



ELSEVIER

ChemExpTM
INDIA

**Advance R&D innovations with Elsevier
research solutions**



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ELSEVIER

OUR SHARED PURPOSE

TO ACCELERATE
SCIENCE TO
IMPROVE HEALTH

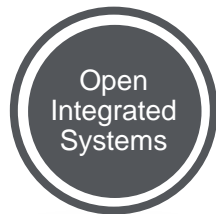
A Knowledge & Information
Analytics Company



OUR PROMISE

Partners in propelling research
and innovation forward to
transform the way you bring
new medicines to the world

OUR KEY DIFFERENTIATORS



140+

years of scientific
knowledge curation

RELX

\$1.4bn
on technology annually

~30,000
employees

Serving customers in

180+
countries

Partnering with

90%

of top Pharma
companies



Elsevier's Innovative solutions with multifunctional approach



Intellectual Property

- Patent registration and litigation
- Prior art, FTO...



Pharma/non-pharma chemical R&D/manufacturing



Data Science/ Bio-/Cheminformatics

- Develop machine learning algorithms
- In-silico screens for safety, efficacy...



Pharmacovigilance

- Monitor drug safety
- Risk mitigation



Non-clinical R&D

- Assess safety, pharmacology, DMPK
- Clinical trial risk mitigation



Business Development/ Market Research

- Identify unmet medical needs
- In-licensing



Clinical R&D

- Clinical trial design
- Evaluate safety, efficacy, dosage



Knowledge Management

- Provide and integrate content
- Foster innovation



Medical Affairs/MSL

- Generate evidence
- Engage with healthcare ecosystem



Regulatory affairs

- Regulatory submissions
- Develop regulatory strategy

Insights tailored to
your needs

Reaxys[®]
Scopus[®]
Embase[®]
EmBiology
ScienceDirect
PharmaPendium[®]
Professional Services
SciBite: TERMite/CENTree

Click on departments for more information

Click on solutions for more information



NOT EXHAUSTIVE

Challenges to the pharma/chemical sector in India



Global economy

Price control and market dynamics



Sustainability

Regulatory Compliance and Quality Standards



Import dependence,



Competitive threat

R&D investment

Surge in technology price



IPR issue



Pricing Pressure in Export Markets



Challenges to the pharma/chemical sector in India



Global economy

Cost control and market dynamics



Import dependence

R&D investment



IPR issue



Sustainability

Regulatory Compliance and Quality Standards



Competitive threat

Surge in technology price



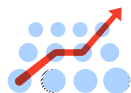
Pricing Pressure in Export Markets



What if there is a **better way** to be
More efficient in Route of Synthesis (ROS)
designing?

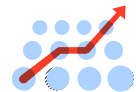


Innovation intelligence with dedicated data and information access



Impact of Exhaustive Dataset

- Confidence in handling competitive intelligence/novelty search
- Cost-effective, time-bound, and sustainable approach
- Stay ahead on the competitive scale
- Acceleration of business growth to the next level

