INTRODUCING REAXYS

PIOTR GOLKIEWICZ
LIFE SCIENCES SOLUTIONS CONSULTANT
CENTRAL-EASTERN EUROPE

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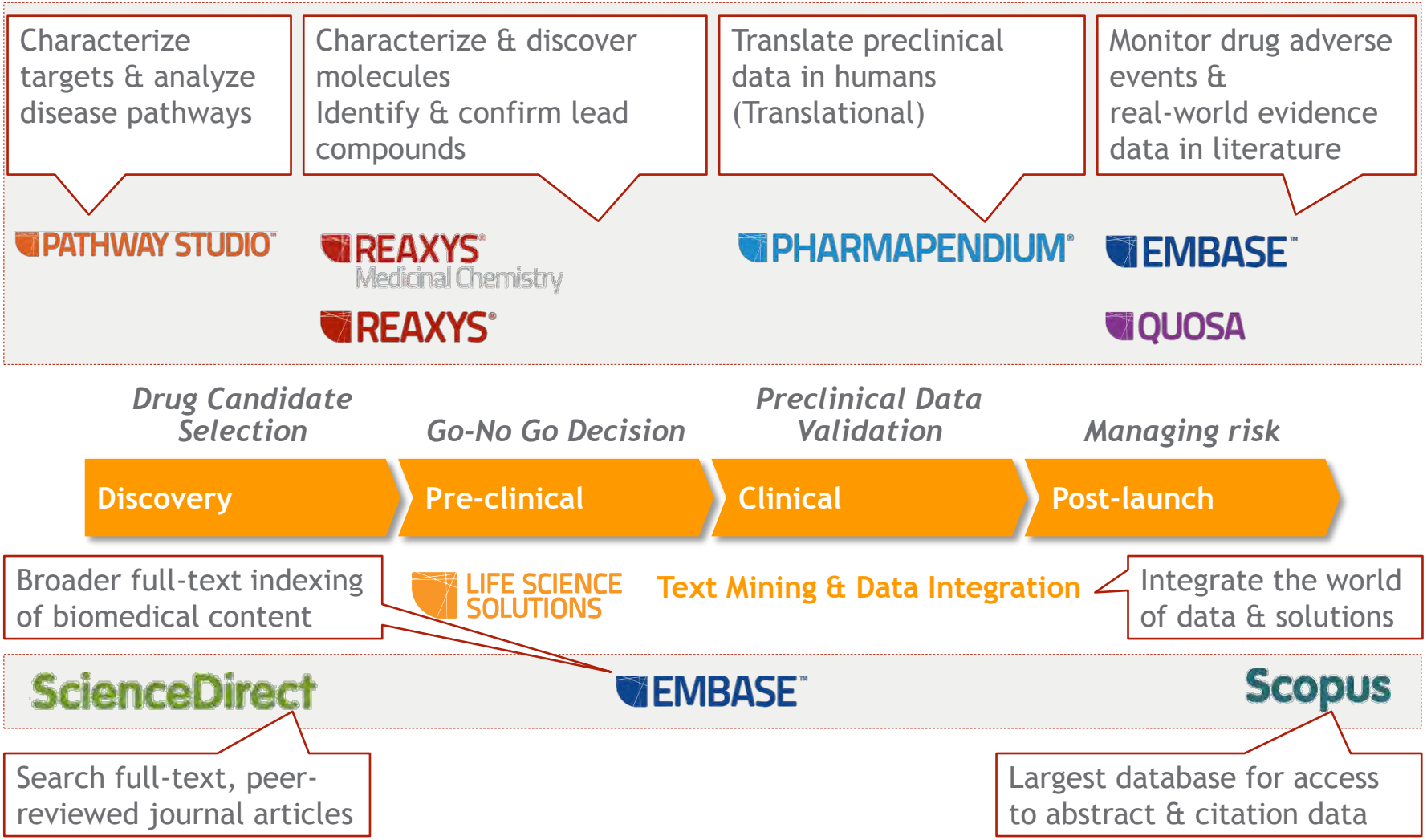
SERVING THE LIFE SCIENCES SPACE

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN



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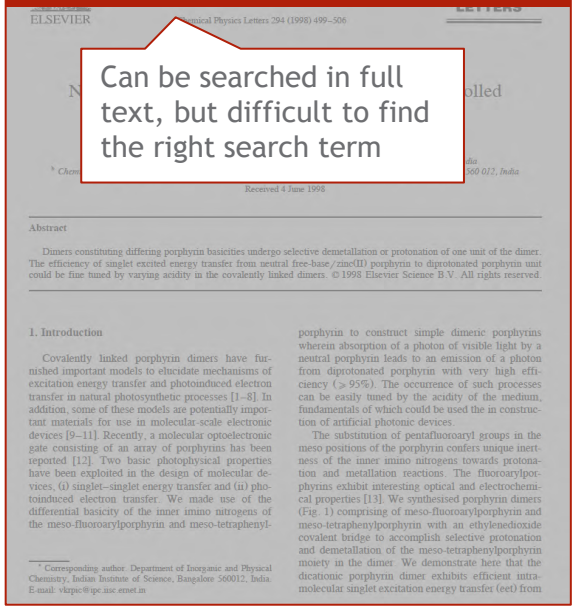
WHAT'S IN A TYPICAL CHEMISTRY DOCUMENT (PUBLICATION OR PATENT)?

Scientific topic, author



ELSEVIER

Chemical Physics Letters 294 (1998) 499–506

LETTERS

Received 4 June 1998

Abstract

Dimers constituting 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-fluoroarylporphyrin 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 (> 95%). The occurrence of such processes can be easily tuned by the acidity of the medium, fundamentals of which could be used the in construction of artificial photonic devices.

The substitution of pentafluoroaryl groups in the meso positions of the porphyrin confers unique inertness of the inner imino 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-tetraphenylporphyrin with an ethylenedioxide 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 (eet) from

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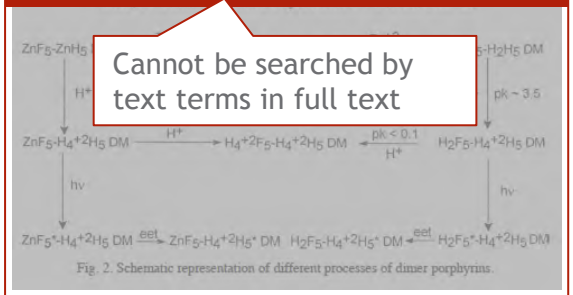
Can be searched in full text, but difficult to find the right search term

Chemical reactions



ZnF_5-ZnH_5 DM

H^+

pk ~ 3.5

ZnF_5-H_4+$^2H_5$ DM $\xrightarrow{H^+}$ H_4+$^2F_5$-H_4+$^2H_5$ DM $\xleftarrow[H^+]{pk < 0.1}$ H_2F_5-H_4+$^2H_5$ DM

hν

hν

ZnF_5*-H_4+$^2H_5$ DM $\xrightarrow{eet}$ ZnF_5-H_4+$^2H_5$* DM H_2F_5-H_4+$^2H_5$* DM $\xleftarrow{eet}$ H_2F_5*-H_4+$^2H_5$ DM

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

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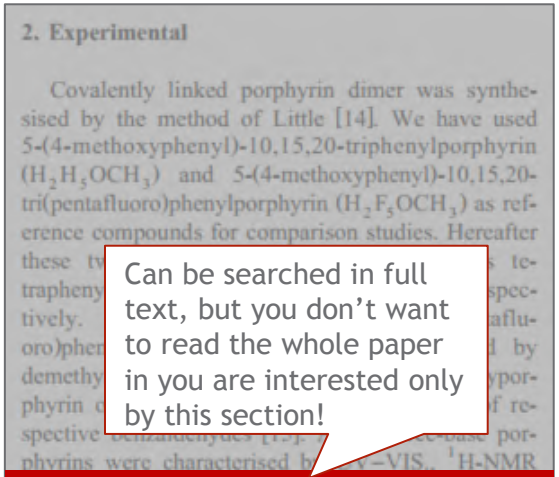
Experimental procedures

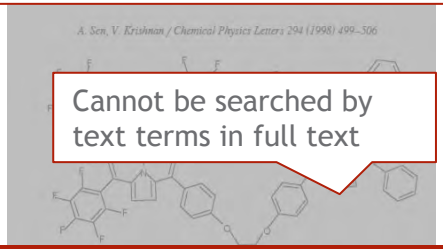


2. Experimental

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(pentafluoro)phenylporphyrin ($H_2F_5OCH_3$) as reference compounds for comparison studies. Hereafter these tw… te-traphen… spec-tively. …aflu-oro)phen… by demethy… …ypor-phyrin … f re-spective … por-phyrins were characterised b… –VIS, ^{1}H-NMR

Can be searched in full text, but you don't want to read the whole paper in you are interested only by this section!

Chemical structure



A. Sen, V. Krishnan / Chemical Physics Letters 294 (1998) 499–506

Cannot be searched by text terms in full text

Chemical spectra

Fig. 3. The fluo… MeOH. v/v): (1) ZnF_5OCH_3, (2) ZnH_4OCH_3, (3) intermolecular mixture of ZnF_5OCH_3 and ZnH_4OCH_3 and (4) ZnF_5–ZnH_5 DM. Inset shows the comparison of the corrected excitation spectrum (solid line) and absorption … (dotted line) of the (a) intermolecular mixture of ZnF_5OCH_3 and ZnH_4OCH_3 and (b) ZnF_5–ZnH_5 DM.

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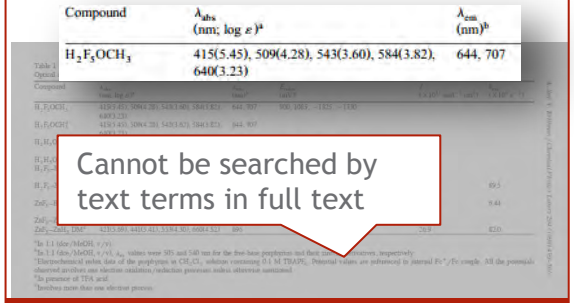
Substances and their physicochemical properties



Compound	λ_{abs} (nm; log ε)[a]	λ_{em} (nm)[b]
$H_2F_5OCH_3$	415(5.45), 509(4.28), 543(3.60), 584(3.82), 640(3.23)	644, 707

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Chemistry as the organizing principle

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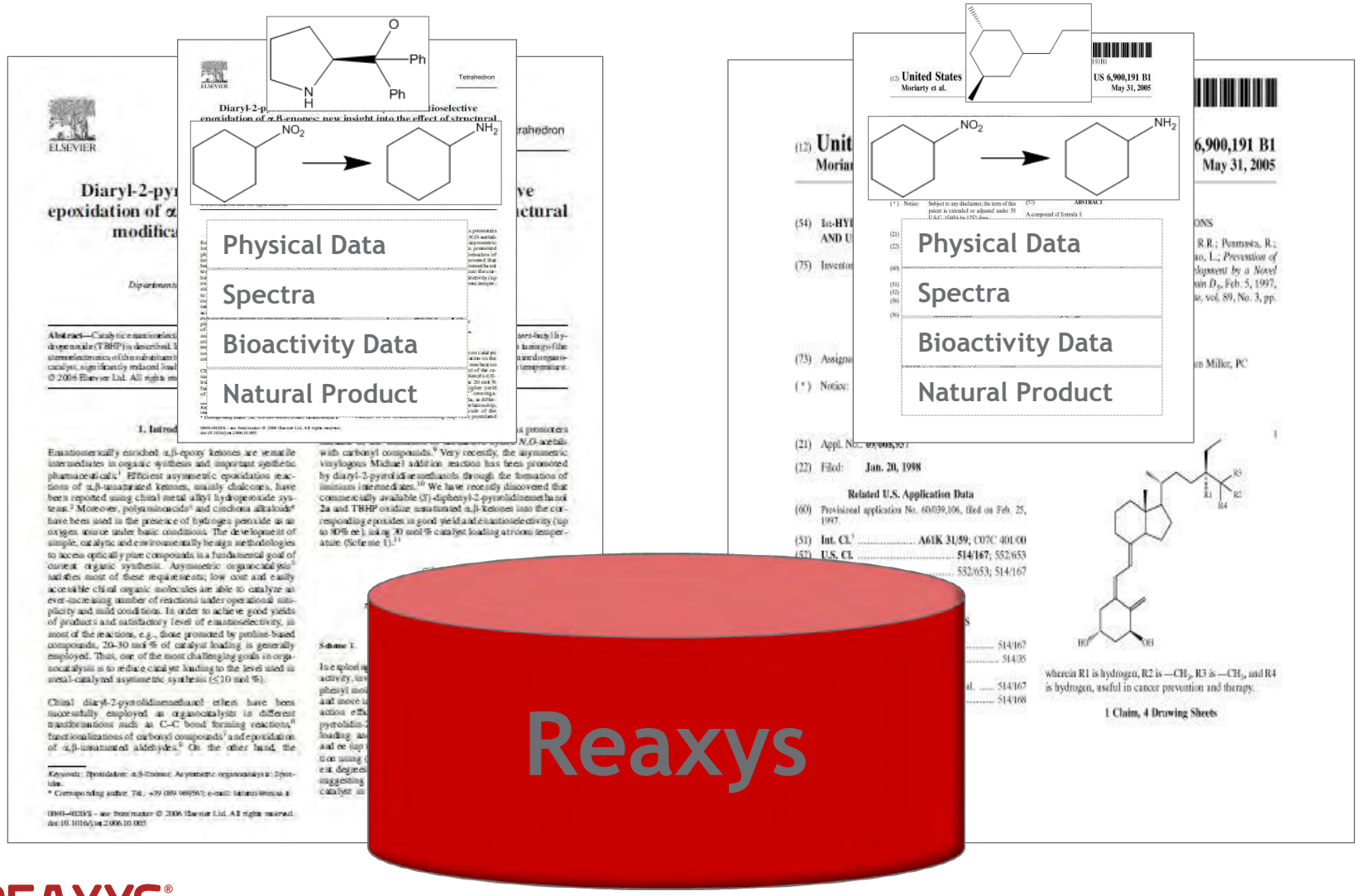
With experimental data from journal articles and patents



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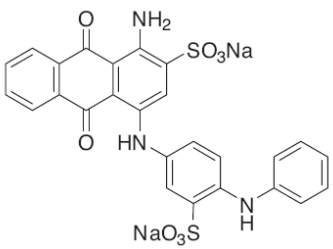
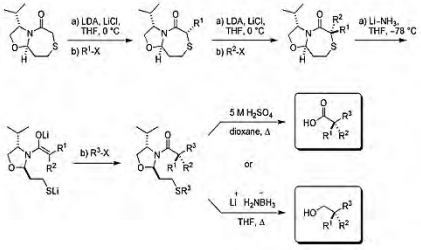
CHEMISTRY AS THE ORGANIZING PRINCIPLE



Chemical Structures



Chemical Syntheses

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

High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet $P2Y_{12}$ Receptors

Younis Baqi,[†] Kerstin Atzler,[†] Meryem Köse,[†] Markus Glänzel,[‡,§] and Christa E. Müller*[,†]

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

Received March 16, 2009

Anthraquinone derivatives related to the moderately potent, nonselective $P2Y_{12}$ receptor antagonist reactive blue 2 (6) have been synthesized and optimized with respect to $P2Y_{12}$ receptor affinity. A radioligand binding assay utilizing human blood platelet membranes and the $P2Y_{12}$ receptor-selective antagonist radioligand [^{3}H]2-propylthioadenosine-5′-adenylic acid (1,1-dichloro-1-phosphonomethyl-1-phosphonyl) anhydride ([^{3}H]PSB-0413) was applied for compound testing. 1-Amino-2-sulfoanthraquinone derivatives bearing a (*p*-phenylamino)anilino substitution in the 4-position and an additional acidic function in the *meta*-position of the aniline ring showed high $P2Y_{12}$ receptor affinity. These new anthraquinone derivatives became accessible by a recently developed copper(0)-catalyzed Ullmann coupling reaction of 1-amino-4-bromoanthraquinone derivatives with anilines in phosphate 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 change. 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.[4] 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

presumably act as covalent, possibly allosteric antagonists at $P2Y_{12}$ receptors[9] (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 $P2Y_{12}$ antagonists that are lacking the drawbacks associated with the standard $P2Y_{12}$ antagonists such as clopidogrel and other thienotetrahydropyridine derivatives. Several groups have recently been developing competitive, reversible $P2Y_{12}$ 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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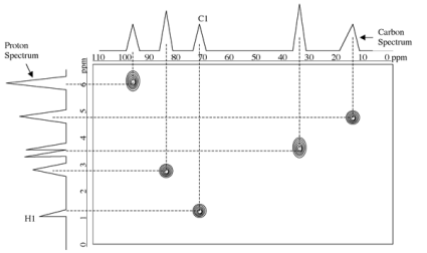
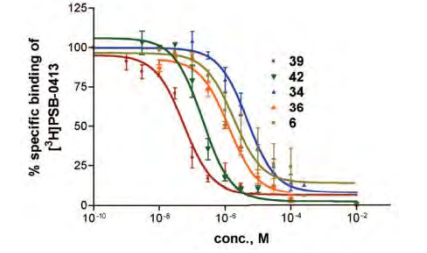
[†] PharmaCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn.
[‡] Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg.
[§] Present address: Elsevier Pharma Biotech Group, Elsevier Information Systems GmbH, Theodor-Heuss-Allee 108, D-60486 Frankfurt (Main), Germany.

10.1021/jm9003297 CCC: $40.75
Published on Web 05/22/2009



Physicochemical Properties



Pharmacology

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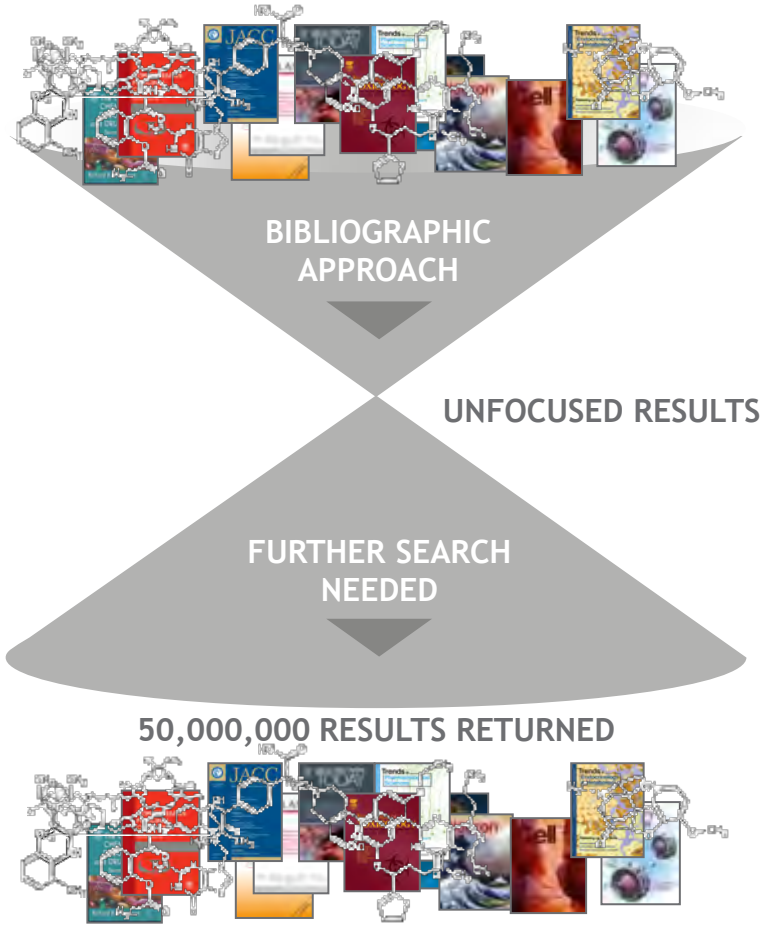
OTHER DATABASES



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

Searching for classes of substances in Reaxys

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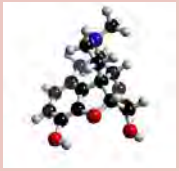
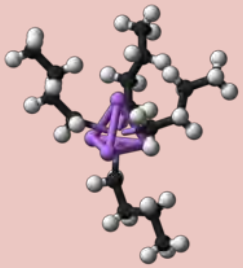
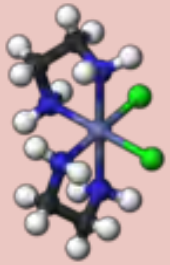


CLASSIC ORGANICS



ORGANOMETALLICS

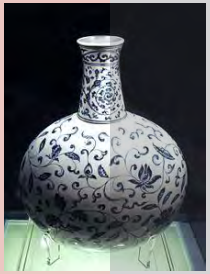
COORDINATION COMPOUNDS



CLASSIC INORGANICS

ALLOYS & METALS

CERAMICS



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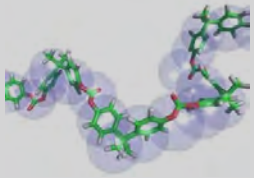
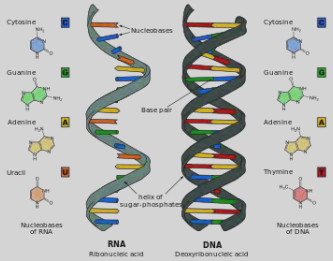
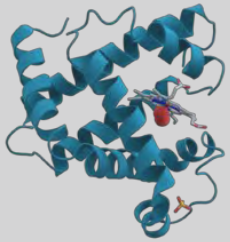
POLYMERS







NUCLEIC ACIDS & PROTEINS

Search Substances Context

Search Literature Context

WHAT IS REAXYS 2015?

