ECR-1771

Research

Teaching & Learning

Content and Features in Reaxys

Presented By :
Ravindra Gupta
Solution Manager – Life Science Division
Elsevier- ANZ /SA

New Reaxys : 1 solution-7databases+ Predictive AI + Gen AI + Chemdraw

Reaxys is the largest database for experimentally validated (not calculated) substance properties and reaction data, presented with chemistry as the organizing principle.

Reaxys Base

New modules -AI powered

Bioactivity Database
>46 million experimental bioactivity data points

Reaxys Target & Bioactivity

Target Database
> 40.000 targets incl. species information

Bibliographic Database
>112 million records
(from ~18,000 journal titles)

Substance Database
>278 million substances (total integrated content)
~ 107 million substances (unique)

Patent Database
105 patent offices in 170 patent classes, 42M patents

Reaxys®

Reaxys AI
Beta testing

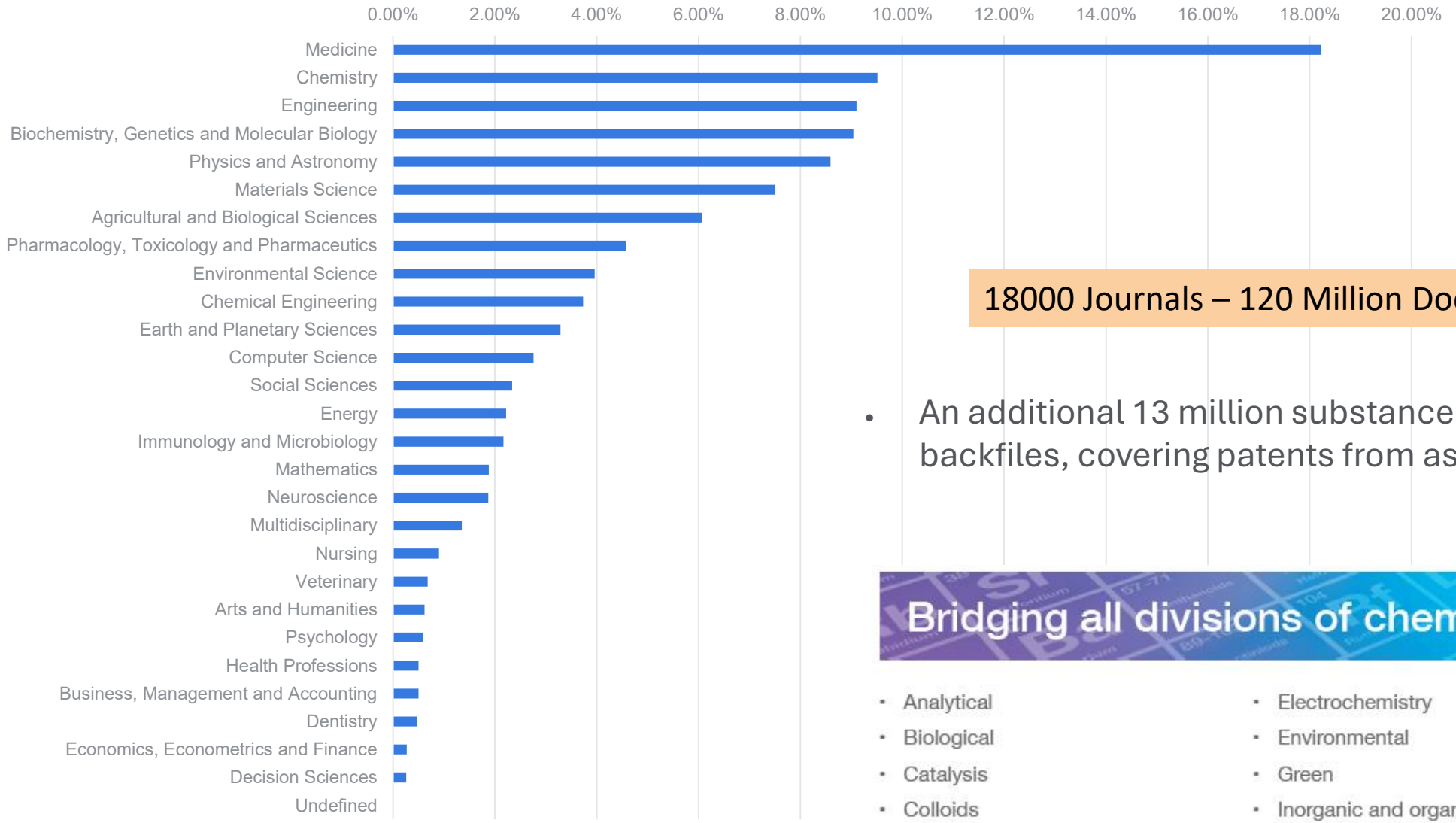
Chemical Reaction database
>65 million reactions

Property Database
> 500 million experimental properties in > 500 fields in > 130 subject areas

Predictive AI Retrosynthesis
Pending.AI / IKTOS

Reaxys®

New Reaxys –Multidisciplinary tool with largest data



***"Reaxys law"**:*
Chemistry information doubles every 140 months (11.6 years)
+7.1% annually

18000 Journals – 120 Million Documents

- An additional 13 million substances from our patent backfiles, covering patents from as far back as 2000.

