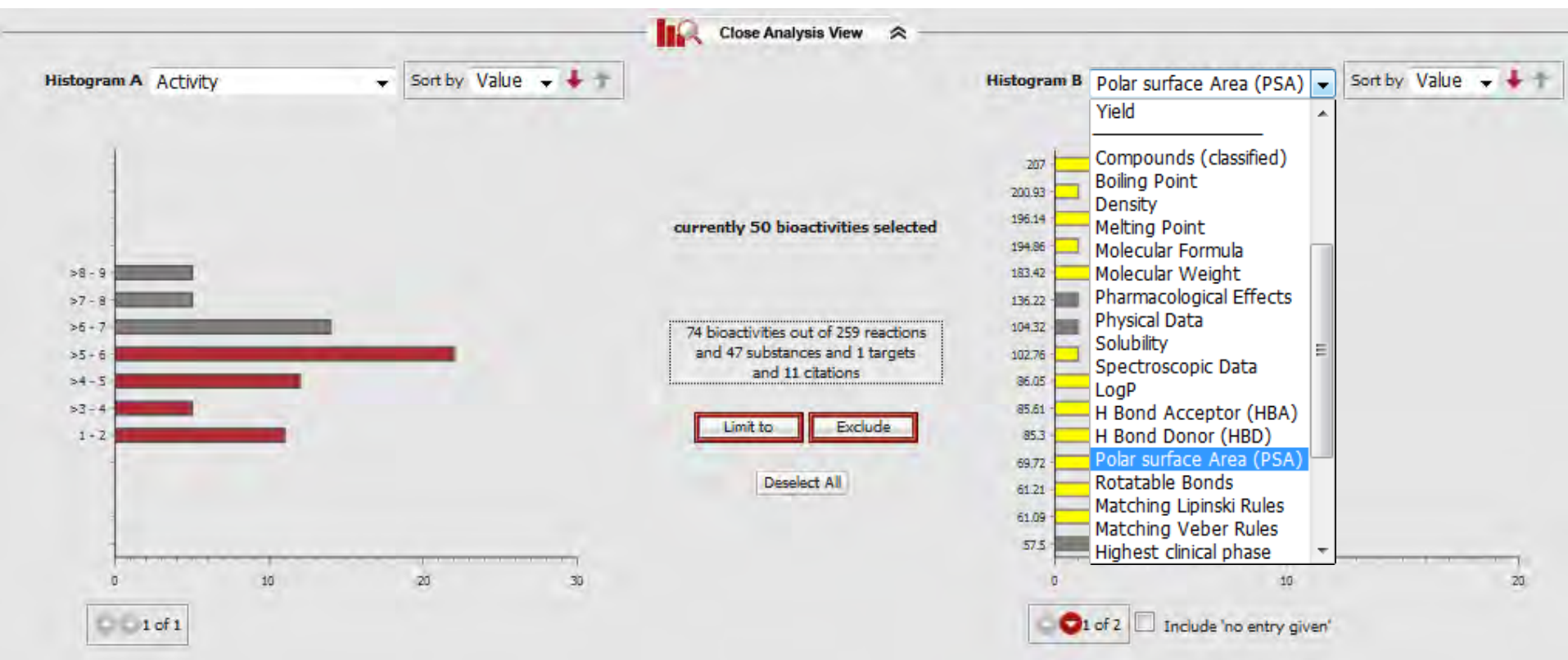
Clear Query

Search Bioactivities

ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR



ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR



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.

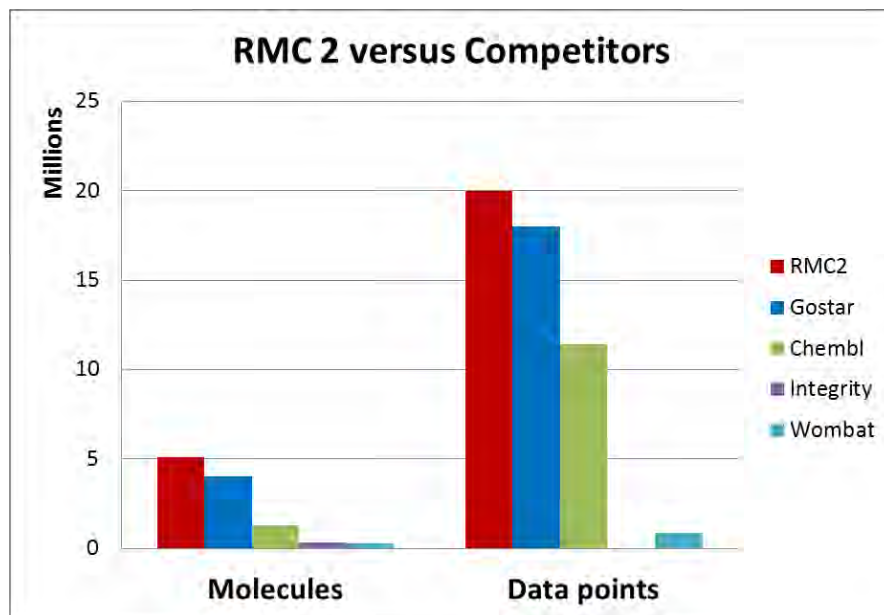
Articles and Journals

- >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

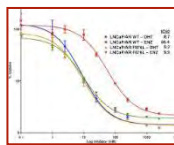
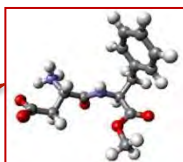
Output to

| | | | |
|---------------------------------------|--|---|--|
| <input type="radio"/> Substances Grid | <input checked="" type="radio"/> Substances Report Table | <input type="radio"/> Substances Reactions Table | <input type="radio"/> Substances Citations Table |
| <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 checked="" type="radio"/> Microsoft Excel | <input type="radio"/> Electronic Lab Notebook | <input type="radio"/> SD/Molfile |
| | | | <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...

