



# Reaxys: Where chemistry adventures begin!

---

Katarzyna Gaca, Ph.D.  
[katarzyna@gaca.cat](mailto:katarzyna@gaca.cat)



# Agenda

---

- Elsevier: general information
- How to navigate in an ocean of information?
- How is Reaxys different?
- Articles on-line today...and tomorrow!
- Chemistry research – what do you need to know?
- Reaxys – let's search!
- Supporting your educational needs
- Who uses Reaxys? What do our customers say?
- Development plans
- Summary



# Elsevier: general information

---



- Publishing House Elzevir was established in 1580 by Lowys Elzevir at the Leiden University in the Netherlands.



- Following the publishing traditions established by Lowys Elzevir, Jacobus George Robbers started the present Elsevier publishing house in 1880.

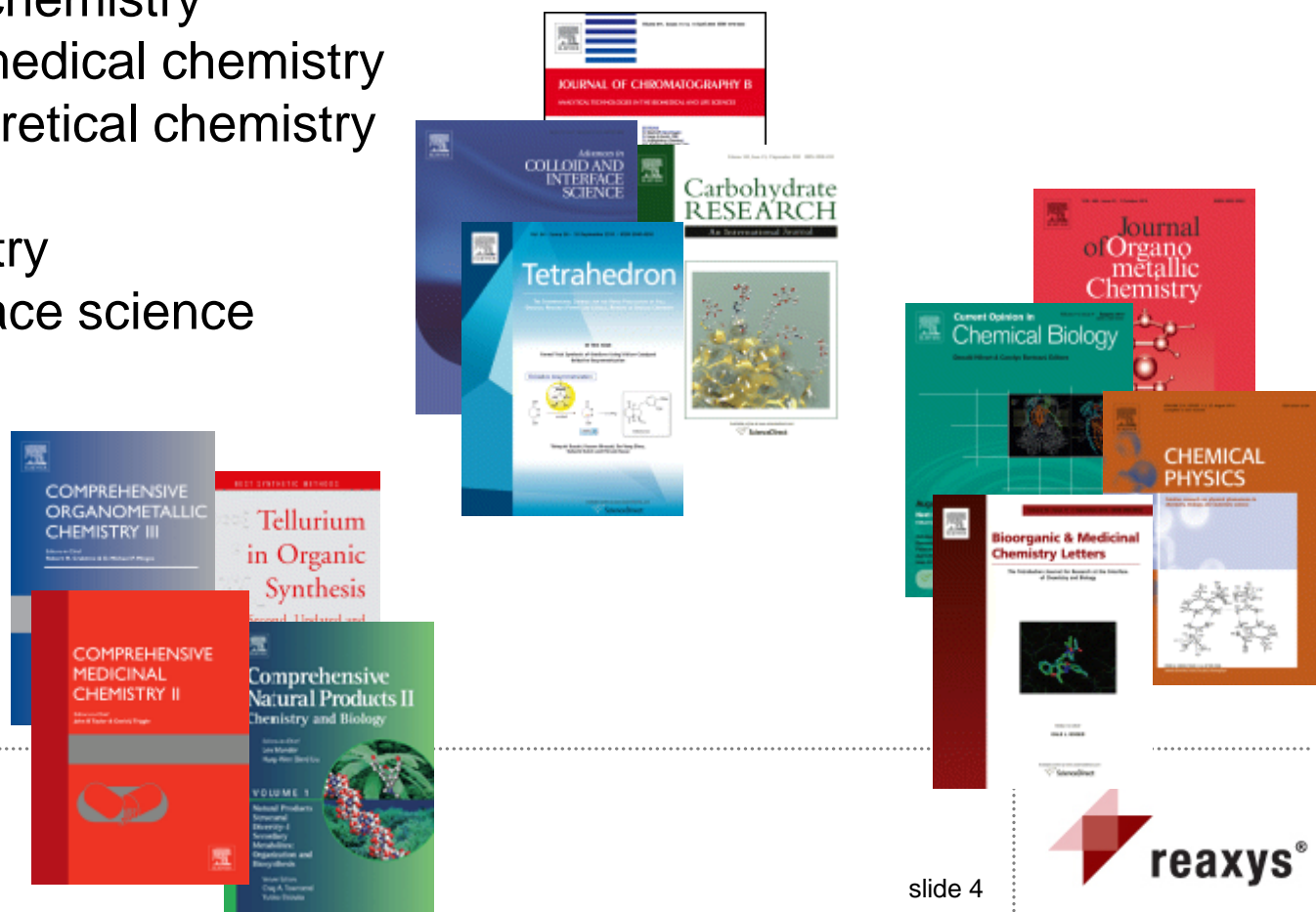


- Among many authors associated with Elsevier one can find Galileo, Erasmus, Descartes, Alexander Fleming, Julius Verne...