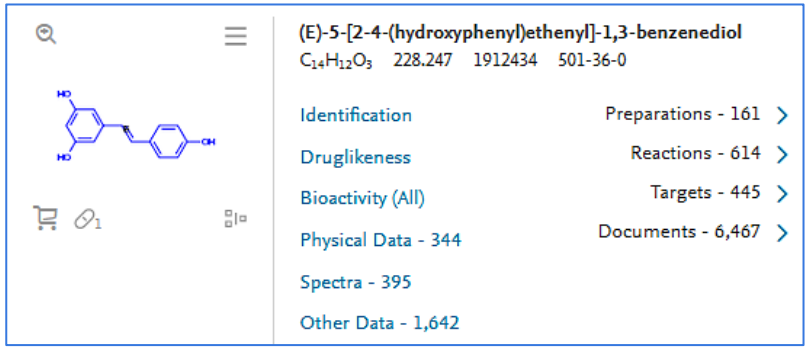
Bridging all divisions of chemistry

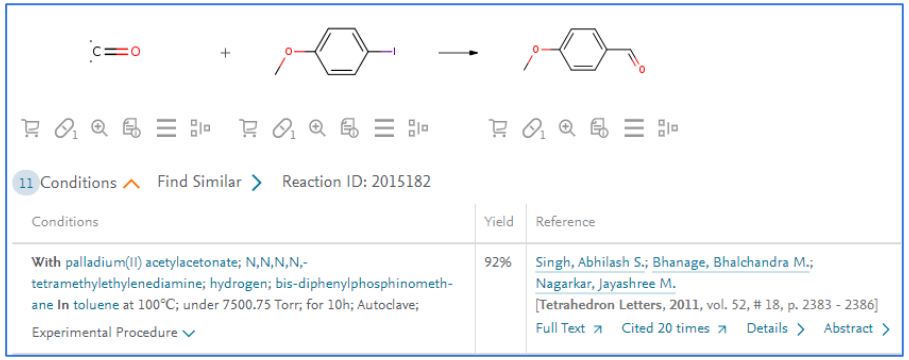
- Analytical
- Biological
- Catalysis
- Colloids
- Computational
- Electrochemistry
- Environmental
- Green
- Inorganic and organometallic
- Materials
- Medicinal
- Organic
- Physical
- Polymer
- Supramolecular

CONSUME INFORMATION EFFECTIVELY WITH REAXYS

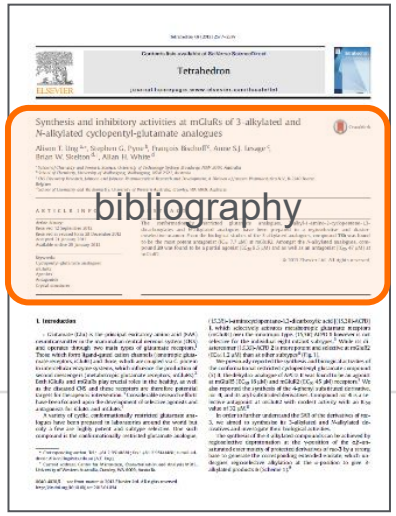
Its not just Indexing, data is excerpted /curated as well

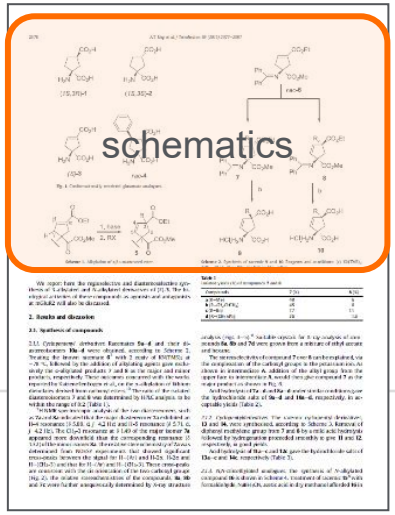
Each substance & reaction record is an **organized**, **searchable**, **multi-sourced** compilation of information

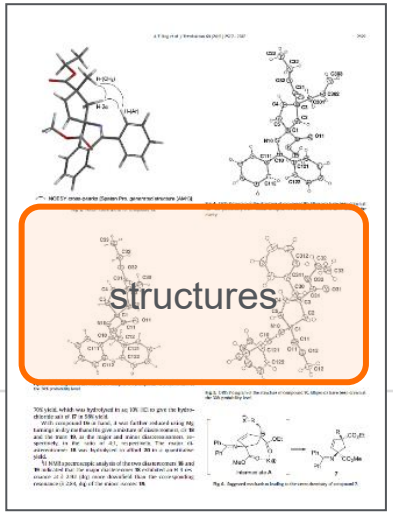


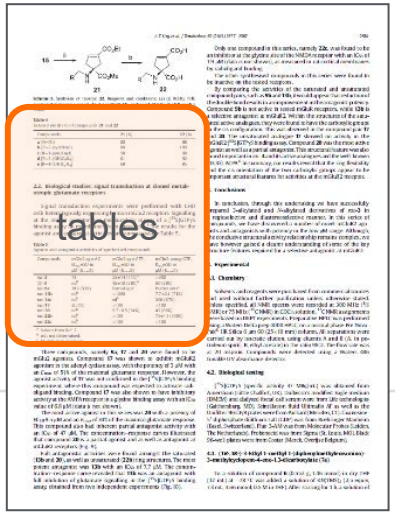


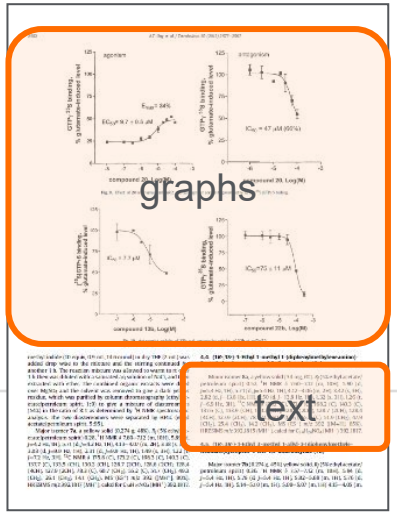
The data are professionally excerpted and indexed from various formats and multiple publications and patents











ELSEVIER

Text Search

- Named Reaction – Suzuki coupling reaction
- Substance – Atorvastatin
- Concept – drug action, effect
- Property – melting point, NMR,
- Document – articles , conference
- Author –
- Any key word-
- Any small query
- **Text to structure search**

Structure Search

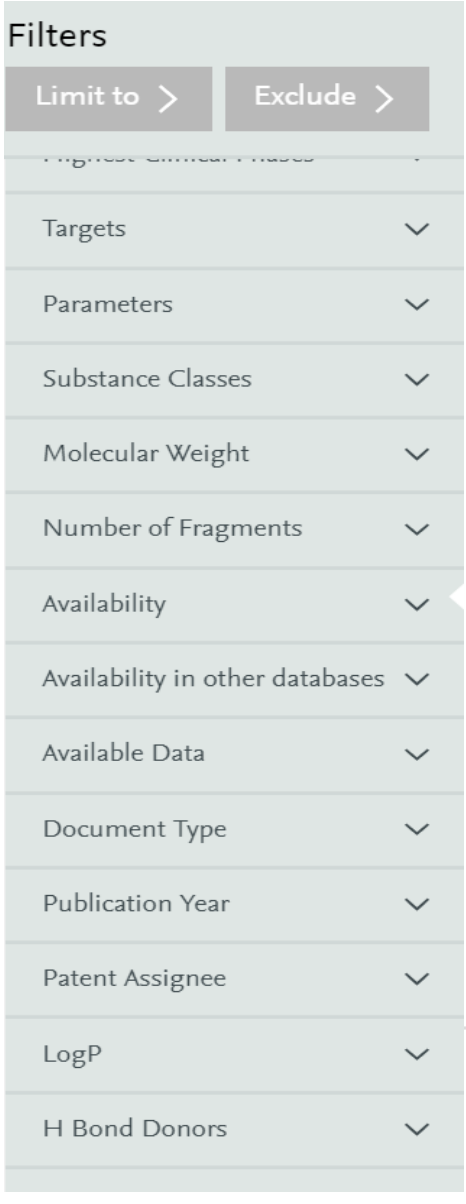
- High specificity
- Allow to paly around atoms, groups etc
- Markush search
- discovery of new compounds
- enables the modification of existing lead compounds
- Crucial for patent analysis/IP clearance