CONTENT: MANY DATABASES ALL IN ONE

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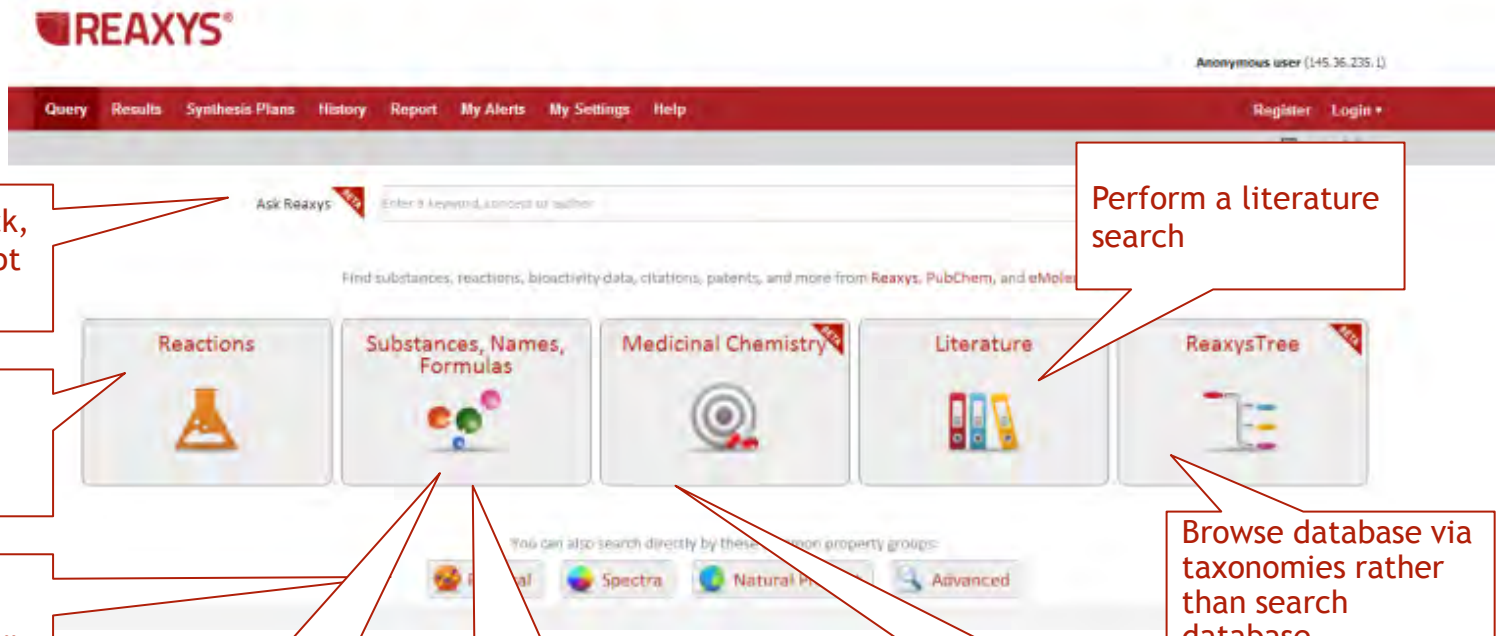
HOW YOU THINK HOW YOU WORK

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



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

Open Reaction search form

Data search form by "property"

Open a structure search form

Search using chemical identifiers

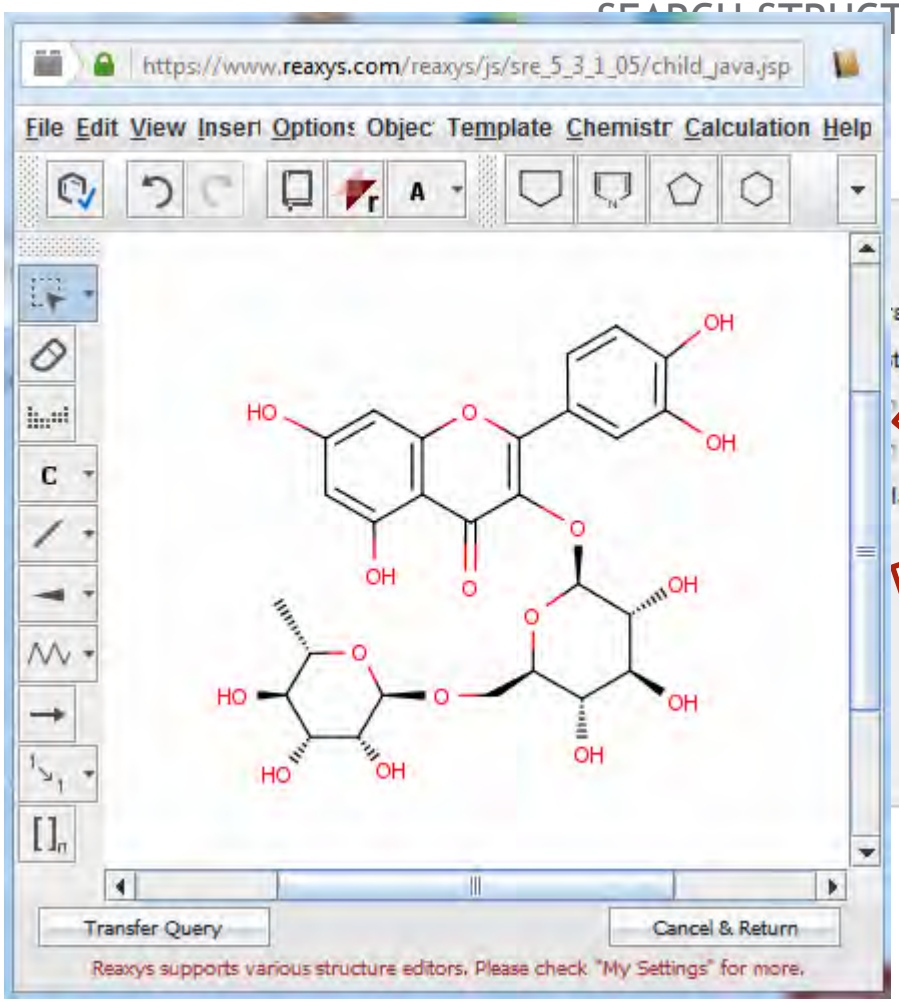
Access detailed Biodata, and MedChem specific features

Browse database via taxonomies rather than search database

Perform a literature search

SEARCH SUBSTANCES

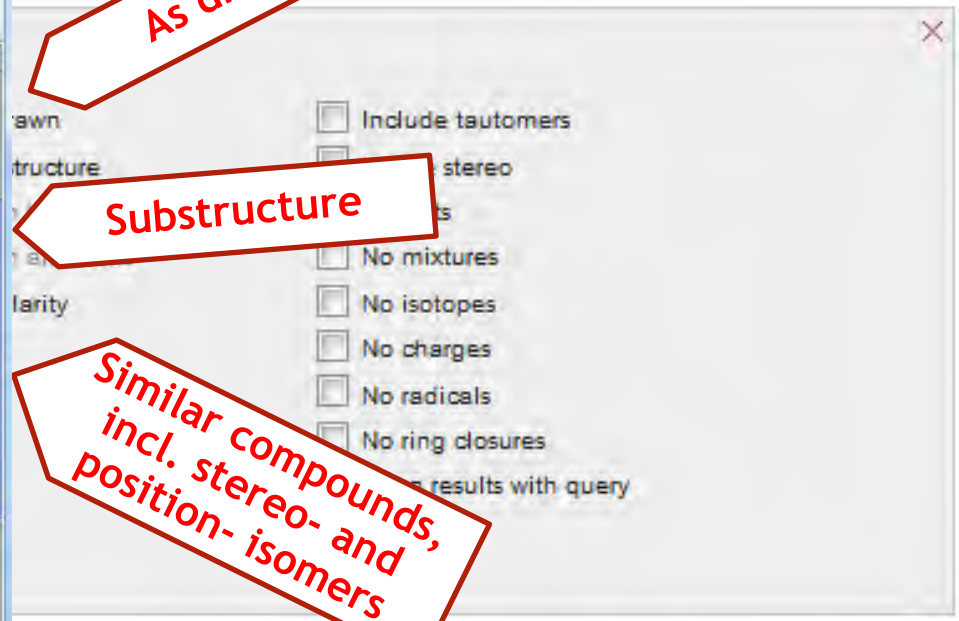
SEARCH STRUCTURE, NAME, OR FORMULA – IN FULL, OR IN PART



As drawn

Substructure

Similar compounds, incl. stereo- and position- isomers



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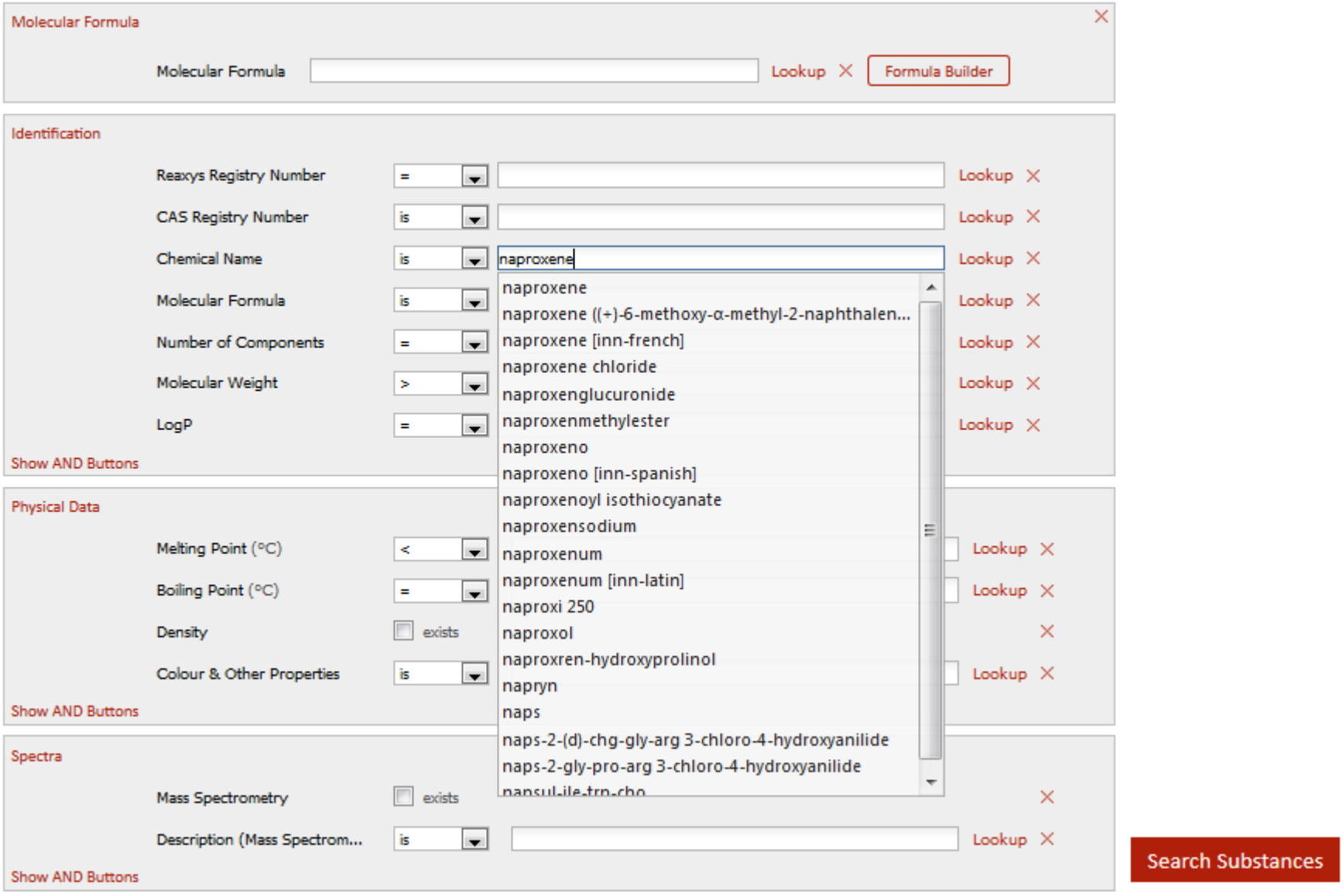
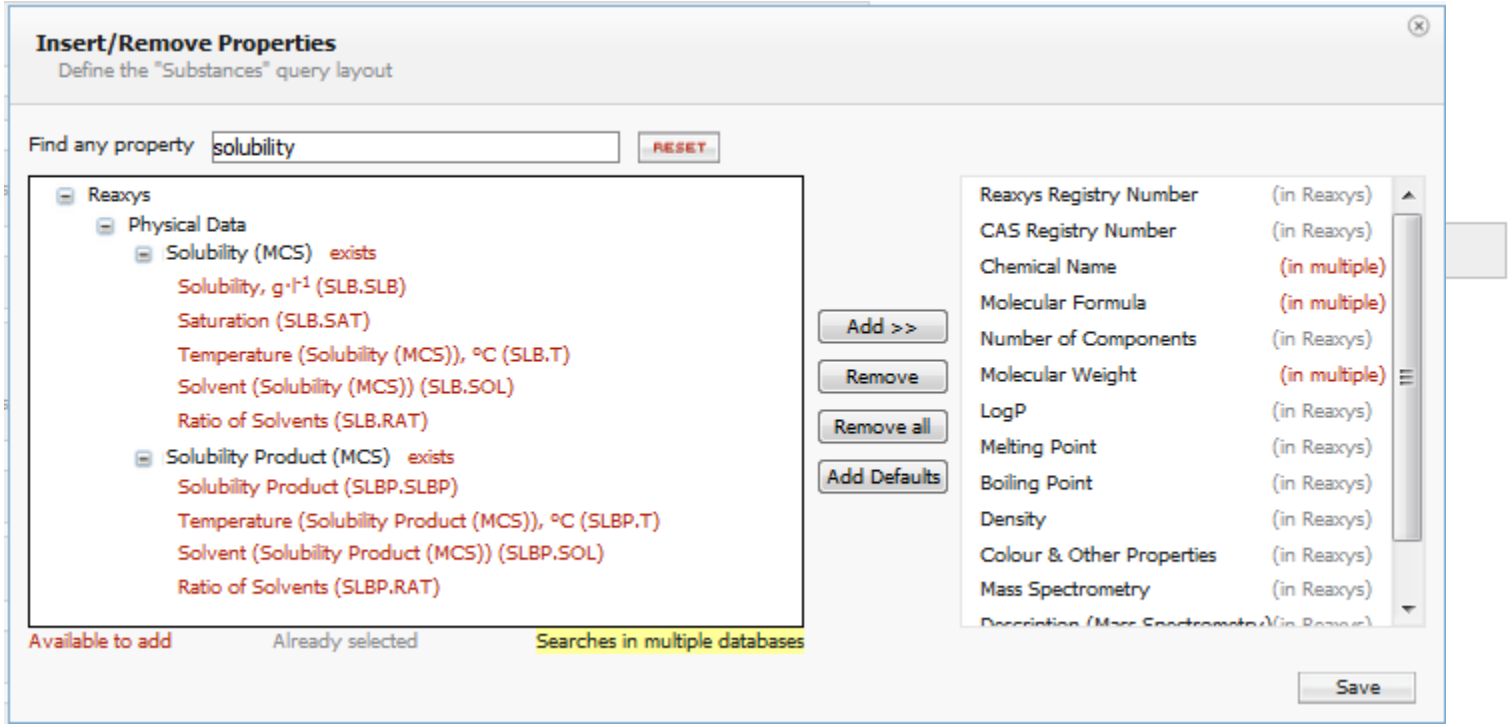
SEARCH SUBSTANCES

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



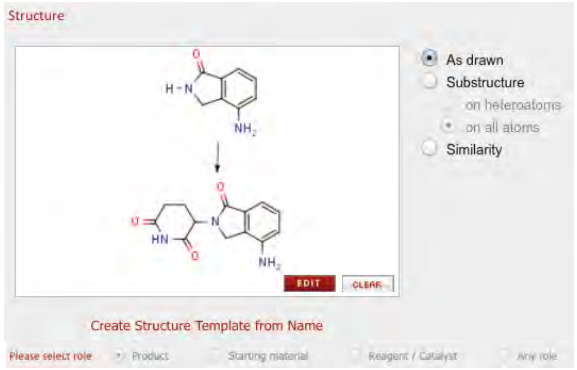
ADD OR REMOVE SEARCH FIELDS



SEARCH REACTIONS

SEARCH BY STRUCTURE, DATA, OR TYPE

STRUCTURE



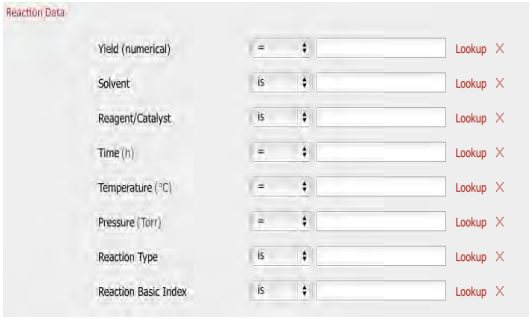
Atom mapping

Bond forming/breaking

Search reactions by structure

✔✔✔

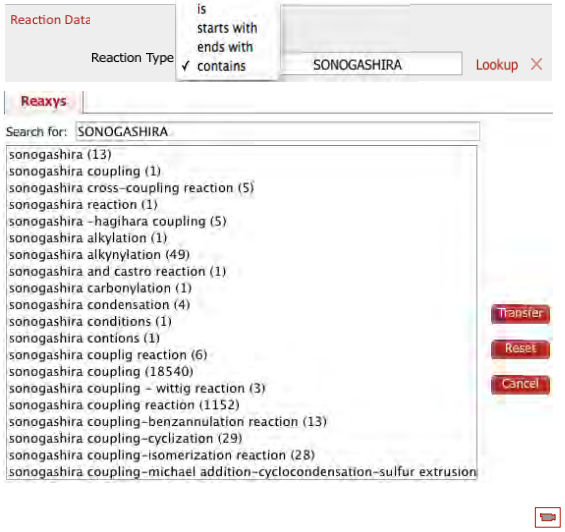
DATA



Search reactions by reaction conditions

✔✔✔

TYPE



Search reactions by type or name

✔✔✔

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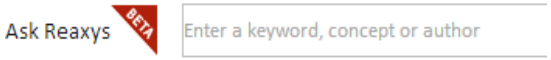
HOW YOU THINK HOW YOU WORK

SEARCH LITERATURE

OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

Ask Reaxys

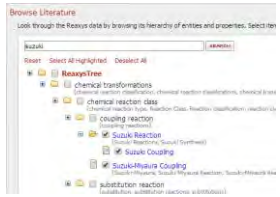


Ask Reaxys provides new user experience for text searching: content better discoverable, answers more immediately available

Intelligent interpretation of topic query

✔✔✔

Reaxys Tree

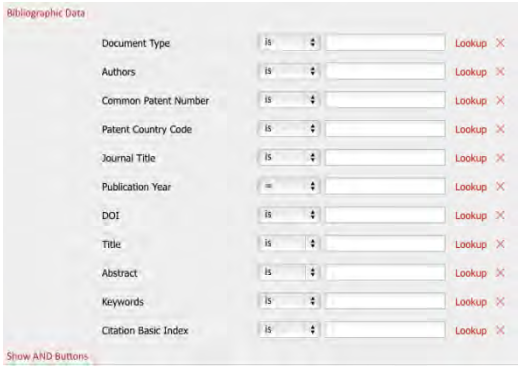


ReaxysTree lets users “browse” the database by taxonomies: helps with search precision and answer comprehension

