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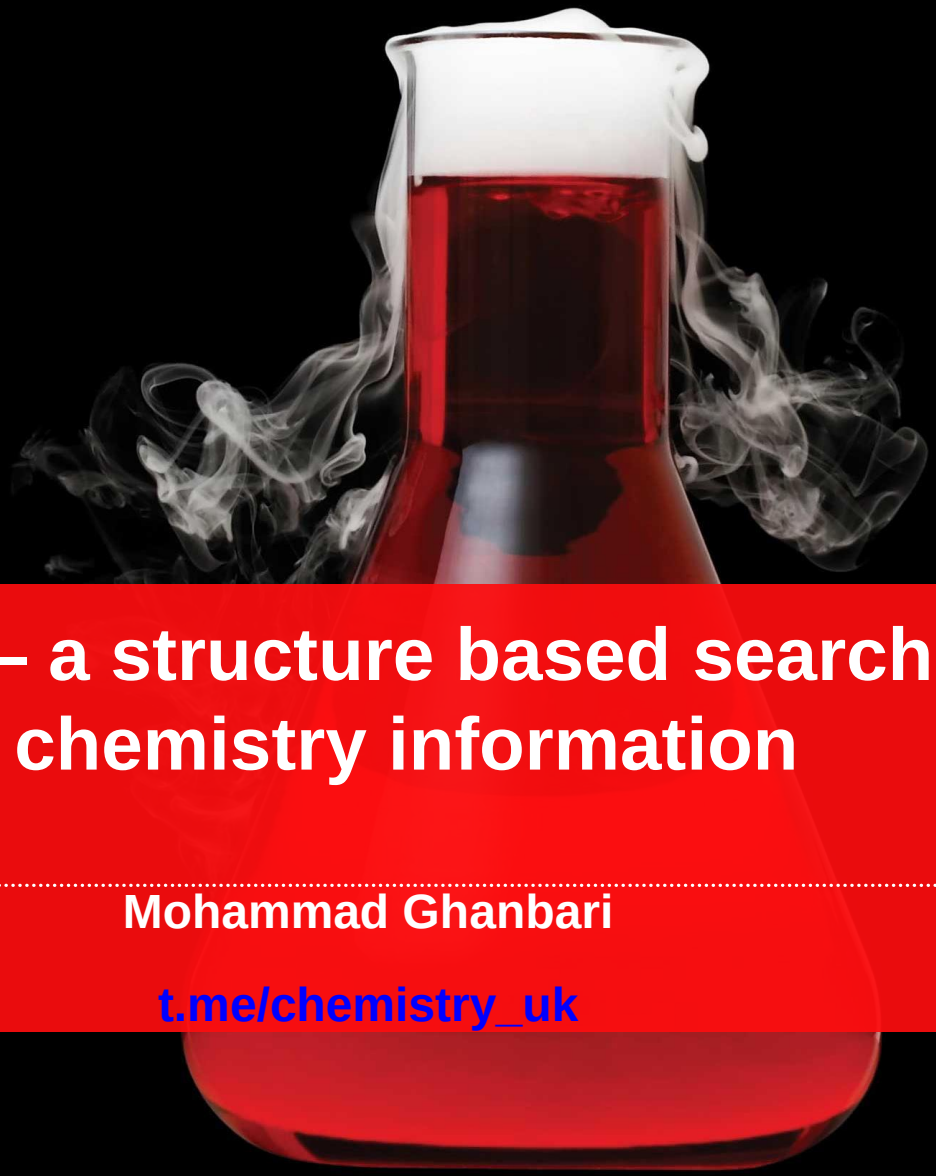

Reaxys – a structure based search and retrieval chemistry information

Mohammad Ghanbari

t.me/chemistry_uk

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Agenda

1. About Reaxys

- Concept of design
- Coverage
- Who is it for
- Community's response

2. Using Reaxys to…

- Find properties, reactions, patent information, citations…
- Plan a synthetic scheme
- Create your own report, library of compounds…

3. Demonstration

- www.reaxys.com
- Tips and tricks

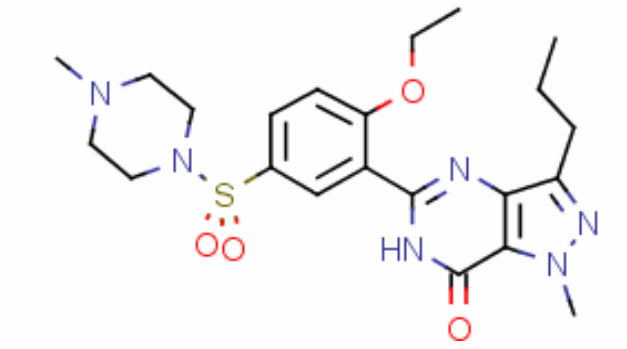
4. Summary

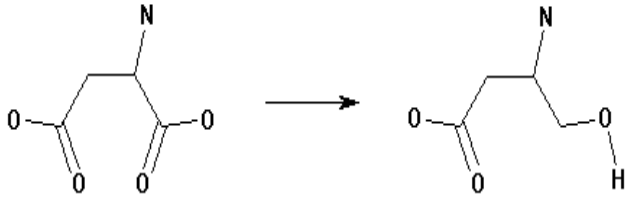
- Trial duration and access model
- Online training centre
- Customer support

1. 1 - Concept of Design

What does a Chemist want to know?

1. **What is this?**
   - Is it novel? Patented?
   - What are its physical characteristics (weight, melting point, etc)?
2. **What does it do?**
   - Is it a reagent? Solvent?
   - What is its bioactivity? Pharmacology?
   - Is it toxic?
3. **How can I make it?**
   - How can I change it?
   - How can I make it better?





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1. 1 - Concept of Design

Where do you go to find answers?