Advance search

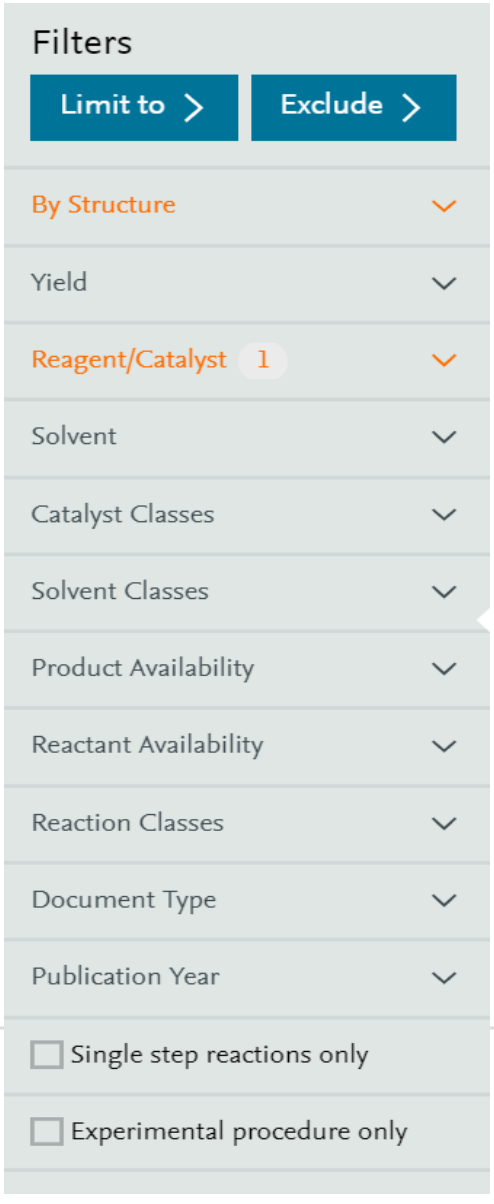
- Customized search,
- Complex Query Search
- Combination search
- 500+ properties- Query lets
- Batch search/grouping
- Search with Boolean operator
- Exclusion search
- Remove duplication