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

✔✔✔

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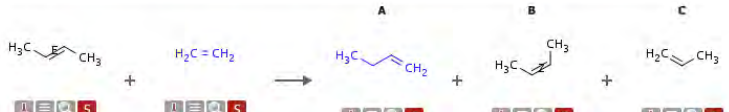
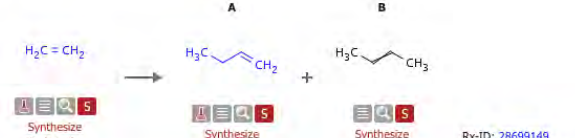
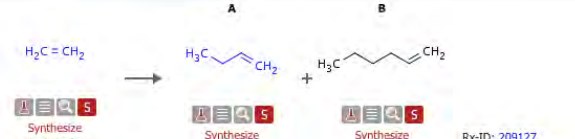
Ask Reaxys preparation of 1-butene from ethylene **Search**

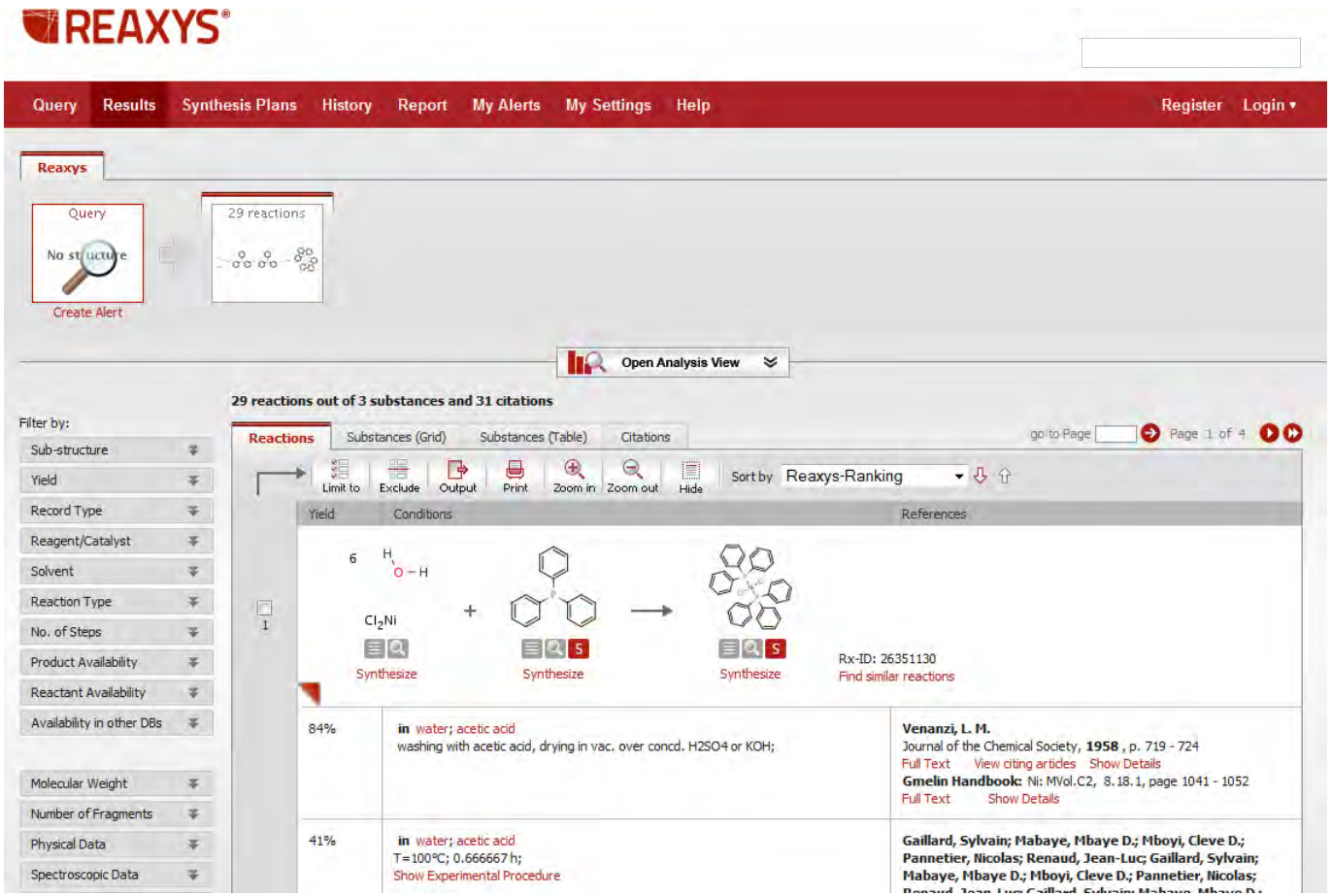
Reactions (96) | Substances (81) | Citations (190) — go to Page — Page 1 of 11

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

	Yield	Conditions	References
1			Rx-ID: 38295231 Find similar reactions
	C: 55%	T=450°C; P=750.075 Torr; 10 h; AutoclaveInert atmosphere; 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
		Reagent/catalyst; Show Experimental Procedure	**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		 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		 Rx-ID: 209127 Find similar reactions	
	A: 90% B: 6%	**With** $[Ph_2PC_6H_4C(OB(C_6F_5)3)O\text{-}\kappa^2P,O](\eta^3\text{-}CH_2CMeCH_2)$ **in** toluene T=0°C; oligomerization; P=2280.15 Torr; 1 h; Product distribution; Further Variations:TemperaturesPressures;	**Komon, 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}$NiBr_2$; 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

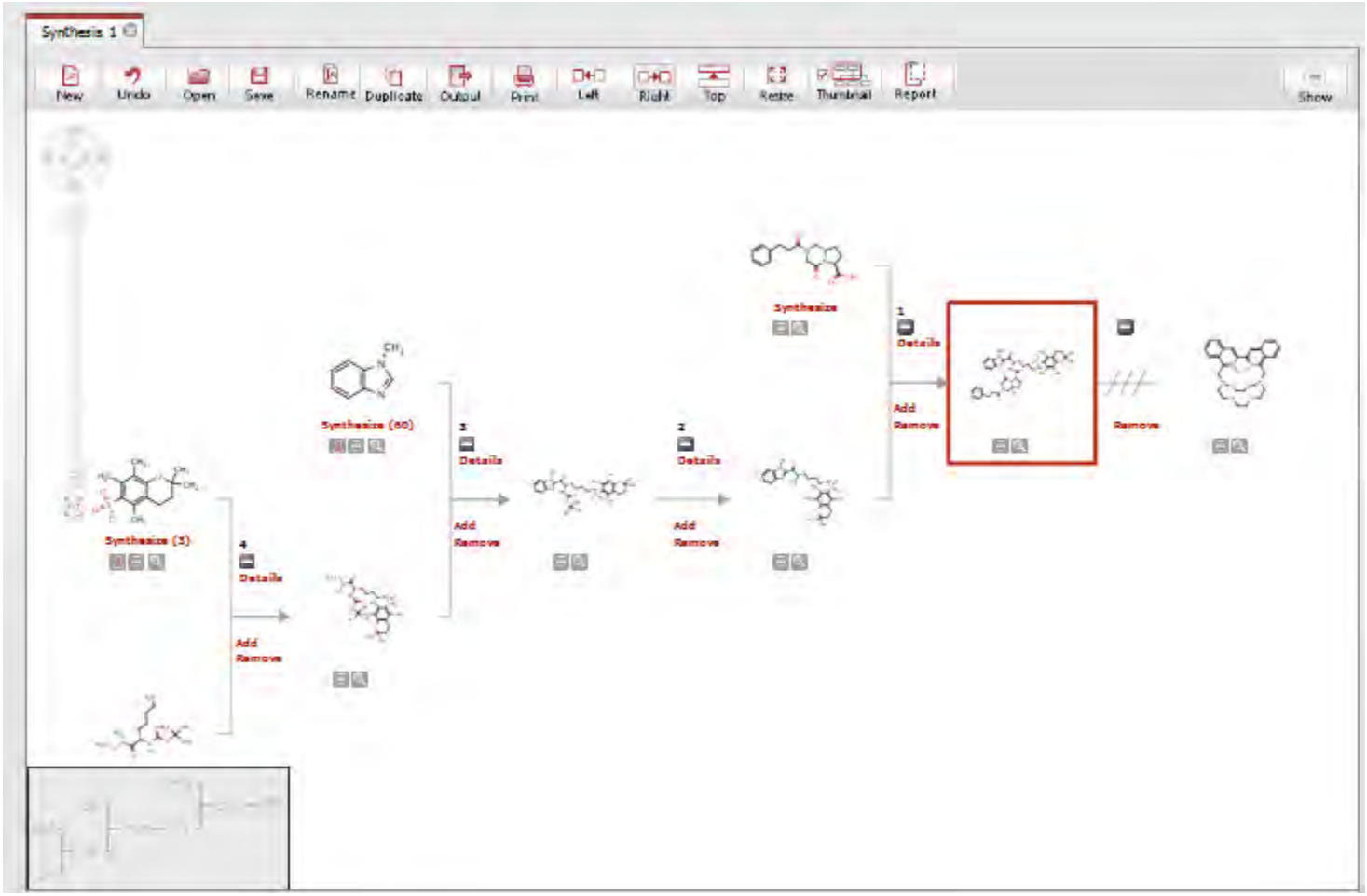
REA
HOW YOU TH

MAKE A COMPOUND



SYNTHESIS PLAN:

AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES



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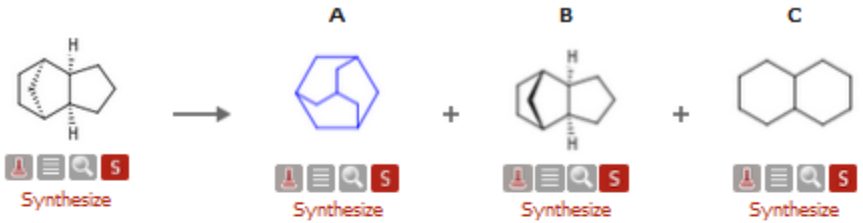


Rx-ID: 27727760
Find similar reactions

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-Mi
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 4.65 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.
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 proce
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
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
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_{g}
and/or MCPD diners. 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 v
reaction time is too long 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 rin
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 isome

TI02 - 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)

- 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)

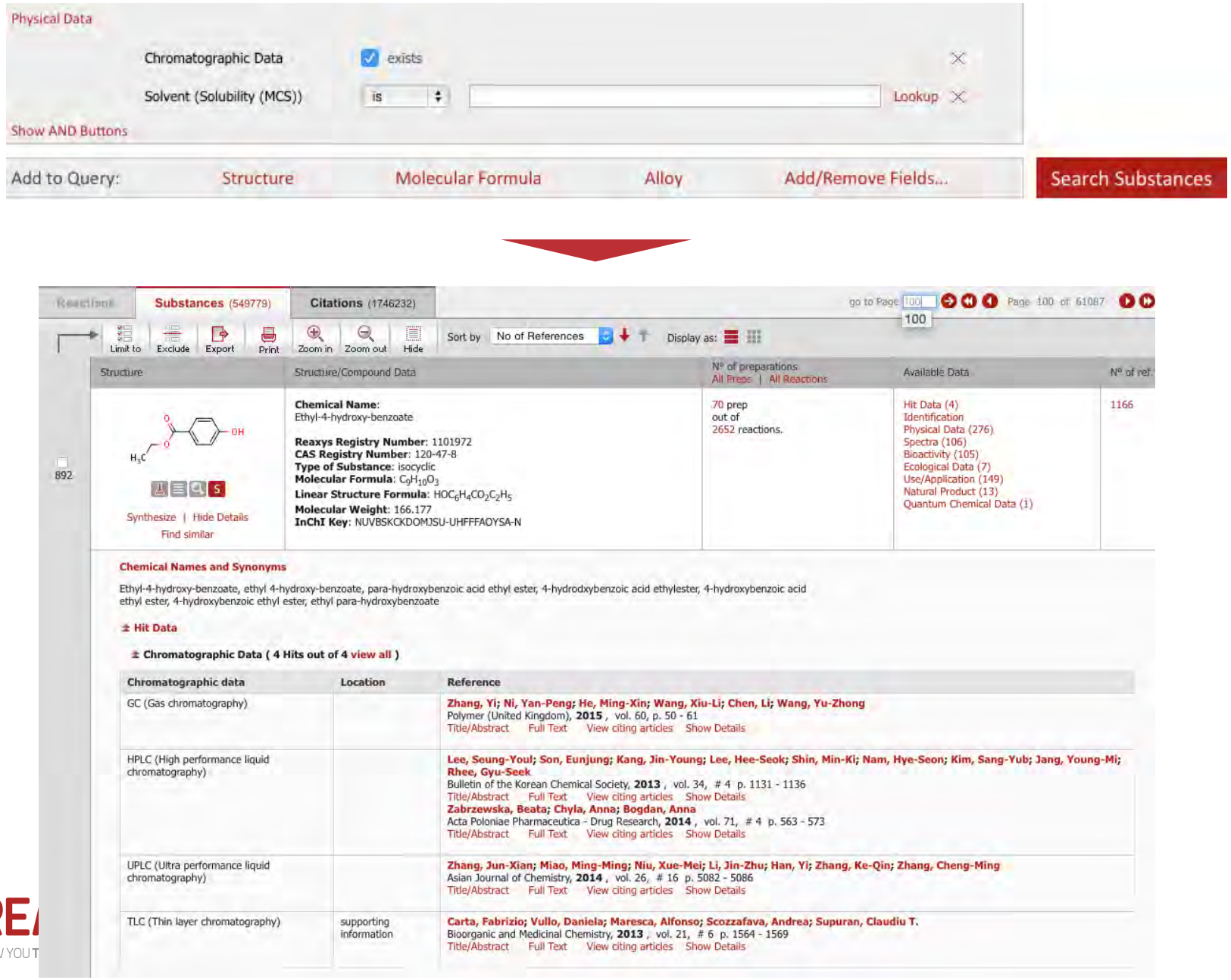
Structure	Structure/Compound Data	N° of preparations All Preps | All Reactions	Available Data	Target	N° of re
O_2Ti Synthesize | Hide Details	**Chemical Name:** Titanium(IV) oxide **Reaxys Registry Number:** 4360545 **Type of Substance:** Glass or Ceramic materialCoordination compoundIsotope or isotope containing compoundSolid solution **Molecular Formula:** O_2Ti **Linear Structure Formula:** O_2Ti **Molecular Weight:** 79.8788 **InChI Key:** QWWIMOOFEDJKFN-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

Use (1555)

Use Pattern	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 DENKO Masahiro; LI D Patent: WO2013 Title/Abstract
photocatalytic material in antimicrobial composition	Paragraph 34	SHOWA DENKO Masahiro; LI D Patent: WO2013 Title/Abstract
photocatalytic material in antiviral composition	Paragraph 34	SHOWA DENKO 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

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 Chemica Title/Abstract Full Text Vi
Density of states	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-à, Hartree-Fock)		Feng, Ningdong; Wang, Qian Feng Journal of the American Chemica Title/Abstract Full Text Vi
Atom distances, angles Potential energy function, potential curve Vibrational constants	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhuang, Jia; Li, Zhen Hua; F Journal of Physical Chemistry A, Title/Abstract Full Text Vi
Molecular orbitals Electronic energy levels	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-à, Hartree-Fock)		El-Shafei, Ahmed; Hussain, Journal of Materials Chemistry, 2 Title/Abstract Full Text Vi
Electronic energy levels	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Lu, Xiaoqing; Wei, Shuxian; Journal of Organometallic Chemis Title/Abstract Full Text Vi
Density of states Band structure	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Munnix, S.; Schmeits, M. Physical Review B: Condensed M Full Text View citing articles Sarkar; Ghosh; Maiti; Chatto Physica B: Condensed Matter, 2 Title/Abstract Full Text Vi
Band structure Density of states UV/VIS wave lengths	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Guo; Zhang; Liang Physica B: Condensed Matter, 2 Title/Abstract Full Text Vi
Density of states Molecular orbitals Electronic energy levels Band structure	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhao, Dongqiu; Huang, Xiao Applied Physics Letters, 2011 , Title/Abstract Full Text Vi
Population analysis, charge distribution Density of states Band structure	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Shi, Weimei; Chen, Qifeng; X Journal of Solid State Chemistry, Title/Abstract Full Text Vi
Band structure Effective masses Population analysis, charge distribution UV/VIS wave lengths	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhang, Rui-Shuo; Liu, Yong; Journal of Alloys and Compounds Title/Abstract Full Text Vi
Density of states UV/VIS wave lengths	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Zhang, Zhi-Kun; Bai, Mei-Lin Chemical Communications, 201 Title/Abstract Full Text Vi
Atomization energy	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)		Shinzato, Yoshifumi; Yukawa Journal of Alloys and Compounds Title/Abstract Full Text Vi West, Richard H.; Beran, Gr Journal of Physical Chemistry A, Title/Abstract Full Text Vi Hirate; Morinaga; Yukawa; Journal of Alloys and Compounds Title/Abstract Full Text Vi


Physical Data
Chromatographic Data
exists
Solvent (Solubility (MCS))
is
Lookup
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Add to Query:
Structure
Molecular Formula
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Add/Remove Fields...
Search Substances
Substances (549779)
Citations (1746232)
Limit 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.
Chemical Name:
Ethyl-4-hydroxy-benzoate
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
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
Synthesize | Hide Details
Find similar
Chemical Names and Synonyms
Ethyl-4-hydroxy-benzoate, ethyl 4-hydroxy-benzoate, para-hydroxybenzoic acid ethyl ester, 4-hydrodxybenzoic 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-Youl; Son, Eunjung; Kang, Jin-Young; Lee, Hee-Seok; Shin, Min-Ki; Nam, Hye-Seon; Kim, Sang-Yub; Jang, Young-Mi; Rhee, Gyu-Seek
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

FIND: A polymer shape

Comb polymer

EXAMPLE: Comb shaped polyacrylates

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

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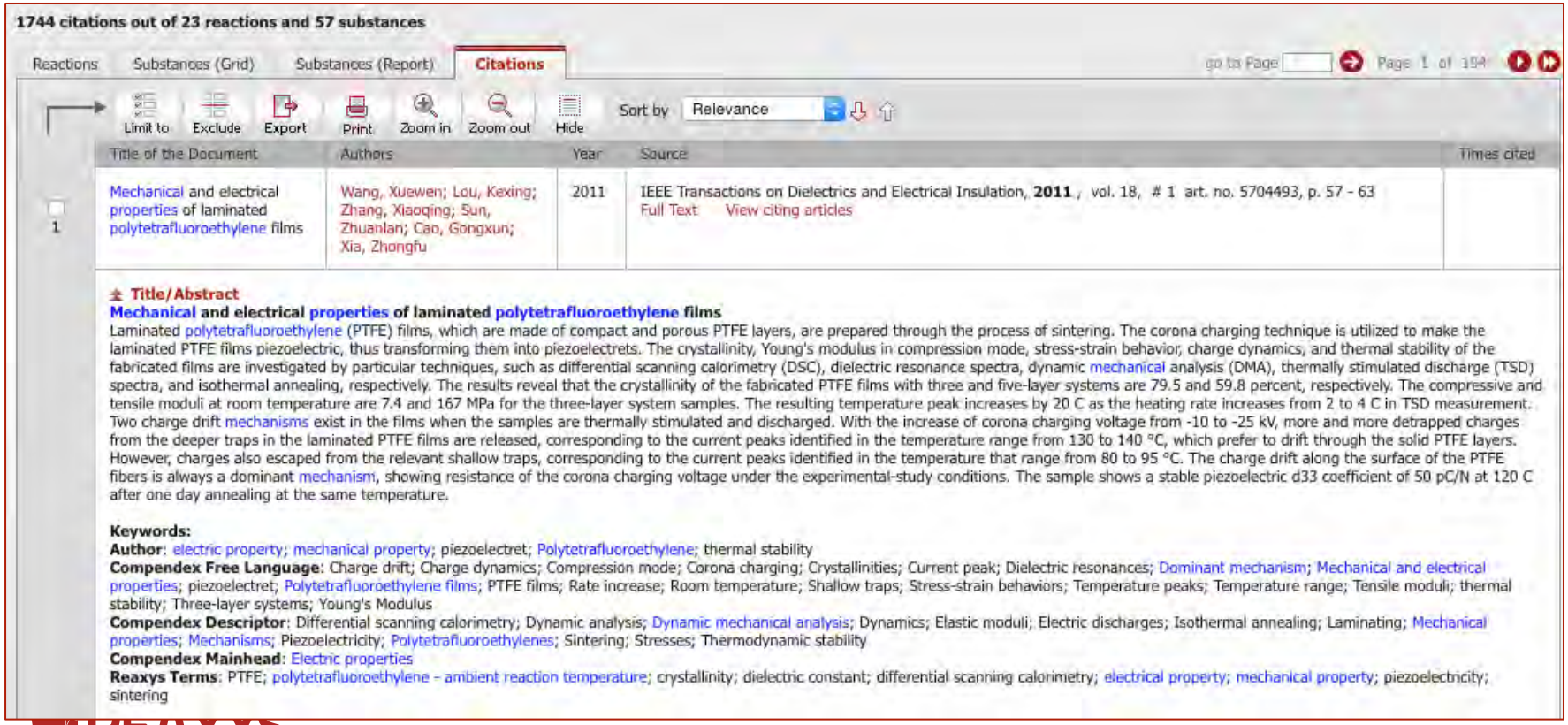
FIND: Property of a Polymer