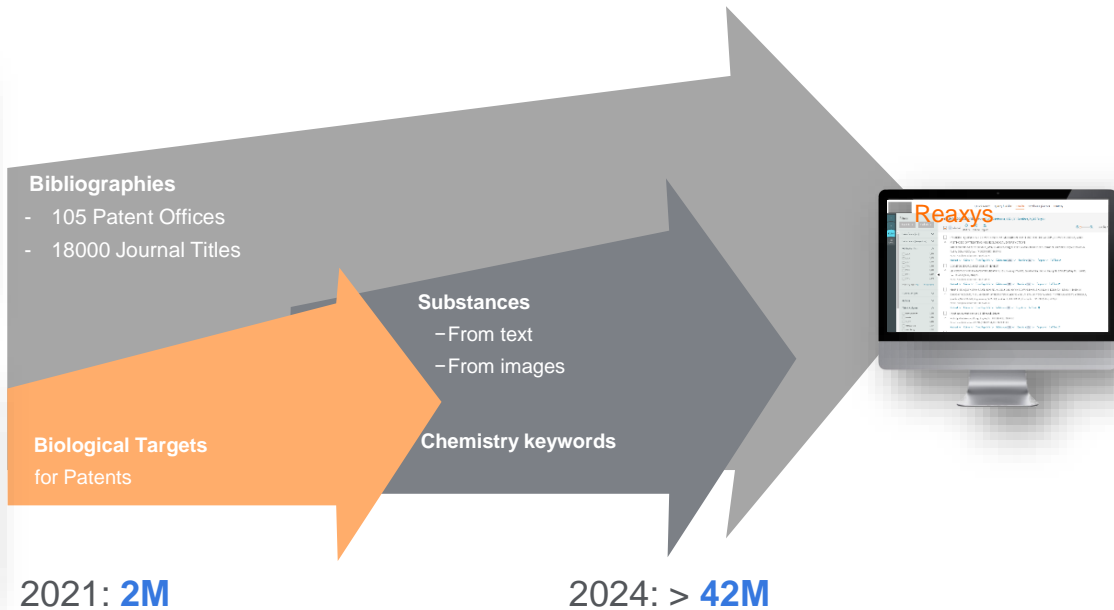
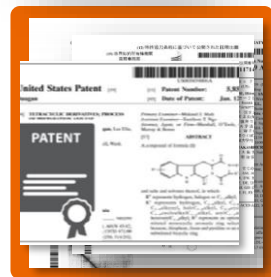
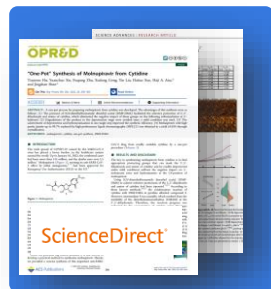


Next Step:
Join
accelerating
business
growth
journey with
Reaxys.com

The image shows a computer monitor in a laboratory setting. The monitor displays the Reaxys search results page for the query "atenolol". The page features a navigation bar with options like "Quick search", "Query builder", "Results", "Retrosynthesis", "History", and "Alerts". Below the search bar, the results are categorized into three sections: "Substances" (128 results), "Documents" (32,232 results), and "Commercial Substances" (8 results). Each section includes a "View Results" button. The Reaxys logo is visible in the top left corner of the page, and the Elsevier logo is in the bottom left. The RELX Group logo is in the bottom right. A person wearing blue gloves is visible at the bottom left, typing on a keyboard.

Category	Count	Actions
Substances	128	View Results
Documents	32,232	View Results
Commercial Substances	8	View Results

Application of award-winning programmatic extraction technologies to Patents and journals expansion



1- High quality, comprehensive content

Meet the team



Dr. Nina Kaun



Dr. Michael Maier



>42 M
Patents

113 M
Documents

105
Patent
Offices

173
IPC
subclasses

46 M
Bioactivity
data

18 K
Journals

> 1 Bn
Experimental
Facts

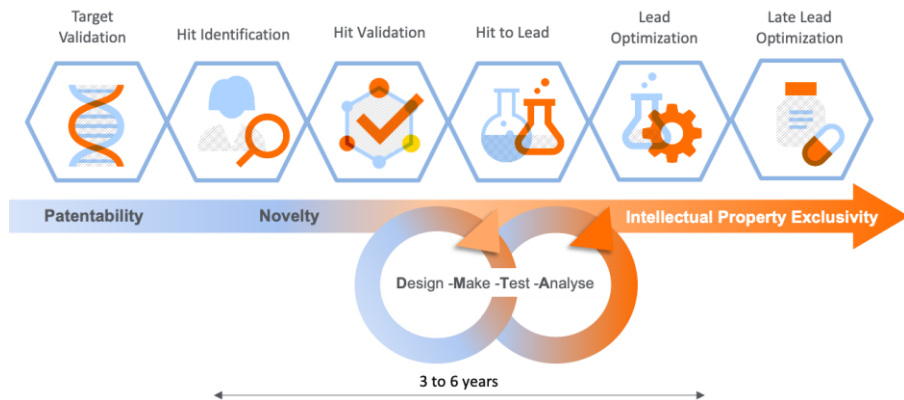
Winners of Cypher
Data Science
Excellence Awards
2022



ELSEVIER

Ensure your projects are designed competitively and remain patentable throughout the discovery years

- Reaxys offers **fast** and **comprehensive** access to **patents** for Novelty search & Competitive Intelligence



- ✓ Confidently assess the **IP landscape** of a **biological target**, check the **novelty of the compounds** in your pipeline and stay on top of **emerging competitors**



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Capture relevant results for target validation with our **target (gene/protein) indexing** for priority patent offices



Do competitive deep-dives with our **advanced search** for **patent assignee**



Patents and **substances** available **5 days** after publication. Stay up-to-date with **email alerts**.

