

CAS 解决方案与核心能力 数据挖掘与分析：基于 AI 解锁科研新视角

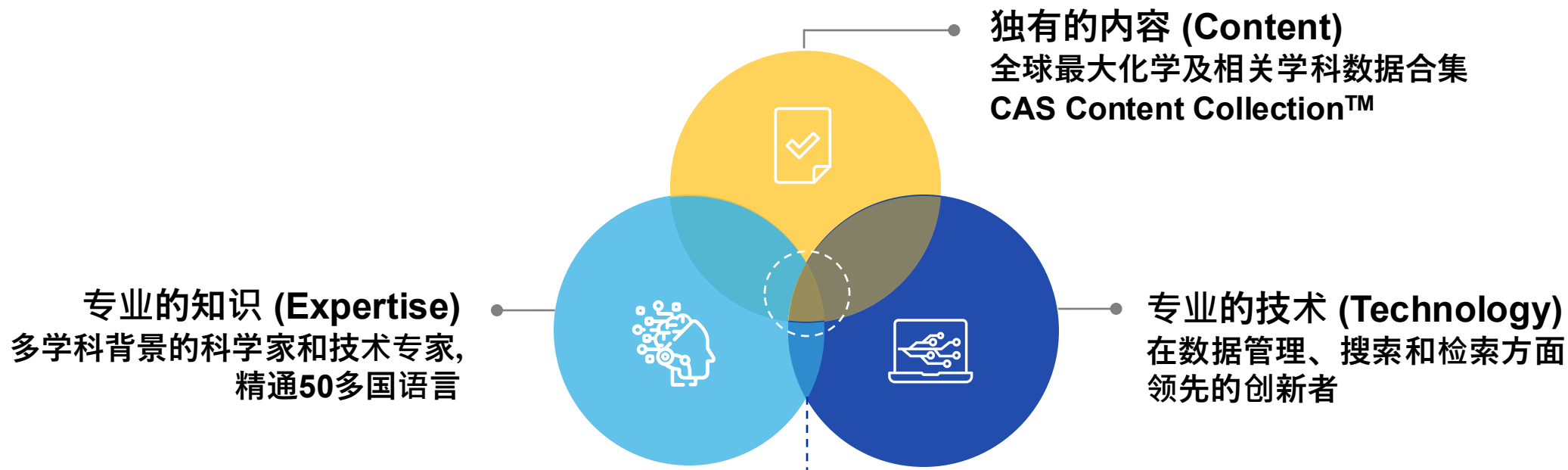


China@acs-i.org

美国化学文摘社中国代表处

2/25/2026

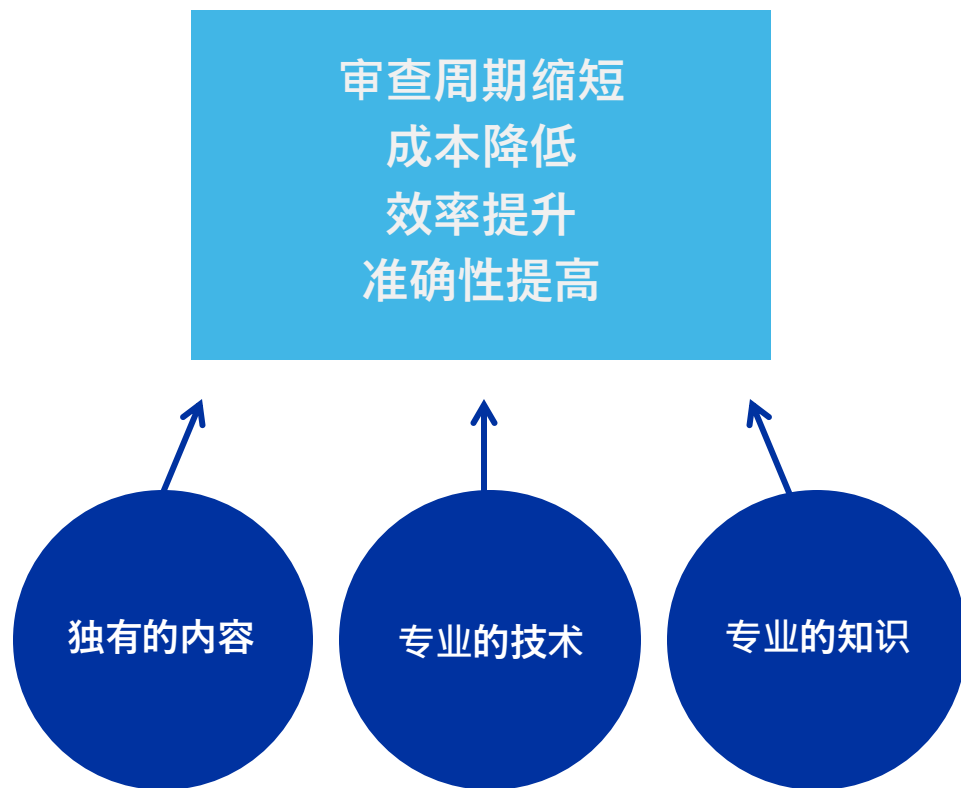
CAS 产品和服务的独特性： 独有内容、领域专家、专业技术



历经百年, CAS始终如一, 承担着连接全球
科学知识的工作

CAS专业现有技术能力

与您的目标一致的创新



由科学家策划的结构化内容

- CAS内容合集 (CAS Content Collection™)
- 覆盖超150年科技发展
- 收录50多种语言文献
- 涵盖专利与非专利出版物

面向复杂科学专利数据的可训练技术

- 用于现有技术检索的AI/ML算法
- 专利分类指派与转换支持

无与伦比的人类专业能力

- 跨学科的深厚科学/技术知识
- CAS检索专家预先筛选
- 专业级专利检索与分析服务

CAS全方位助力创新之旅，确保项目成功与效益最大化



CAS SciFinder Discovery Platform™

以最大化的效益加速科学发现，加快产品上市。

CAS BioFinder Discovery Platform™

利用集成的生物和化学数据与分析解决方案，帮助您满怀信心地推进药物研发工作。

STN IP Protection Suite™

寻找新市场，确保您的知识产权受到保护。

CAS Custom ServicesSM

CAS 定制服务为您提供数据、分析和洞察，帮助您发现机会，最大化投资回报率。

以专利WO2018152134为例

丰富的增值标引信息：

163 Substances

625 Reactions

15 Patent Family Members

3 Formulations

1 Markush structure

18 SAR data points

141 ADME data points

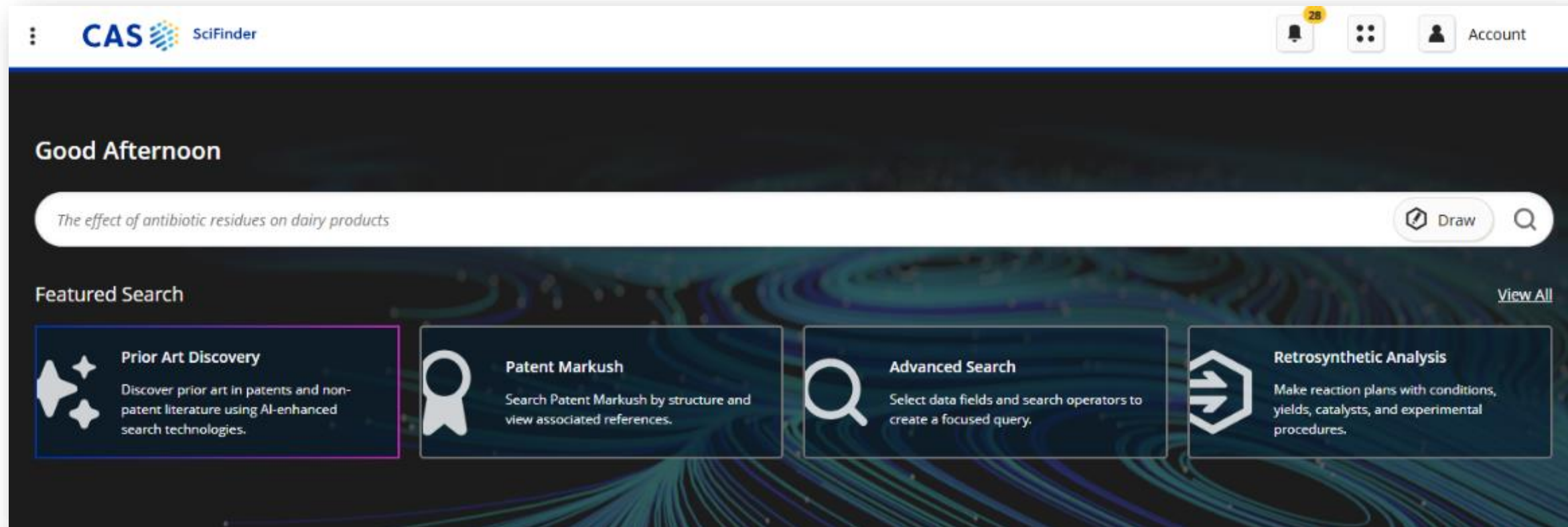


CAS 的 AI 应用策略

- 应用于 CAS 内部数据加工标引，提高内容收录与标引效率
- 增强检索、可视化以及预测相关功能，更准确识别用户检索意图，提供更有针对性的检索结果
- CAS Custom Service定制服务提供AI支持，整合用户数据，构建预测模型，助力AI加速工作流程