EXAMPLE: Mechanical Properties of Polytetrafluoroethylene

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)



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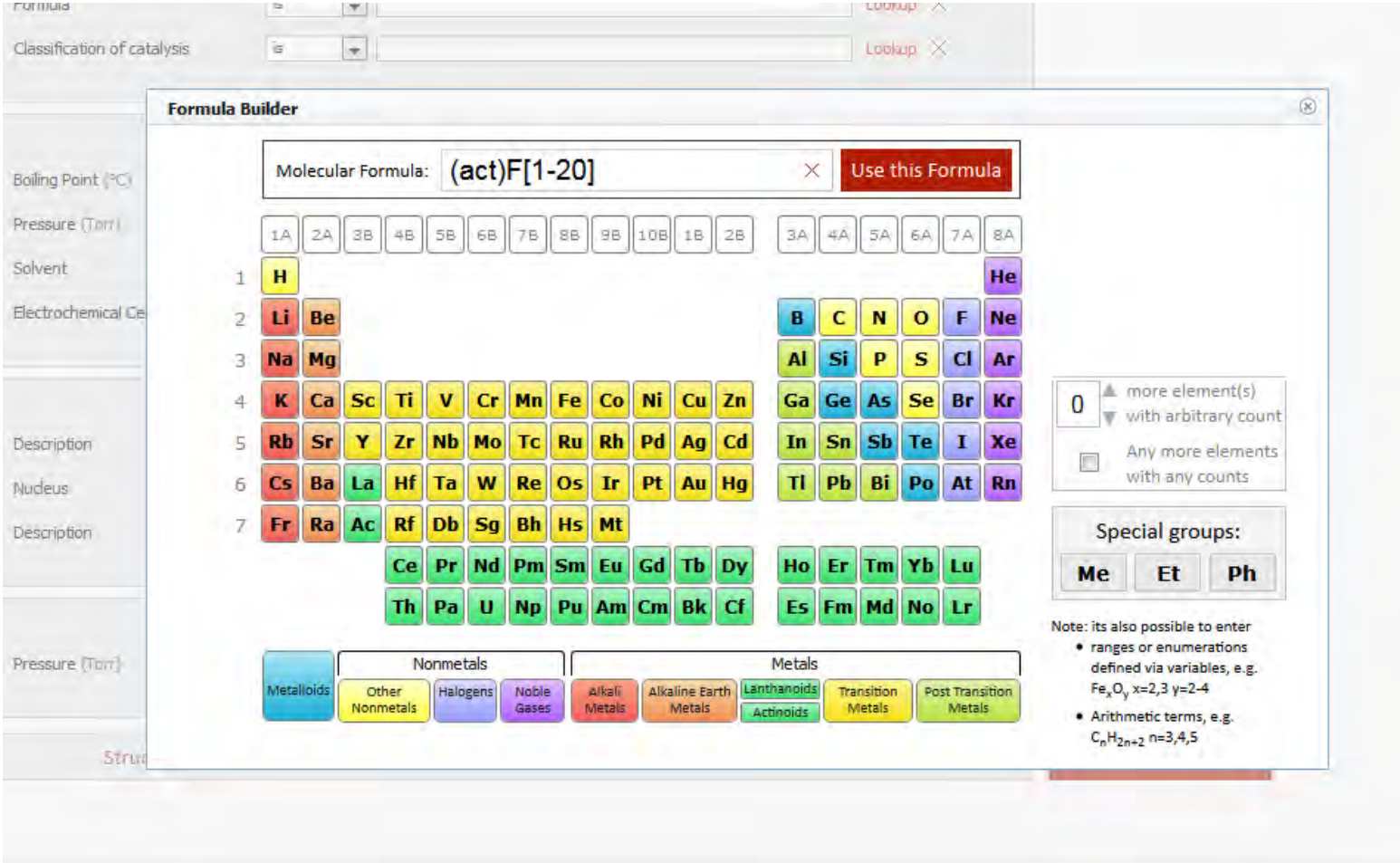
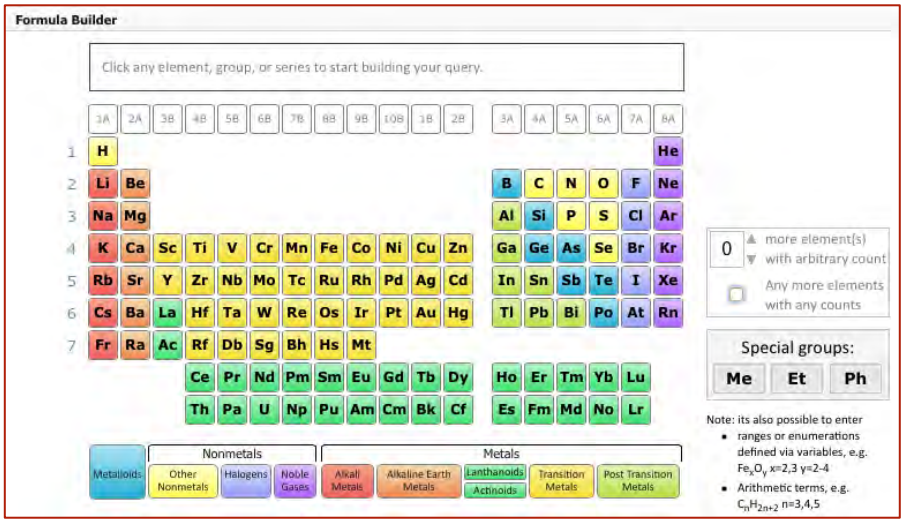
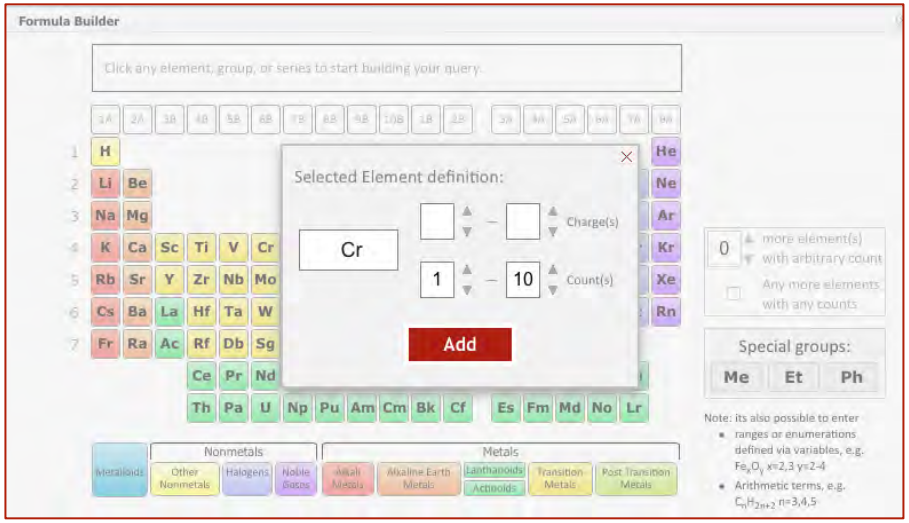
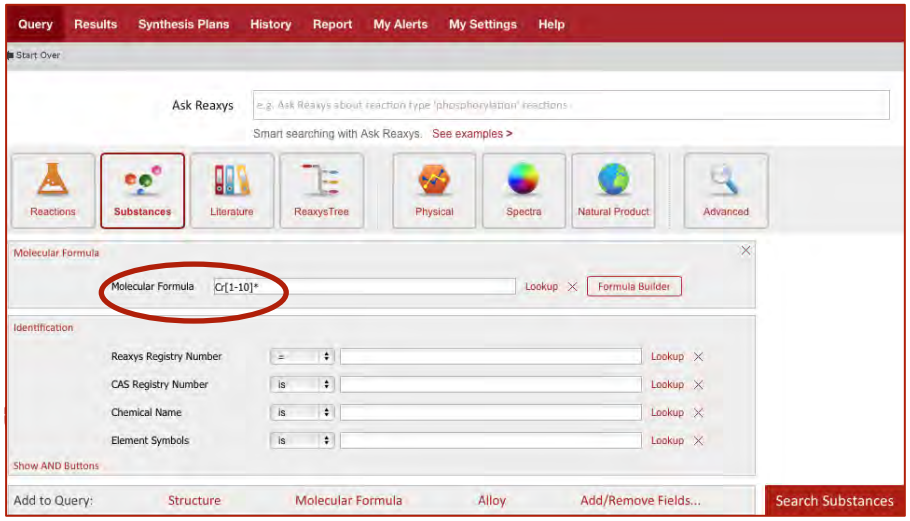
MOLECULAR FORMULA BUILDER

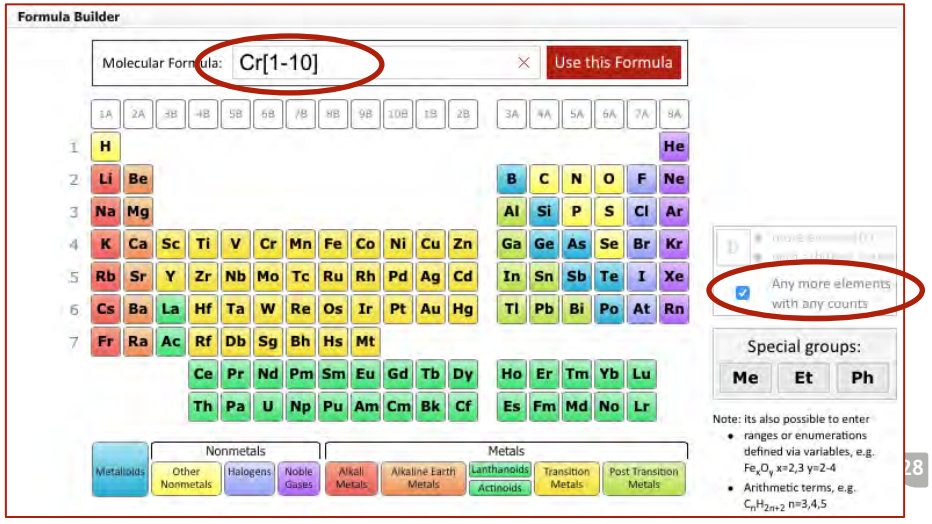


Chrome compounds

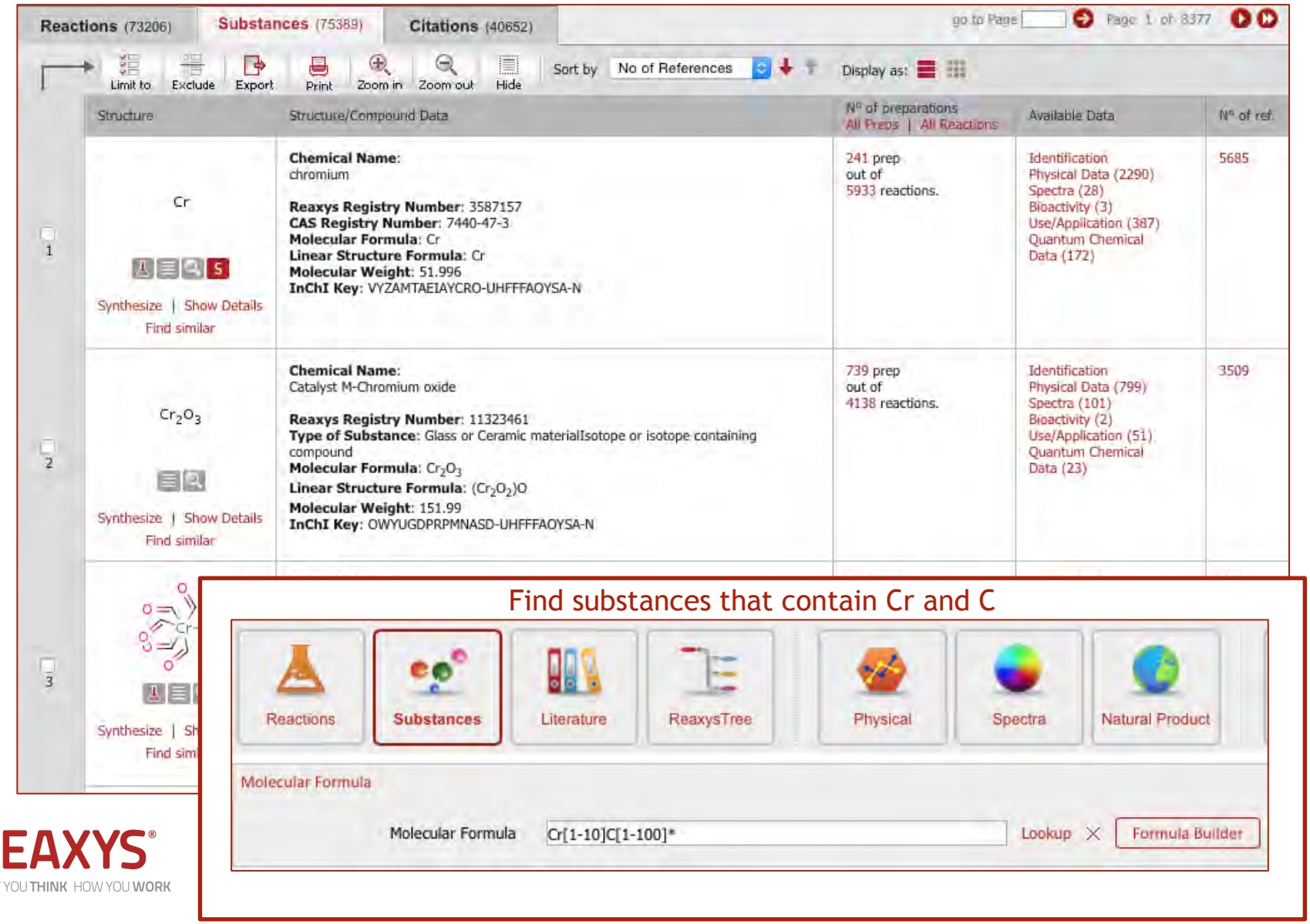








CHROME COMPOUNDS



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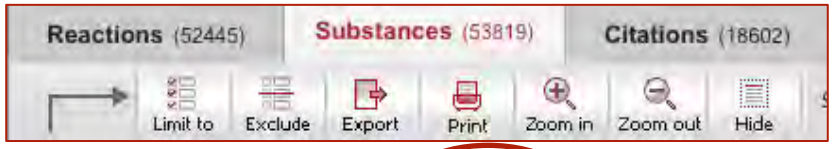
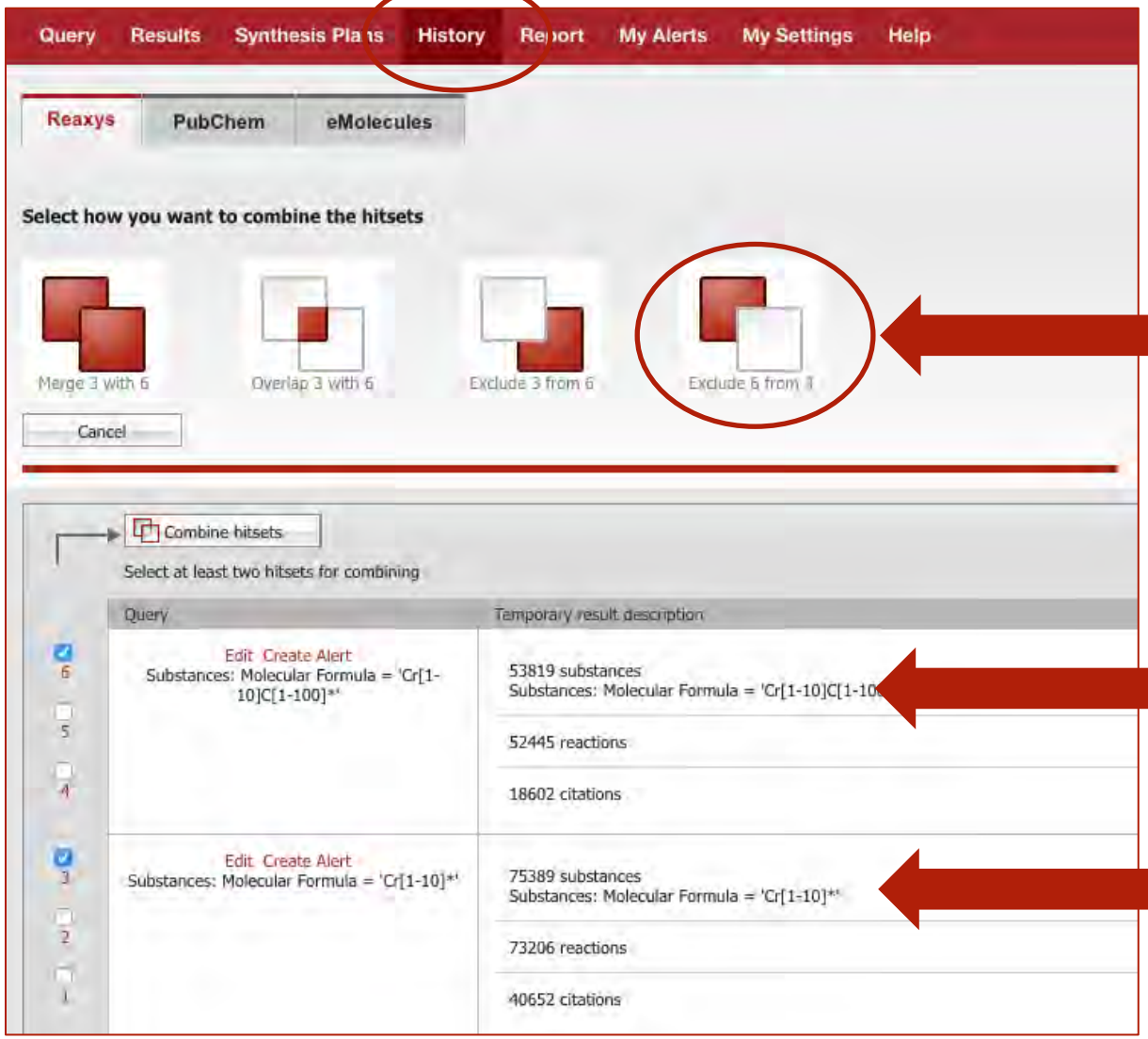