Patent information is easily discoverable in Reaxys' Document results page

1- High quality English translation of abstracts and claims easily accessible in the UI - as it is the case for this Japanese patent

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



Filters

5.78 K
Preview

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

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 A1; 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

Chemical structures of substituted pyrazoloazepin-4-ones.

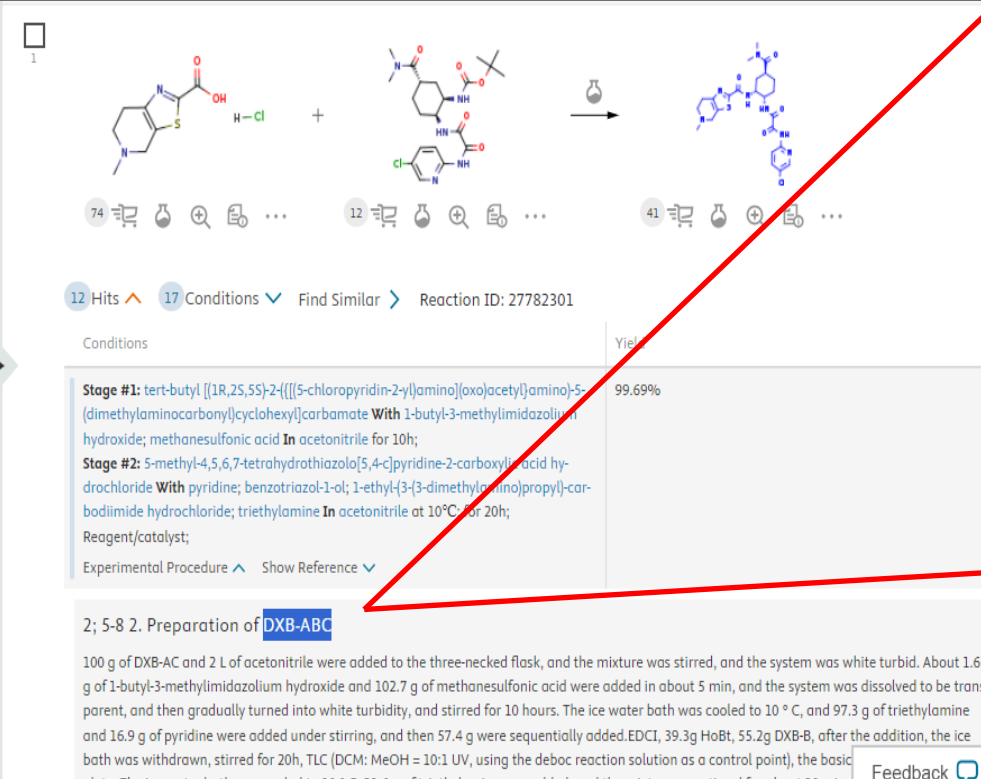
Show Less + Show next 50

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

High-quality English translation of experimental protocols e.g. Edoxaban



1

74

12

41

12 Hits **17** Conditions Find Similar > Reaction ID: 27782301

Conditions	Yield
Stage #1: tert-butyl [(1R,2S,5S)-2-(((5-chloropyridin-2-yl)amino)(oxo)acetyl)amino]-5-(dimethylaminocarbonyl)cyclohexyl]carbamate With 1-butyl-3-methylimidazolium hydroxide; methanesulfonic acid In acetonitrile for 10h;	99.69%
Stage #2: 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carboxylic acid hydrochloride With pyridine; benzotriazol-1-ol; 1-ethyl-3-(3-dimethylamino)propyl]-carbodiimide hydrochloride; triethylamine In acetonitrile at 10°C for 20h;	
Reagent/catalyst:	

Experimental Procedure **DXB-ABC** Show Reference

2; 5-8 2. Preparation of DXB-ABC

100 g of DXB-AC and 2 L of acetonitrile were added to the three-necked flask, and the mixture was stirred, and the system was white turbid. About 1.66 g of 1-butyl-3-methylimidazolium hydroxide and 102.7 g of methanesulfonic acid were added in about 5 min, and the system was dissolved to be transparent, and then gradually turned into white turbidity, and stirred for 10 hours. The ice water bath was cooled to 10 ° C, and 97.3 g of triethylamine and 16.9 g of pyridine were added under stirring, and then 57.4 g were sequentially added. EDCI, 39.3g HoBt, 55.2g DXB-B, after the addition, the ice bath was withdrawn, stirred for 20h, TLC (DCM: MeOH = 10:1 UV, using the deboc reaction solution as a control point), the basic