CAS SciFinder[®] 智能检索 (SearchSense)

界面直观简洁，节省查找各选项时间



多功能检索框更新，高级检索功能现以磁贴形式呈现于检索栏下方

智能检索——AI Summary

在文献结果页面查看AI Summary——AI技术对CAS数据进行的提炼和总结，更快理解研究结果

AI Summary

Based on the search results, here's a summary of key findings related to crown ether and lithium and salts:

The search results highlight various aspects of crown ether-like lithium salts, including their synthesis, properties, and applications. One study describes the formation of amorphous solid electrolytes using cryptands or crown ethers with lithium salts, while another examines the transport rates of metal cations through bulk liquid membranes containing crown ethers. Additionally, research has been conducted on the design of asymmetric ether-like lithium salts to improve the performance of lithium metal batteries. Another study presents a nanofiltration membrane with crown ether as exclusive Li⁺ transport channels for efficient extraction of lithium from salt lake brine. Furthermore, the isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions are discussed, along with the computerized conductometric determination of stability constants of complexes of crown ethers with alkali metal salts and neutral molecules in polar solvents.

Key Findings:

1. Amorphous Solid Electrolytes:

- Amorphous solid electrolytes can be formed by the interaction of cryptands or crown ethers with lithium salts when the cavity size of the macrocycle does not match the diameter of the lithium cation. (1)

2. Metal Cation Transport Rates:

- The transport rates of metal cations through bulk liquid membranes containing crown ethers depend on the cation concentration in the source salt solution phase and the anion type. (2)

3. Lithium Metal Battery Performance:

- Designing an asymmetric ether-like lithium salt can improve the fast-cycling performance of lithium-metal batteries, particularly for practical lithium-metal batteries with high cathode loading. (3)

4. Nanofiltration Membranes:

- A nanofiltration membrane with crown ether as exclusive Li⁺ transport channels, generated by crown ethers, can efficiently extract lithium from salt lake brines with high Mg²⁺/Li⁺ mass ratio. (4)