All carbon + chromium-containing substances

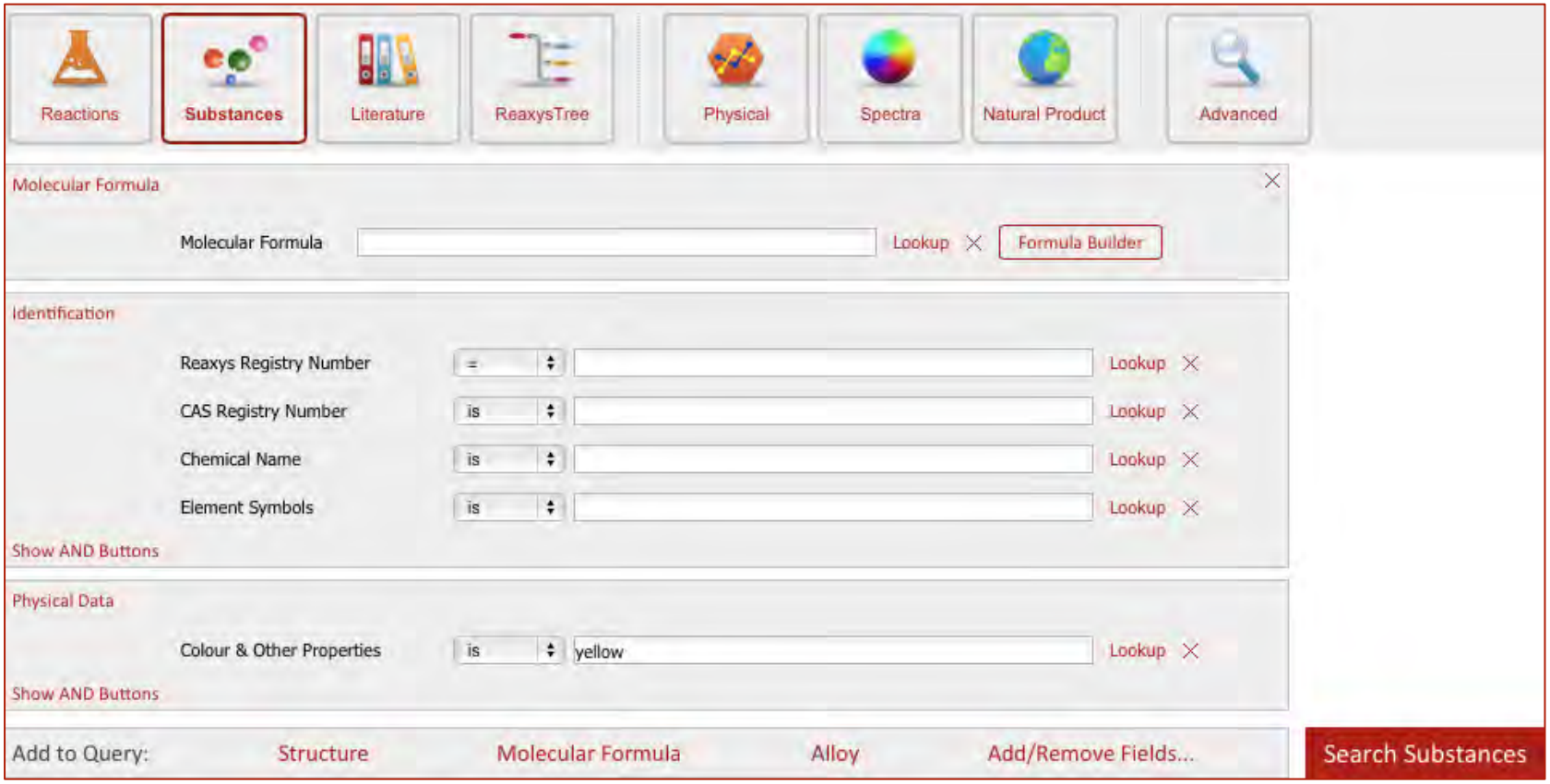


All "inorganic" chromium-containing substances

All carbon + chromium-containing substances

All chromium-containing substances

CHROME COMPOUNDS (Yellow Inorganics)



> 900,000
YELLOW SUBSTANCES

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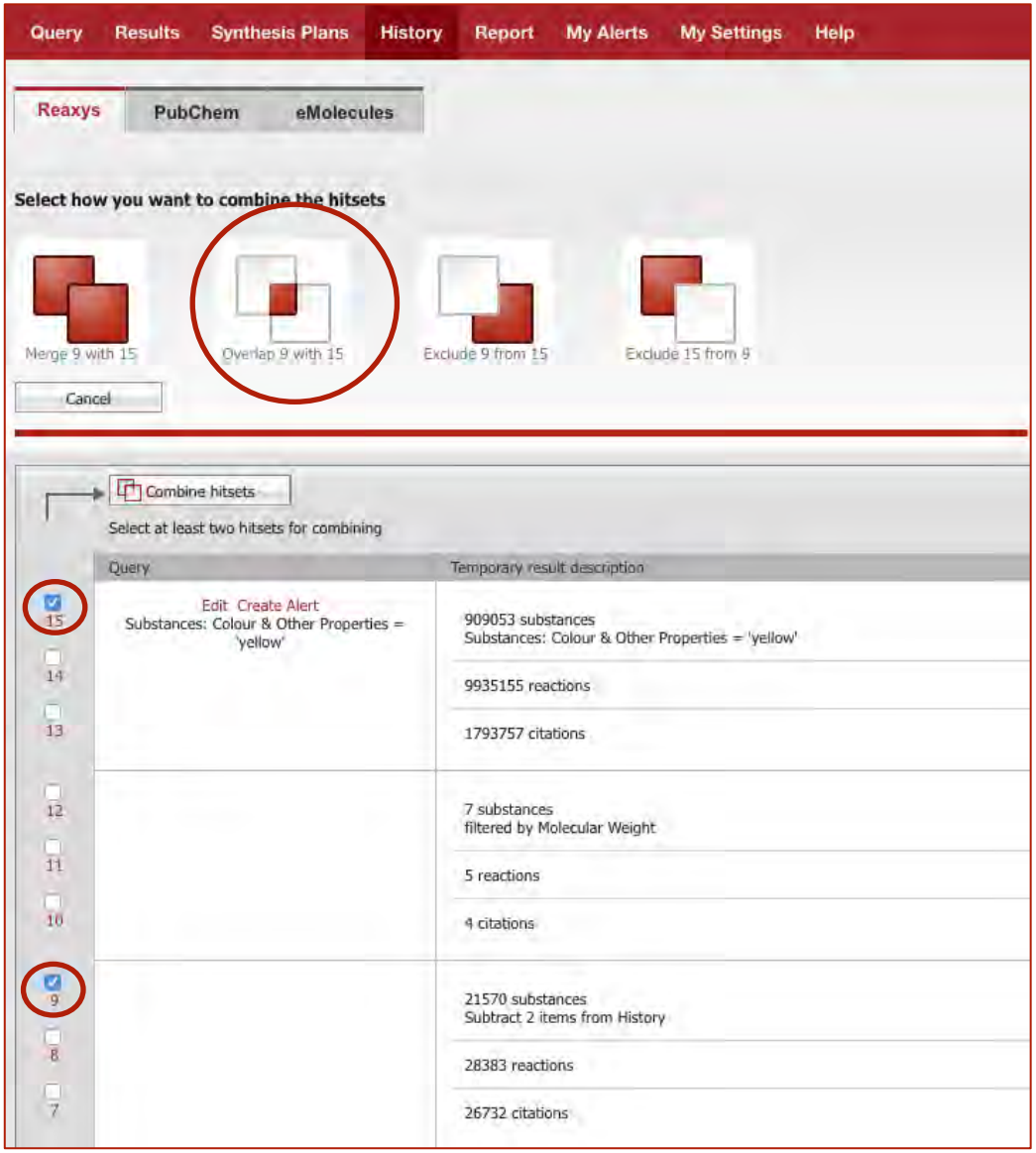
HOW YOU THINK HOW YOU WORK

CHROME COMPOUNDS (Yellow Inorganics)



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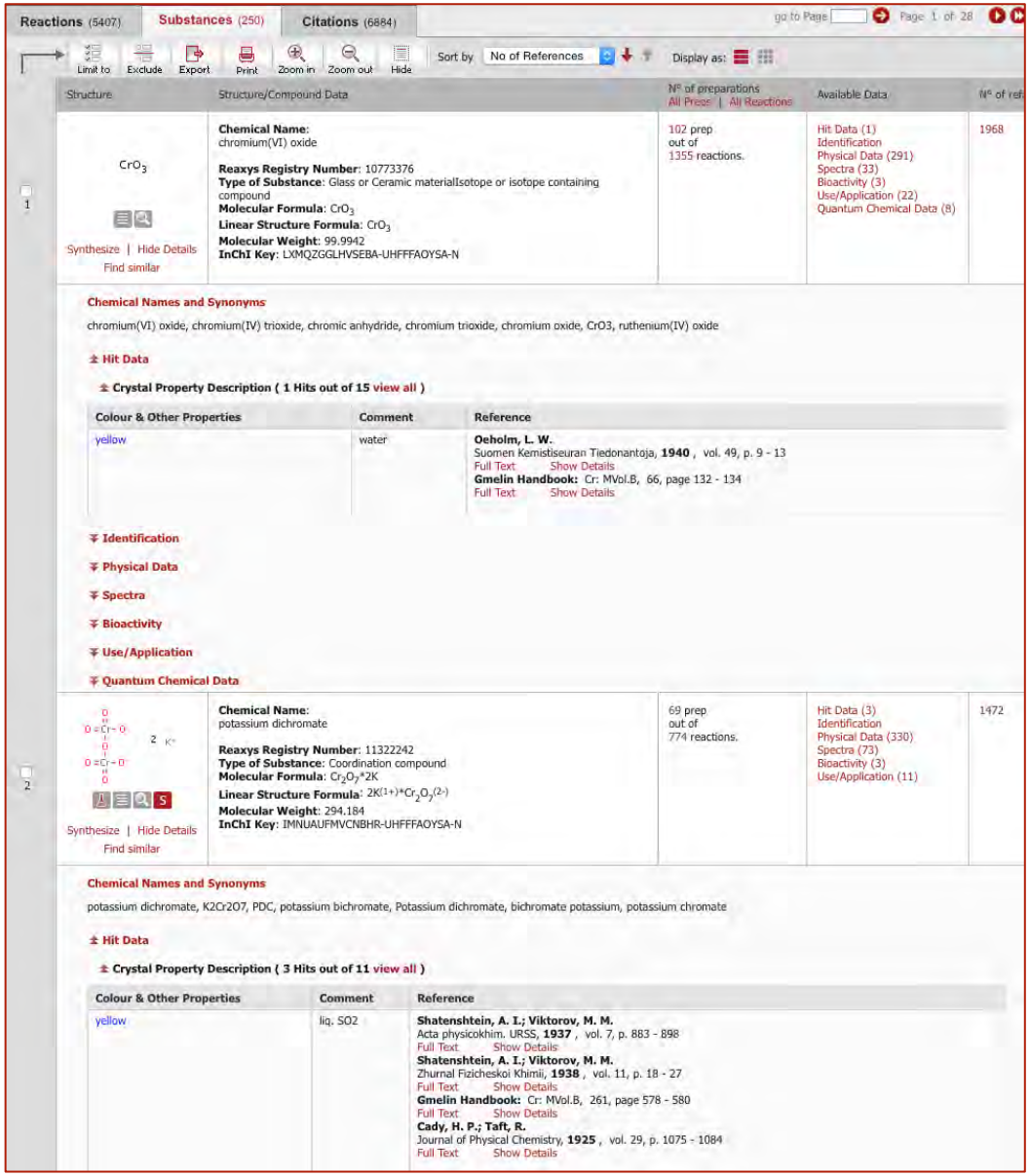
CHROME COMPOUNDS (Yellow Inorganics)



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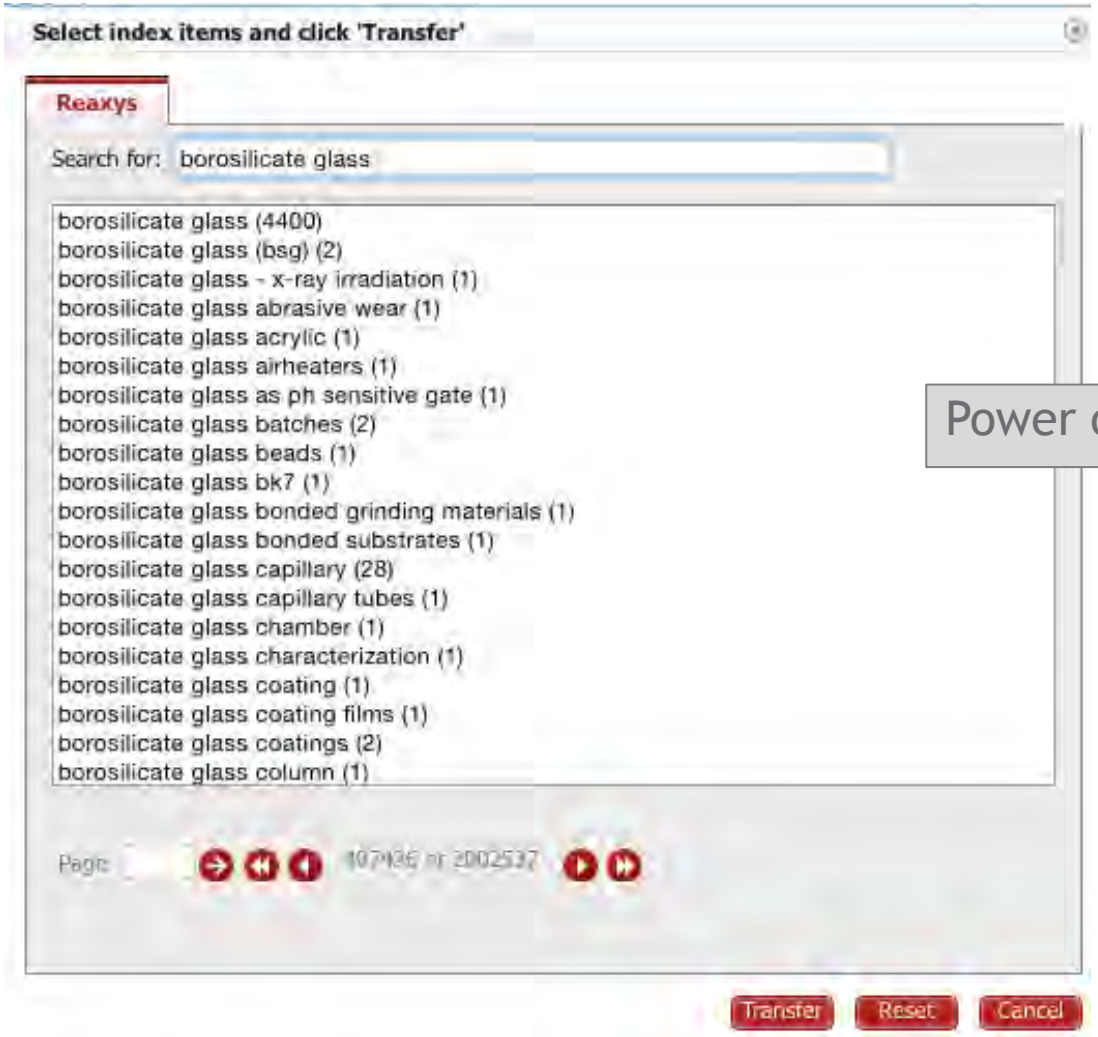
borosilicate glass



Power of lookup

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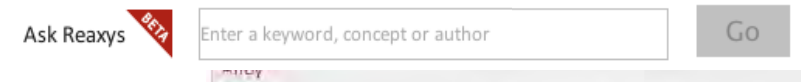
ALLOYS

USING THE ALLOY QUERY FORM

INITIAL ALLOY SEARCH OPTIONS



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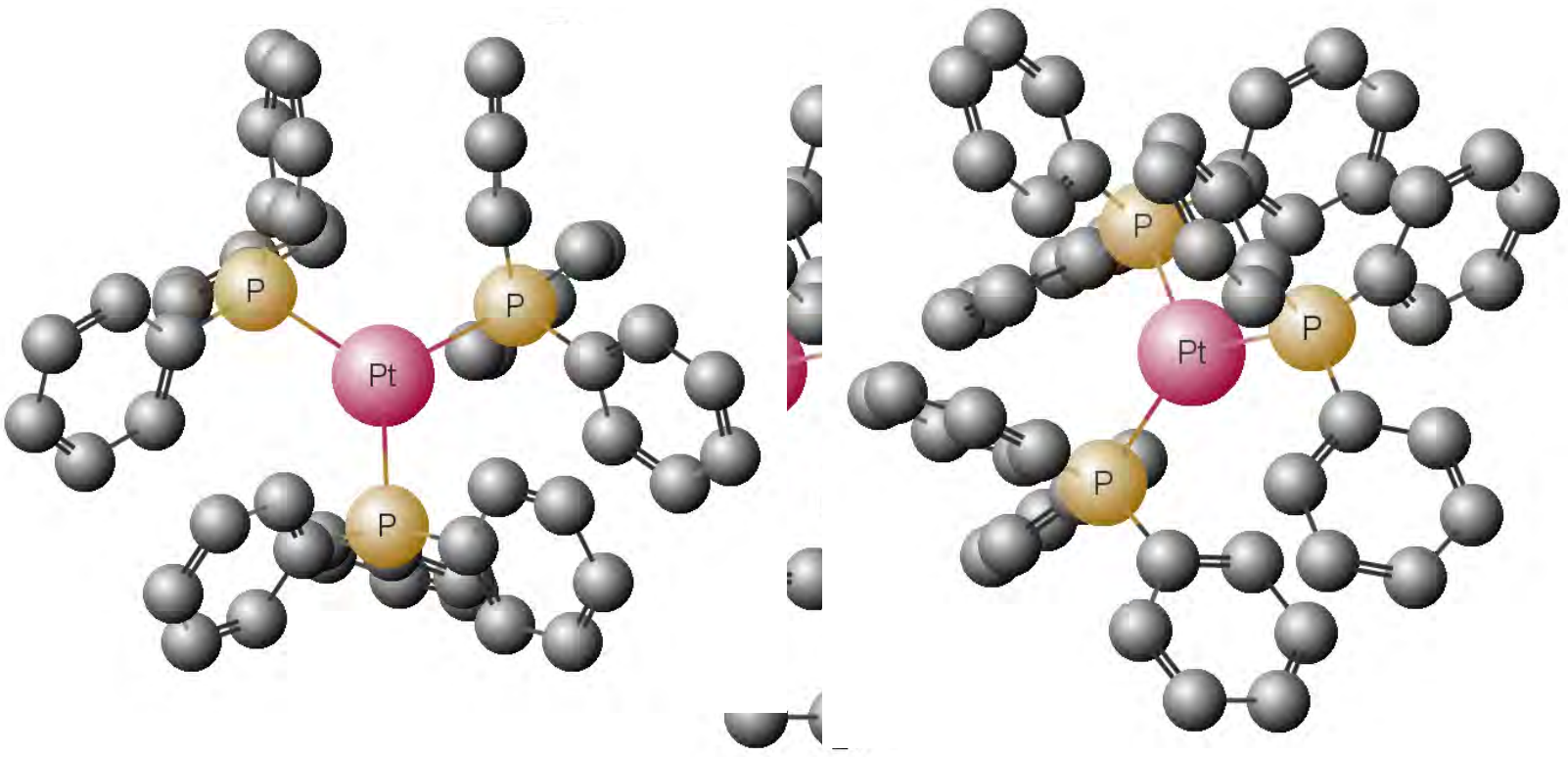
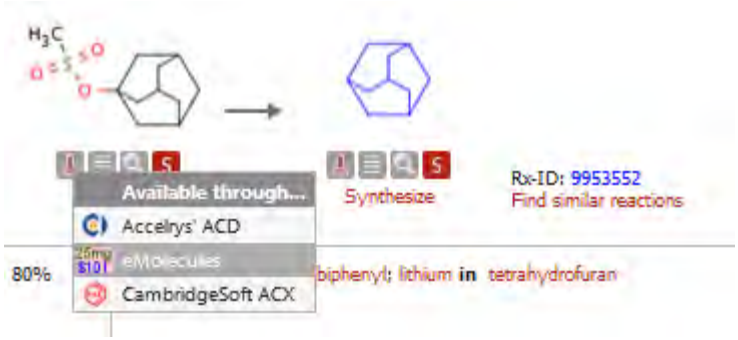
ROTATE 3D VIEW



CHECK COMMERCIAL AVAILABILITY



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SUPPORTS DIFFERENT STRUCTURE EDITORS

REAXYS®

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

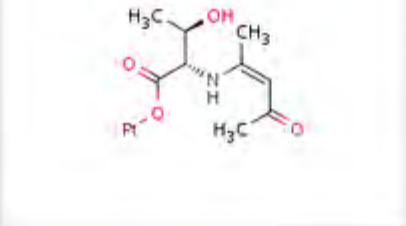
Reaxys uses Dotmatic's Elemental as default structure and reaction query editor, if no other editor is selected