Filters options based on result type

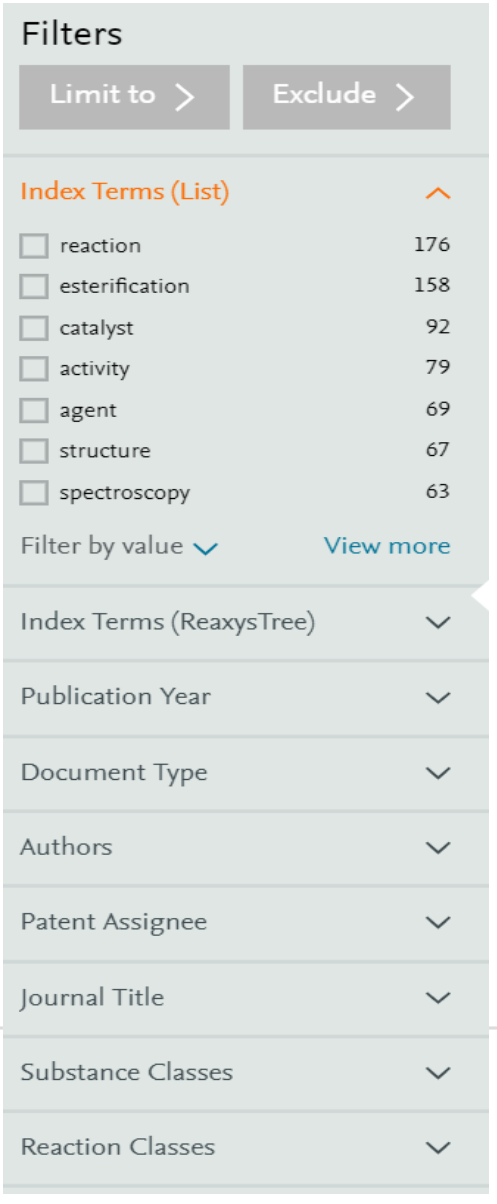
Substances



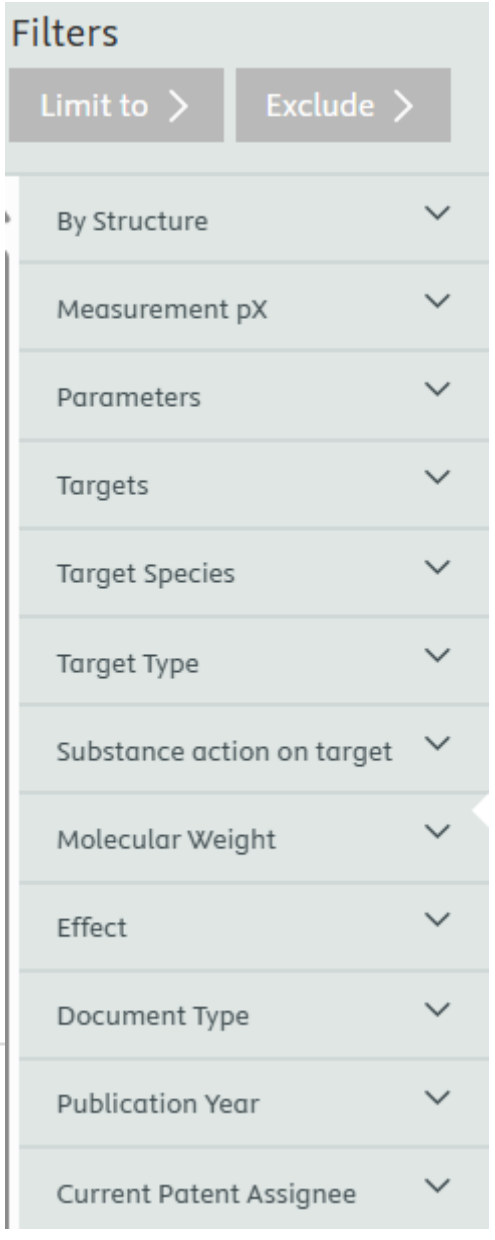
Reactions



Documents



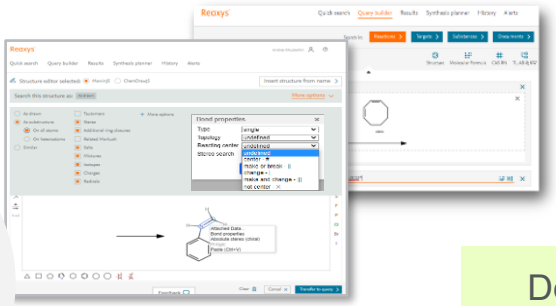
Drug Target



Using Reaxys each step of the way on the path to publication

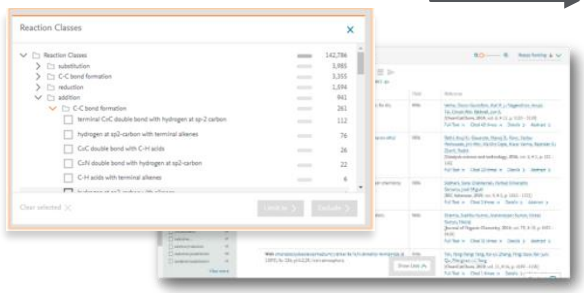
Reaxys®

Use the highly flexible structure and reaction editor to perform document searches on your topic of interest



Novel idea generation

Project proposal / grant presentation



Reaxys®

Use structure search and advance filtering to design a new catalytic system

Design of new substance

Design of new synthetic sequence / method

Reaxys®

Use advance structure and text search to identify the best synthetic methods to synthesise your catalytic system

Synthesis of (new) substance

Purification identification characterization

Application testing

Reaxys®

Use over 500 excerpted properties and advance query builder search capability to compare isolation methods, identify, and characterise your products

Reaxys®

Use over 500 excerpted properties to compare applicability of your products

Reporting, publication and dissemination

Proposal | Design | Execution | Assessment | Dissemination

Students who use Reaxys are better prepared for the digital future

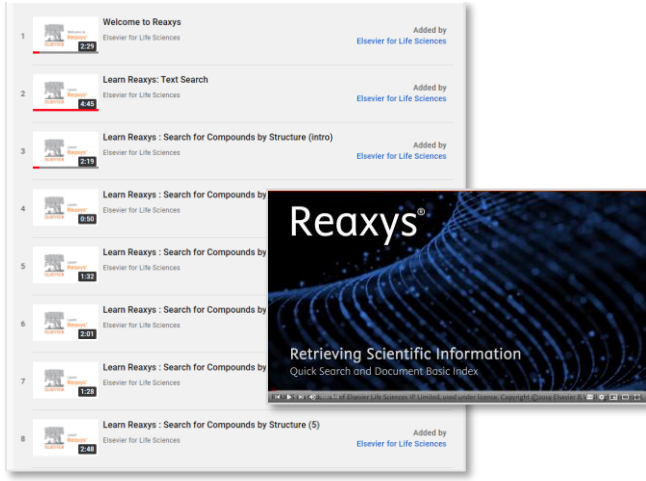
Teaching & Learning

Students need…

- To gain chemistry **digital literacy** skills
- To have engaging **Online learning resources**
- To be well **prepared for the future** job in academia or industry

Reaxys helps by…

- **Reaxys Education Program** provides 20 videos on YouTube designed to support learning **chemistry concepts** with Reaxys
- Reaxys Retrosynthesis is a vital tool when teaching advanced courses
- ReactionFlash app makes learning named reactions easy and fun, by providing access to over 1000 Named Reactions and examples in Reaxys



ELSEVIER

Reaxys Academy- Online Certificate Training course

How it works | Reaxys 101 | Chemistry 101 | Teaching 101

Welcome to Reaxys Academy, your gateway to keeping up with chemical research and designing better experiments!

Unlock your potential with Reaxys, the ultimate chemical platform. Our courses are designed to boost your confidence and refine your skills through comprehensive video instruction.

Discover how to embark on this journey below, take your chemical research to new heights. Complete the self-paced course, take a quiz and earn a certificate you can showcase.

ELSEVIER

Reaxys Academy and Reaction Flash App

[Reaxys User Academy | Elsevier]

ReactionFlash™ gives access to over 1’000 Named Reactions, their mechanisms and examples published in peer-reviewed literature.

Predictive AI delivering best-in-class predictive retrosynthesis technology

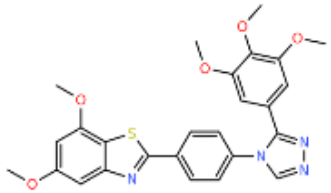
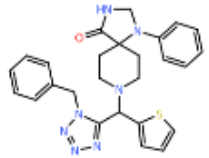
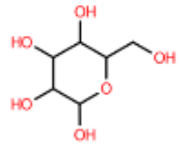
Reaxys: Predictive Retrosynthesis

Retrosynthetic analysis is the process of breaking down a target molecule into intermediates and purchasable precursors using disconnections that can be made using chemical reactions.