Google scholar beta

SciFinder SCHOLAR

SCIRUS
search engine for science

PubChem

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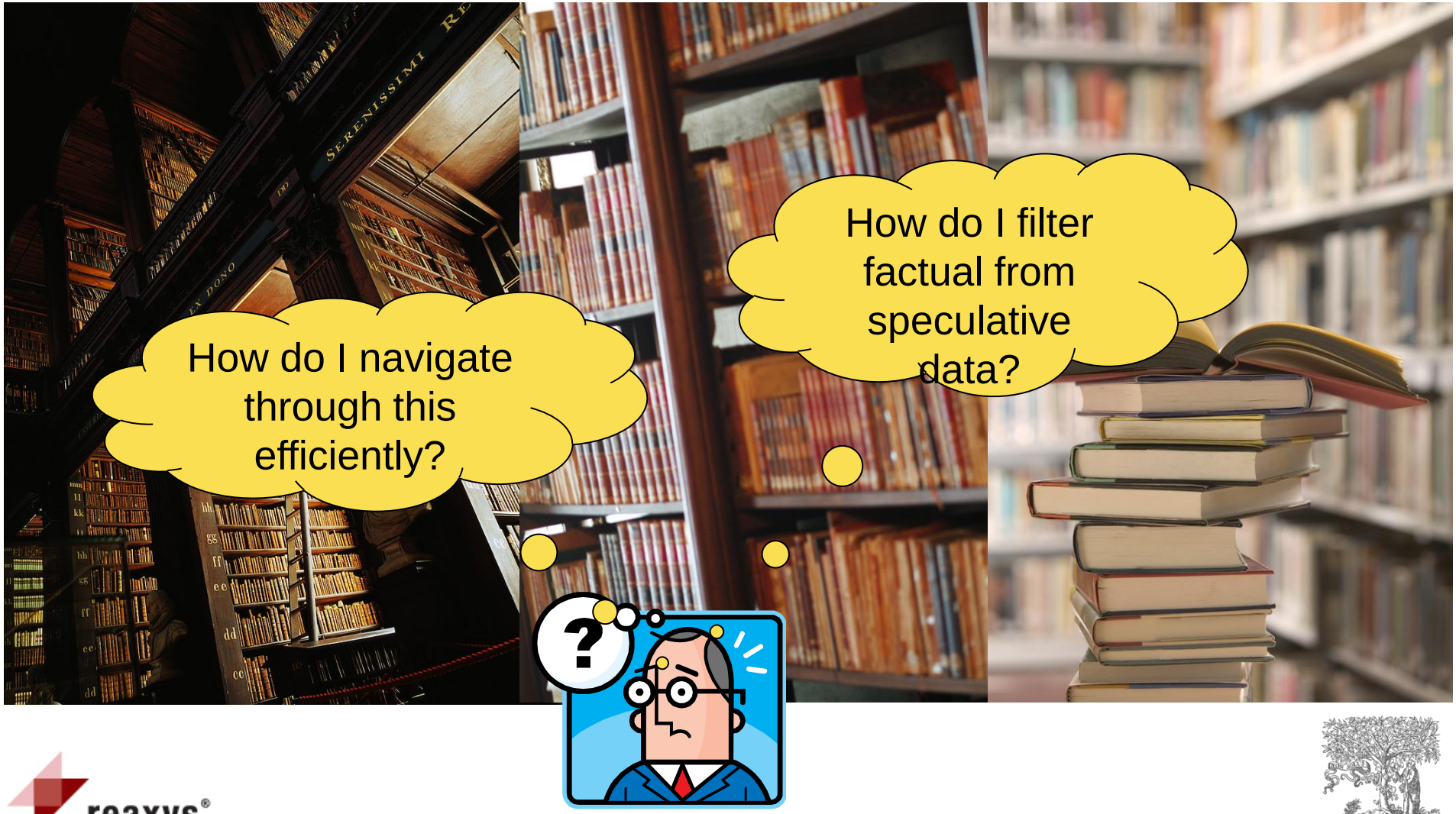
Information Explosion

5



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Information explosion

How much time will it take to filter through all these to find the relevant information?

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1. 1 - Concept of Design

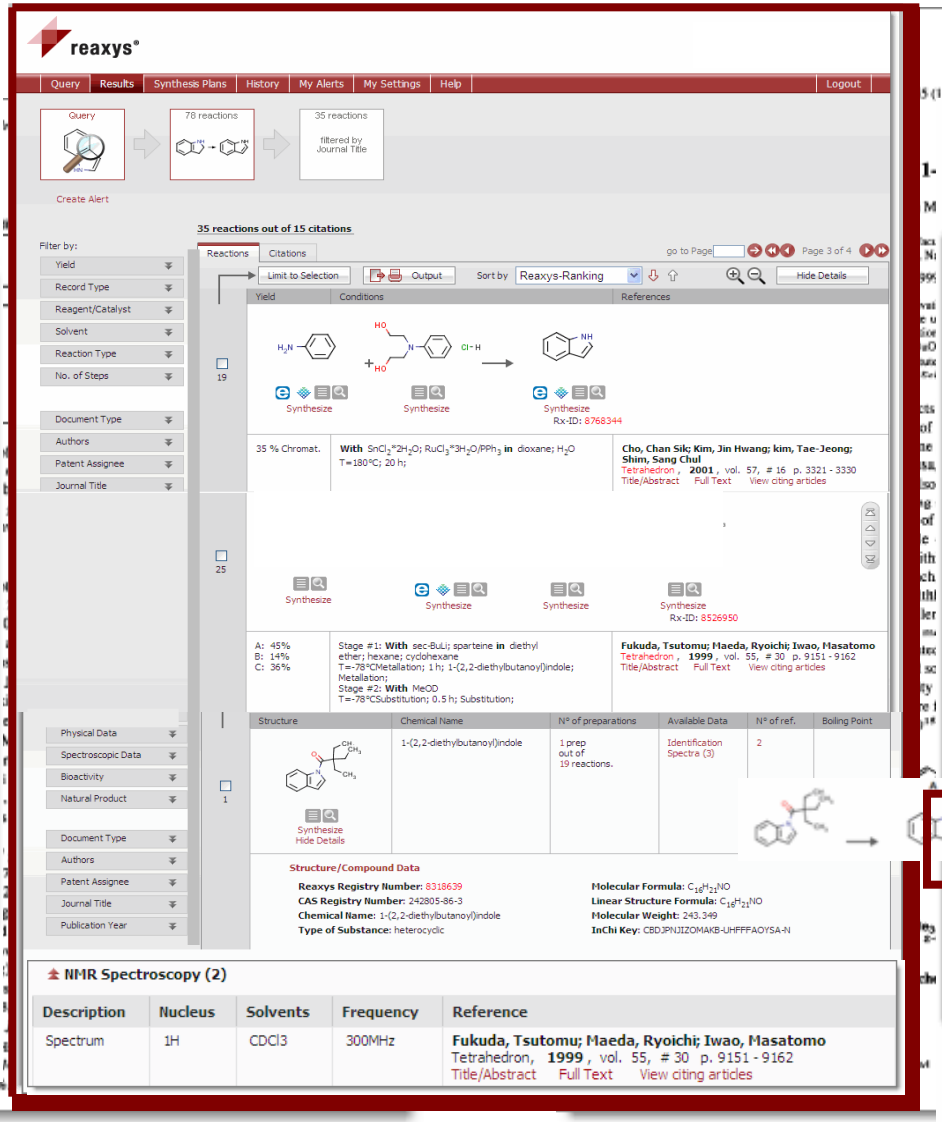
Designed with **chemistry as the organising principle** to **reduce your time** to get to the **relevant results**

