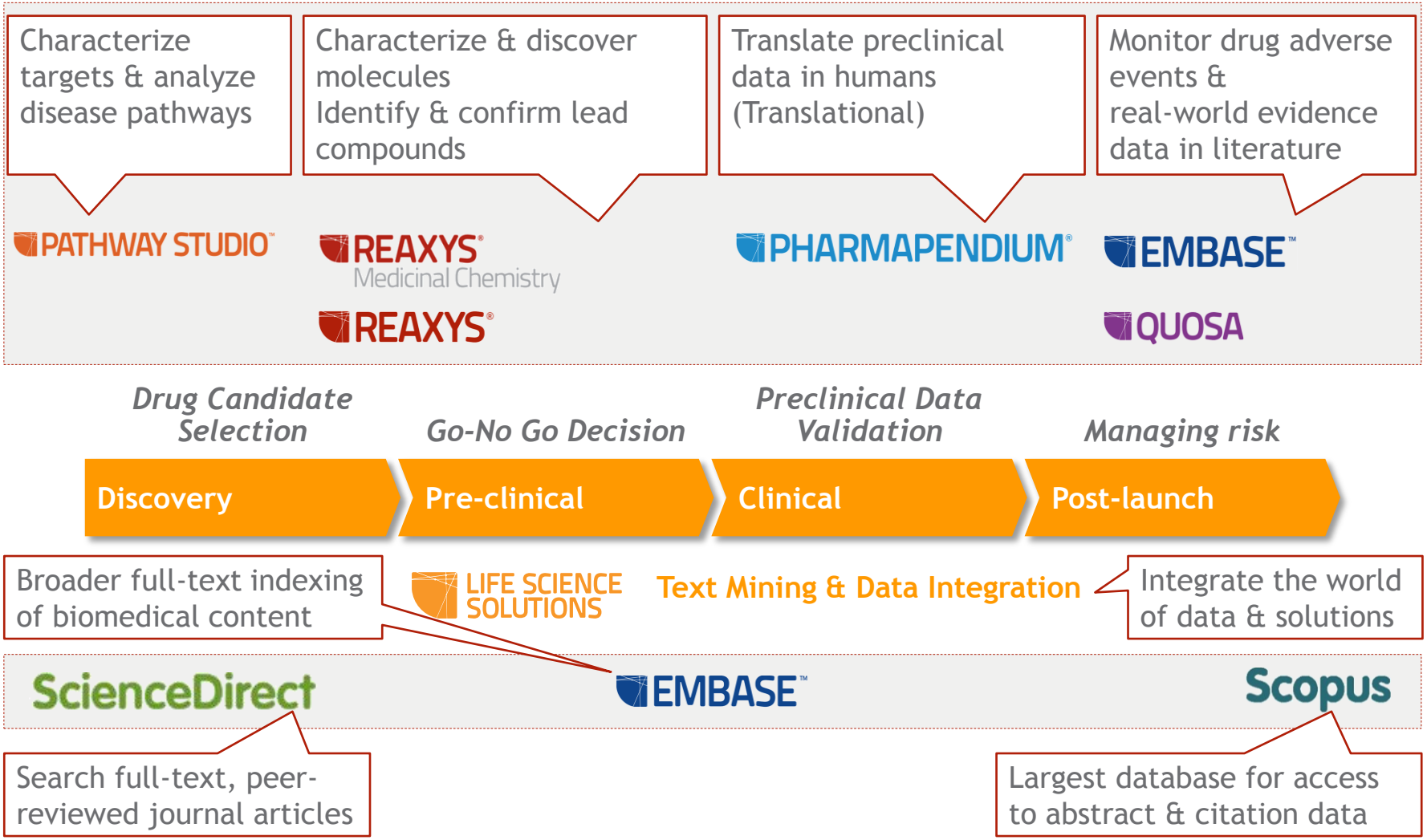
PIOTR GOŁKIEWICZ
SOLUTION SALES MANAGER
LIFE SCIENCES
CENTRAL-EASTERN EUROPE
AND RUSSIA

INTRODUCING REAXYS

REAXYS®
HOW YOU THINK HOW YOU WORK

SERVING THE LIFE SCIENCES SPACE

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN



REAXYS®
HOW YOU THINK HOW YOU WORK

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

Scientific topic, author

ELSEVIER Chemical Physics Letters 294 (1998) 499–506

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

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.

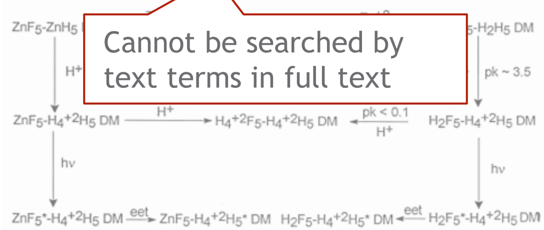
1. Introduction

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

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

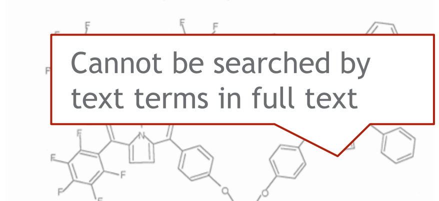
Chemical reactions



Cannot be searched by text terms in full text

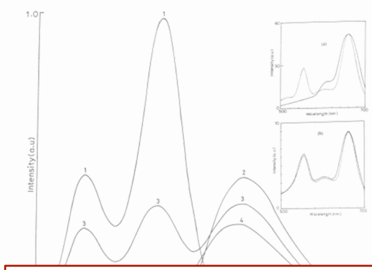
Fig. 2. Schematic representation of different processes of dimer porphyrins.

Chemical structure



Cannot be searched by text terms in full text

Chemical spectra



Cannot be searched by text terms in full text

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… tripheny… tively. … oro)pher… demethy… phyrin c… spective … phyrins were characterised b… V–VIS, ¹H-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!