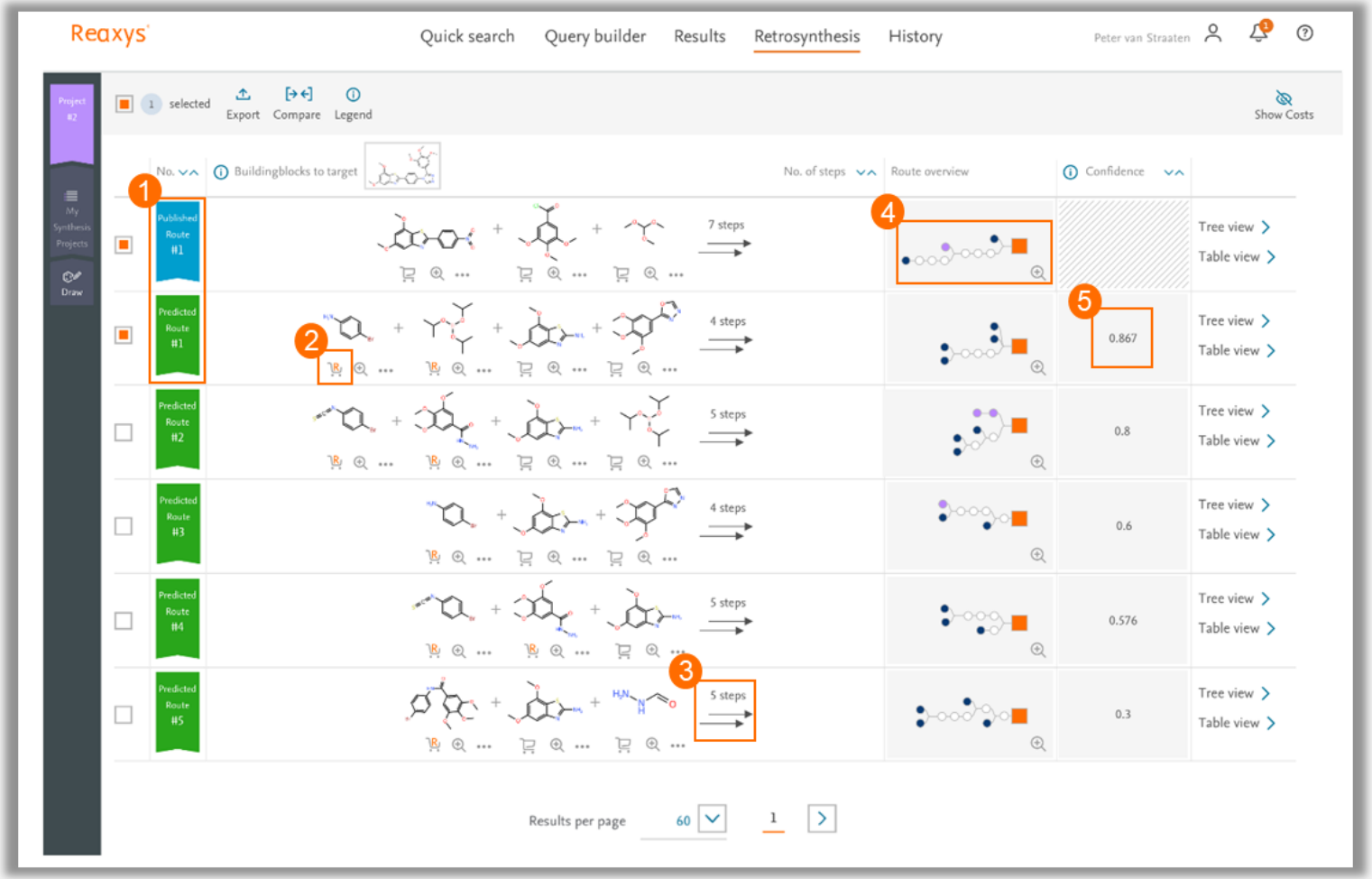
My Synthesis Projects

Draw

1 selected | Export | Edit | Delete | Hide Parameters

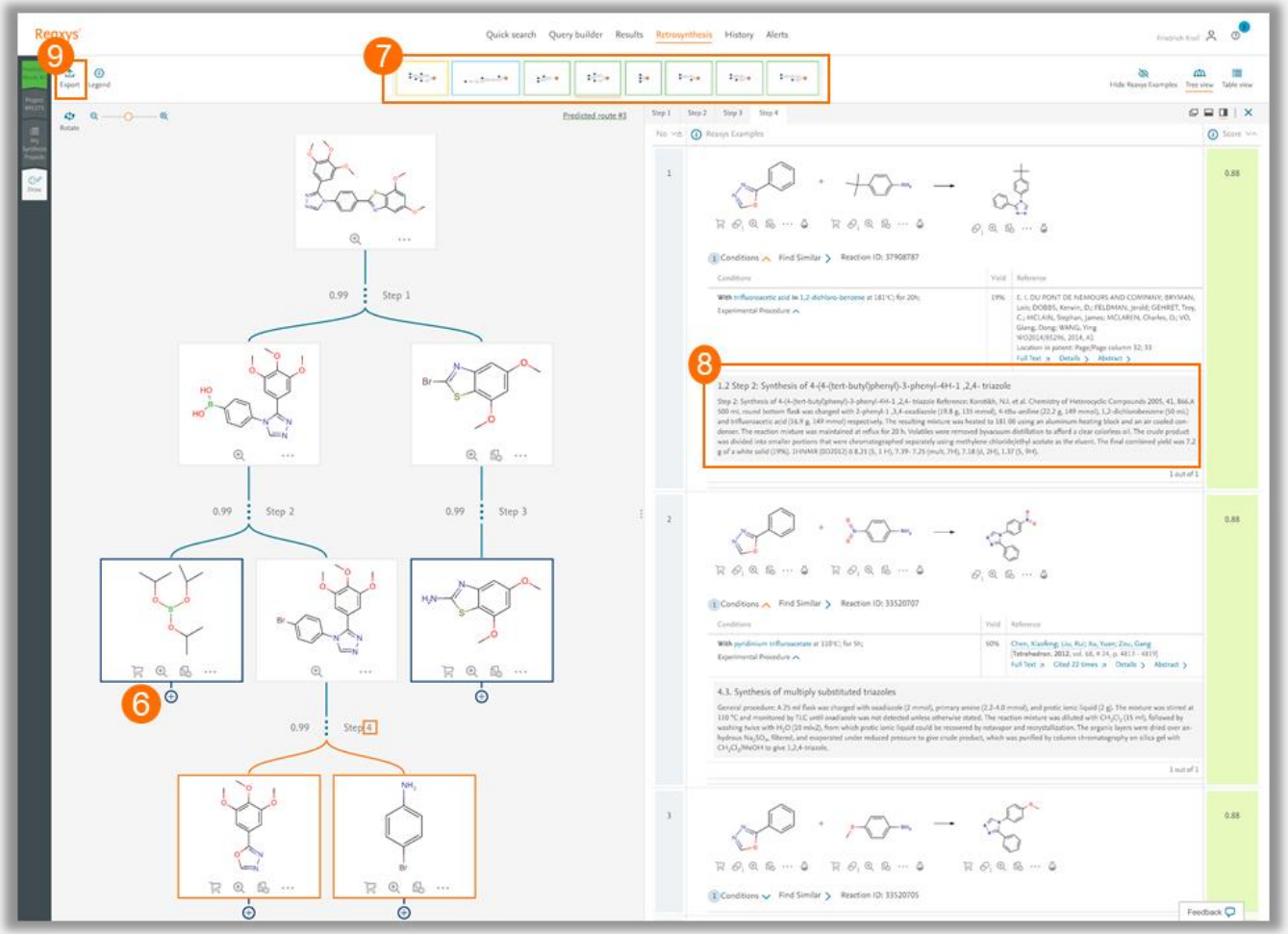
	No.	Date/Time	Projectname	Structure	Parameters Predicted	Parameters Published	No. of routes
☑	3	25 Sep 2020 09:25	Project #8		**5** synthesis plans created. **3** steps with identical reaction. **3** identical building blocks. **15 min** processing time. **SA, LN, RX, EM** Used building blocks.	**1** synthesis plans created. **5** Max alternative branches. **5** Max number of steps. **Stop** at building blocks. **50%** default yieid.	View Results 5 1
☐	2	25 Nov 2019 09:25	Project #7		**3** synthesis plans created. **5** steps with identical reaction. **5** identical building blocks. **10 min** processing time. **SA, RX** Used building blocks.	**5** synthesis plans created. **5** Max alternative branches. **5** Max number of steps. **Stop** at building blocks. **50%** default yieid.	View Results 3 0
☐	1	25 Nov 2019 09:25	Project #3		**16** synthesis plans created. **3** steps with identical reaction. **5** identical building blocks. **5 min** processing time. **SA, RX** Used building blocks	**5** synthesis plans created. **5** Max alternative branches. **5** Max number of steps. **Stop** at building blocks. **50%** default yieid.	No Results