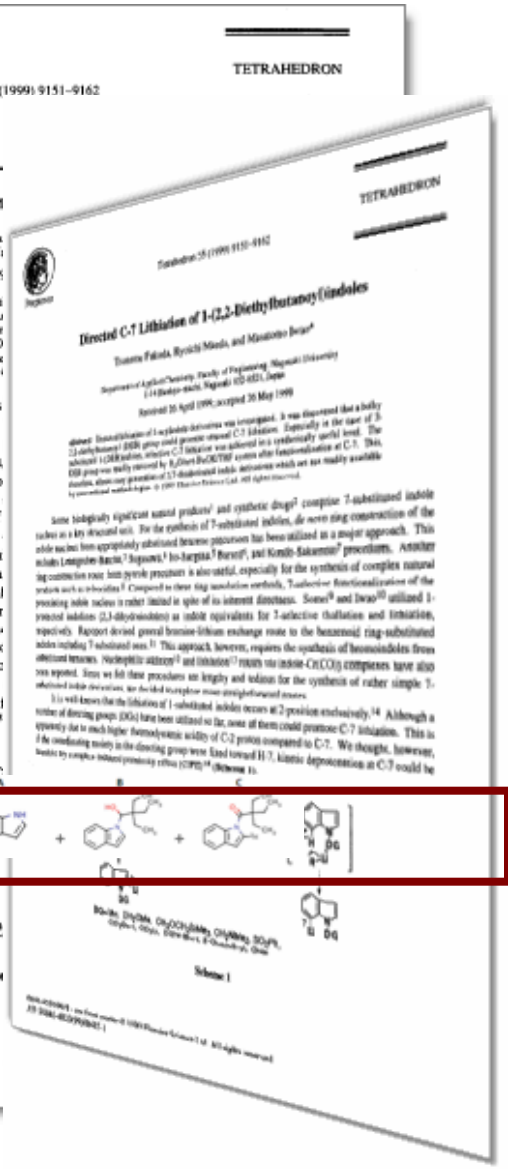
- Reaxys is an extensive repository of experimentally validated structural, chemical, and physical data
- **Designed** around chemists workflows **to improve efficiency;**
- **Simple web-based interface** makes it easy to work with, and easily accessible;
- Functionality that allow chemists to query and filter by property data, design the optimum synthesis route, and view multi-step reactions.
- **A synthesis planner** lets chemists plan the synthesis of compounds and to compare alternative synthetic routes. Identify the shortest potential path, generate a list of reagents, et cetera.

Reaxys extracts valuable chemical properties and reaction details from journals and patents.....

1H NMR

300 MHZ





- Mutarotation exists
- Circular Dichroism exists
- Optical Rotatory Dispersion exists
- Magnetic Susceptibility exists
- Magnetic Data exists
- Static Dielectric Constant exists
- Dielectric Constant exists
- Electrical Data exists
- Electrochemical Behaviour exists
- Dissociation Exponent exists
- Isoelectric Point pH exists
- Electrochemical Characteristics exists
- Flash Point exists
- Autoignition exists
- Explosion Limits exists
- Further Information exists
- Solubility (MCS) exists
- Solubility Product (MCS) exists
- Solution Behaviour (MCS) exists
- Critical Micelle Concentration (MCS) exists
- Henry Constant (MCS) exists
- Partition octan-1-ol/water (MCS) exists
- Liquid/Vapour Systems (MCS) exists
- Azeotropes (MCS) exists
- Complex Phase Equilibria (MCS) exists
- Liquid/Liquid Systems (MCS) exists
- Liquid/Solid Systems (MCS) exists
- Mechanical & Physical Properties (MCS) exists
- Transport Phenomena (MCS) exists
- Energy Data (MCS) exists
- Electrical Data (MCS) exists
- Optical Data (MCS) exists
- Boundary Surface Phenomena (MCS) exists
- Adsorption (MCS) exists
- Association (MCS) exists

- Spectra exists
  - NMR Spectroscopy exists
  - IR Spectroscopy exists
  - Mass Spectrometry exists

Hundreds of searchable fields

Boiling Point

218 - 222°C

Solubility	Saturation	Temperature	Solvent
0.000341568gl-1	in pure solvent	25°C	H2O

Use Pattern

Antitumor drug

Effect	cell growth; inhibition of
Species or Test-System	acute promyelocytic leukemia NB4 cells of human
Concentration	0.01 - 50 µmol/l

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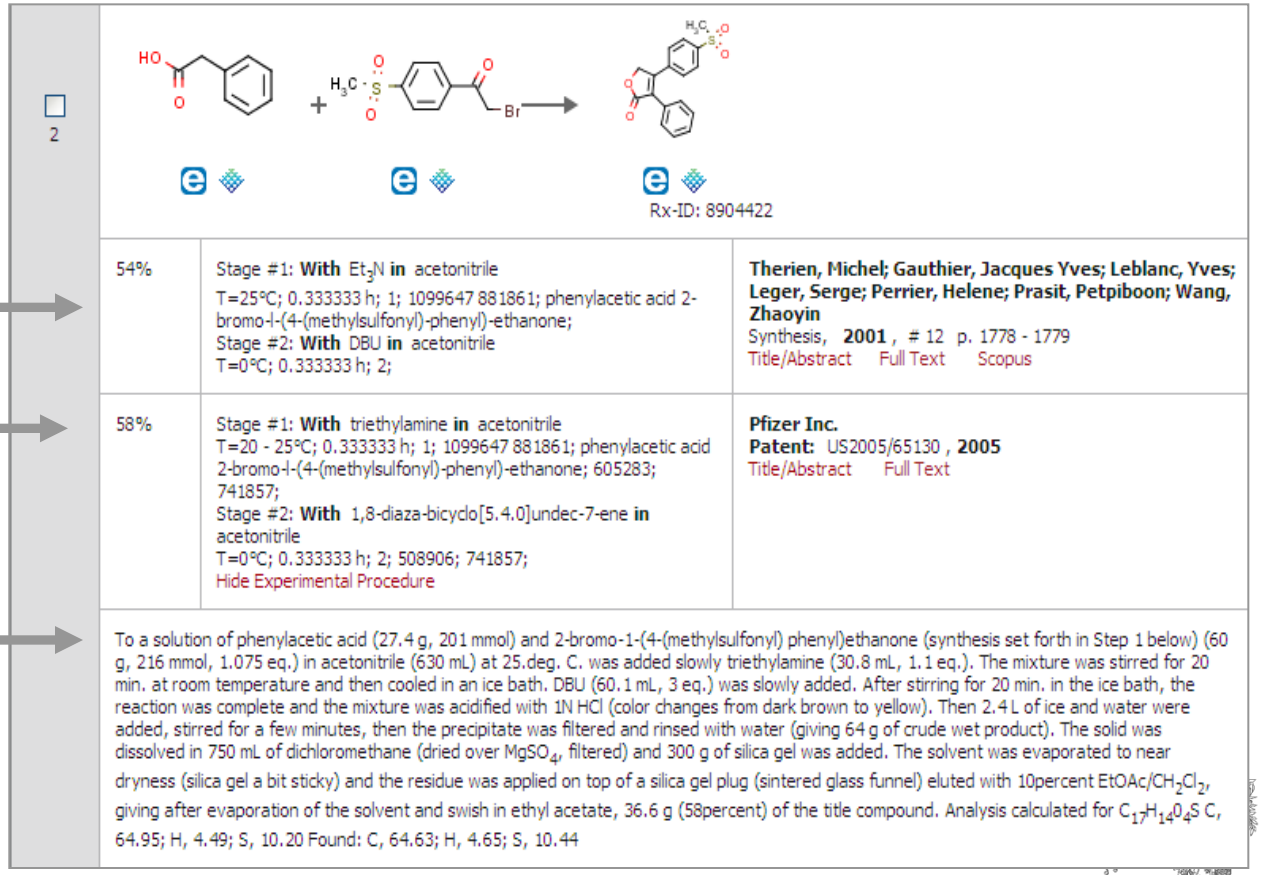
Experimental data and much more at your fingertips