# Elsevier: general information

- Organic chemistry
- Inorganic chemistry
- Organometallics chemistry
- Bio-organic and medical chemistry
- Physical and theoretical chemistry
- Spectroscopy
- Analytical chemistry
- Colloid and interface science
- Electrochemistry
- Sensors

- 30 000 new articles annually
- 50 – 70 new books



# How to navigate in an ocean of information?



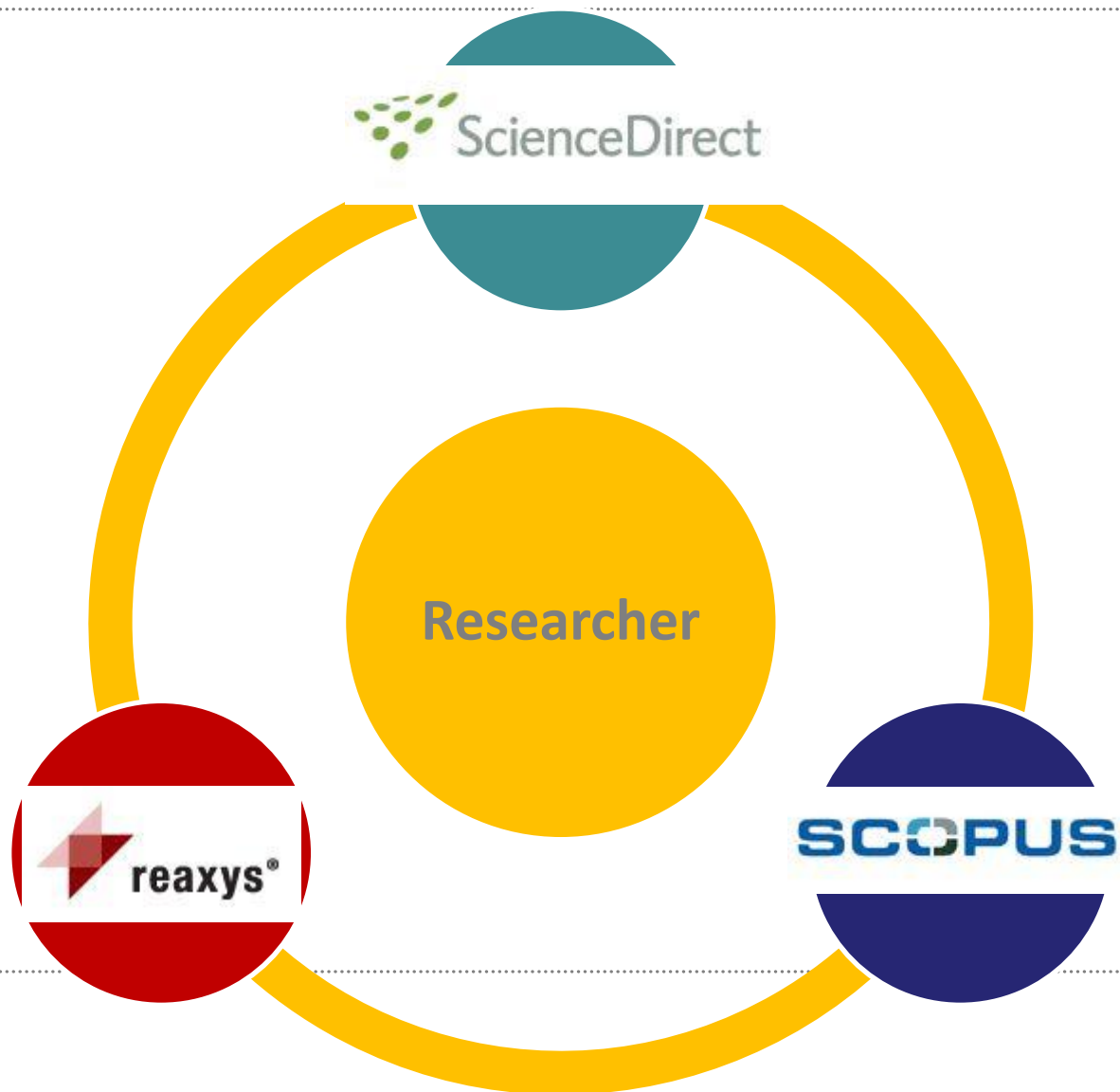
# How to navigate in an ocean of information?