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

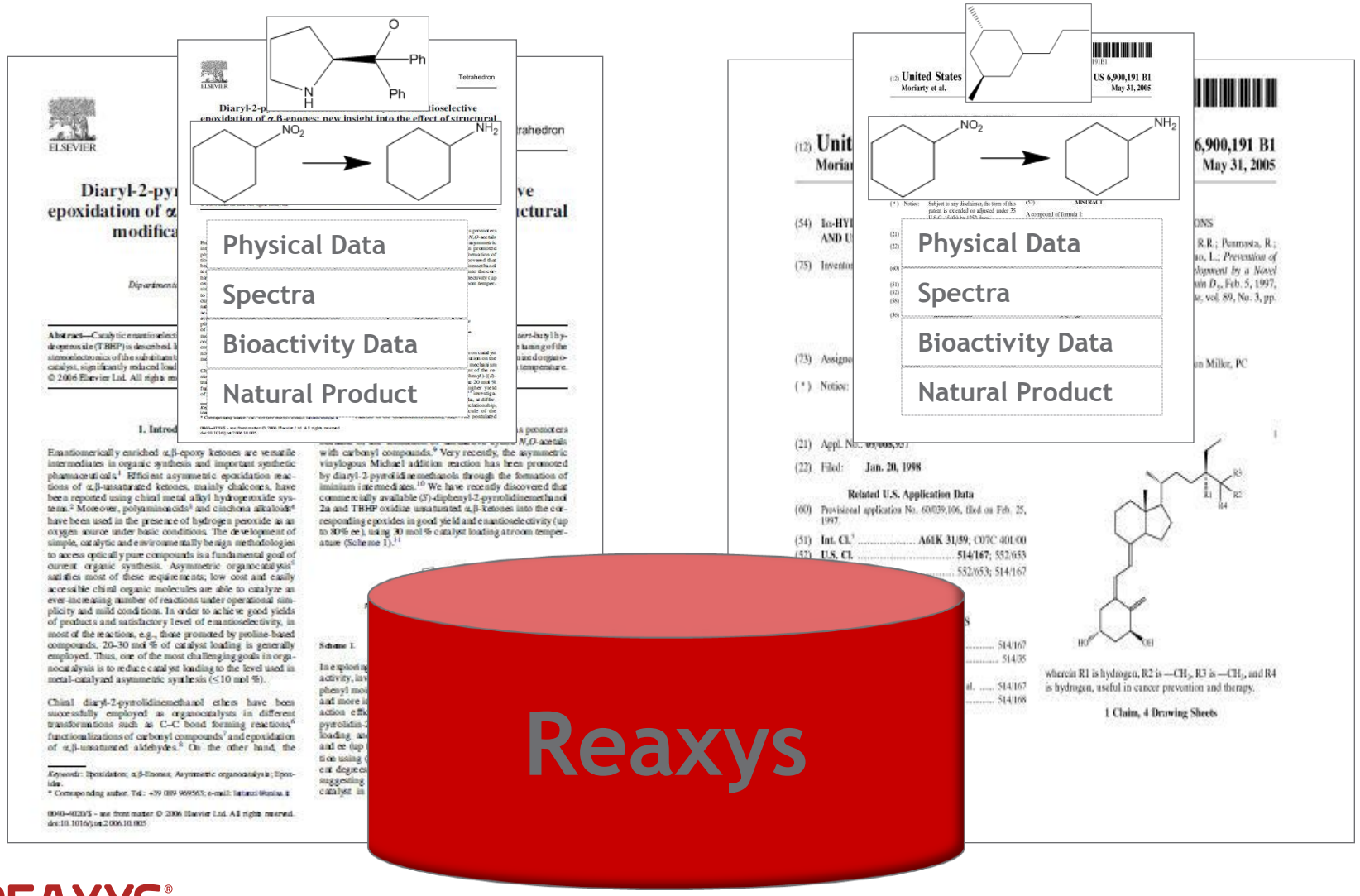
Cannot be searched by text terms in full text

REAXYS® HOW YOU THINK HOW YOU WORK

Chemistry as the organizing principle

REAXYS IS BUILT

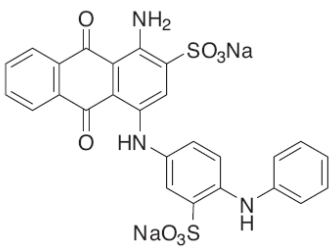
With experimental data from journal articles and patents



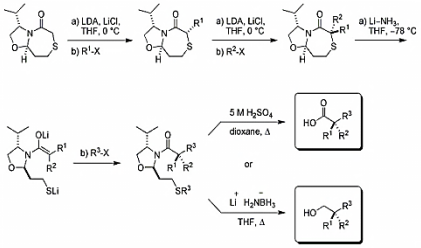
REAXYS®

HOW YOU THINK HOW YOU WORK

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-7910d 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

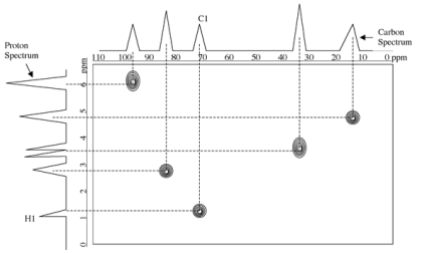
adenylate cyclase through G_i protein and mediates a progressive and sustained aggregation not preceded by shape change. The latter receptor also plays an important role in the potentiation of platelet secretion induced by several agonists, and its congenital deficiency has been shown to result in a 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.