View full experimental details taken directly from the literature

See all related data in a single view

Same transformation with different experimental properties from Patent Chemistry

Full searchable experimental details directly in the database



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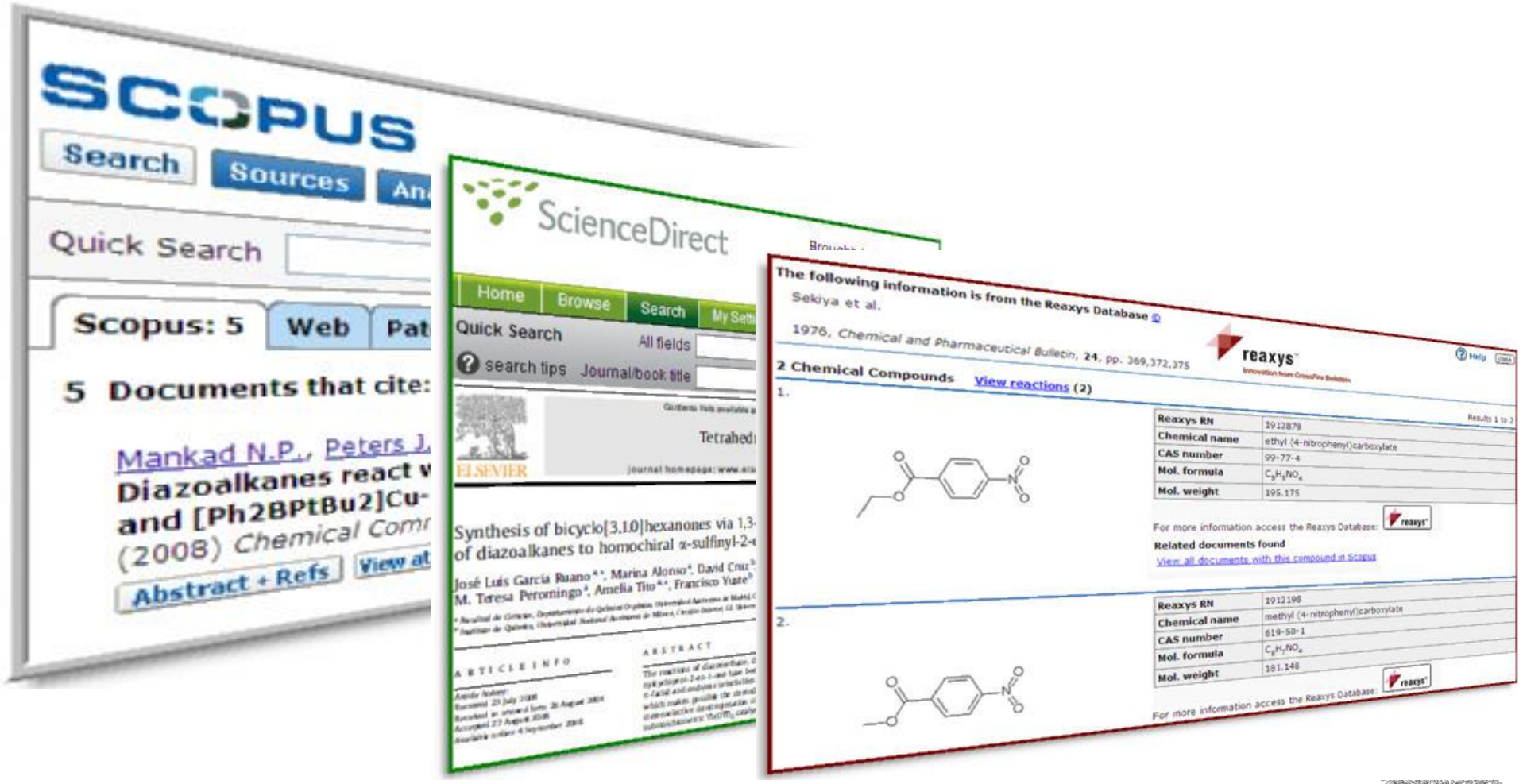
Interoperability with Scopus and Science Direct



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1.2 - COVERAGE

Beilstein

- Beilstein handbook (since 1771)
- Small molecular organic chemistry
- Key journas
- Patent publications 1889 – 1990 (Select)

Gmelin

- Gmelin handbook (since 1772)
- Ceramics, glass, alloys, catalysts, minerals, coordination compounds…
- Physical data, electric, mechanical, magnetic, thermodynamic properties.