# How to navigate in an ocean of information?



# How to navigate in an ocean of information?





# How is Reaxys different?

---

- Actionable, **reliable** and **relevant** physical, chemical and bioactivity data, collected from **journals** and **patents**
- Allows to **efficiently** develop synthesis strategies, to evaluate and compare them with alternative routes, and thus to create a **comprehensive synthesis plan**
- **Relevant** information regarding commercial availability, including pricing and information about suppliers – all within Reaxys

# Articles on-line today..

## Synthesis of unnatural pentahydroxylated pyrrolizidines: 5-*epi*- and 5,7a-di-*epi*-hyacinthacine C<sub>1</sub>

Juan A. Tamayo<sup>a</sup>, Francisco Franco<sup>a</sup> and Fernando Sánchez-Cantalejo<sup>a</sup>

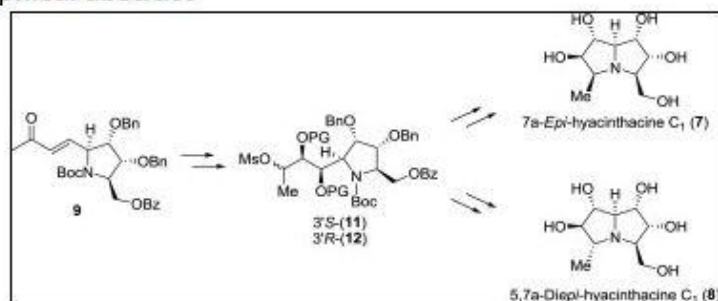
<sup>a</sup> Department of Medicinal and Organic Chemistry, Faculty of Pharmacy, University of Granada, 18071 Granada, Spain

Received 9 June 2010; revised 9 July 2010; accepted 9 July 2010. Available online 16 July 2010.

### Abstract

Stereocontrolled synthesis of 5-*epi*- and 5,7a-di-*epi*-hyacinthacine C<sub>1</sub> (**7** and **8**), two potential glycosidase inhibitors are described using  $\alpha,\beta$ -unsaturated ketone **9** as homochiral starting material. The key step in the synthesis is the highly diastereoselective dihydroxylation reaction of **9**, that allows the obtention of a single bis-hydroxylated ketone (**10**). Further derivatization into two epimeric mesylate esters followed by internal cyclization form the pyrrolizidinic compounds **7** and **8**. This type of compounds can be useful in glycobiology due to their ability to inhibit carbohydrate-processing enzymes.

### Graphical abstract



### Author's Key Structures in this Article

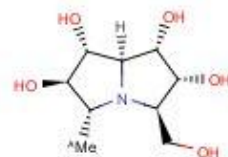
powered by reaxys<sup>®</sup>



[Search in Reaxys](#)



[InChIKey Search](#)



[Search in Reaxys](#)



[InChIKey Search](#)



# ...and tomorrow!

**Table 3. Deprotection of DEB Group**

Entry	Conditions	Yield (%)	Time (h)
1	K <sub>2</sub> CO <sub>3</sub> , MeOH	100	2
2	NaOH, EtOH	100	2
3	NaOH, EtOH	100	2
4	tert-BuOK, H <sub>2</sub> O, THF	100	2
5	tert-BuOK, H <sub>2</sub> O, THF	100	2
6	tert-BuOK, H <sub>2</sub> O, THF	100	2

In conclusion, we discovered the first example of the direct C-7 substitution of 1-(DEB)indoles on indole nitrogen. Direct C-7 substitution of 1-(DEB)indoles were employed as the substrate. Direct C-7 substitution of 1-(DEB)indoles in THF, this method allows easy preparation of a variety of 3-substituted derivatives which are not easily available by using conventional routes.