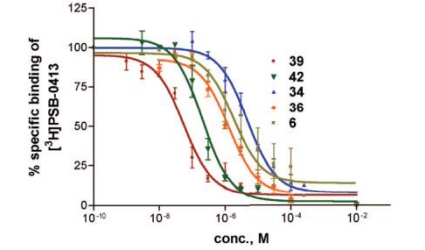
Therefore, it is highly desirable to develop $P2Y_{12}$ antagonists that are lacking the drawbacks associated with the standard $P2Y_{12}$ antagonists such as clopidogrel and other thienotetrahydropyridine derivatives. Several groups have recently been developing competitive, reversible $P2Y_{12}$ antagonists that may be superior to clopidogrel and related drugs. Most approaches started from the adenine nucleotides as lead structures, ADP,

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

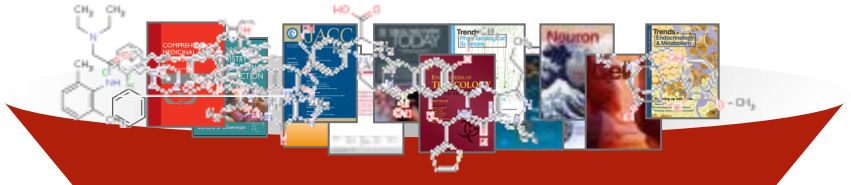
REAXYS®
HOW YOU THINK HOW YOU WORK

STRUCTURED TO HELP YOU SEARCH

OTHER DATABASES

REAXYS

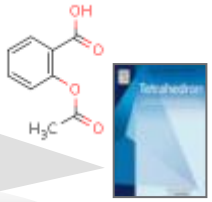
CATALOGUED AND TAXONMISED BY CHEMISTS FOR CHEMISTS



ESSENTIAL TITLES

ACROSS TIME/LITERATURE

USE-CASE DRIVEN



RELEVANT ANSWERS

BIBLIOGRAPHIC APPROACH

UNFOCUSED RESULTS

FURTHER SEARCH NEEDED

50,000,000 RESULTS RETURNED

REAXYS®

HOW YOU THINK HOW YOU WORK

REAXYS INCLUDES

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

REAXYS INCLUDES

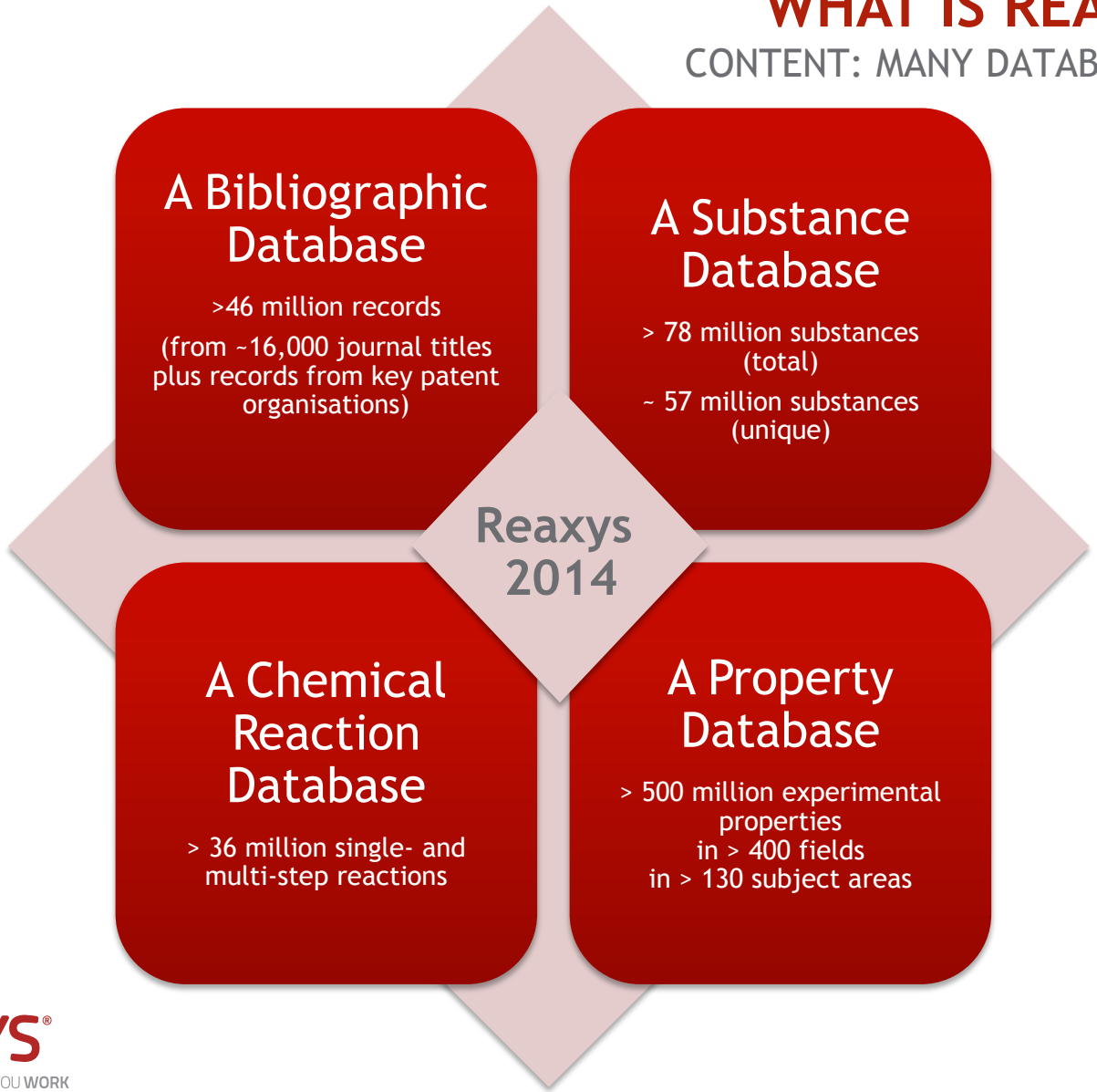
Over 500 million facts

Over 400+ searchable data fields

HIGH QUALITY experimental results

WHAT IS REAXYS 2014?

