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INTRODUCING REAXYS
SERVING THE LIFE SCIENCES SPACE
ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN

- Characterize targets & analyze disease pathways
- Characterize & discover molecules
  Identify & confirm lead compounds
- Translate preclinical data in humans
  (Translational)
- Monitor drug adverse events &
  real-world evidence data in literature

**Pathway Studio**

**REAXYS**

**Medicinal Chemistry**

**REAXYS**

**PharmaPendium**

**EMBASE**

**QuOsa**

**Drug Candidate Selection**
- Discovery
- Pre-clinical

**Go-No Go Decision**
- Clinical

**Preclinical Data Validation**
- Post-launch

**Managing risk**

- Broader full-text indexing of biomedical content
- Text Mining & Data Integration
- Integrate the world of data & solutions

**ScienceDirect**

- Search full-text, peer-reviewed journal articles

**EMBASE**

- Largest database for access to abstract & citation data
WHAT’S IN A TYPICAL CHEMISTRY DOCUMENT (PUBLICATION OR PATENT)?

Scientific topic, author

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

Chemical reactions

Cannot be searched by text terms in full text

Experimental procedures

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

Cannot be searched by text terms in full text

Chemical structure

Cannot be searched by text terms in full text

Chemical spectra

Cannot be searched by text terms in full text
Chemistry as the organizing principle
Physical Data

Spectra

Bioactivity Data

Natural Product
Reaxys excerpts all relevant data even from footnotes and text
OTHER DATABASES

REAXYS
CATALOGUED AND TAXONMISED BY CHEMISTS FOR CHEMISTS

ESSENTIAL TITLES

ACROSS TIME/LITERATURE

USE-CASE DRIVEN

RELEVANT ANSWERS

STRUCTURED TO HELP YOU SEARCH

BIBLIOGRAPHIC APPROACH

UNFOCUSED RESULTS

FURTHER SEARCH NEEDED

50,000,000 RESULTS RETURNED

RELEVANT ANSWERS
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

A Bibliographic Database
> 46 million records
(from ~16,000 journal titles plus records from key patent organisations)

A Substance Database
> 78 million substances (total)
~ 57 million substances (unique)

A Chemical Reaction Database
> 36 million single- and multi-step reactions

A Property Database
> 500 million experimental properties
in > 400 fields
in > 130 subject areas
REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION

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

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

Perform a literature search

Browse database via taxonomies rather than search database

Access detailed Biodata, and MedChem specific features

REAXYS®
HOW YOU THINK HOW YOU WORK
SEARCH REACTIONS
SEARCH BY STRUCTURE, DATA, OR TYPE

STRUCTURE

Data

Type

Atom mapping
Bond forming/breaking

Search reactions by structure

Search reactions by reaction conditions

Search reactions by type or name

✔✔✔

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SEARCH LITERATURE
OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

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

Intelligent interpretation of topic query

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

Browse through taxonomies

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

Use truncation/proximity if you like
SEARCH PROPERTIES
>500 MILLION EXPERIMENTAL PROPERTIES, >400 FIELDS, >130 SUBJECT AREAS

PRE-PROGRAMMED
- Physical
- Spectre
- Natural Product

BUILD YOUR OWN

MedChem

PROPERTIES
✔✔✔ easy to set up

CONTENT
✔✔✔ easy to search

FIELDS
✔✔✔
MAIN NEW FEATURES & FUNCTIONALITIES
OUR GOAL: MAKE CONTENT MORE DISCOVERABLE, MORE EASILY!

Ask Reaxys

Enter a keyword, concept or author

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

Reaxys Tree

ReaxysTree

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
AUTOMATES THE UNDERLYING PROCESSES IN CREATING SYNTHESIS ROUTES
SHOW EXPERIMENTAL PROCEDURE

With AlCl₃, aluminium chloride in dichloromethane
T = 0 - 20°C; 18 h

Hide Experimental Procedure

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 glass bottle, followed by adding 40 g of dichloromethane thereto to dissolve the nitrogen and stirring in the ice bath. Subsequently, 10 g of AlCl₃ 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. The above saturated KCl solution washing procedure is repeated for three times. 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 upper layer in the separatory funnel. The above saturated KCl solution washing procedure is repeated for three times. Subsequently, the mixture washed with the saturated KCl solution is washed with 100 ml of deionized water, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the lower layer in the deionized water washing procedure is repeated for three times. Subsequently, the lower layer is distilled to remove dichloromethane and water. The bottoms is collected, and determined by chemical analysis. The chemical analysis is composed of 85.7 wt percent of exo-THDCPD, 0.5 wt percent of endo-THDCPD, 1.2 wt percent of Decalin, 5.8 wt percent of adamantane, 1.3 wt percent of exo-THMDCPD, and the other two-stage hydro-treated and saturated C₇ and/or C₈ hydrocarbon homologous. The bottoms has a volumetric heating value of 39.17 MJ/L, a density of 0.9339 at 15°C, and a viscosity of 3.52 cSt at 20°C and more than 26.7 cSt at -20°C. In this example, the isomerization reaction is very slow so that portions of exo-THDCPD is further isomerized to adamantane which will increase the viscosity of the high energy fuel. Under such a violent reaction conditions, a small amount of THDCPD will be ring-opened to Decalin (the side product) with relatively less volumetric heating value as well as density. Therefore, the isomerization reaction of this example is not suitable for preparing the high energy fuels because the freezing point of the isomerization reaction.
SUPPORTS DIFFERENT STRUCTURE EDITORS

### Structure editor

Editors that do not require a plugin to be installed:
- Dotmatics Elemental
- ChemAxon MarvinSketch  *(Note: requires Java to be installed)*
- GGA Ketcher

Reaxys uses Dotmatics’ 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
  - Off

- E/Z Labels
  - Off

- Display Atom Valence
  - On
  - Off
REPORTING:
GATHER AND PREPARE THE INFORMATION
and... what is your reaction?

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REAXYS®
HOW YOU THINK. HOW YOU WORK