**Experimental**

Melting points were determined with a Yanagimoto micro melting point apparatus and an accurate IR spectra were obtained with a Perkin Elmer Spectrum 2000 instrument. <sup>1</sup>H NMR spectra were recorded at 300 MHz on a Varian Gemini-300 instrument, at 300 MHz on a Varian Gemini-300 instrument. The differential NMR measurements were carried out on a JEOL JNM-GX400 instrument. All spectra were expressed as ppm down field from tetramethylsilane used as an internal standard (δ value = 0 ppm). High resolution mass spectra were recorded on a JEOL JMS-EX200 instrument. Elemental analyses were performed at the microanalytical laboratory in Nagasaki University. Column chromatography was conducted on silica gel 60, 70-230 mesh ASTM (E.Merck), unless otherwise mentioned. Flash chromatography was conducted on silica gel 60, 230-400 mesh ASTM (E.Merck). Solvents were dried (Na/benzophenone) and distilled under nitrogen or argon if necessary. Anhydrous solvents were purchased from Aldrich Chemical Co., Inc. All reagents were used as they are (H<sub>2</sub>) were purchased from Aldrich Chemical Co., Inc. All high-boiling solvents were distilled over CaH<sub>2</sub>. 2,5-dimethylbenzyl alcohol, 3-phenylacetyl chloride (1) was synthesized according to the literature procedure.<sup>13</sup>

1-(4-(2,5-dimethylbenzyl)oxy)indole (2). Indole (1.07 g, 5.14 mmol) was added to a solution of NaH (0.97 g, 10.28 mmol) in THF (10 mL) and cooled to 0 °C. After stirring, 3-phenylacetyl chloride (1) (1.07 g, 5.14 mmol) was added dropwise and the mixture was stirred for 1 h, the mixture was washed successively with water, 10% NaOH solution, and water. The mixture was dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated in vacuo to give pure 2 (2.37 g, 98%) as colorless oil. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.84 (d, J = 7.4 Hz, 1H), 7.74 (d, J = 7.4 Hz, 1H), 7.54 (d, J = 7.4 Hz, 1H), 7.44 (d, J = 7.4 Hz, 1H), 7.34 (d, J = 7.4 Hz, 1H), 7.24 (d, J = 7.4 Hz, 1H), 7.14 (d, J = 7.4 Hz, 1H), 7.04 (d, J = 7.4 Hz, 1H), 6.94 (d, J = 7.4 Hz, 1H), 6.84 (d, J = 7.4 Hz, 1H), 6.74 (d, J = 7.4 Hz, 1H), 6.64 (d, J = 7.4 Hz, 1H), 6.54 (d, J = 7.4 Hz, 1H), 6.44 (d, J = 7.4 Hz, 1H), 6.34 (d, J = 7.4 Hz, 1H), 6.24 (d, J = 7.4 Hz, 1H), 6.14 (d, J = 7.4 Hz, 1H), 6.04 (d, J = 7.4 Hz, 1H), 5.94 (d, J = 7.4 Hz, 1H), 5.84 (d, J = 7.4 Hz, 1H), 5.74 (d, J = 7.4 Hz, 1H), 5.64 (d, J = 7.4 Hz, 1H), 5.54 (d, J = 7.4 Hz, 1H), 5.44 (d, J = 7.4 Hz, 1H), 5.34 (d, J = 7.4 Hz, 1H), 5.24 (d, J = 7.4 Hz, 1H), 5.14 (d, J = 7.4 Hz, 1H), 5.04 (d, J = 7.4 Hz, 1H), 4.94 (d, J = 7.4 Hz, 1H), 4.84 (d, J = 7.4 Hz, 1H), 4.74 (d, J = 7.4 Hz, 1H), 4.64 (d, J = 7.4 Hz, 1H), 4.54 (d, J = 7.4 Hz, 1H), 4.44 (d, J = 7.4 Hz, 1H), 4.34 (d, J = 7.4 Hz, 1H), 4.24 (d, J = 7.4 Hz, 1H), 4.14 (d, J = 7.4 Hz, 1H), 4.04 (d, J = 7.4 Hz, 1H), 3.94 (d, J = 7.4 Hz, 1H), 3.84 (d, J = 7.4 Hz, 1H), 3.74 (d, J = 7.4 Hz, 1H), 3.64 (d, J = 7.4 Hz, 1H), 3.54 (d, J = 7.4 Hz, 1H), 3.44 (d, J = 7.4 Hz, 1H), 3.34 (d, J = 7.4 Hz, 1H), 3.24 (d, J = 7.4 Hz, 1H), 3.14 (d, J = 7.4 Hz, 1H), 3.04 (d, J = 7.4 Hz, 1H), 2.94 (d, J = 7.4 Hz, 1H), 2.84 (d, J = 7.4 Hz, 1H), 2.74 (d, J = 7.4 Hz, 1H), 2.64 (d, J = 7.4 Hz, 1H), 2.54 (d, J = 7.4 Hz, 1H), 2.44 (d, J = 7.4 Hz, 1H), 2.34 (d, J = 7.4 Hz, 1H), 2.24 (d, J = 7.4 Hz, 1H), 2.14 (d, J = 7.4 Hz, 1H), 2.04 (d, J = 7.4 Hz, 1H), 1.94 (d, J = 7.4 Hz, 1H), 1.84 (d, J = 7.4 Hz, 1H), 1.74 (d, J = 7.4 Hz, 1H), 1.64 (d, J = 7.4 Hz, 1H), 1.54 (d, J = 7.4 Hz, 1H), 1.44 (d, J = 7.4 Hz, 1H), 1.34 (d, J = 7.4 Hz, 1H), 1.24 (d, J = 7.4 Hz, 1H), 1.14 (d, J = 7.4 Hz, 1H), 1.04 (d, J = 7.4 Hz, 1H), 0.94 (d, J = 7.4 Hz, 1H), 0.84 (d, J = 7.4 Hz, 1H), 0.74 (d, J = 7.4 Hz, 1H), 0.64 (d, J = 7.4 Hz, 1H), 0.54 (d, J = 7.4 Hz, 1H), 0.44 (d, J = 7.4 Hz, 1H), 0.34 (d, J = 7.4 Hz, 1H), 0.24 (d, J = 7.4 Hz, 1H), 0.14 (d, J = 7.4 Hz, 1H), 0.04 (d, J = 7.4 Hz, 1H). Found: C, 78.22; H, 8.80; N, 5.54%.