CONTENT: MANY DATABASES ALL IN ONE



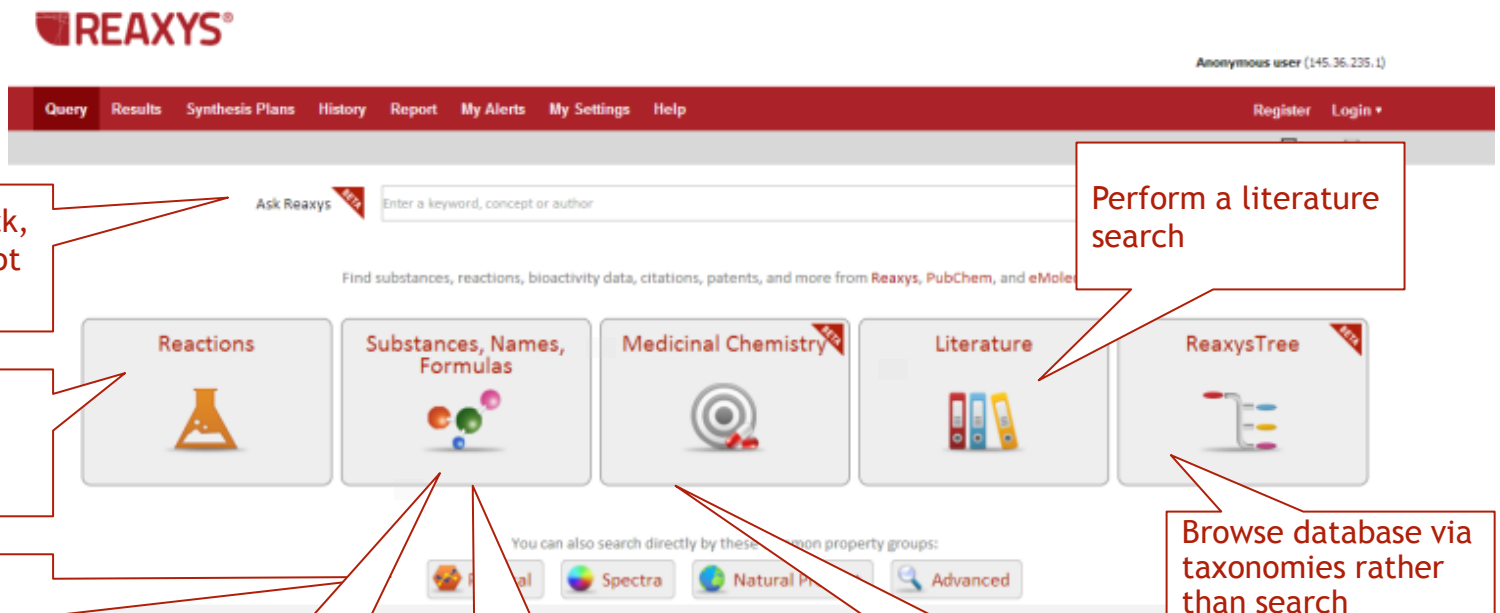
REAXYS®
HOW YOU THINK HOW YOU WORK

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

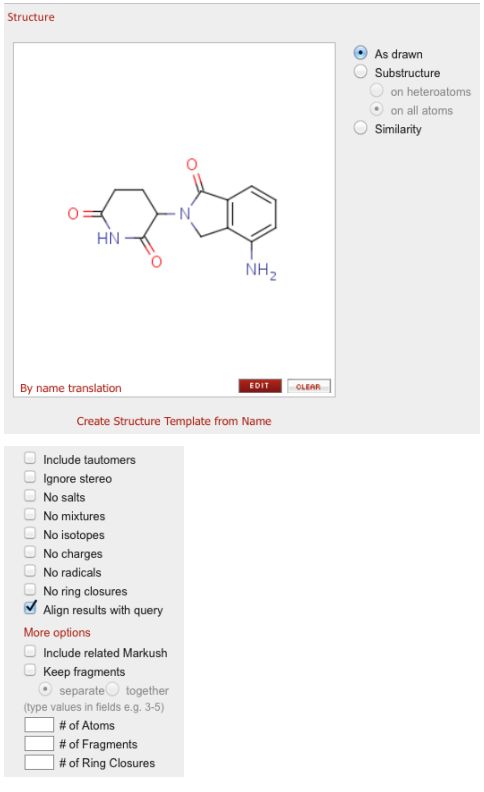
Browse database via taxonomies rather than search database

Perform a literature search

SEARCH SUBSTANCES

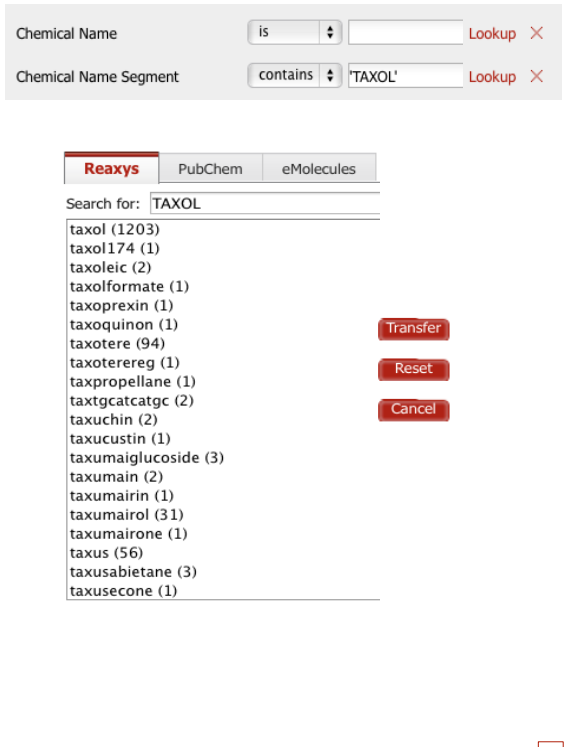
SEARCH STRUCTURE, NAME, OR FORMULA – IN FULL, OR IN PART