Patent Chemistry

- 1976 till present: World Patent Office (1978 <), USPTO (1976 <), & EPO (1978 <)
- English language patents
- IPC C07, A61K, A01N and C09B

1.2 - COVERAGE

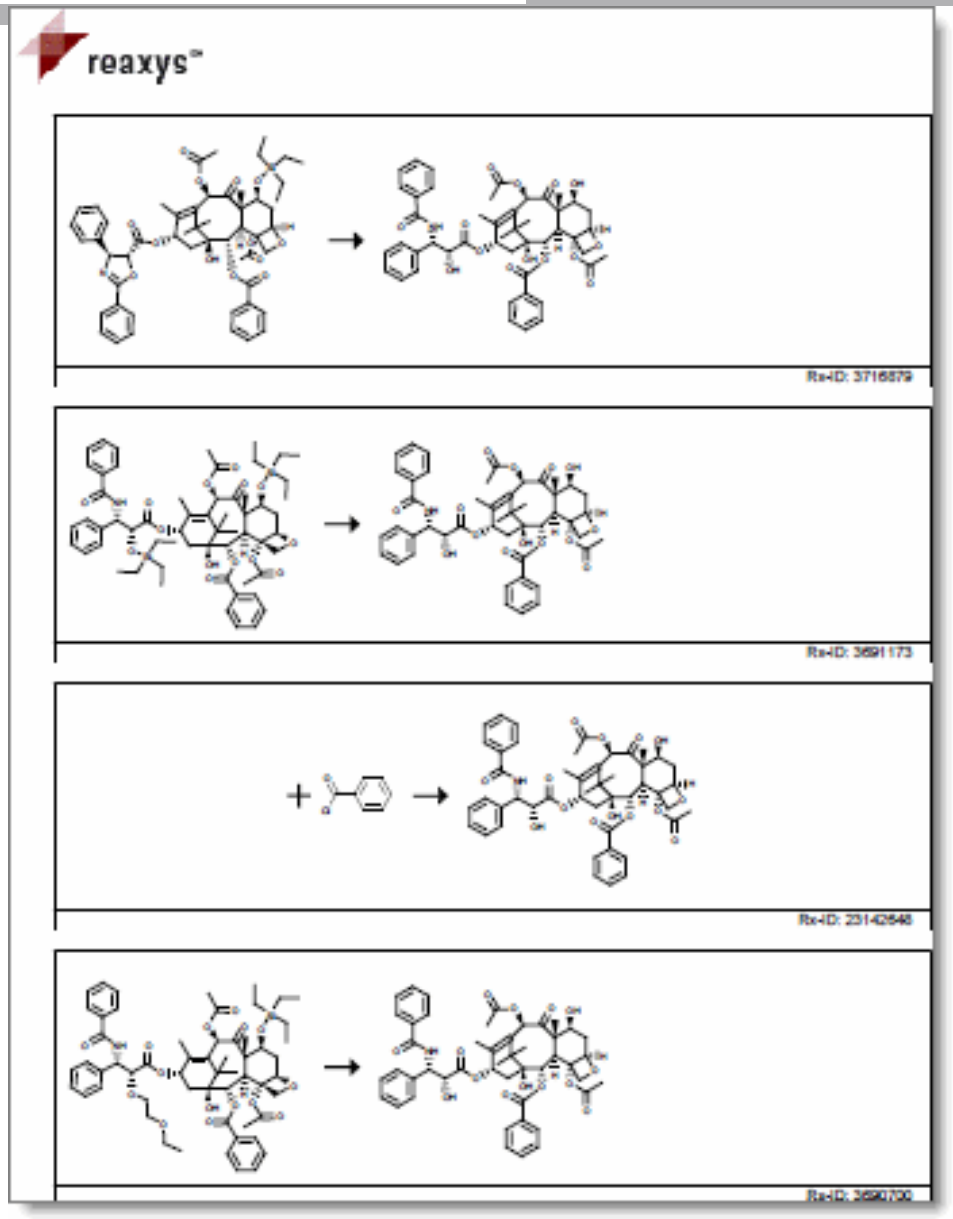
- **Experimentally validated** content built upon more than 100 years tradition with Beilstein and Gmelin.
- An **extensive repository** of experimentally validated **structural, chemical, and physical** data
- Abstract sources and extracting data **relevant** to synthetic chemists
- Excerpted by trained chemists, Quality checked by trained chemists, process managed and overseen by PhD chemists

.....And gives you what no other database has.....

28.6 million Reactions

18.017.396 Substances

4.118.881 Citations



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1.3 Who is it for?

Anyone who needs accurate and instant information on chemical synthesis, structural, spectroscopic, biological, chemical & physical property data

- Medicinal Chemists
- Synthetic Chemists
- Process Engineers
- Chemical Engineers
- Material Scientists

Note: Reaxys may not be very intuitive for chemistry specialties that are not listed here, however, it may still contain very valuable data.

1.4 Reaxys users feedback

"I welcome Reaxys to the chemistry information world, so do my users. If you have not tried it, please give yourself a chance, and I hope, and I know, you will like it**"**

Norah Xiao – University of Southern California (2/2010 Library Connect Article)

"Reaxys is a powerful tool in the armory of structure-based literature searching. It will be very **useful both for teaching and research and deserves to be widely used**."

Prof Jonathan Goodman – University of Cambridge (12/2009 article in Journal of Chemical Information & Computing)

"You guys should be proud to be involved in **something that will change the chemistry world**"

Prof Xue Chen Li – Hong Kong University (letter to Elsevier)

"Having had access to Reaxys this past few months have been such a boon to our efforts. We are now even more enthralled with this program. To say that this is a **powerful tool for getting information quickly and reliably** is an understatement.