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右加入

4/9 页

1.66g 氢氧化1-丁基-3-甲基咪唑, 102.7g 甲磺酸, 体系溶解至透明, 后逐渐变为白色混浊, 搅拌10h。冰水浴降温至10℃, 搅拌下加入97.3g 三乙胺和16.9g 吡啶, 然后依次加入57.4g EDCI、39.3g HoBt、55.2g DXB-B, 加毕后, 撤冰浴, 搅拌反应20h, TLC (DCM:MeOH=10:1UV, 用脱boc反应液作对照点) 基本反应完全。冰水浴降温至10℃, 加入21.6g 三乙胺, 搅拌30min左右。抽滤, 用100ml 乙腈淋洗。滤饼45℃鼓风干燥, 得类白色固体, 收率97%, 纯度98.05%;

[0052] 3、DXB-ABC的精制

[0053] 向5L三口瓶中加入DXB-ABC粗品和2L二氯甲烷, 搅拌20-30min, 固体基本溶解。抽滤, 滤液转入10L瓶, 搅拌下加入4L正己烷, 搅拌30min, 抽滤。滤饼45℃鼓风干燥, 得浅黄至类白色固体粉末;

[0054] 将上述类白色固体加入2L瓶, 加入1275ml 甲醇, 室温搅拌10-15h, 抽滤, 滤饼45℃鼓风干燥至恒重, 得浅黄至类白色固体;



What do you need to consider for effective molecule design?

Make data driven decisions and find new ways of designing novel and safe compounds under tight timelines with Reaxys' Target & Bioactivity insights integrated into Reaxys.com

[Quick search](#) Query builder Results Retrosynthesis History Alerts


Search substances, reactions, documents and bioactivity data
in Reaxys, Reaxys Medicinal Chemistry, PubChem and Commercial Substances

Search Reaxys






Find >

Cell Lines Name, e.g. HEK293

AND

 Draw

Content Overview | Latest update: 19. April 2024 >

282M	65M	113M	42M	46M
 Substances	 Reactions	 Documents	 Patents	 Bioactivities



Our content is **manually curated and harmonized** by a team of experts from over **600K citations 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+
species



21k+
Cell lines



36K+
Biological
targets

Easy access to relevant bioactivity seamlessly integrated into Reaxys.com

The screenshot displays the Reaxys.com interface for searching and analyzing bioactivity data. On the left, a 'Filters' sidebar includes categories like 'Measurement pX', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', 'Number of Fragments', 'Availability', and 'Availability in other databases'. The main search results area shows '0 selected' items and a search for 'imatinib' with its chemical structure and molecular formula $C_{29}H_{31}N_7O$. Below the search results, a table lists parameters for imatinib, with two rows highlighted in green: pX (7.47) and IC50 (35). A 'Heatmap settings' dialog box is open, showing a list of targets and a 'Full Screen' display mode. A 'Bioactivity Visualization' window is also visible, showing a radar chart comparing the substance's properties against Lipinski/Verber rules. The interface includes various icons for actions like 'Limit To', 'Exclude', 'Export', and 'Preparations'.

1 Druglikeness

2 Bioactivity (All)

- ✓ In vitro: Efficacy - 6151
- ✓ In vivo: Animal Model - 612
- ✓ Metabolism - 455
- ✓ Pharmacokinetic - 795
- ✓ Toxicity/Safety Pharmacology - 2626

Heatmap settings

Value of X-axis: Targets

Value of Y-axis: Bioassays, Targets, Target Species, Biological Species, Effects, Parameter, Cell Lines, Substances

Value of Cells: Cell, Effect

Show substances: Ba/F3 cell line (cytotoxic agent), GIST-T1 cell line (antineoplastic agent)

Display mode: Normal Full Screen

Always show settings

Apply

Cell	Effect
Ba/F3 cell line	cytotoxic agent
GIST-T1 cell line	antineoplastic agent