**Fact**

**reaxys**

Query Results Synthesis Plans History My Alerts My Settings Help Logout

Query 70 reactions 35 reactions filtered by Journal Title

Sort by Reaxys-Ranking

References

Synthesize

With SnCl<sub>4</sub>·2H<sub>2</sub>O; RuCl<sub>2</sub>·3H<sub>2</sub>O/PPPh<sub>3</sub> in dioxane; H<sub>2</sub>O T=180°C; 20 h;

Choi, Chan Sil; Kim, Jin Hwang; Kim, Tae-Jeong; Shim, Sang Chul  
Tetrahedron, 2001, vol. 57, # 16 p. 3321-3330  
Title/Abstract Full Text View citing articles

Stage #1: With sec-BuLi; sparteine in diethyl ether; hexane; cyclohexane; T=-78°C;Metalation; Stage #2: With MeOD T=-78°C;Substitution; O, S; Substitution;

Physical Data Spectroscopic Data Bioscience Publications

N<sup>o</sup> of preparations Available Data N<sup>o</sup> of ref. Boiling Point

1 prep out of 3 reactions. Identification Spectra (3) 2

Molecular Formula: C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O  
Molecular Structure Formula: C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O  
Molecular Weight: 243.349  
InChI Key: CBDJPNJIZOMAKS-UHFFFAOYSA-N

NMR Spectroscopy (1)

Description	Nucleus	Solvents	Frequency	References
Spectrum	<sup>1</sup> H	CDCl <sub>3</sub>	300MHz	Fukuda, Tsutomu; Maeda, Ryoichi; Iwao, Masatomo Tetrahedron, 1999, vol. 55, # 30 p. 9151-9162 Title/Abstract Full Text View citing articles