Dr. Aileen Bongat – National Institutes of Health

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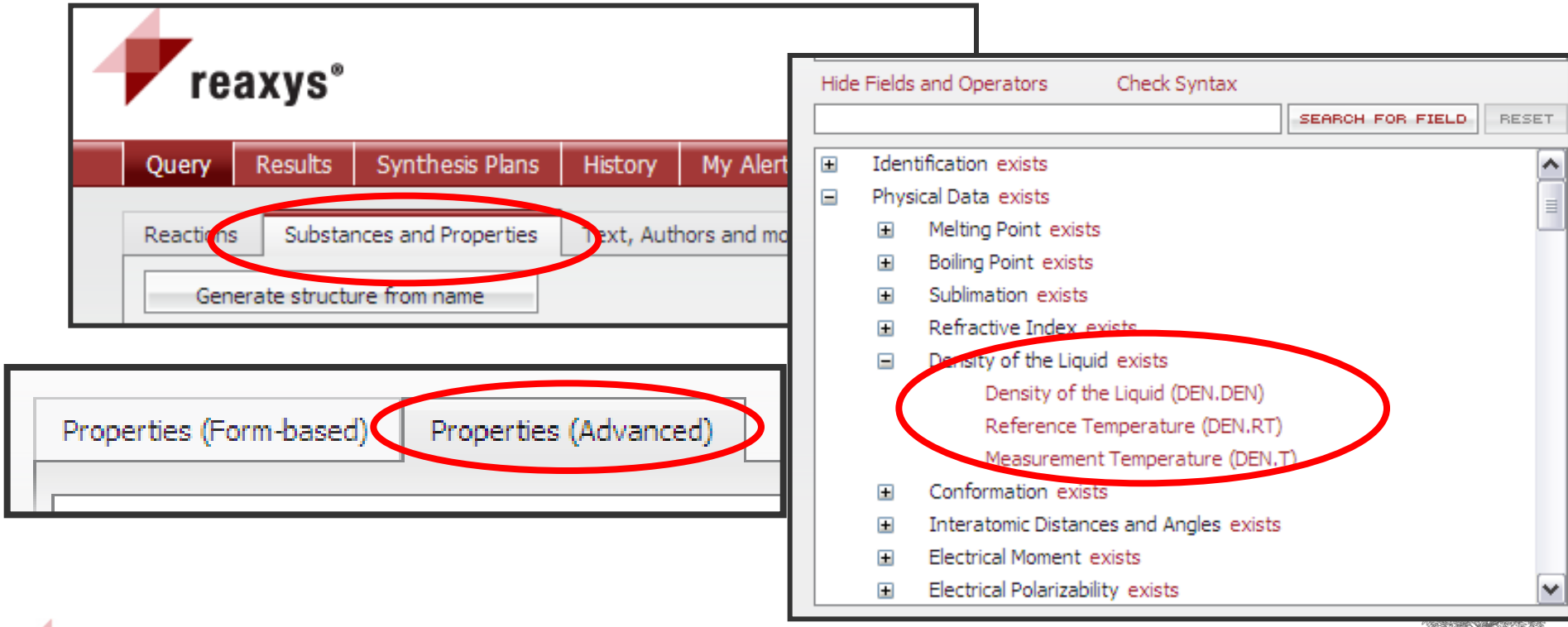
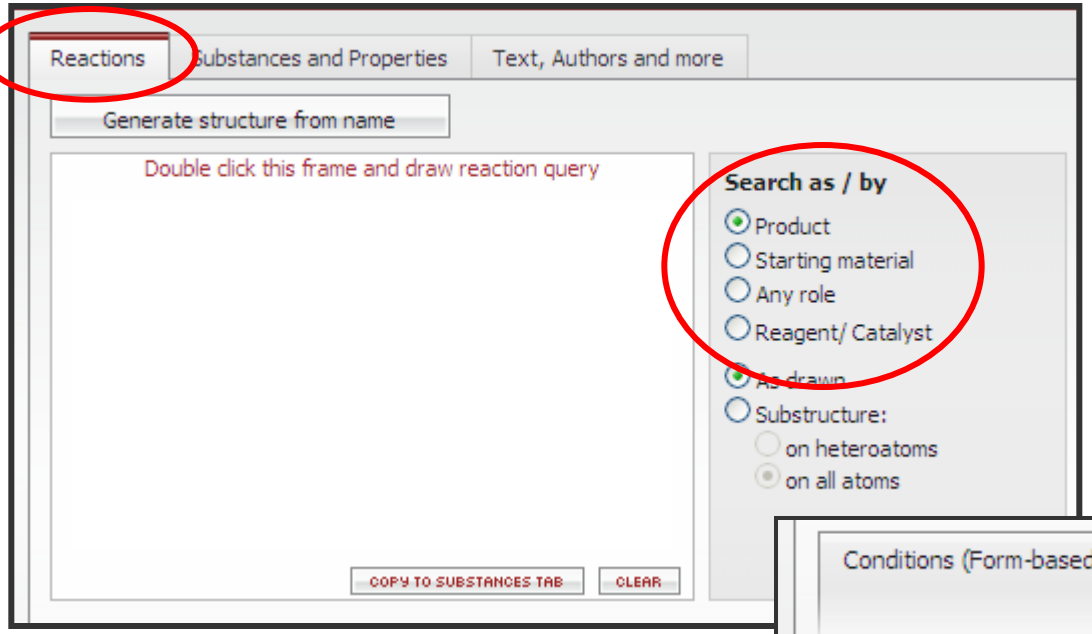
2.1. Finding physical properties

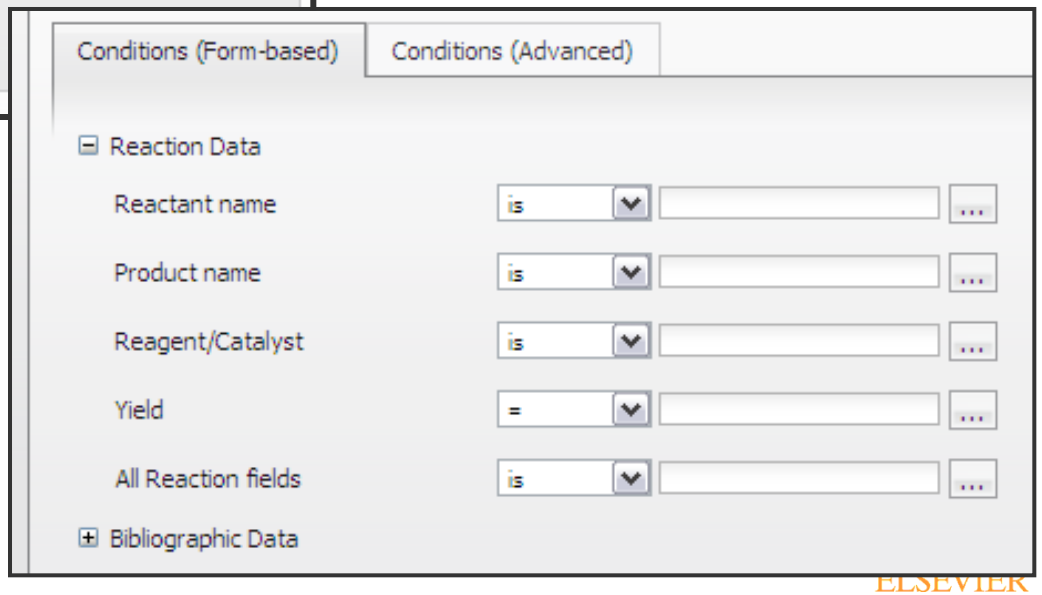
Example: Search for substances with…

- Density 0.9 – 1.1 g/cc at 20 degree celsius
- Viscosity 0.02 – 0.12P at 20 degree celsius
- Surface tension 55 – 65 dyn/cm



