



Content and Features in Reaxys

Presented By :
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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 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



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 | • Electrochemistry | • Medicinal |
| • Biological | • Environmental | • Organic |
| • Catalysis | • Green | • Physical |
| • Colloids | • Inorganic and organometallic | • Polymer |
| • Computational | • Materials | • 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

(E)-5-[2-(4-(hydroxyphenyl)ethenyl)-1,3-benzenediol]
C₁₄H₁₂O₃ 228.247 1912434 501-36-0

Identification Preparations - 161 >

Druglikeness Reactions - 614 >

Bioactivity (All) Targets - 445 >

Physical Data - 344 Documents - 6,467 >

Spectra - 395

Other Data - 1,642

11 Conditions Find Similar > Reaction ID: 2015182

Conditions	Yield	Reference
With palladium(II) acetylacetonate; N,N,N,N,-tetramethylethylenediamine; hydrogen; bis-diphenylphosphinomethane in toluene at 100°C; under 7500.75 Torr; for 10h; Autoclave;	92%	Singh, Abhilash S.; Bhanage, Bhalchandra M.; Nagarkar, Jayashree M. [Tetrahedron Letters, 2011, vol. 52, # 18, p. 2383 - 2386]

Experimental Procedure >

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

Synthesis and inhibitory activities at mGluRs of 3-allylated and N-allylated cyclopentyl-glutamate analogues

Alison E. Ling^{a,b}, Stephen G. Fyfe^a, Duncan Beckett^a, Anne S.J. Smart^a, Robert W. Stratton^a, Alan H. Wright^a

bibliography

schematics

structures

tables

graphs

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

Filters	
Limit to >	Exclude >
Targets	▼
Parameters	▼
Substance Classes	▼
Molecular Weight	▼
Number of Fragments	▼
Availability	▼
Availability in other databases	▼
Available Data	▼
Document Type	▼
Publication Year	▼
Patent Assignee	▼
LogP	▼
H Bond Donors	▼

Reactions

Filters	
Limit to >	Exclude >
By Structure	▼
Yield	▼
Reagent/Catalyst 1	▼
Solvent	▼
Catalyst Classes	▼
Solvent Classes	▼
Product Availability	▼
Reactant Availability	▼
Reaction Classes	▼
Document Type	▼
Publication Year	▼
<input type="checkbox"/> Single step reactions only	
<input type="checkbox"/> Experimental procedure only	