STRUCTURE



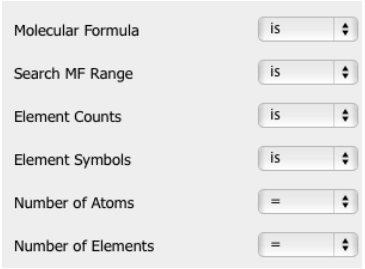
As Drawn ✔
Substructure ✔
Similarity ✔

CHEMICAL NAME

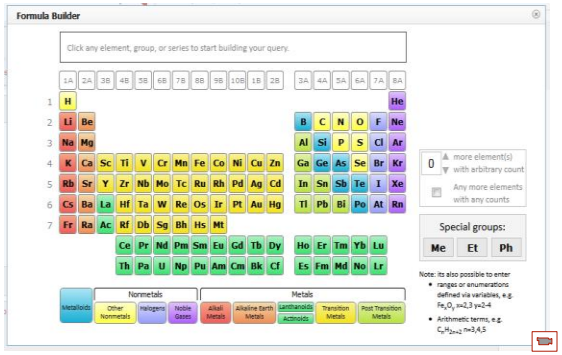


Chemical Name ✔
Part of Chemical Name ✔
Reaxys helps on the way ✔✔

FORMULA



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

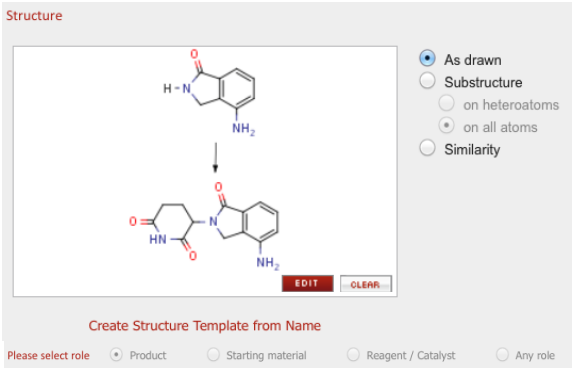


Formula ✔
Part of Formula ✔
Reaxys helps on the way ✔✔

SEARCH REACTIONS

SEARCH BY STRUCTURE, DATA, OR TYPE

STRUCTURE



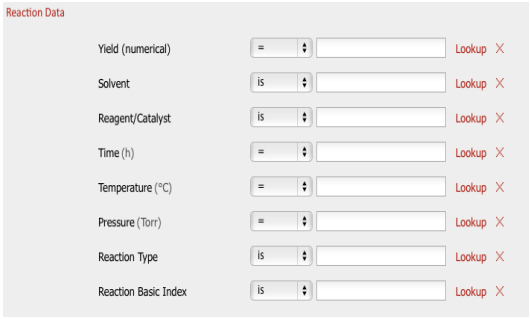
Atom mapping

Bond forming/breaking

Search reactions by structure

✔✔✔

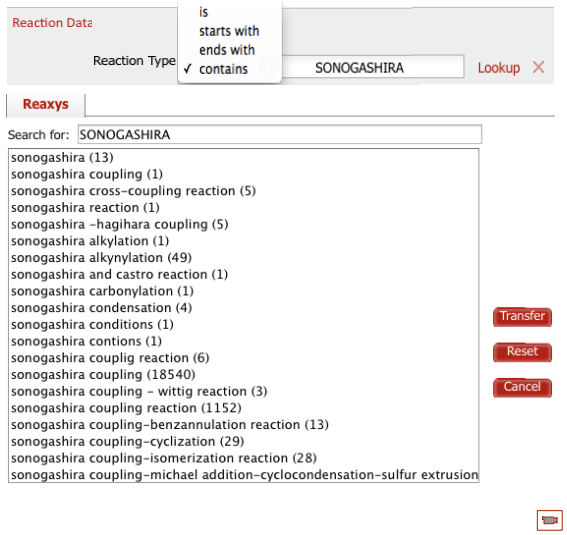
DATA



Search reactions by reaction conditions

✔✔✔

TYPE



Search reactions by type or name

✔✔✔

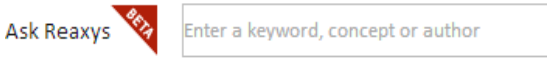
REAXYS®

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

✔✔✔

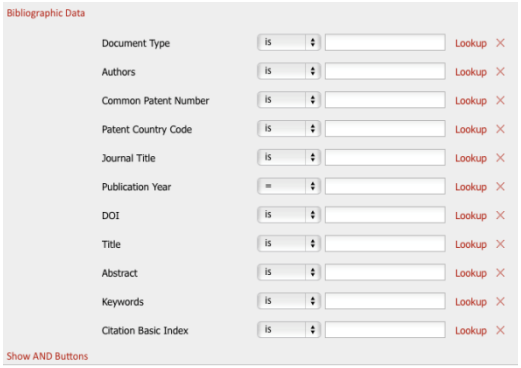
Reaxys Tree

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