Reaxys Retrosynthesis provides an easy to use and intuitive interface



1. View published, predicted & customized routes in one view
2. Commercially available starting materials needed for synthesis
3. Number of steps in the route
4. Interactive and graphical route overview to asses complexity
5. Scoring system for route ranking

Reaxys Retrosynthesis provides an easy to use and intuitive interface



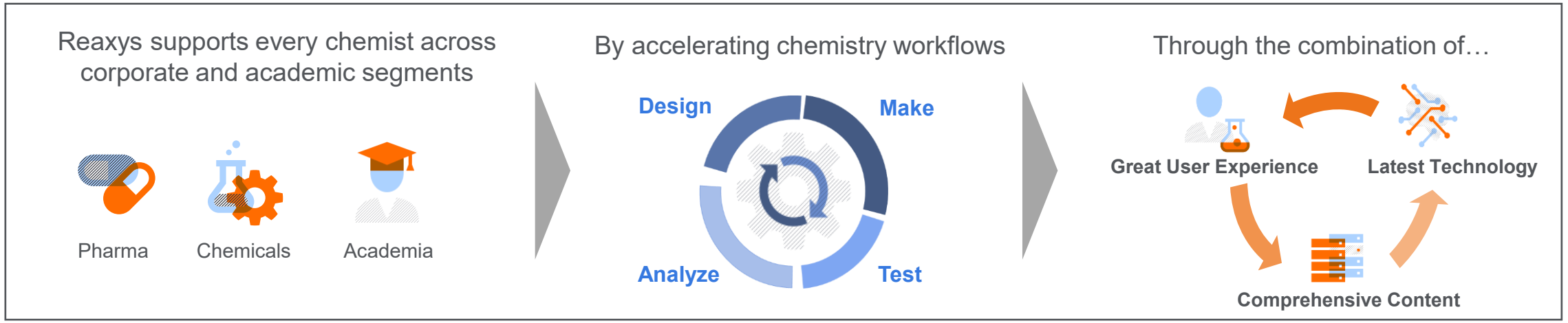
6 Edit your route by clicking ⊕ select from published or predicted steps to create a new customised route

7 No need to navigate between multiple windows

8 Literature references of published routes that informed predicted routes including experimental procedures

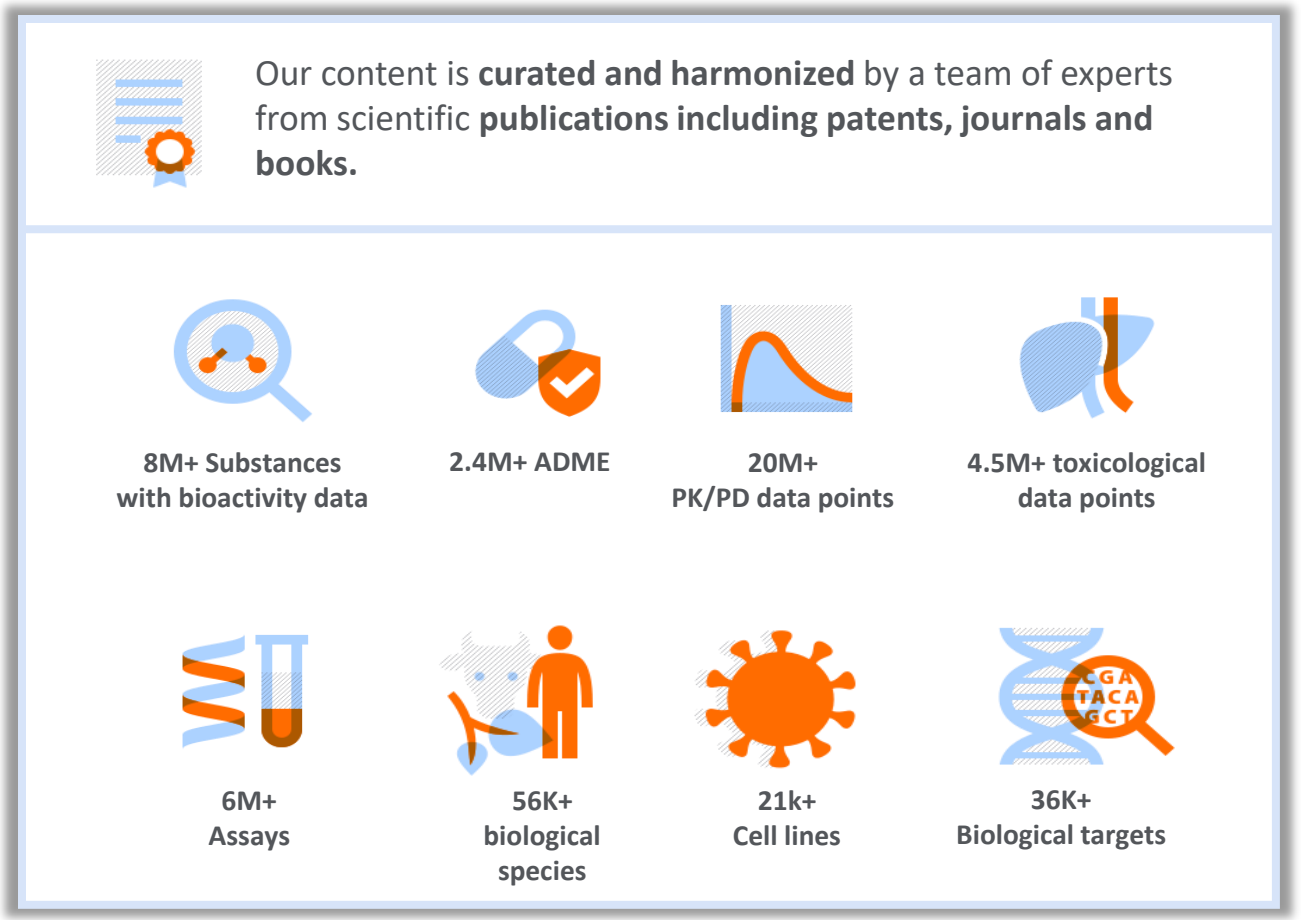
9 Export All/Selected Results in multiple formats (PDF, DOC, XLS, XML, RD, SD) for sharing, adding to ELNs etc.