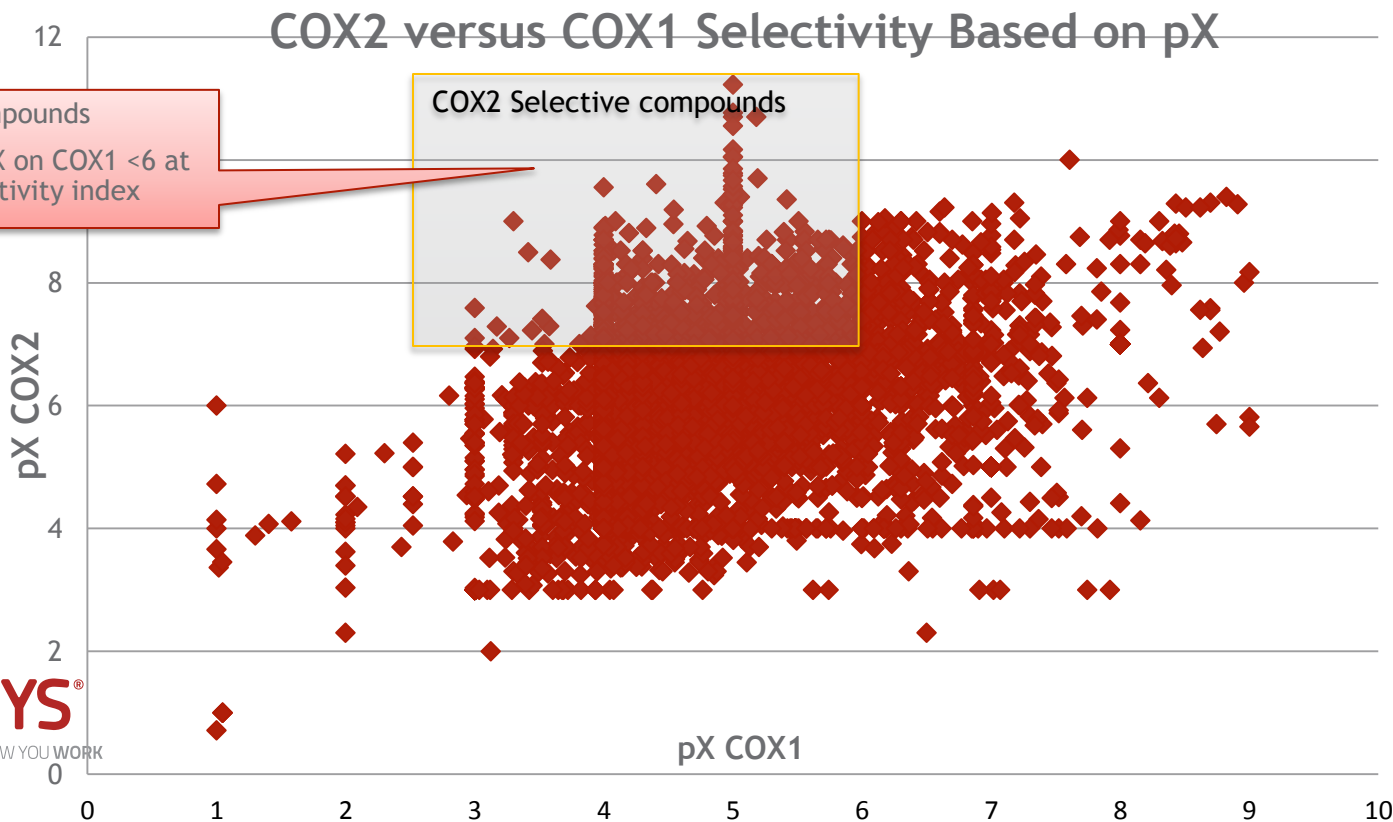
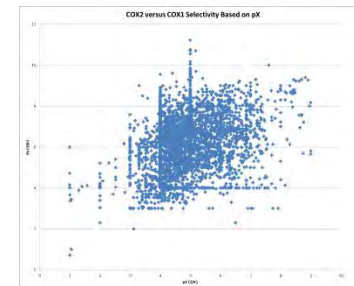
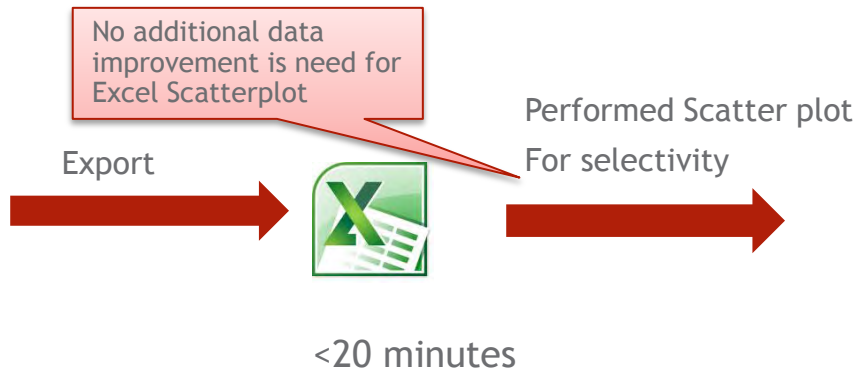


RMC2 EXCEL EXPORT AND SCATTER PLOT GENERATION

TARGET SELECTIVITY



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



and...
what is
your
reaction?

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