**Verified and confirmed experimental data instantly available**

**Vast number of available data – up to 400 fields!**

**Citation**

**Structure**

**Reaction**

TETRAEDRON

Direct C-7 Lithiation of 1-(DEB)indoles

Yoshino, Takashi; Ryoichi, Maeda; Masatomo, Iwao  
Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, 1-8 Bunkyo-2-chou, Nagasaki 852-8581, Japan  
Received 26 April 1999; accepted 26 May 1999

Abstract: Direct lithiation of 1-(DEB)indoles was investigated. It was discovered that a highly substituted 1-(DEB)indole group could promote direct C-7 lithiation. Specifically, on the case of 3-(2,5-dimethylbenzyl)oxyindole, direct C-7 lithiation was observed in a reasonably high yield. The substituted 1-(DEB)indoles, which are C-7 lithiation was observed in a reasonably high yield. This C-7 lithiation was easily achieved by 2,2,6,6-tetramethylpiperidine (TEMPO) system after deprotonation at C-2. This C-7 lithiation was easily achieved by 2,2,6,6-tetramethylpiperidine (TEMPO) system after deprotonation at C-2. This C-7 lithiation was easily achieved by 2,2,6,6-tetramethylpiperidine (TEMPO) system after deprotonation at C-2.

Some biologically significant natural products and synthetic drugs<sup>1</sup> comprise 7-substituted indole moieties as a key structural unit. The synthesis of 7-substituted indoles, however, is a major objective. This article describes the synthesis of 7-substituted indoles from 1-(DEB)indoles. A number of authors have reported the synthesis of 7-substituted indoles from 1-(DEB)indoles. Some<sup>2</sup> and Iwao<sup>3</sup> utilized 1-(DEB)indoles as starting materials in the synthesis of 7-substituted indoles. Iwao<sup>3</sup> reported direct C-7 lithiation of 1-(DEB)indoles to give 7-substituted indoles. This approach, however, requires the synthesis of 7-substituted indoles from 1-(DEB)indoles. This approach, however, requires the synthesis of 7-substituted indoles from 1-(DEB)indoles. This approach, however, requires the synthesis of 7-substituted indoles from 1-(DEB)indoles.

It will be known that the lithiation of 1-substituted indoles occurs at 2-position exclusively.<sup>4</sup> Although a variety of direct C-7 lithiation has been utilized on the case of 1-(DEB)indoles, direct C-7 lithiation. This is the first example of direct C-7 lithiation of 1-(DEB)indoles. We thought, however, that a simple lithiation procedure