Reaxys strategy is to be the most comprehensive, intuitive and innovative chemistry information system supporting customers' chemistry use cases and digital transformation needs, driving commercial success and strengthening our competitive positioning



Monitor and Design			Make		Test and Analyze	
Competitive Intelligence	Novelty search	SAR, ADMET	Synthesis planning	PhysChem properties	Product analysis	Pharmacological profiling

Reaxys Target and Bioactivity Data



Patent information

is easily discoverable in Reaxys'

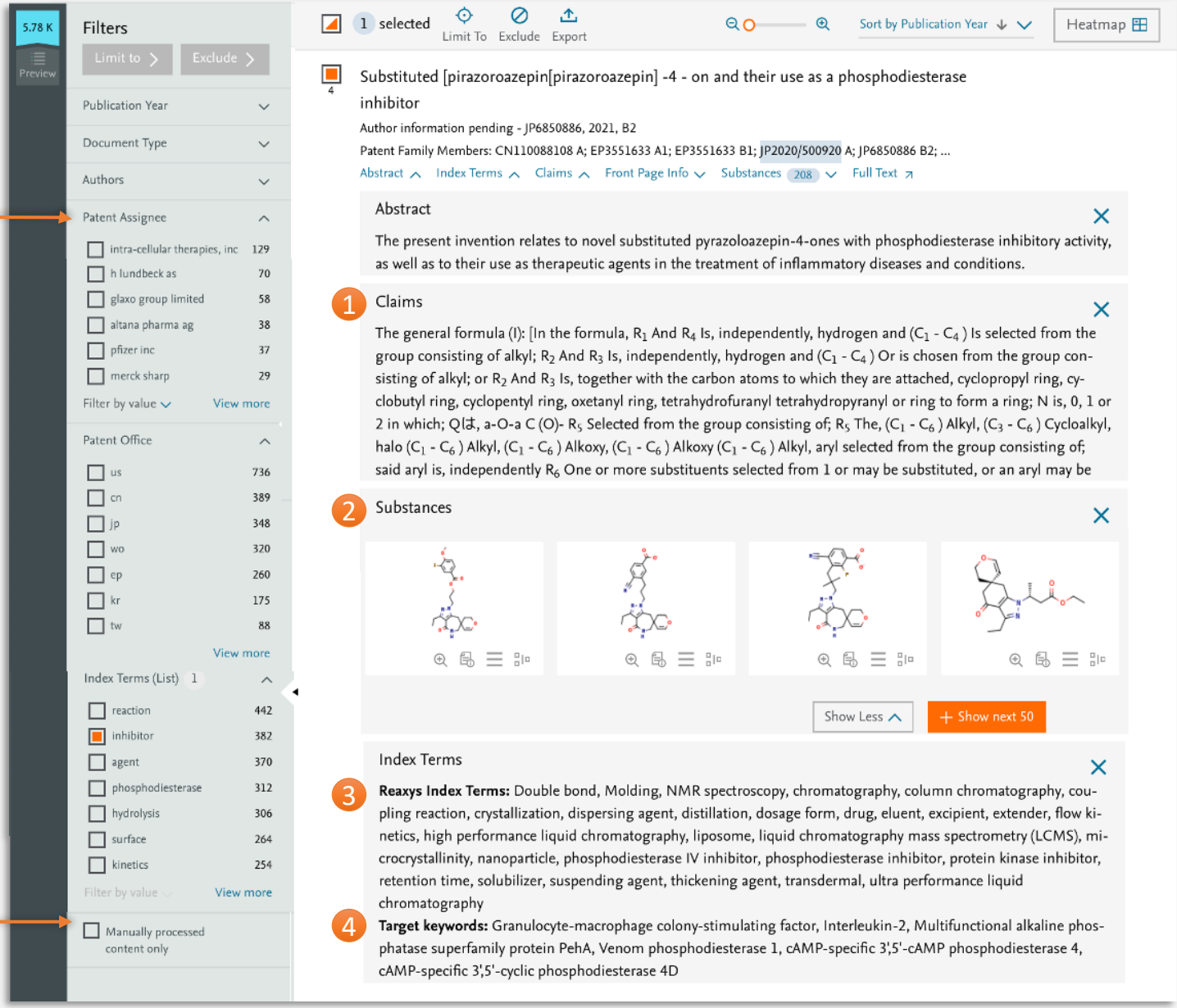
1- High quality English translation of abstracts and claims easily accessible in the UI - as it is the case for this Japanese patent. Chinese language patents have been translated mostly manually.

2- Substance excerption of all compounds from the full patent body. Common solvents and reagents excluded for fast access to the most important compounds in the patent.

3- Reaxys Indexed Terms extract chemistry relevant concepts to enhance patent search and discovery.

4- Primary target indexing, including target synonym expansion, to access all relevant patents on a given biological target.