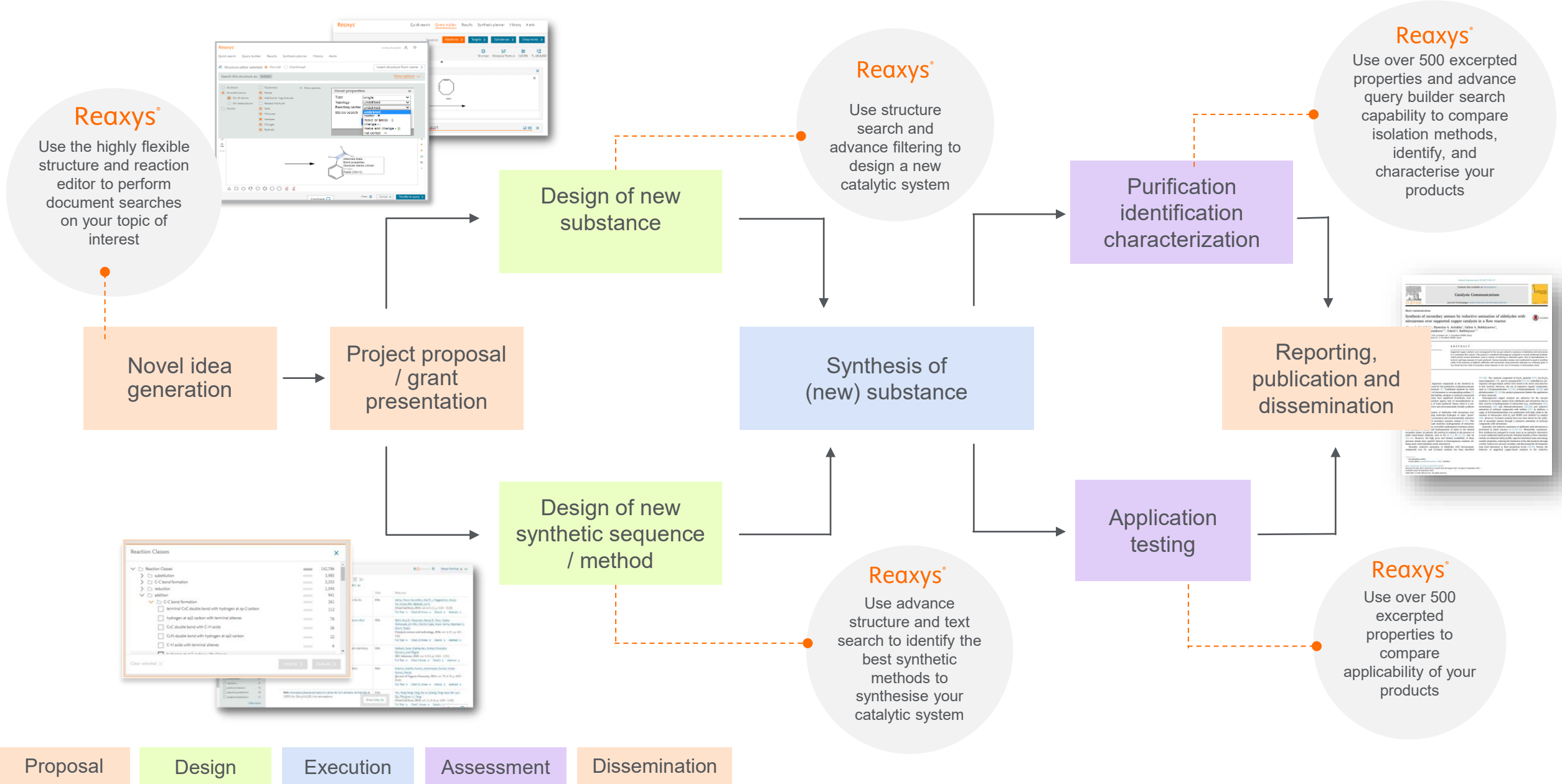
Documents

Filters	
Limit to >	Exclude >
Index Terms (List)	▲
<input type="checkbox"/> reaction	176
<input type="checkbox"/> esterification	158
<input type="checkbox"/> catalyst	92
<input type="checkbox"/> activity	79
<input type="checkbox"/> agent	69
<input type="checkbox"/> structure	67
<input type="checkbox"/> spectroscopy	63
Filter by value ▼	View more
Index Terms (ReaxysTree)	▼
Publication Year	▼
Document Type	▼
Authors	▼
Patent Assignee	▼
Journal Title	▼
Substance Classes	▼
Reaction Classes	▼

Drug Target

Filters	
Limit to >	Exclude >
By Structure	▼
Measurement pX	▼
Parameters	▼
Targets	▼
Target Species	▼
Target Type	▼
Substance action on target	▼
Molecular Weight	▼
Effect	▼
Document Type	▼
Publication Year	▼
Current Patent Assignee	▼

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



Students who use Reaxys are better prepared for the digital future

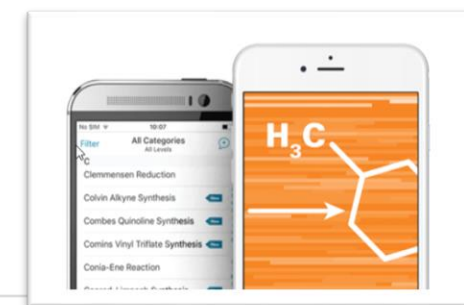
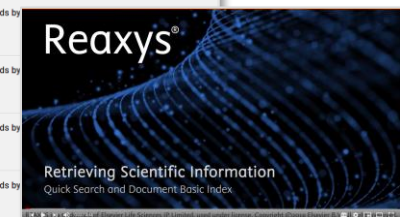
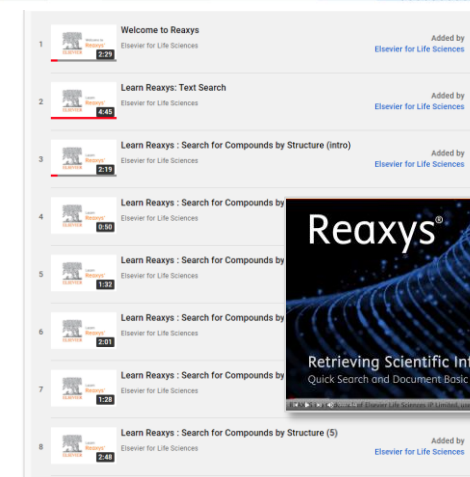