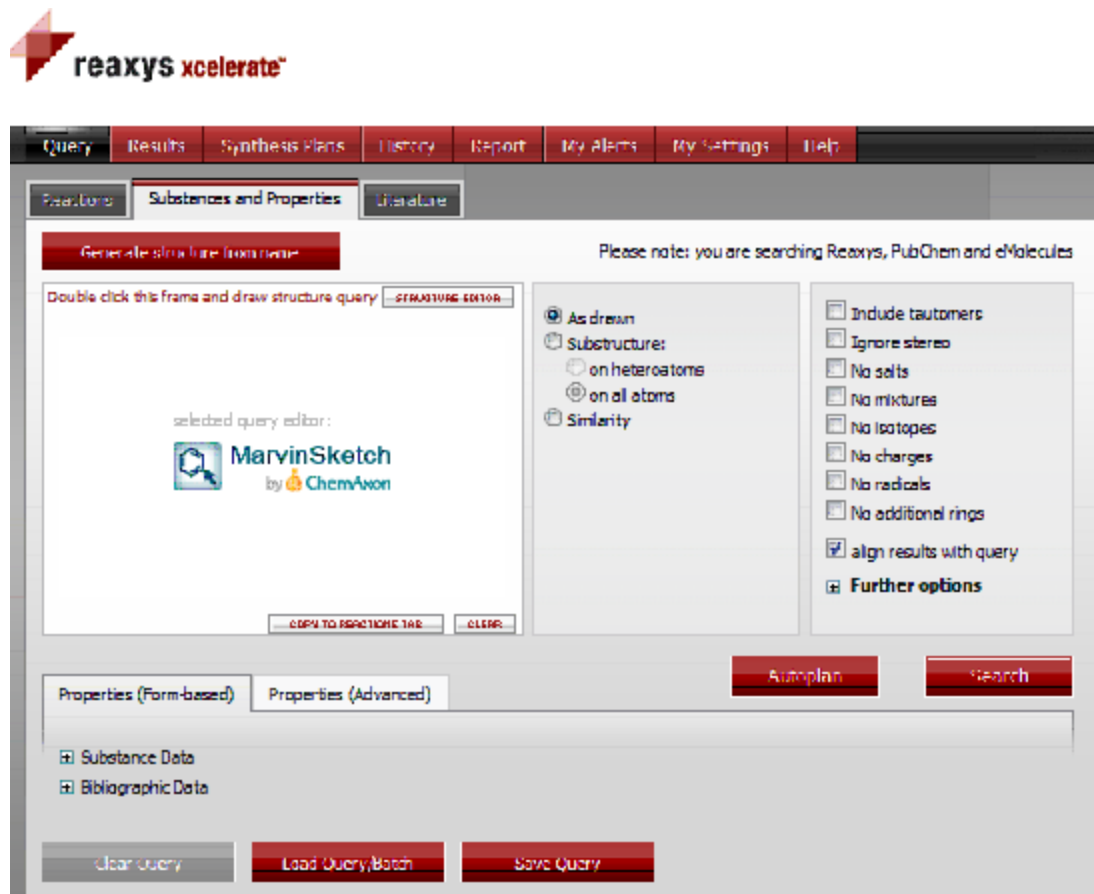


# Chemistry research – what do you need to know?

Things you usually want to know when you start researching a new substance:

- How can it be **synthesised**?
- What are the **reaction conditions**, **yields**? Are any **patents** available?
- What are the **starting materials**? Do I have to **purchase** them or can I **synthesise** them on my own?
- How can I **identify** this substance? Is there any **physical data or spectra** available?
- Does this substance **react** with others? If yes, then with **which**? **How** does that happen – what are the **conditions**, what are the **products**?
- What are **the practical applications** of this substance? Is it **bioactive**?
- Are there any other substances of **similar properties**, and are these **comparable**?
- Where can I **read more** about this substance? Which are the **key publications**?

# Reaxys – let's search!



The screenshot shows the Reaxys xcelerate search interface. At the top, there is a navigation bar with tabs for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this is a sub-navigation bar with tabs for Features, Substances and Properties, and Literature. The main content area is titled "Generate structure from name" and includes a note: "Please note: you are searching Reaxys, PubChem and eMolecules".

The interface is divided into several sections:

- Structure Editor:** A large central area with the text "Double click this frame and draw structure query" and a "STRUCTURE EDITOR" button. Below this, it says "selected query editor:" and displays the "MarvinSketch by ChemAxon" logo.
- Options Panel:** A panel on the right with various search options:
  - As drawn
  - Substructures:
    - on heteroatoms
    - on all atoms
  - Similarity
  - Include tautomers
  - Ignore stereo
  - No salts
  - No mixtures
  - No isotopes
  - No charges
  - No radicals
  - No additional rings
  - align results with query
  - Further options

Buttons for "COPY TO APPLICATION CLIPBOARD" and "CLEAR" are located below the structure editor.

At the bottom of the interface, there are tabs for "Properties (Form-based)" and "Properties (Advanced)". Below these are checkboxes for "Substance Data" and "Bibliographic Data". A "Clear query" button is on the left, and "Load Query/Batch" and "Save Query" buttons are on the right. A red "Autoplan" button and a red "Search" button are also present.

# Supporting your educational needs

Teaching

Learning

Testing

Evaluating

**Faculty**

"I need an easily digestible introduction to chemistry"

**Faculty**

"I need to explain the principles behind a reaction and show live examples"

**Faculty**

"I need reliable references and easy access to experimental data for effective class preparation"

**Librarian**

"I need a simple system to introduce chemistry information search principles"

**PhD organic/inorganic chemist**

"I need a system where I can put into practice learning in practical lab work"

**Department Head**

"I need greater student retention in chemistry programs"

**Student**

"I need something to make sense of chemistry"

**Librarian**

"I need researchers in my institution to have access to the best possible chemistry information"



# Who uses Reaxys?

Reaxys is used by **over 1000** universities and research institutions, including majority of the universities which are in the top 50 ARWU list. These are – among many others:

University of California, Berkeley

Harvard University

University of Cambridge

Stanford University

Massachusetts Institute of Technology (MIT)

University of Oxford

...and of course Semmelweis University!