2.2. Finding reactions





- Search by end product, starting material or catalyst/reagent.
- Search by name or draw a structure

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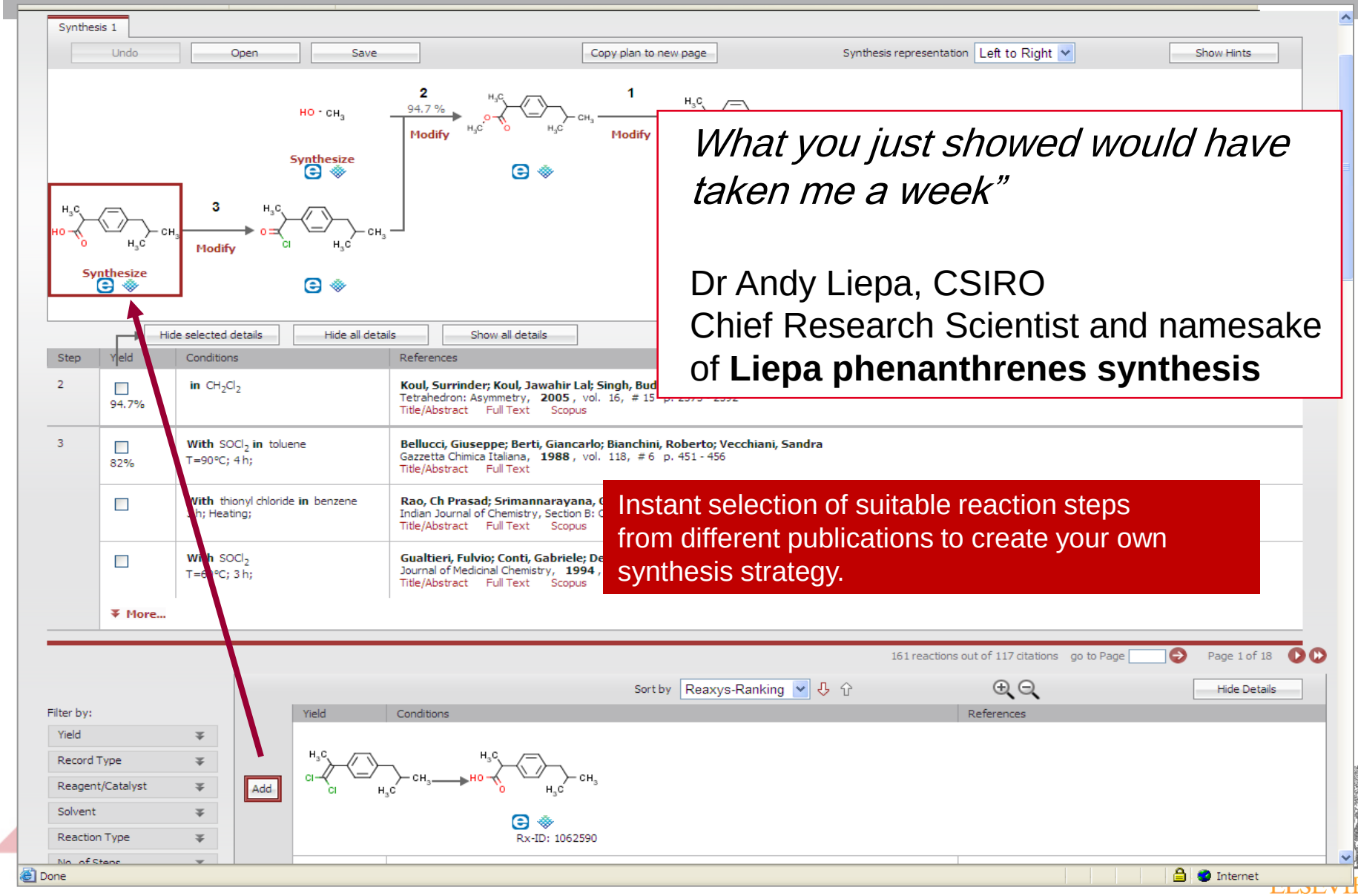
2.3 Synthesis Planner

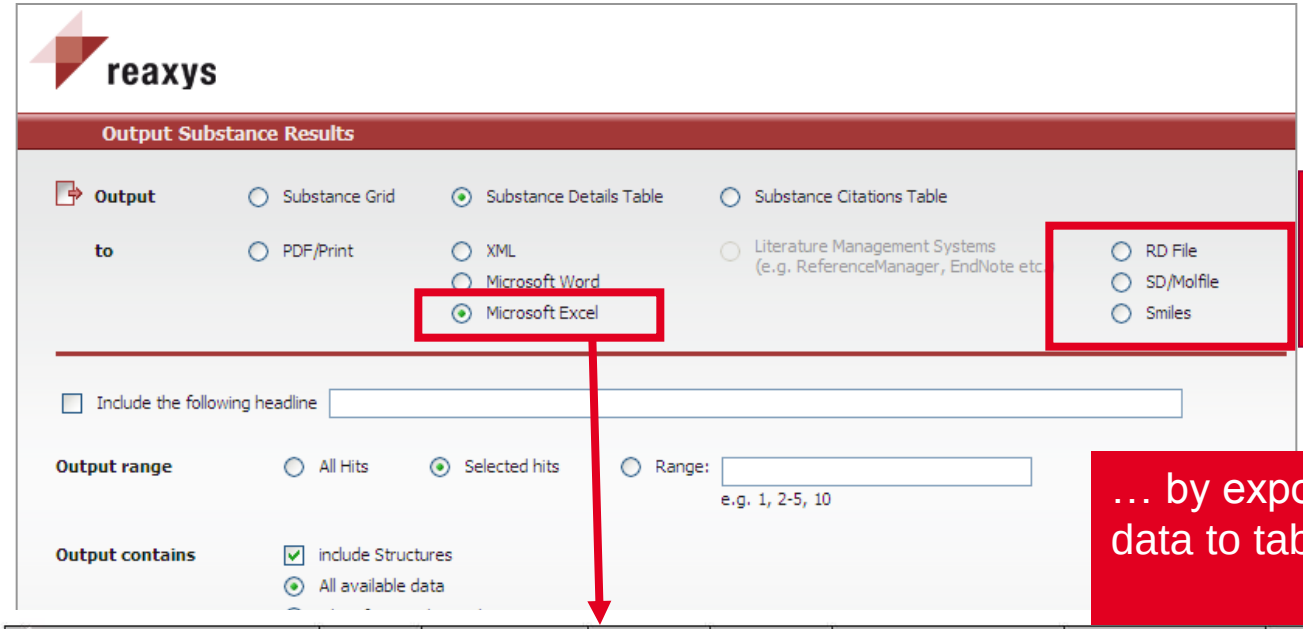


What you just showed would have taken me a week"

Dr Andy Liepa, CSIRO
Chief Research Scientist and namesake of **Liepa phenanthrenes synthesis**

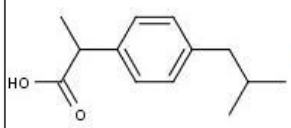
Instant selection of suitable reaction steps from different publications to create your own synthesis strategy.