Students need...

- 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



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.



Reaxys Academy

Introductory chemistry training for students and educators



Reaxys Academy Certificate of Completion



Reaxys 101

Reaxys Academy

ELSEVIER

Nancy Rubino

has successfully completed the requirements for the
Reaxys Academy module on
Reaxys 101

November 2022

Date

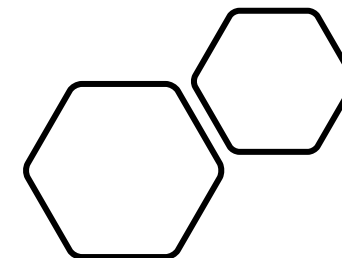
Reaxys®

Ivan Krstic

Ivan Krstic, PhD
Senior Director of Reaxys Product
Management
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.

1 selected

Export

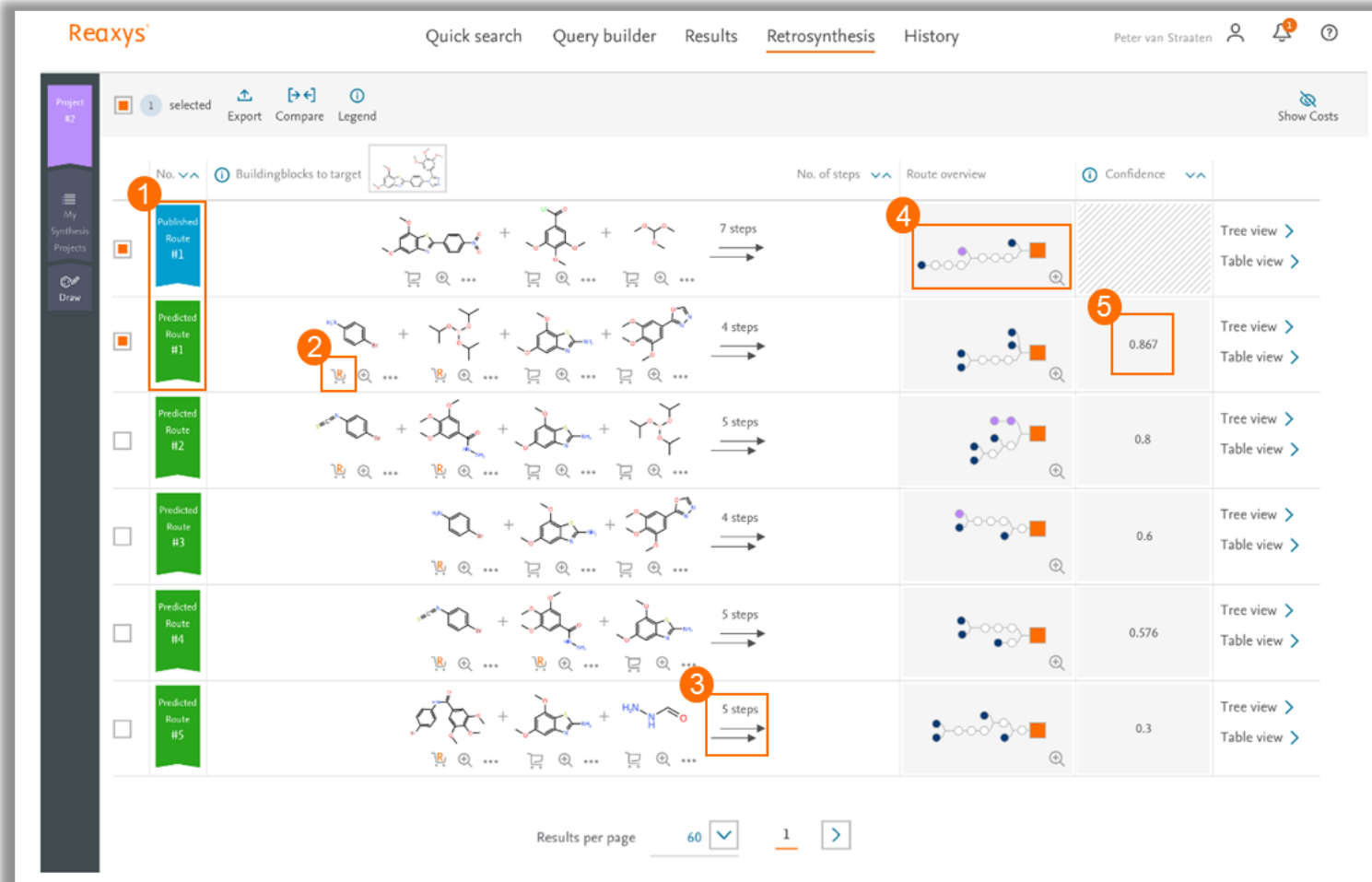
Edit

Delete

Hide Parameters

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

Reaxys Retrosynthesis provides an easy to use and intuitive interface



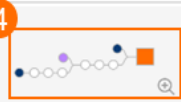

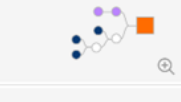



Reaxys

Quick search Query builder Results Retrosynthesis History

Peter van Straaten

1 selected Export Compare Legend

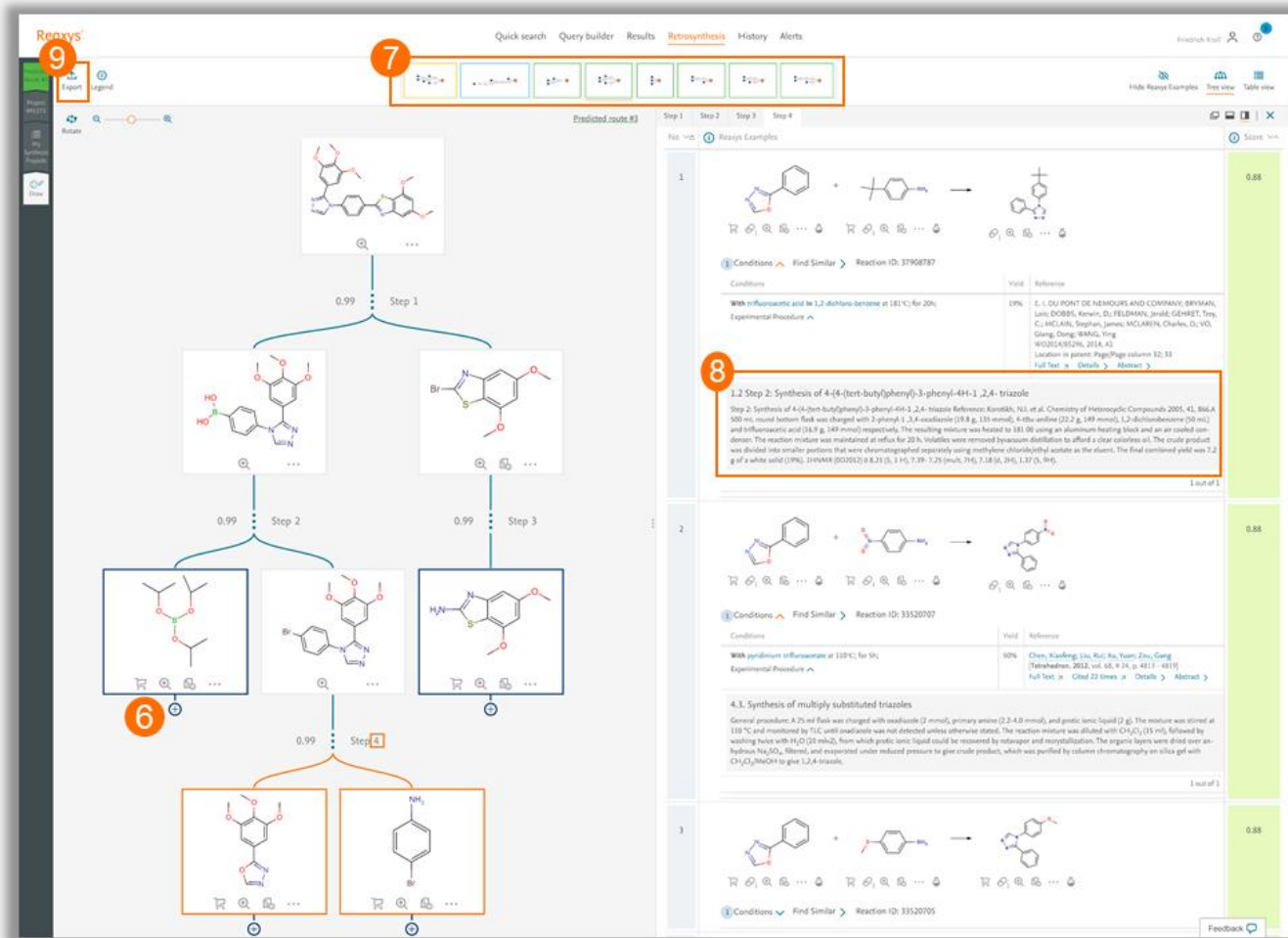
Show Costs

No. of steps	Route overview	Confidence	
7 steps			Tree view > Table view >