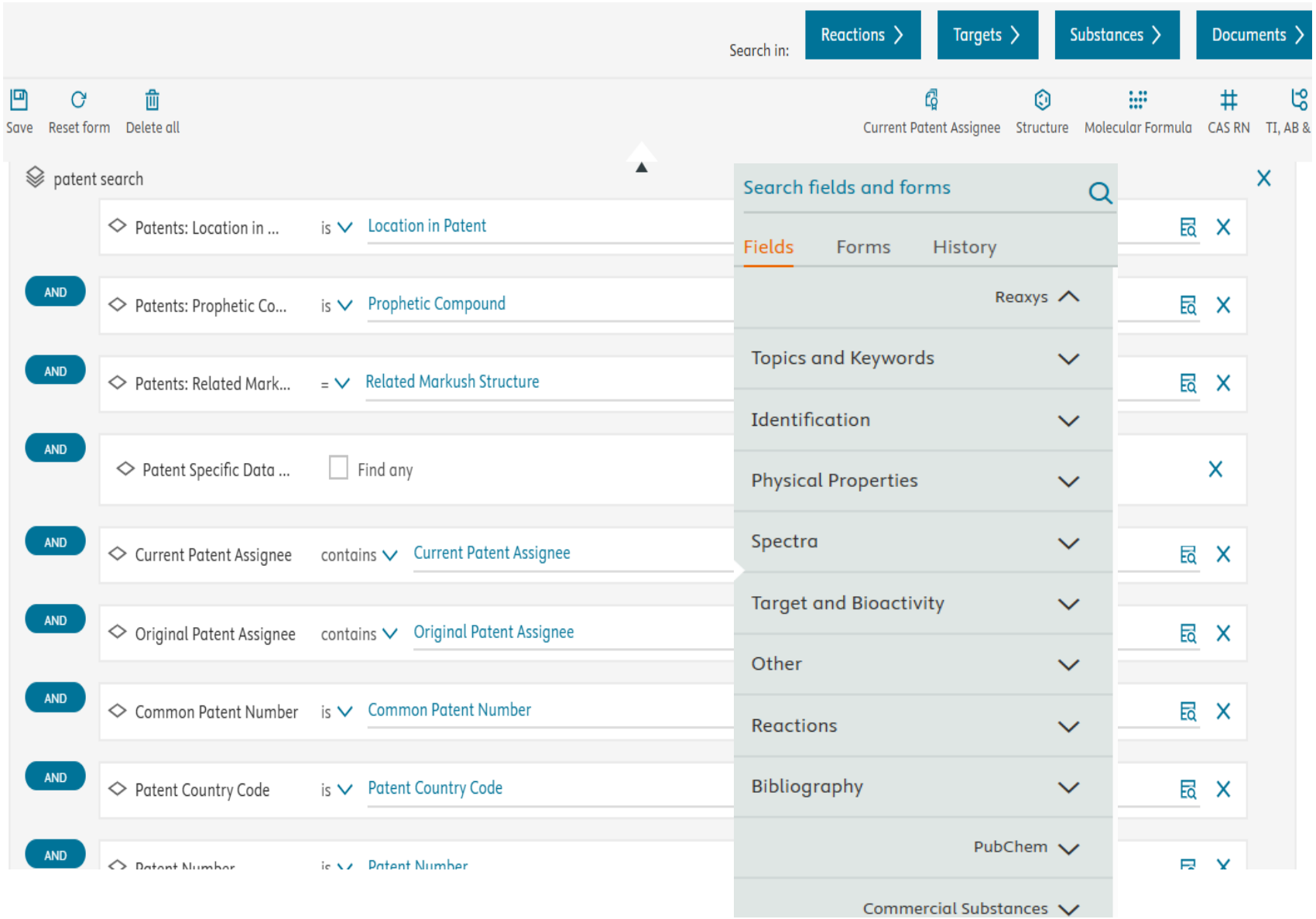
New filters to facilitate navigation of results sets
Patent Office, Patent Assignee and
Manually processed patents



New Way of finding Information :Targeted and precise search

Query Builder :

- Search with multiple keywords and values
- Customized search,
- Complex Query Search
- Specific Search
- 500+ properties
- Combination and Batch search
- Exclusion search
- Create my form
- Export and import the forms
- Combine structure + key word+ reaction + property



Reaxys: Fields (Query Builder)

ELSEVIER

Deeply indexed extracted data available for use

Reaxys is the world's largest repository of substance property data.

Ground stability and transport data are just two of the >500 fields available in Reaxys.

Melting point
Boiling point
Sublimation
Refractive index
Density
Adsorption
Association
Autoignition
Bound Surface Phenomena
Viscosity
Circular Dichromism
Complex Phase Equilibria
Compressibility
Conformation
Critical Density
Critical Micelle Concentration
Critical Pressure
C
C
Electrical Data
Electrical Moment
Electrochemistry Data
Electron Binding
Energy Barriers
Energy Data

Transport data

Enthalpy of Formation
Enthalpy of Sublimation
Flash Point
Gas Phase
Dissociation Energy
Crystal System
Crystal Phase
Heat Capacity

Stability in Soil

Isoelectric Point
Kinematic Viscosity
Liquid Phase
Magnetic Data
Mechanical Properties
Molecular Deformation
Optical Data
Thermochemical Data
Solubility
Solution Behavior
Sound Properites
Static Dielectric Constat
Surface Tension
Transition Points
Transport Data

NMR Spectroscopy
IR Spectroscopy
Mass Spectroscopy
UV/VIS Spectroscopy
ESR Spectroscopy
NQR Spectroscopy
Raman Spectroscopy
Luminscence Spectroscopy
Fluorescence Spectroscopy
Exposure Assessment
Bioaccumulation
Biomagnification
Biodegradation
Abiotic Degradation
Stability in Soil
Oxygen Demand
Uses
Isolation from Natural Prod.
Reaction Yield
Reaction Conditions
Reaction Type
Named Reaction
Pharmacological Data
Route of Administration
Concentration

Target
Substance Effect
Substance Action on Target
Substance Dose
Bioassay
Animal Model
Organs/Tissue
Cells/Cell Lines
Measurment Parameter
Endpoint of Effect
Ecotoxicology Data
Dielectric Constant
Dissociation Exponent
Dynamic Viscosity
Electrolytic Conductivity
Enthalpy of Fusion
Enthalpy of Vaporization
Explosion Limits
Interactomic Distance/Angle
Kinematic Viscosity
Liquid/Solid Systems
Liquid/Vapor Systems
Metarotation

And many more...