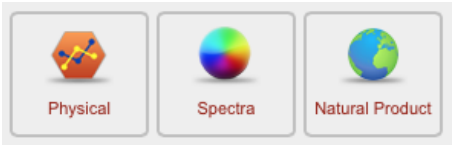
✔✔✔

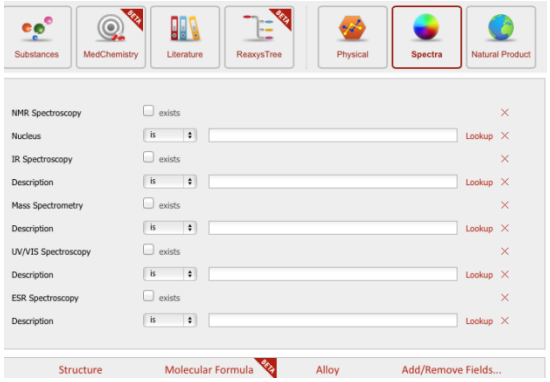
REAXYS®
HOW YOU THINK HOW YOU WORK

SEARCH PROPERTIES

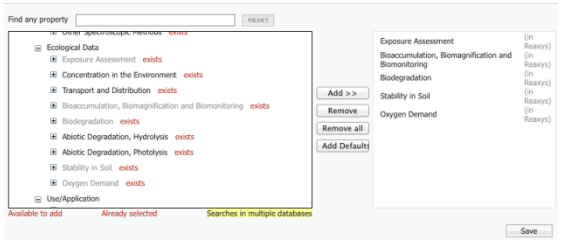
>500 MILLION EXPERIMENTAL PROPERTIES, >400 FIELDS, >130 SUBJECT AREAS

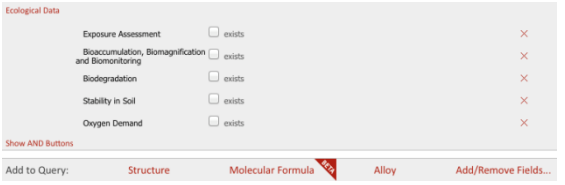
PRE-PROGRAMMED



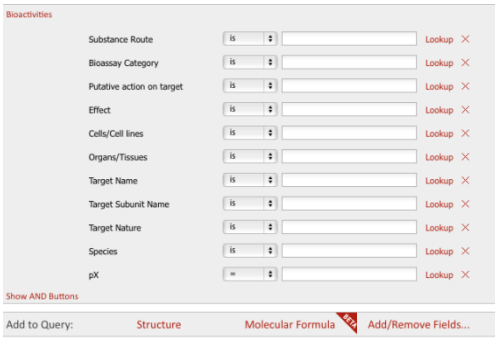


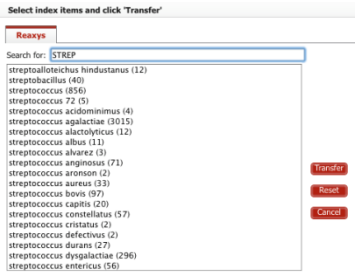
BUILD YOUR OWN





MedChem





PROPERTIES ✔✔✔ easy to set up

CONTENT ✔✔✔ easy to search

FIELDS ✔✔✔

REAXYS®
HOW YOU THINK HOW YOU WORK

MAIN NEW FEATURES & FUNCTIONALITIES

OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

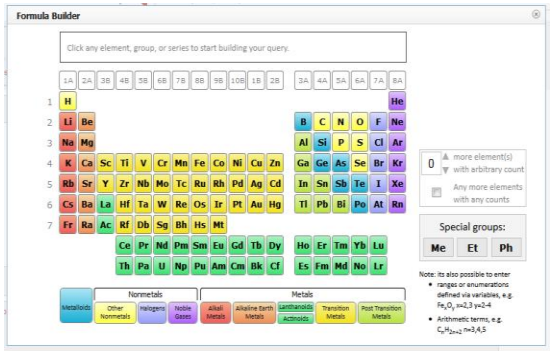
Ask Reaxys

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

Reaxys Tree

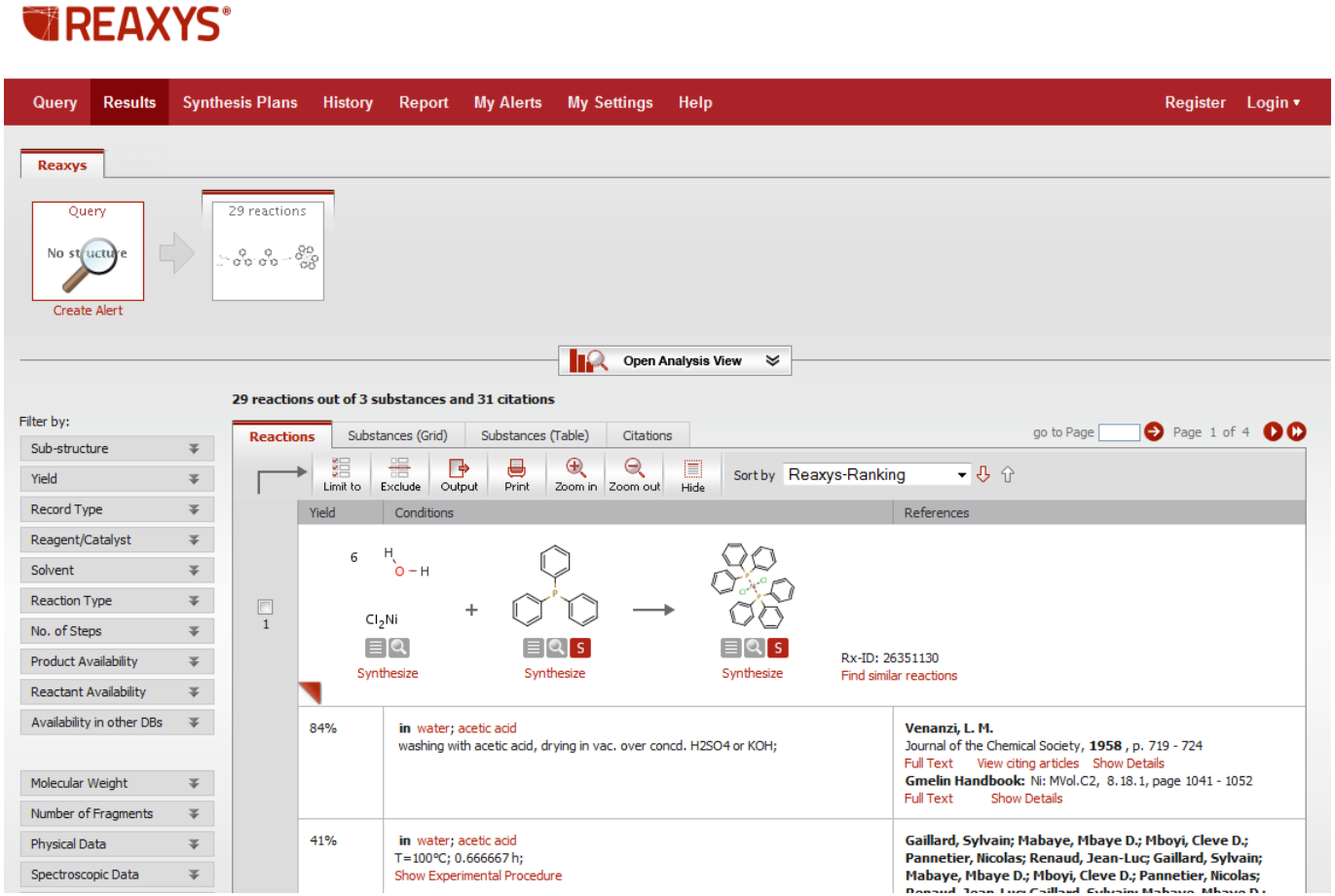
ReaxysTree lets users "browse" the database by taxonomies: helps with search precision and answer comprehension