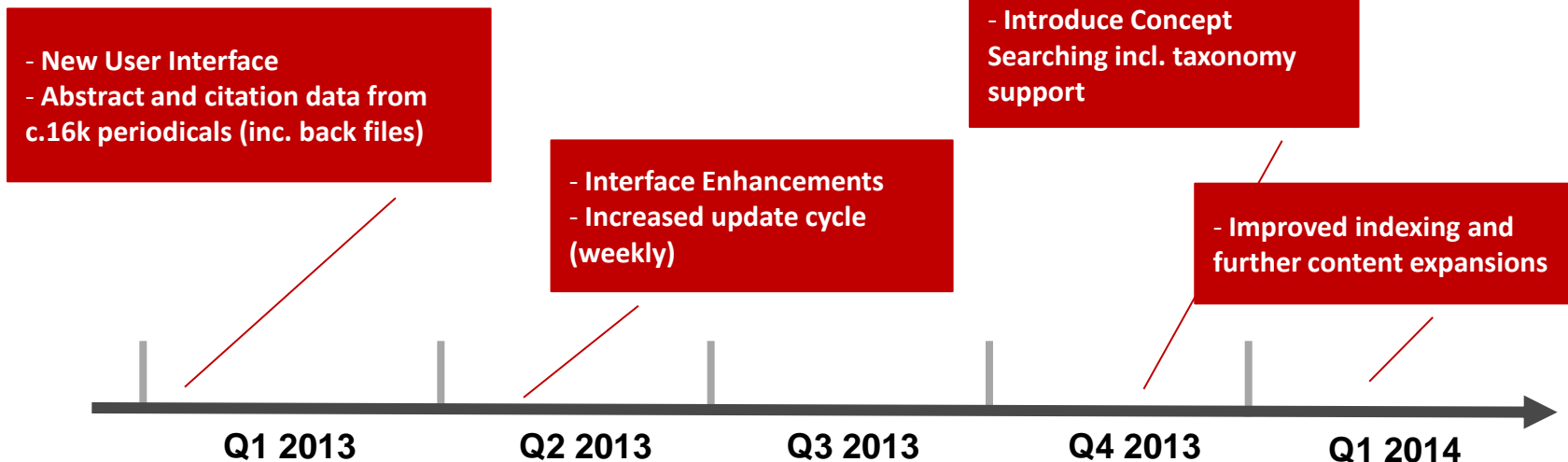
\* wg. ARWU

slide 15



# Reaxys development

Current coverage	2013 onwards
400 journals	15,973 periodicals: chemistry, life sciences, engineering, pharmacology, environmental sciences & more (including journal articles, book series & conference proceedings)
Relevant chemistry patents	Relevant chemistry patents
Historical data (from 1771)	Historical data (from 1771)





# Reaxys development

Bibliographic  
search

Experimentation

Writing/  
publication



## Project initiation

Concept searching, topic identification, literature search, identify partners/collaborators/competitors, evaluate potential risk/benefit, novelty check



## Project progress

Find ways how to make compounds, solve daily problems, modify experiments, use experimental data to verify results



## Project end

Last novelty check, confirm findings, prepare publication/report, ongoing status monitoring

# Summary

Reaxys is a very broad and deep repository of **experimental, verified and reliable** reaction and substance data.

- **Exact data** within your reach – all in one place
- **Shorter time** spent on **searching** and reading full-text articles and patents – irrelevant and unreliable data is rejected
- **Efficient access** to relevant, actionable results
- **No limits** on the number of users
- Access via web browser – from your institution or home:  
[www.reaxys.com](http://www.reaxys.com)



**Thank you kindly for your attention!**

**I will be happy to answer your questions.**

---

**Contact: Dr inż. Katarzyna Gaca, [katarzyna@gaca.cat](mailto:katarzyna@gaca.cat)**