2.4 Creating your own reports



SD-/RD-/XML-formats to load structures and data into other systems

… by exporting structures with their data to tables: XLS, WORD, PDF

reaxys Structure	Reaxys RegNo	CAS Registry Number	Pharmacological Data: Effect	Species or Test-System	Method	Further Details	Type	Value of Type	References
	2049713	15687-27-1; 51146-56-6; 51146-57-7; 58560-75-1	enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1	enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20α-hydroxysteroid dehydrogenase	IC50	29 µmol/l	Journal; Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M.; Biochemical Pharmacology; vol. 75; 2; (2008); p. 484 - 493;

3. Live demonstration

www.reaxys.com

@chemistry_uk

Reaxys – a workflow tool for chemists

Validated and Experimental Data only

- Journals – physical properties; bioactivity; natural product; yields, reaction conditions, popular reagents / solvents; catalysts; commercial availability.

- Patents – experimental procedures and spectroscopic data (NMR; IR; MS; UV/VIS).

Synthesis planner:

- Plan multi-step synthesis, compare alternative synthetic routes. Make quick decision on the most appropriate pathway.

Reaxys Ranking, Filtering & Analysis tools:

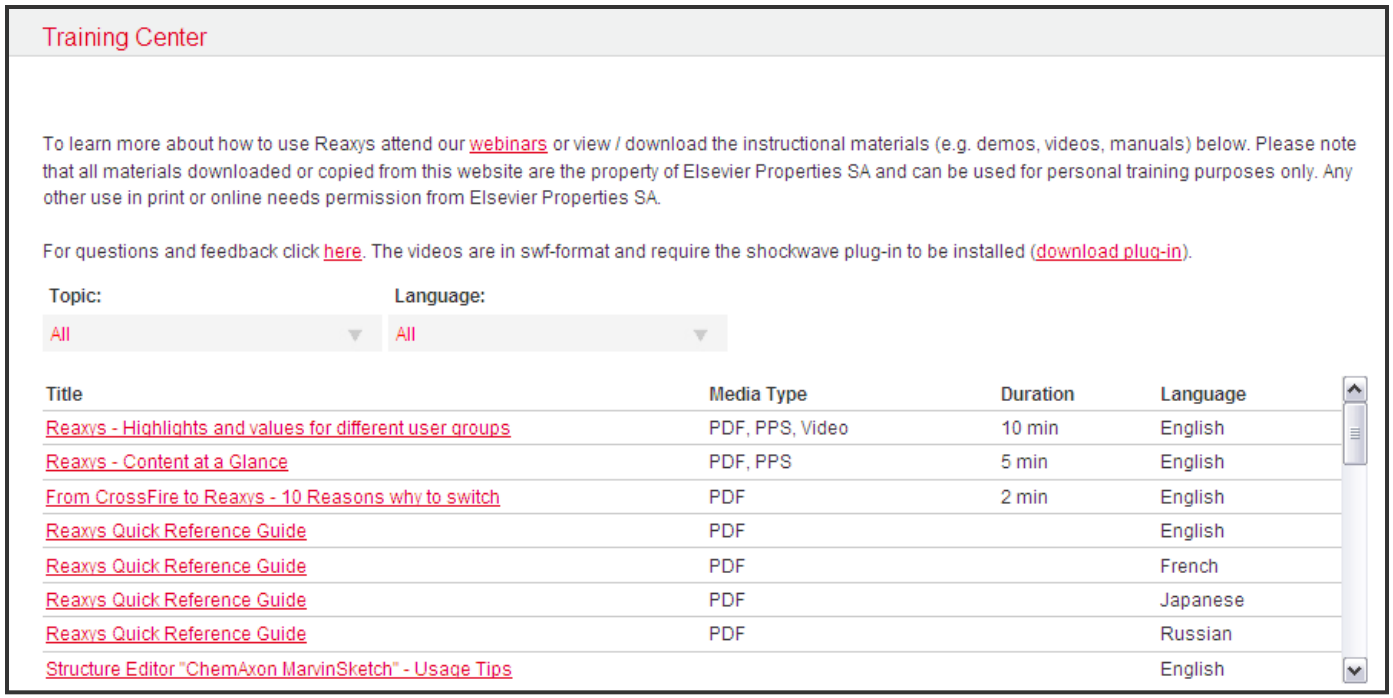
- It's easy to find, filter and analyze data.

Institutional wide, unlimited access:

- So you can obtain the information you need when you need it.

Trial duration and access model

- Trials are available
- Unlimited access model – anyone can log in at any time when within the institute's IP range.
- Training center to support the trial: http://www.info.reaxys.com/training-center
- http://china.elsevier.com



Training Center

To learn more about how to use Reaxys attend our webinars or view / download the instructional materials (e.g. demos, videos, manuals) below. Please note that all materials downloaded or copied from this website are the property of Elsevier Properties SA and can be used for personal training purposes only. Any other use in print or online needs permission from Elsevier Properties SA.

For questions and feedback click here. The videos are in swf-format and require the shockwave plug-in to be installed (download plug-in).

Topic: All

Language: All

Title	Media Type	Duration	Language
Reaxys - Highlights and values for different user groups	PDF, PPS, Video	10 min	English
Reaxys - Content at a Glance	PDF, PPS	5 min	English
From CrossFire to Reaxys - 10 Reasons why to switch	PDF	2 min	English
Reaxys Quick Reference Guide	PDF		English
Reaxys Quick Reference Guide	PDF		French
Reaxys Quick Reference Guide	PDF		Japanese
Reaxys Quick Reference Guide	PDF		Russian
Structure Editor "ChemAxon MarvinSketch" - Usage Tips			English

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Customer Support

helpdesk (Ph.D Chemists answer your questions):

jpinfo@reaxys.com
cninfo@elsevier.com

+81 – 3 – 5561 5034
+86 - 10 – 8520 8800

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Questions?

Thank you!

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