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

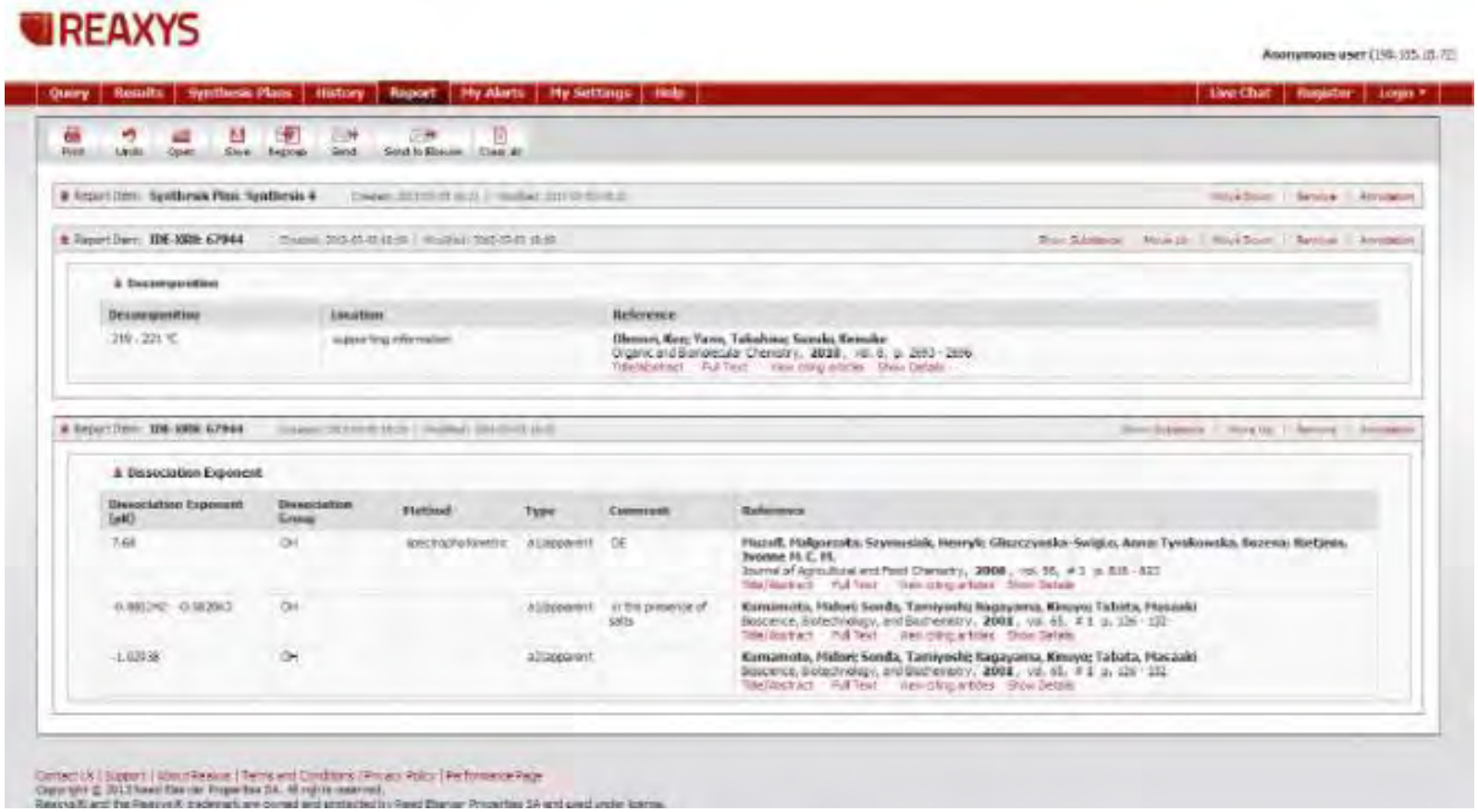
R/S Labels
- On All
- Absolute Stereo
- None

E/Z Labels
- On
- Off

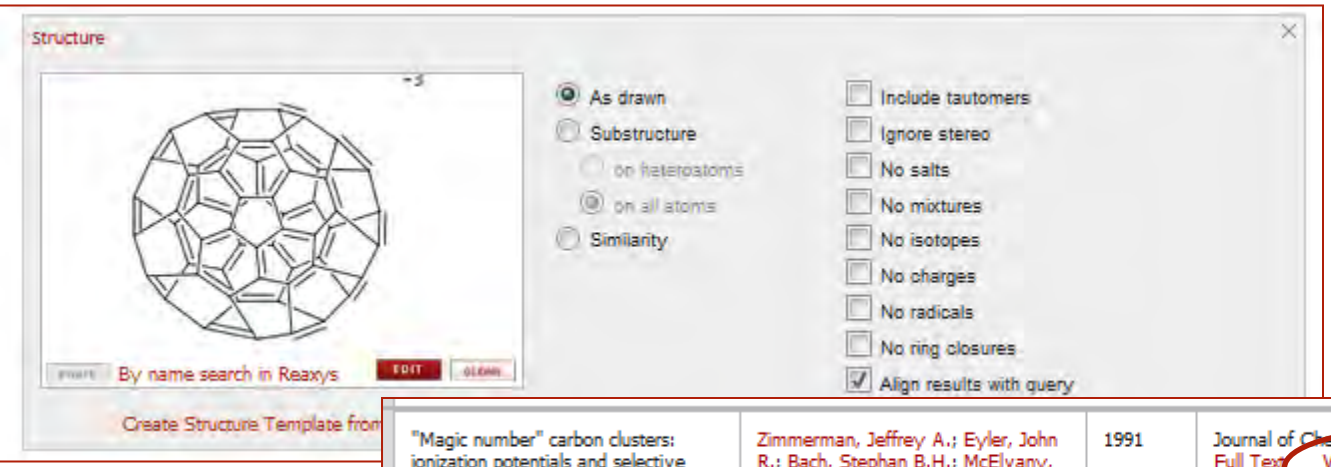
Display Atom Valence
- On
- Off

REPORTING:

GATHER AND PREPARE THE INFORMATION



INTEROPERABILITY



"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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Year

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

Author Name

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

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

REAXYS MEDICINAL CHEMISTRY

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.

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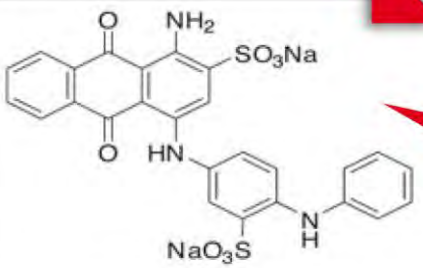
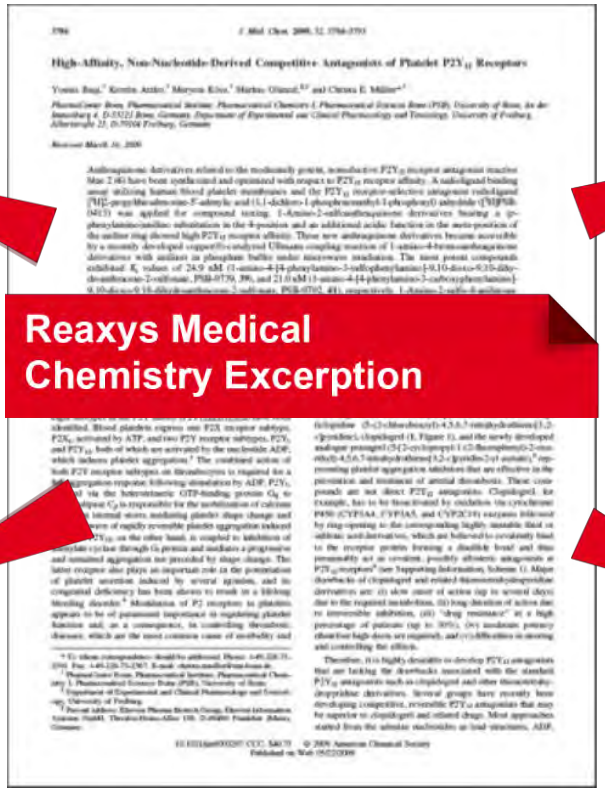
ESSENTIAL INFORMATION: 100+ EXPERIMENTAL FIELDS

Chemical Structures

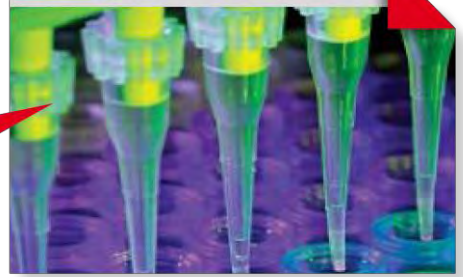




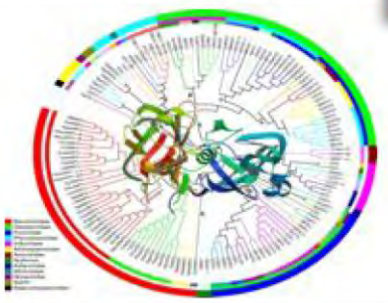
High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet $P2Y_{12}$ Receptors

Reaxys Medical Chemistry Excerption

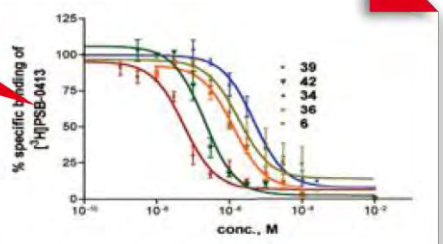
Bioassays: Cell lines, Species



Druggable Proteins



Quantitative Results



Reaxys Medicinal Chemistry excerpts all the relevant Quantitative data

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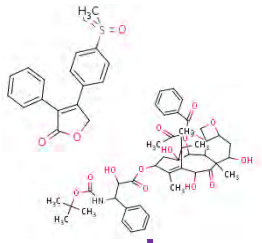
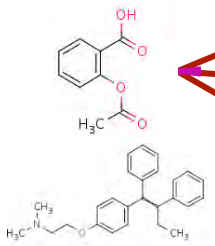
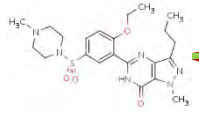
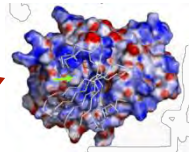
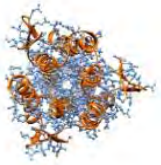
… BUT IT'S NOT THAT SIMPLE, MEDICINAL CHEMISTS FOR INSTANCE NEED TO COLLECT, ORGANIZE AND COMPARE INFORMATION FROM DIFFERENT SOURCES… THIS IS TIME CONSUMING AND ERROR PRONE

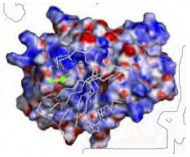


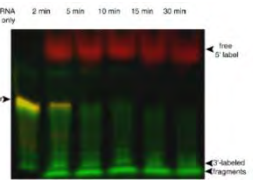


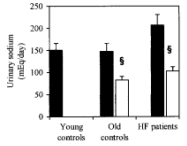


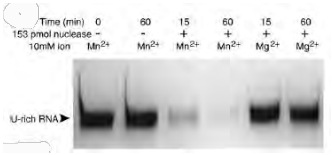


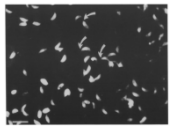


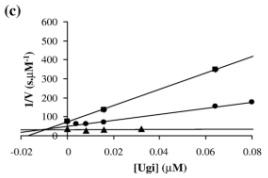












Entry	Compound	R^2	R^3	mPGES-1 Inhibition IC_{50}, μM[a]
1	14	^{i}Pr	H	1.1 (3)
2	15	H	^{i}Pr	4.3 (2)
3	16	H	H	3.2 (2)
4	17	F	H	2.6 (3)
5	18	^{t}Bu	H	0.33 (2)
6	19	^{i}Pr	H	0.60 (5)

[a] Mean of two or more experiments, ± 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 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 synoviocytes (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 ($PGF_{2\alpha}$) (2% FBS)	2.0 (49)	2.4 (3)

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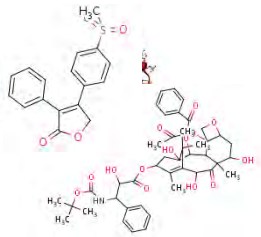
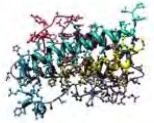
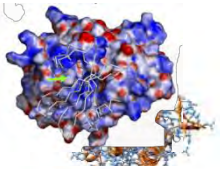
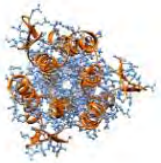
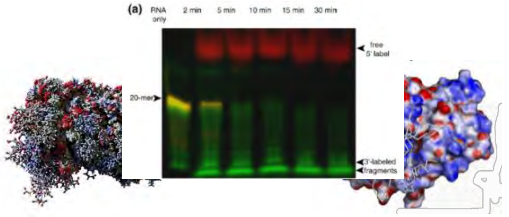
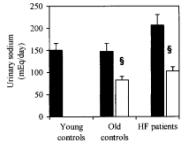


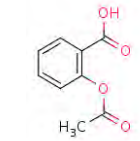


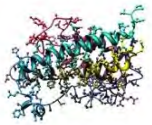


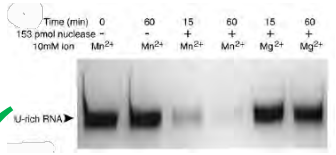


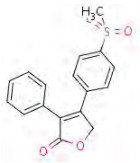


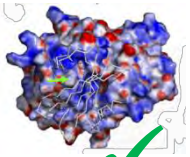


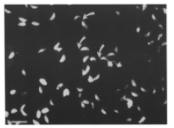


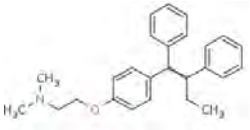


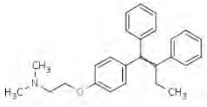


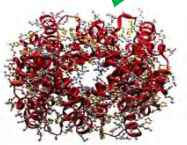


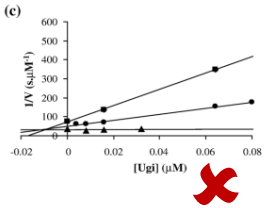


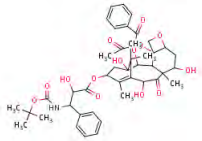


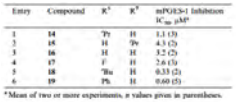


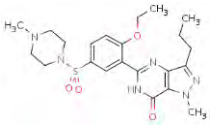


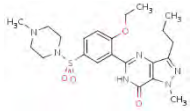












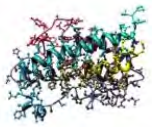
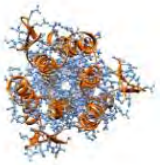
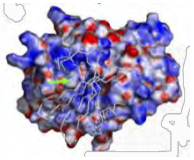
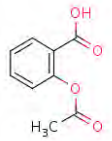
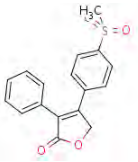
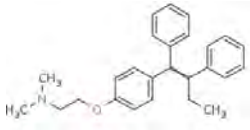
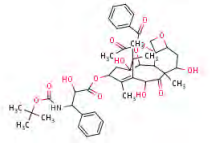
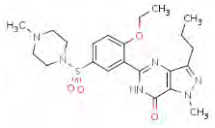
Entry	Compound	R^4	R^5	mPGES-1 Inhibition IC_{50}, μM[a]
1	14	^iPr	H	1.1 (3)
2	15	H	^iPr	4.3 (2)
3	16	H	H	3.2 (2)
4	17	F	H	2.6 (3)
5	18	^tBu	H	0.33 (2)
6	19	^iPr	H	0.60 (5)

[a] 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

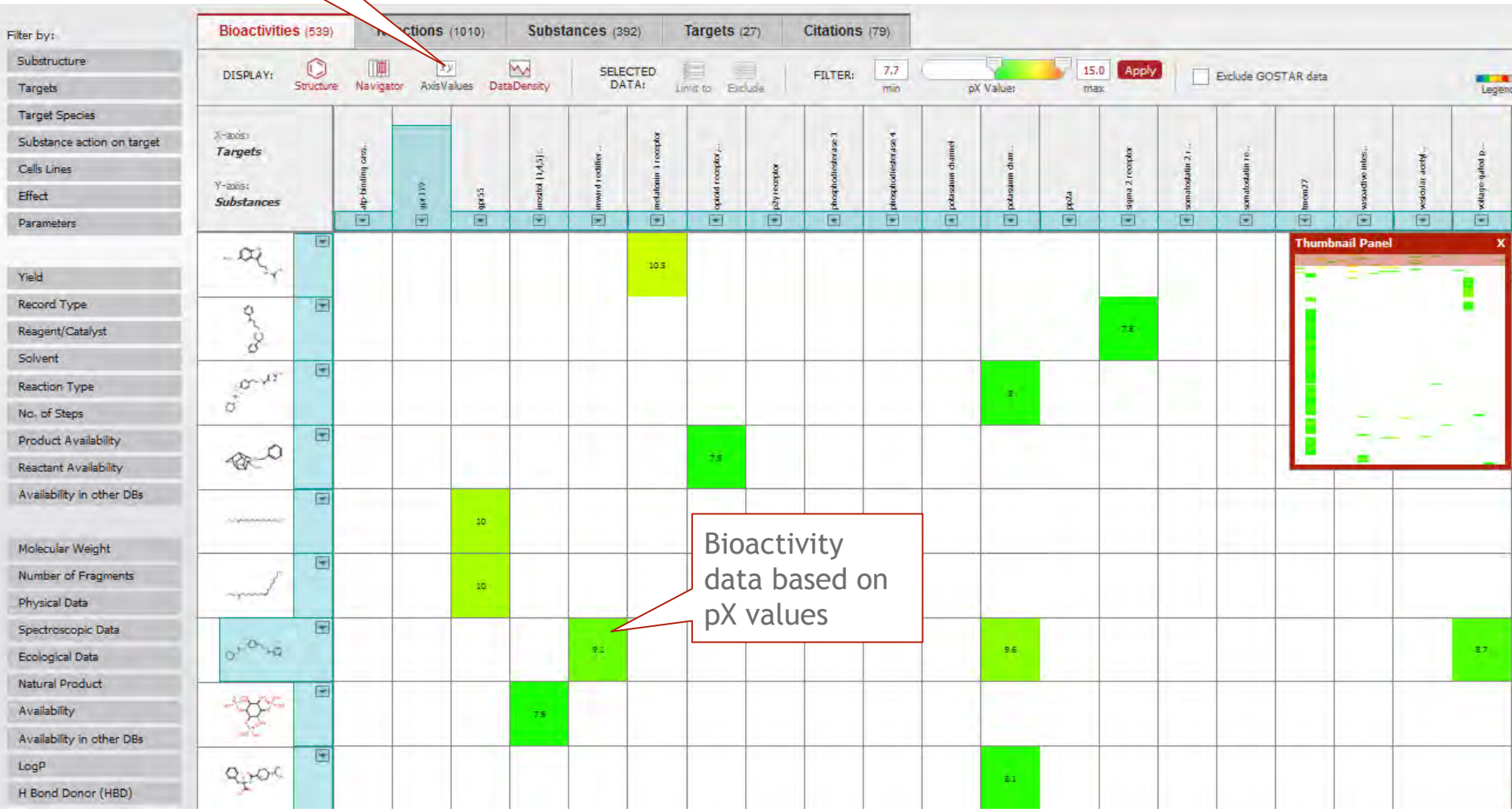
Enzyme or cell assay	Inhibition potency IC_{50}, μM[a]	
	23	**30**
Human mPGES-1	0.007 (9)	0.003 (8)
Human mPGES-2	>1 (3)	>1 (3)
Thromboxane synthase	1.4 (3)	0.95 (3)
FLAP binding	>1 (3)	>1 (3)
Human synoviocytes (PGE_2) (2% FBS)	0.61 (4)	0.25 (3)
A549 cells (PGE_2) (2% FBS)	0.49 (49)	0.27 (3)
A549 cells (PGE_2) (50% FBS)	8.0 (49)	5.8 (3)
A549 cells ($PGF_{2\alpha}$) (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



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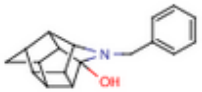
Heatmap Cell Details Substance 1 of 1

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-azahexacyclo[5.4.1.02,6.0.05,9.08,11]dodecan-3-ol

Reaxys Registry Number: 1476838
CAS Registry Number: 33226-57-2
Type of Substance: heterocyclic
Molecular Formula: $C_{18}H_{19}NO$
Linear Structure Formula: $C_{18}H_{19}NO$
Molecular Weight: 265.355
InChI Key: YSEXVIPNIGQQMN-UHFFFAOYSA-N

Highest Clinical Phase: Preclinical

Chemical Names and Synonyms

N-benzyl-4-azahexacyclo[5.4.1.02,6.0.05,9.08,11]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