4 steps		0.867	Tree view > Table view >
5 steps		0.8	Tree view > Table view >
4 steps		0.6	Tree view > Table view >
5 steps		0.576	Tree view > Table view >
5 steps		0.3	Tree view > Table view >

Results per page 60 1 >

- 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 assess complexity
- 5 Scoring system for route ranking

Reaxys Retrosynthesis provides an easy to use and intuitive interface



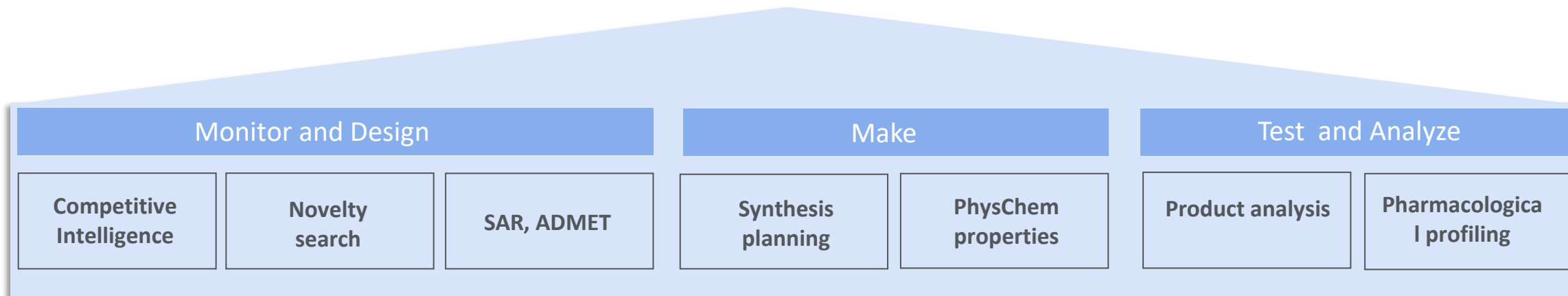
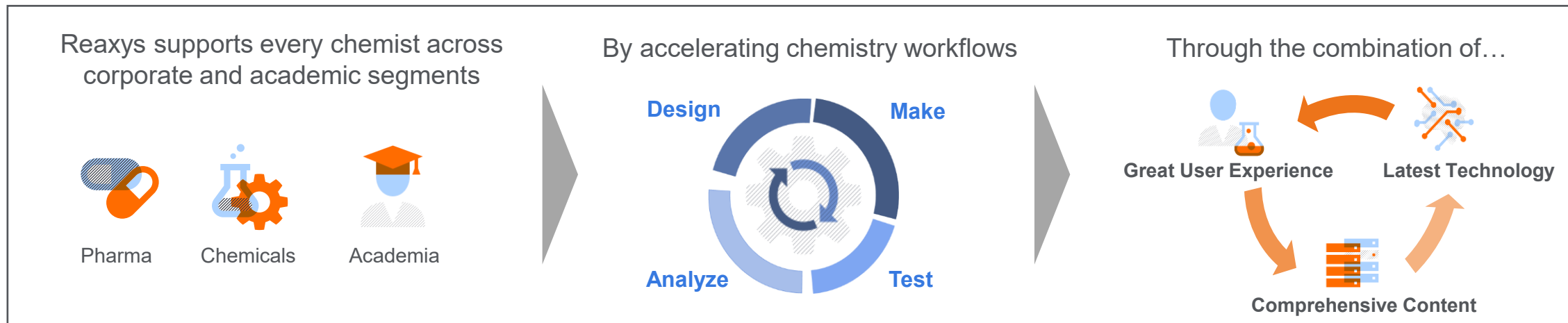
6 Edit your route by clicking ⊕ select from published or predicted steps to create a new customised route