Formula Builder



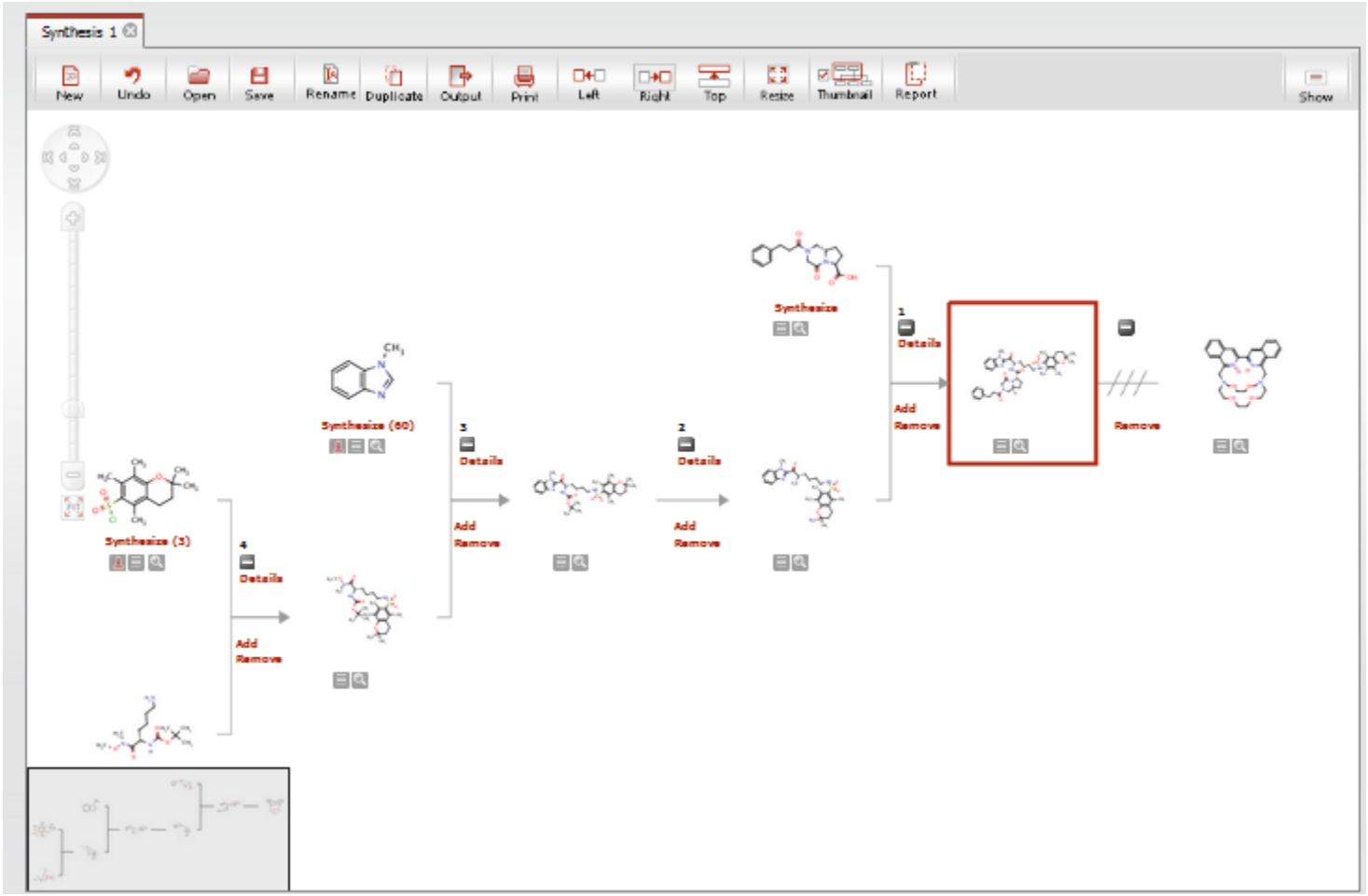
Formula Builder improves the searchability of substances through molecular formulas: easy way to find substances right across the Periodic Table

REAXYS 2014
MAKE A COMPOUND



AUTOPLAN:

AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES



REAXYS®
HOW YOU THINK HOW YOU WORK

SHOW EXPERIMENTAL PROCEDURE

Rx-ID: 27727760
Find similar reactions

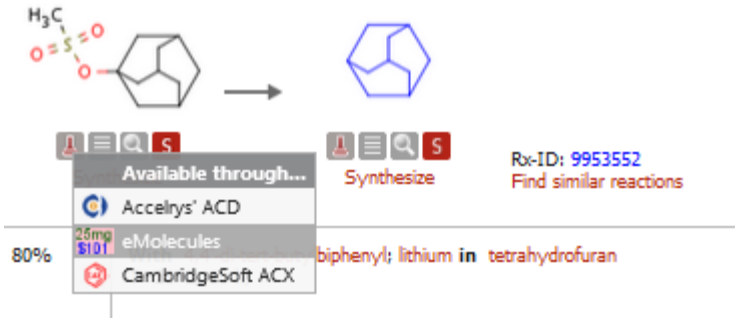
With $AlCl_3$, aluminium chloride **in** dichloromethane
T=0 - 20°C; 18 h;
Hide Experimental Procedure

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

CHECK COMMERCIAL AVAILABILITY



REAXYS®
HOW YOU THINK HOW YOU WORK

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

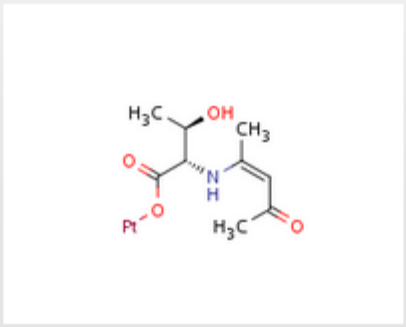
Reaxys uses Dotmatic's Elemental as default structure and reaction query editor, if no other editor is selected

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

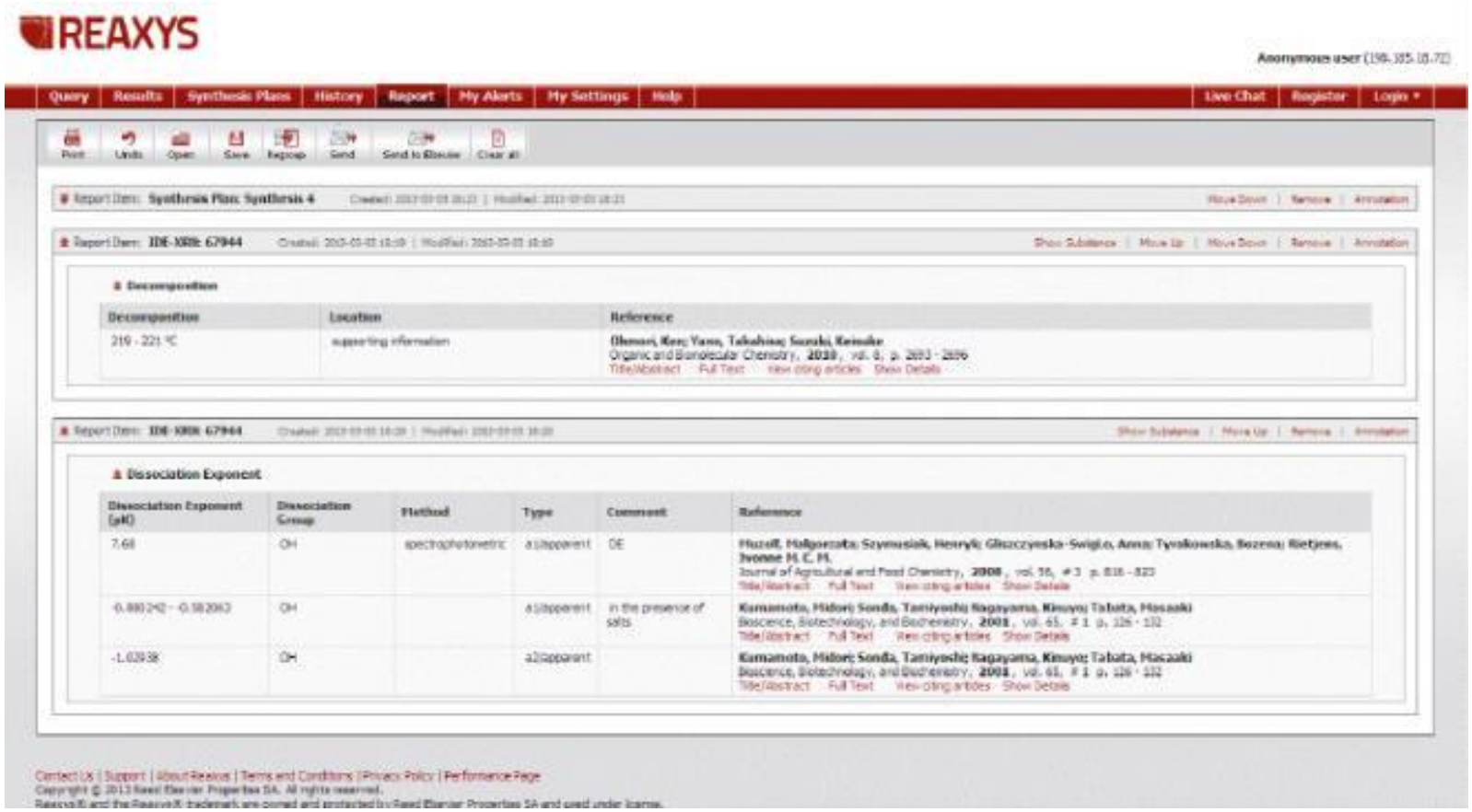
R/S Labels
- On All
- Absolute Stereo
- None

E/Z Labels
- On
- Off

Display Atom Valence
- On
- Off

REPORTING:

GATHER AND PREPARE THE INFORMATION



and... what is your reaction?

PIOTR GOLKIEWICZ

SOLUTION SALES MANAGER LIFE SCIENCES

CENTRAL AND EASTERN EUROPE

P.GOLKIEWICZ@ELSEVIER.COM

MOBILE: +48 695 30 60 17

REAXYS®

HOW YOU THINK HOW YOU WORK