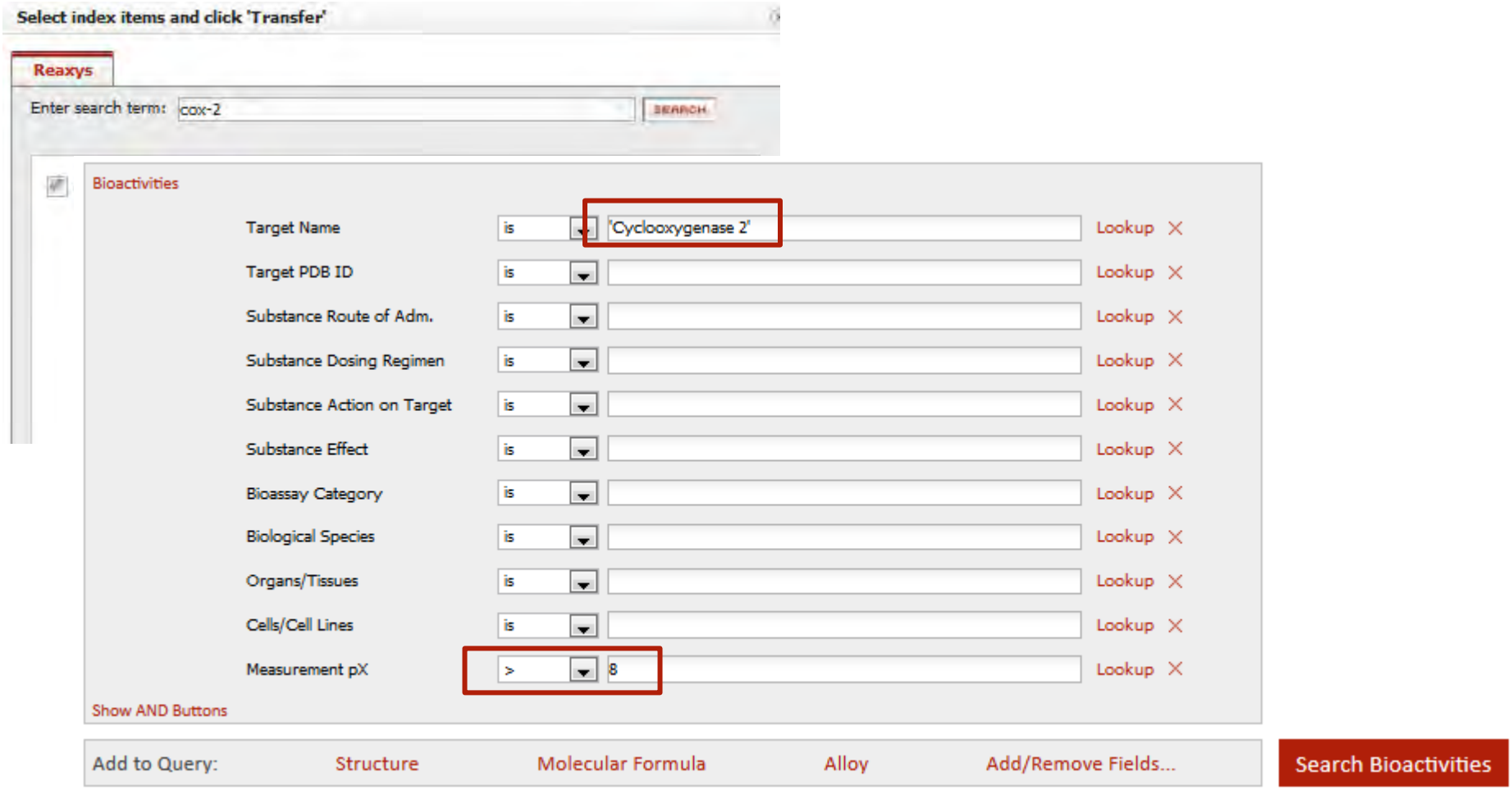
Bioactivity

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

EXAMPLE:
SUBSTANCES ACTIVE ON COX-2



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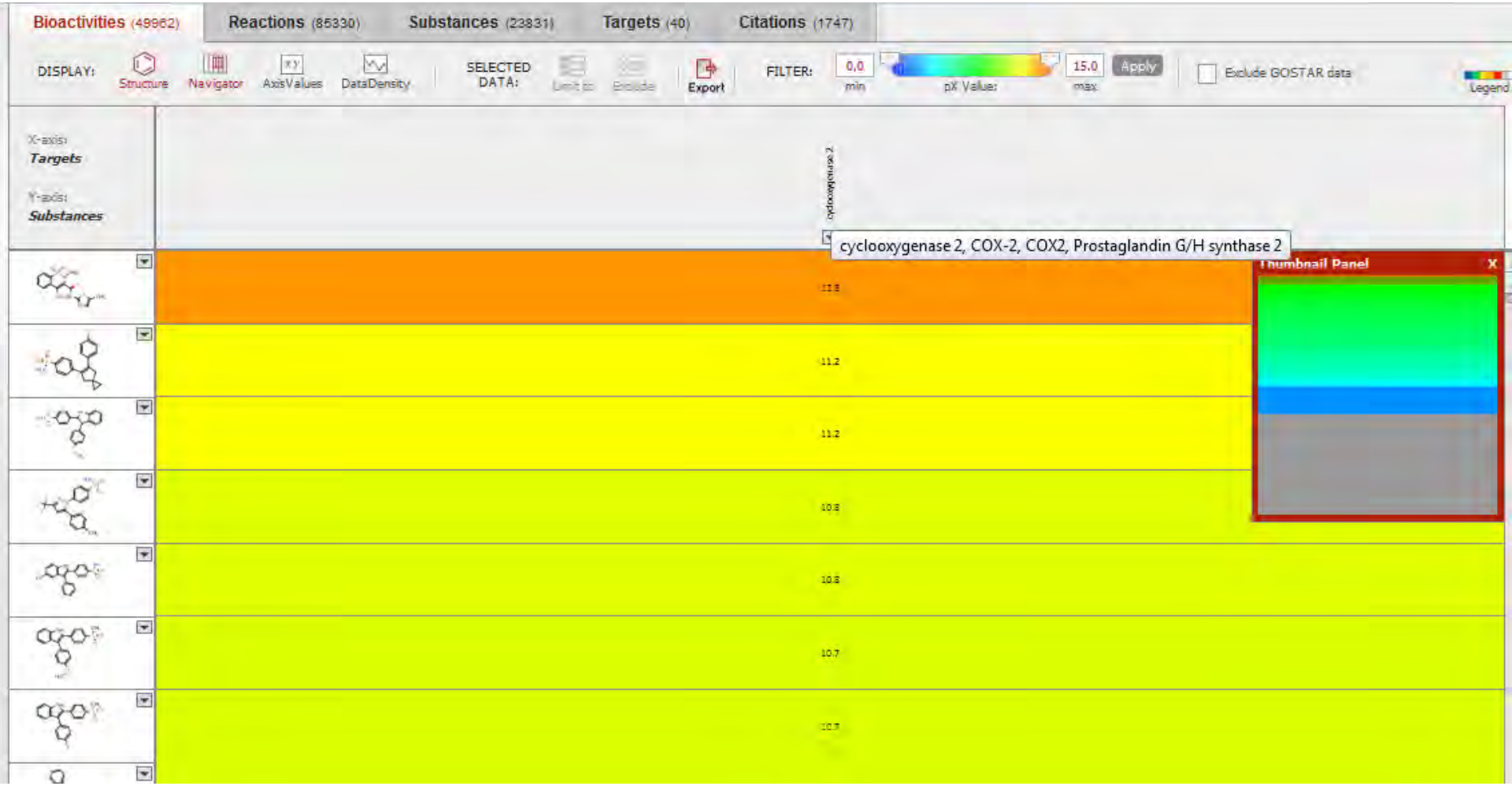
EXAMPLE:
SUBSTANCES ACTIVE ON COX-2



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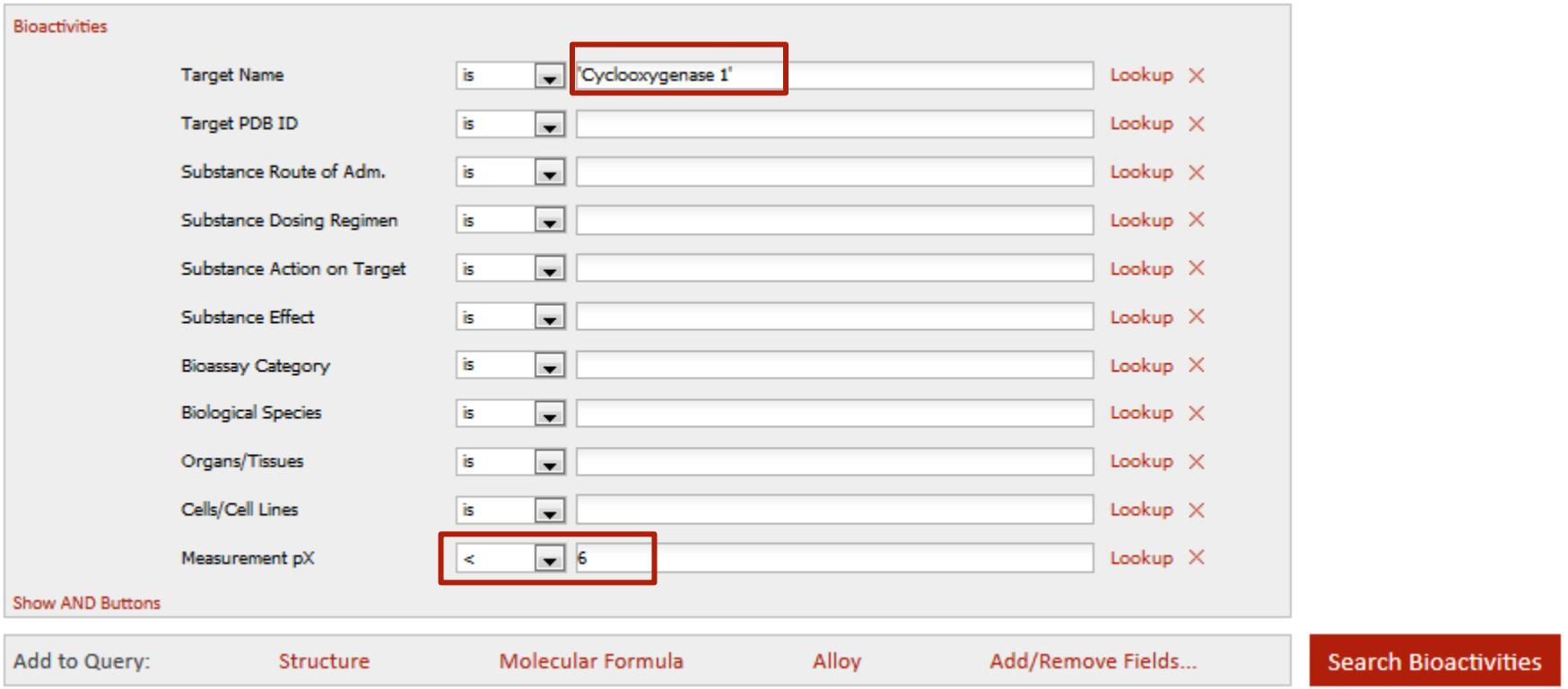
EXAMPLE:
AND NOT ACTIVE ON COX-1



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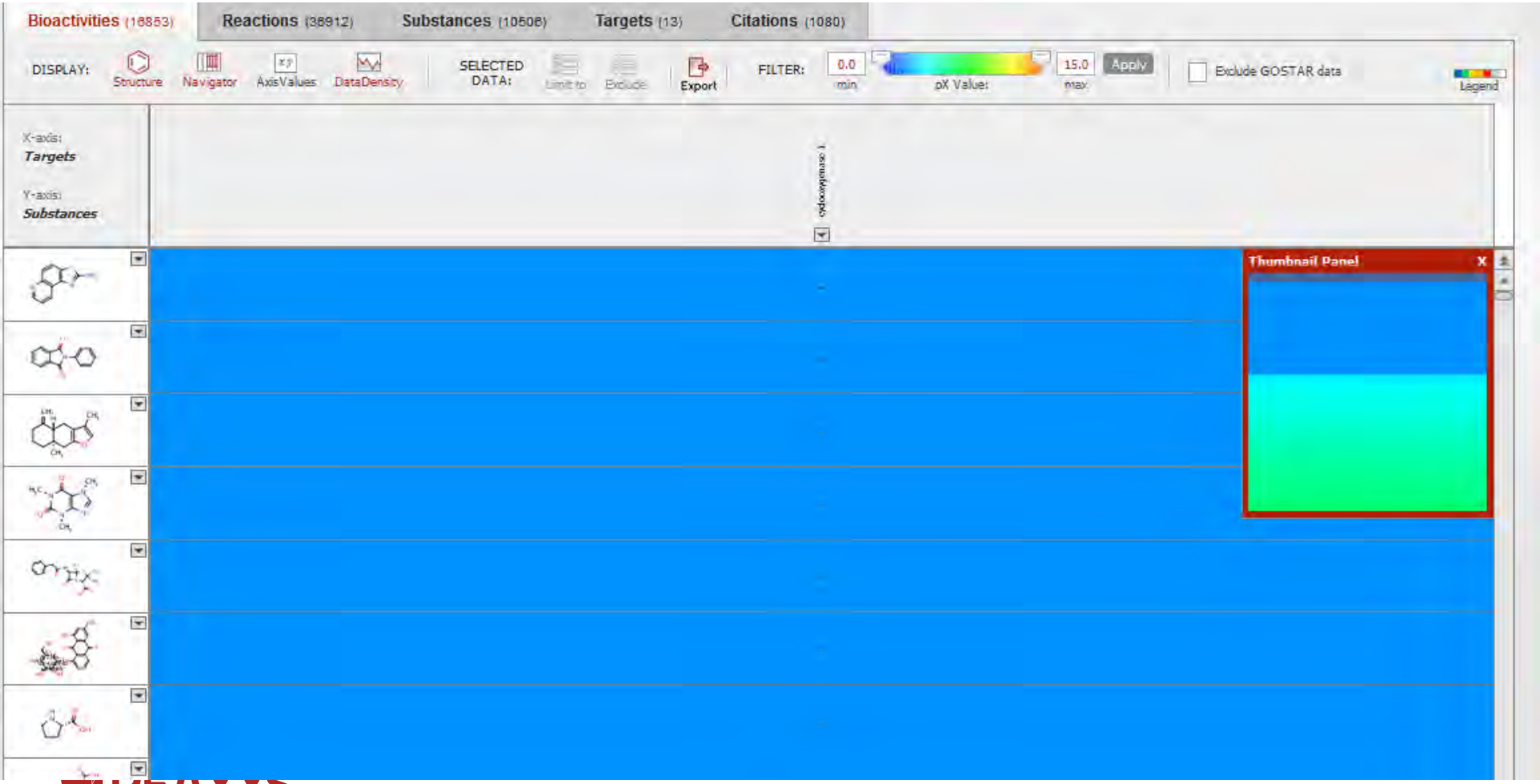
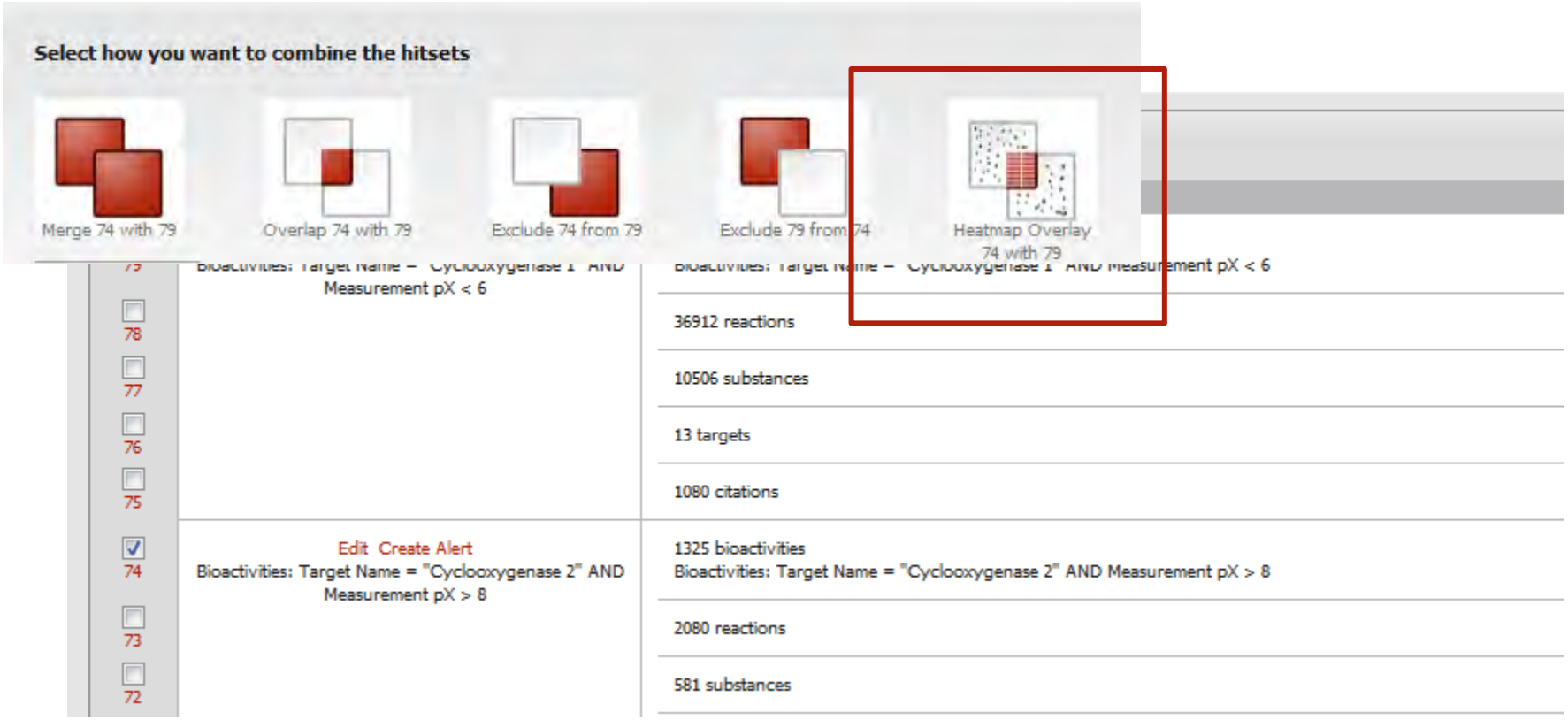
EXAMPLE:
AND NOT ACTIVE ON COX-1



EXAMPLE:
AND NOT ACTIVE ON COX-1



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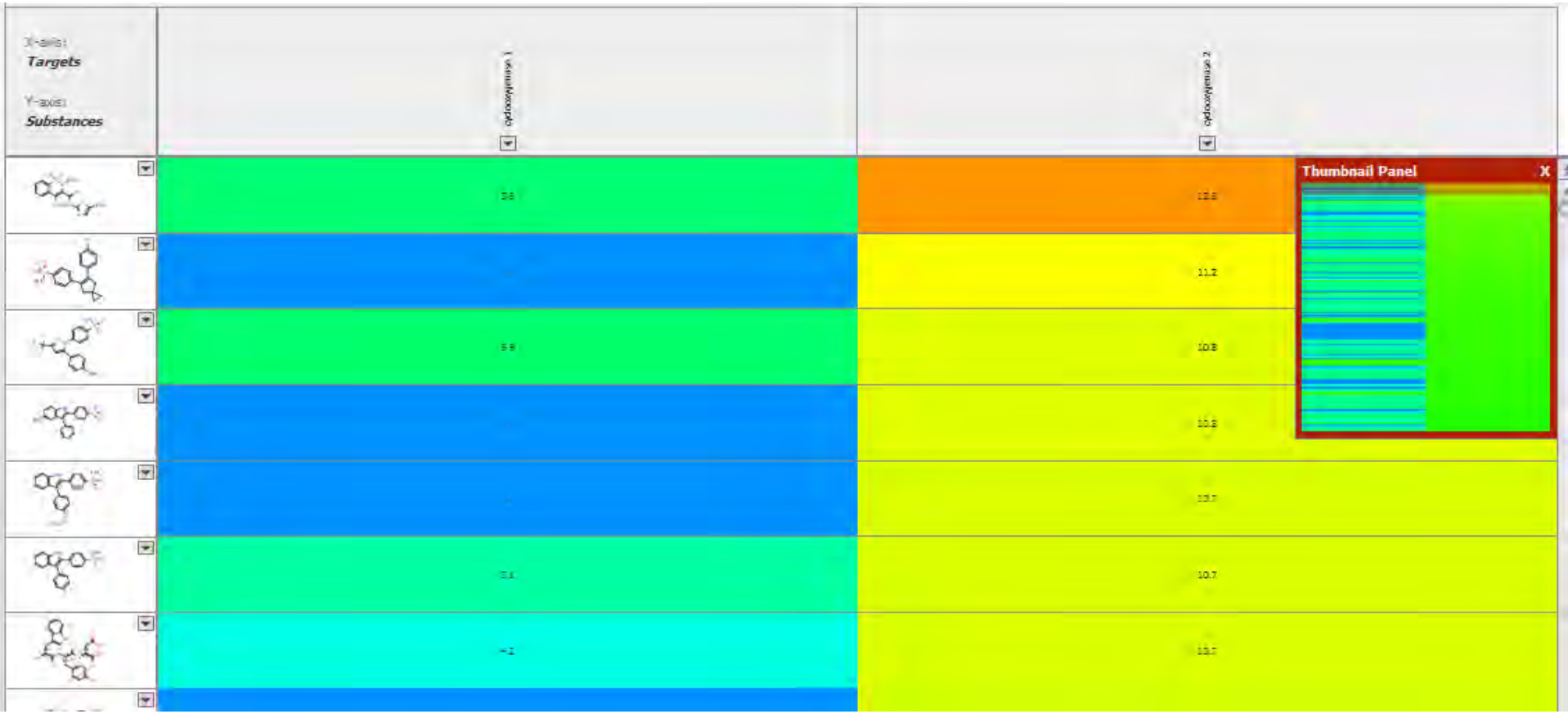
EXAMPLE:
SUBSTANCES ACTIVE SELECTIVELY ON COX-1 AND COX-2