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



Reaxys Target and Bioactivity Data



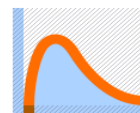
Our content is **curated and harmonized** by a team of experts from scientific **publications** including **patents, journals and books**.



8M+ Substances
with bioactivity data



2.4M+ ADME



20M+
PK/PD data points



4.5M+ toxicological
data points



6M+
Assays



56K+
biological
species



21k+
Cell lines



36K+
Biological targets

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

The screenshot displays the Reaxys patent search interface. On the left, a sidebar contains filters for 'Patent Assignee' and 'Patent Office'. The 'Patent Assignee' filter lists companies like 'intra-cellular therapies, inc' (129), 'h lundbeck as' (70), 'glaxo group limited' (58), 'altana pharma ag' (38), 'pfizer inc' (37), and 'merck sharp' (29). The 'Patent Office' filter lists countries like 'us' (736), 'cn' (389), 'jp' (348), 'wo' (320), 'ep' (260), 'kr' (175), and 'tw' (88). Below these are 'Index Terms (List)' and a 'Manually processed content only' checkbox. The main search results pane shows a single result for a Japanese patent. The title is 'Substituted [pirazoroazepin[pirazoroazepin] -4 - on and their use as a phosphodiesterase inhibitor'. The abstract states: 'The present invention relates to novel substituted pyrazoloazepin-4-ones with phosphodiesterase inhibitory activity, as well as to their use as therapeutic agents in the treatment of inflammatory diseases and conditions.' The claims section provides a detailed description of the general formula (I). The substances section displays four chemical structures. The index terms section lists various chemical and process-related terms. The target keywords section lists specific biological targets and enzymes.

5.78 K

Filters

Limit to > Exclude >

Publication Year

Document Type

Authors

Patent Assignee

☐ intra-cellular therapies, inc 129

☐ h lundbeck as 70

☐ glaxo group limited 58

☐ altana pharma ag 38

☐ pfizer inc 37

☐ merck sharp 29

Filter by value View more

Patent Office

☐ us 736

☐ cn 389

☐ jp 348

☐ wo 320

☐ ep 260

☐ kr 175

☐ tw 88

View more

Index Terms (List) 1

☐ reaction 442

☒ inhibitor 382

☐ agent 370

☐ phosphodiesterase 312

☐ hydrolysis 306

☐ surface 264

☐ kinetics 254

Filter by value View more

☐ Manually processed content only

1 selected Limit To Exclude Export

Search Sort by Publication Year Heatmap

4 Substituted [pirazoroazepin[pirazoroazepin] -4 - on and their use as a phosphodiesterase inhibitor

Author information pending - JP6850886, 2021, B2

Patent Family Members: CN110088108 A; EP3551633 B1; JP2020/500920 A; JP6850886 B2; ...

Abstract Index Terms Claims Front Page Info Substances 208 Full Text

Abstract

The present invention relates to novel substituted pyrazoloazepin-4-ones with phosphodiesterase inhibitory activity, as well as to their use as therapeutic agents in the treatment of inflammatory diseases and conditions.