PSA/10

Matching Lipinski Rules: 4

Veber rules component

Polar Surface Area (PSA)	86.28
Rotatable Bond (RotB)	8
Matching Veber Rules	2

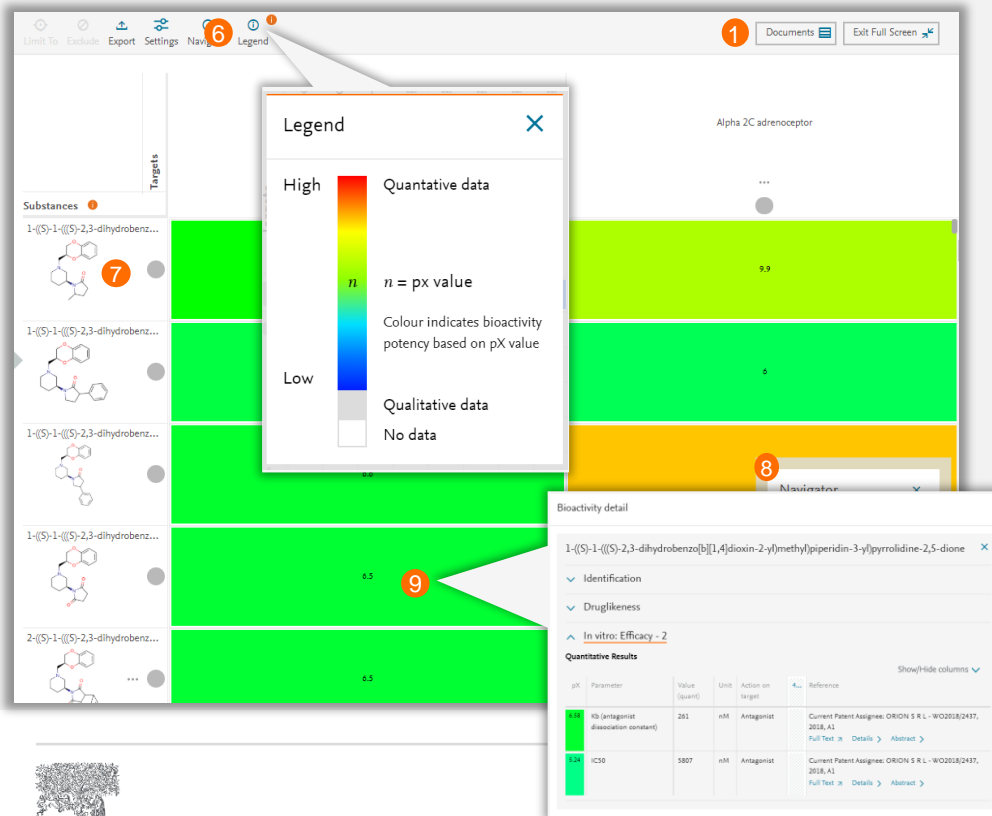
logP

PSA/10

Substance (orange), Lipinski/Veber rules (blue)

- 1** Easily access Druglikeness profiles including Lipinski/Verber rule comparison
- 2** Review bioactivity data in the same window to make informed decisions more rapidly
- 3** Additional relevant filters to optimize your search
- 4** Export your Bioactivity data insights in multiple formats (PDF, DOC, XLS, XML, RD, SD) for further analysis
- 5** The Bioactivity visualization feature, lets take a closer look...

Reaxys' bioactivity visualization feature enables easy comparison of relevant data



1. Seamlessly go between the heatmap and relevant documents for further assessment
6. Access the legend for a quick overview of the potency scale
7. View the chemical structures whilst reviewing the data for quick SAR analysis
8. Evaluate large datasets with an easy to use Navigation bar
9. Click a cell to access all the details for a specific record

Summary: Reaxys for every R&D organization

Impact of Technology-driven data extraction with intelligent AI-based tools

- Cost, time-effective, sustainable end-product; stay ahead of competitors
- Consistent cost monitoring of the ongoing project (ROS)
- Stay ahead on competitive intelligence and novelty search use case
- Medicinal chemistry database for innovative drug discovery
- Acceleration of business growth to the next level



Our information security standards are certified

Reaxys has obtained the ISO 27001 Information Security System Management certification

Your confidentiality is our key priority

You can trust Reaxys to confidently perform searches on proprietary research to strengthen your IP portfolio.

- ✓ Reaxys maintains certified high standards for security practices
- ✓ Reaxys continuously improves its information security practices





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04.05.2024

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