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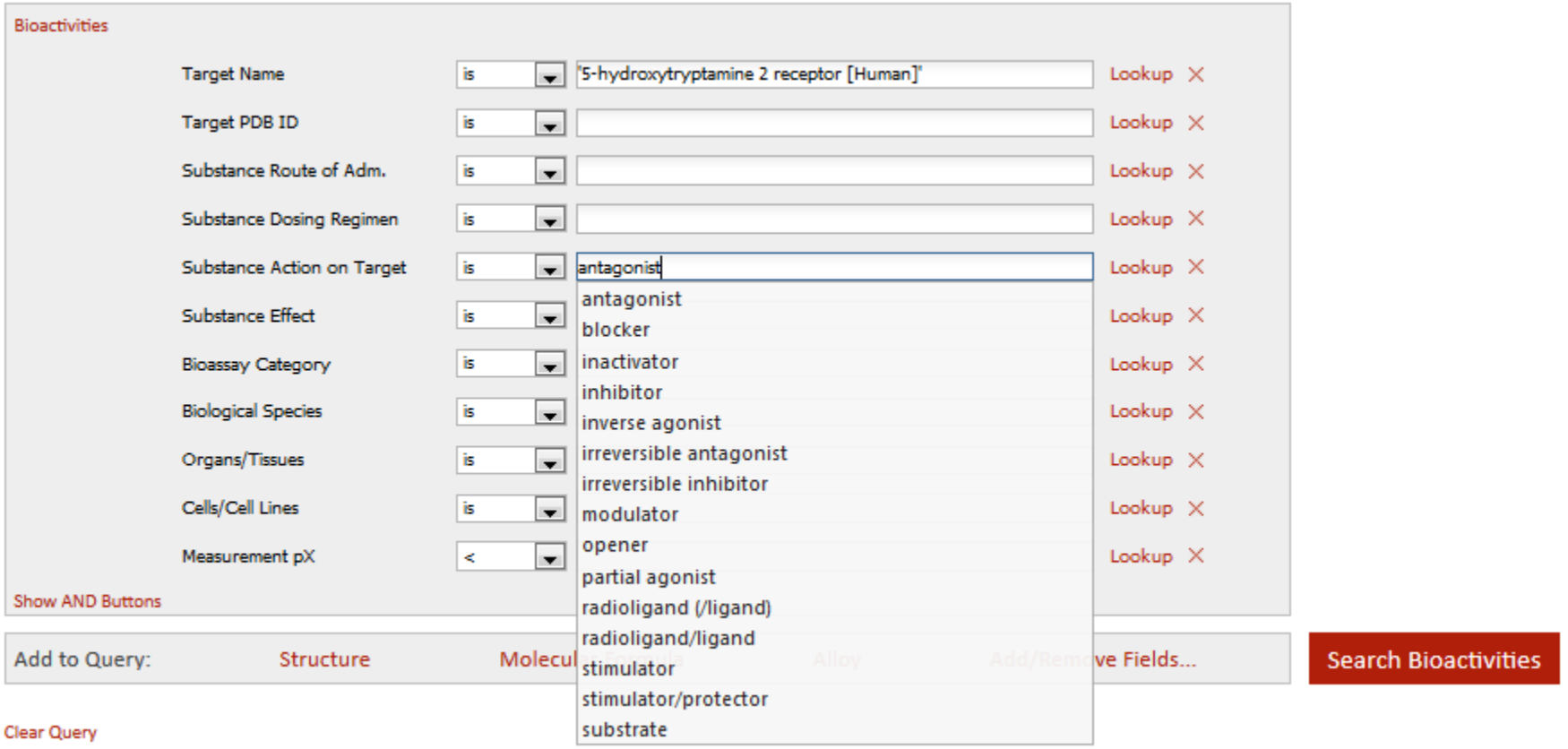
ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR



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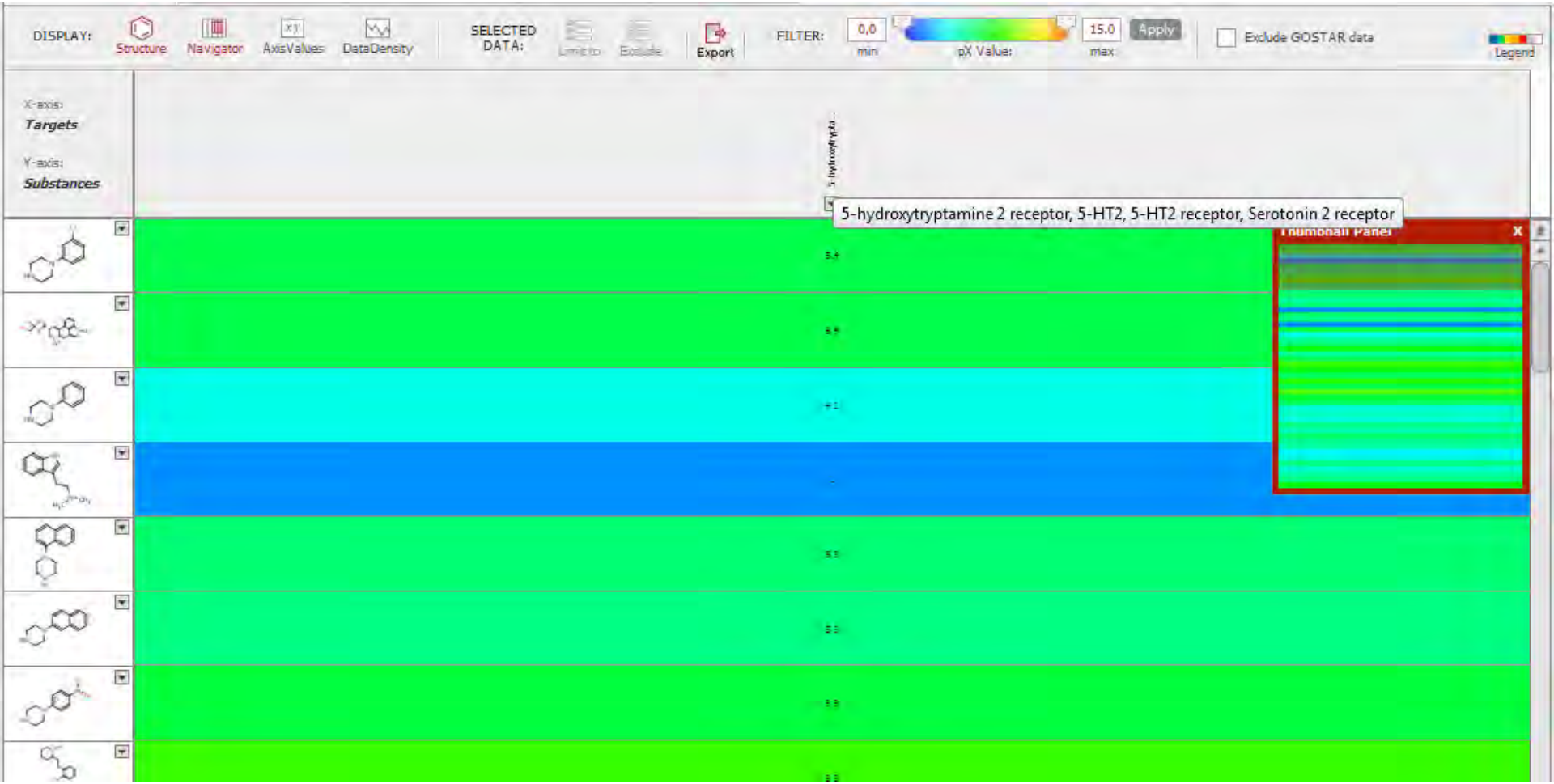
ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR



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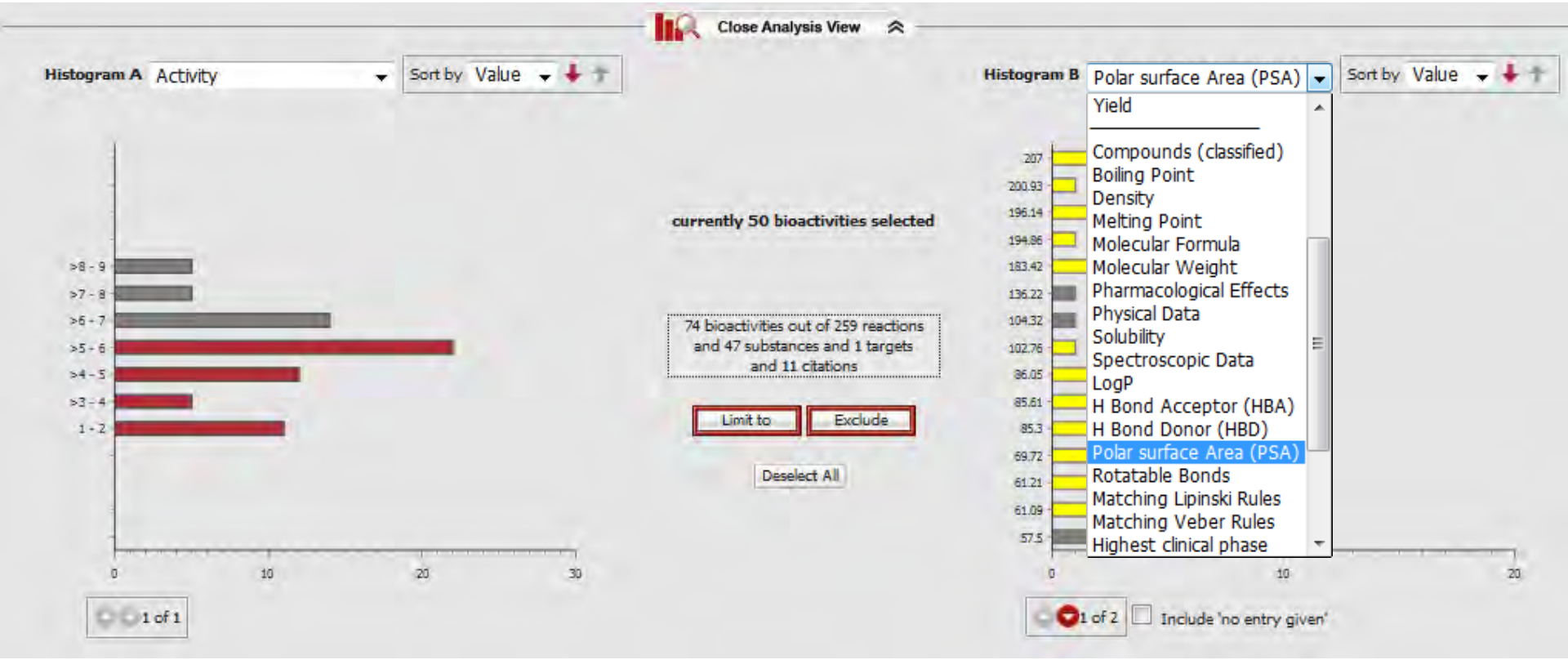
ANTAGONIST WITH LOW ACTIVITY ON 5-HYDROXYTRYPTAMINE RECEPTOR



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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.

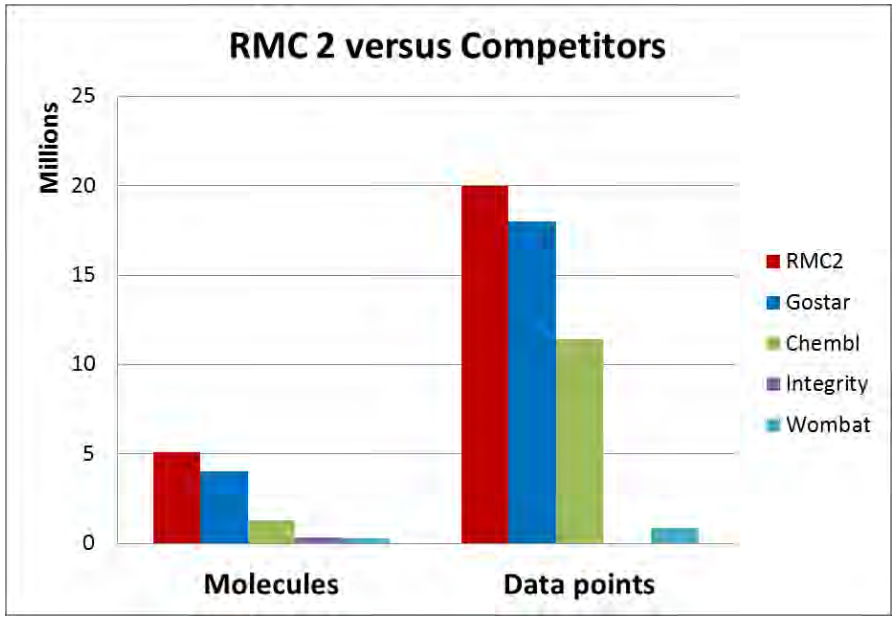
Articles and Journals

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

Drugable Targets

- **>9000 Drugable Targets**

« The most comprehensive medicinal chemistry solution on the market »



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EXPORT CAPABILITIES

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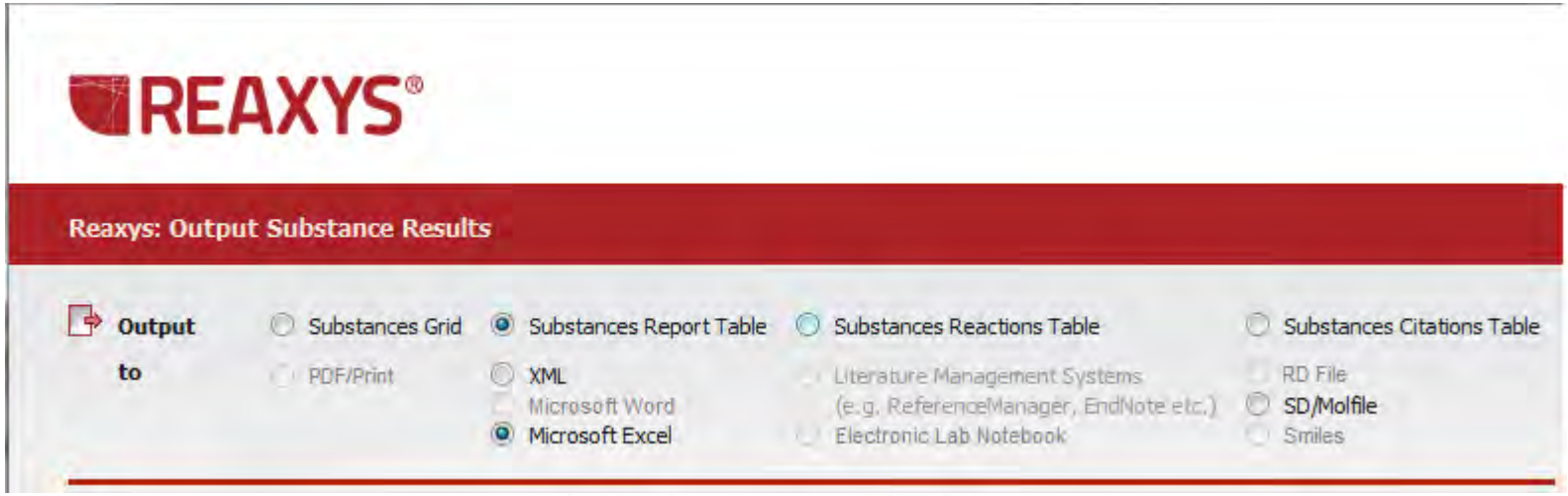
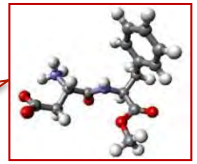
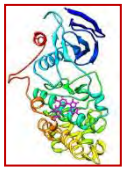
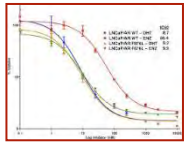
RMC2 EXPORT AND OUTPUT CAPABILITIES



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







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

accelrys® Pipeline Pilot

Spotfire®

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

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RMC2 EXCEL EXPORT AND SCATTER PLOT GENERATION

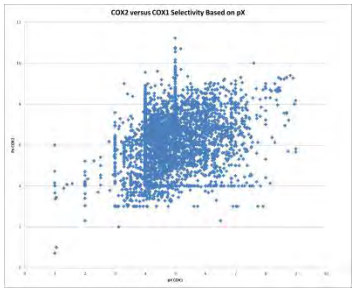
TARGET SELECTIVITY

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

Export

No additional data improvement is need for Excel Scatterplot

Performed Scatter plot For selectivity



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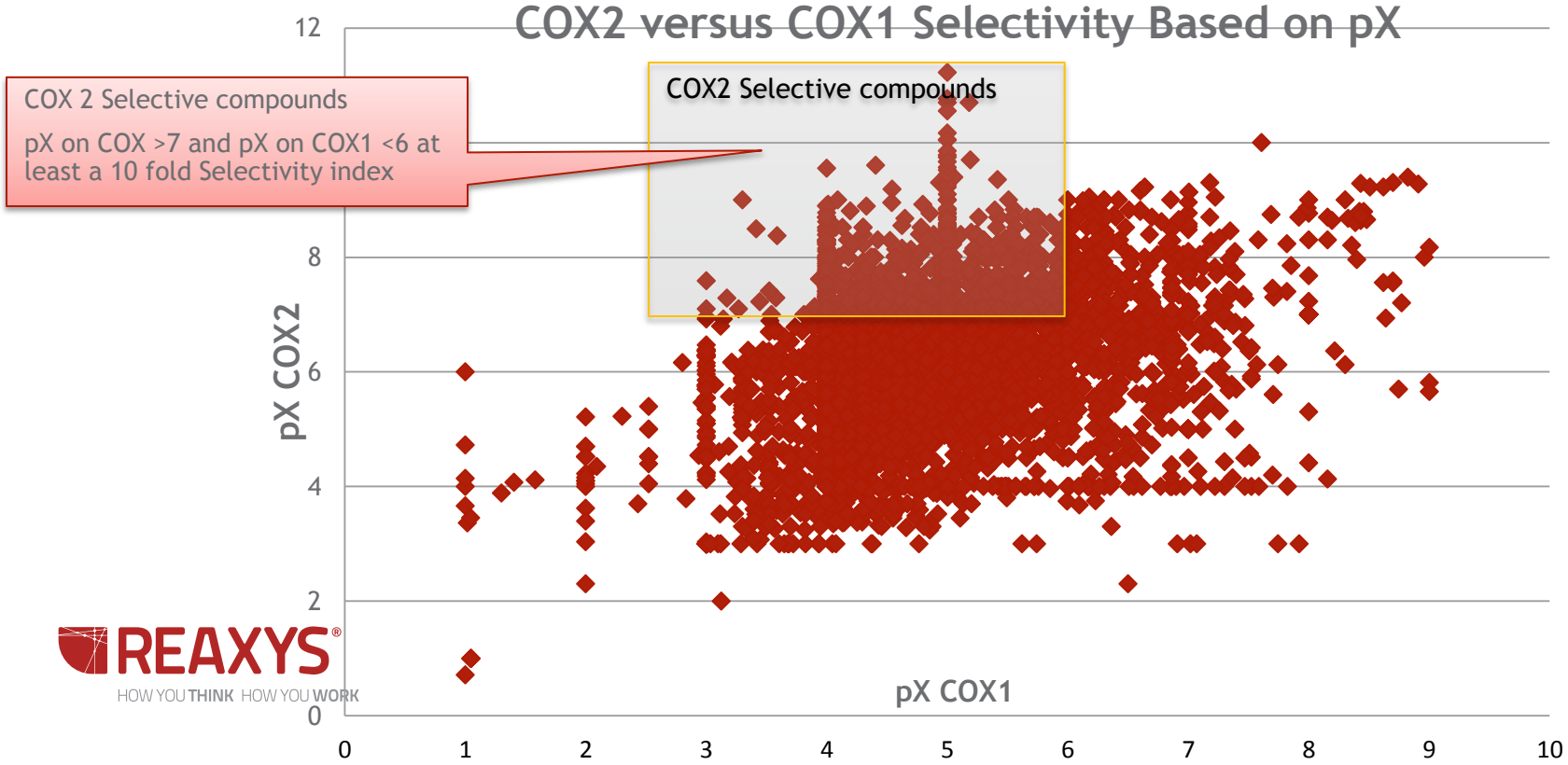

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and... what is your reaction?

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MOBILE: +48 695 30 60 17

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