1 Claims

The general formula (I): [In the formula, R₁ And R₄ Is, independently, hydrogen and (C₁ - C₄) Is selected from the group consisting of alkyl; R₂ And R₃ Is, independently, hydrogen and (C₁ - C₄) Or is chosen from the group consisting of alkyl; or R₂ And R₃ Is, together with the carbon atoms to which they are attached, cyclopropyl ring, cyclobutyl ring, cyclopentyl ring, oxetanyl ring, tetrahydrofuran ring, tetrahydropyran ring or ring to form a ring; N is, 0, 1 or 2 in which; Q is, a-O-a C (O)- R₅ Selected from the group consisting of; R₅ The, (C₁ - C₆) Alkyl, (C₃ - C₆) Cycloalkyl, halo (C₁ - C₆) Alkyl, (C₁ - C₆) Alkoxy, (C₁ - C₆) Alkoxy (C₁ - C₆) Alkyl, aryl selected from the group consisting of; said aryl is, independently R₆ One or more substituents selected from 1 or may be substituted, or an aryl may be

2 Substances

Index Terms

3 Reaxys Index Terms: Double bond, Molding, NMR spectroscopy, chromatography, column chromatography, coupling reaction, crystallization, dispersing agent, distillation, dosage form, drug, eluent, excipient, extender, flow kinetics, high performance liquid chromatography, liposome, liquid chromatography mass spectrometry (LCMS), microcrystallinity, nanoparticle, phosphodiesterase IV inhibitor, phosphodiesterase inhibitor, protein kinase inhibitor, retention time, solubilizer, suspending agent, thickening agent, transdermal, ultra performance liquid chromatography

4 Target keywords: Granulocyte-macrophage colony-stimulating factor, Interleukin-2, Multifunctional alkaline phosphatase superfamily protein PehA, Venom phosphodiesterase 1, cAMP-specific 3',5'-cAMP phosphodiesterase 4, cAMP-specific 3',5'-cyclic phosphodiesterase 4D

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

Search in: Reactions > Targets > Substances > Documents >

Save Reset form Delete all

Current Patent Assignee Structure Molecular Formula CAS RN TI, AB &

patent search

◇ Patents: Location in ... is ▾ Location in Patent

AND ◇ Patents: Prophetic Co... is ▾ Prophetic Compound

AND ◇ Patents: Related Mark... = ▾ Related Markush Structure

AND ◇ Patent Specific Data ... ☐ Find any

AND ◇ Current Patent Assignee contains ▾ Current Patent Assignee

AND ◇ Original Patent Assignee contains ▾ Original Patent Assignee

AND ◇ Common Patent Number is ▾ Common Patent Number

AND ◇ Patent Country Code is ▾ Patent Country Code

AND ◇ Patent Number is ▾ Patent Number

Search fields and forms

Fields Forms History

Reaxys ^

Topics and Keywords ▾

Identification ▾

Physical Properties ▾

Spectra ▾

Target and Bioactivity ▾

Other ▾

Reactions ▾

Bibliography ▾

PubChem ▾

Commercial Substances ▾

Reaxys: Fields (Query Builder)

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
 Critical Temperature
 Critical Volume
 Electrical Data
 Electrical Moment
 Electrochemistry Data
 Electron Binding
 Energy Barriers
 Energy 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 Properties
 Static Dielectric Constant
 Surface Tension
 Transition Points
 Transport Data

Transport data

NMR Spectroscopy
 IR Spectroscopy
 Mass Spectroscopy
 UV/VIS Spectroscopy
 ESR Spectroscopy
 NQR Spectroscopy
 Raman Spectroscopy
 Luminescence 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
 Measurement Parameter
 Endpoint of Effect
 Ecotoxicology Data
 Dielectric Constant
 Dissociation Exponent
 Dynamic Viscosity
 Electrolytic Conductivity
 Enthalpy of Fusion
 Enthalpy of Vaporization
 Explosion Limits
 Interatomic Distance/Angle
 Kinematic Viscosity
 Liquid/Solid Systems
 Liquid/Vapor Systems
 Metarotation

And many more...