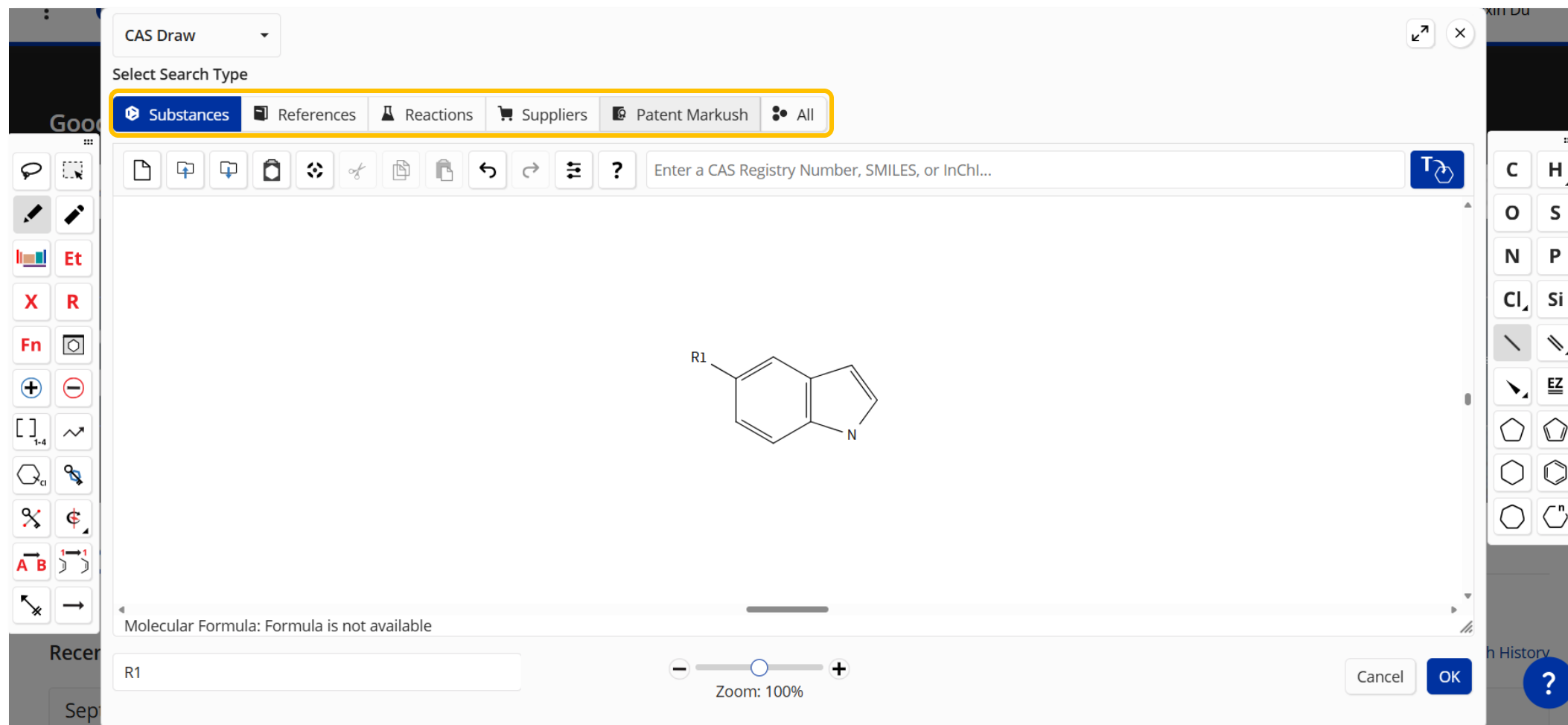
5. Isolation and X-ray Structures:

- The isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions have been reported, providing insight into the molecular structure of these compounds. (9)

Designing an asymmetric ether-like lithium salt to enable fast-cycling high-energy lithium metal batteries

Nature Energy (2023), 8(9), 934-945
| Language: English, Database: CAplus

结构编辑器可直接指定检索类型，提升检索效率



检索类型“画完即选”，灵活选择检索方向

高级检索项自定义检索物质或文献

Advanced Search

Select a search type, and then add multiple search fields to build a query.

[Learn more about Advanced Search.](#)

Substances

References

Clear All

Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.

Draw

-

Molecular Formula

Enter a molecular formula.

×

Examples: C₆H₆ | (C₈H₈)_x | C₂₂H₂₆CuN₂O₅.C₂H₃N

AND

Substance RN

Multiple entries must be delimited by a comma, space, or semicolon.

×

Examples: 57-88-5 | 101600

AND

Component RN

Multiple entries must be delimited by a comma, space, or semicolon.

×

Examples: 120-12-7 | 71432

AND

Chemical Name

Enter chemical name.

×

Examples: 2-(2,6-Dioxo-3-piperidinyl)-1H-isoindole-1,3(2H)-dione | Polypropylene

+ Add Advanced Search Field

Search

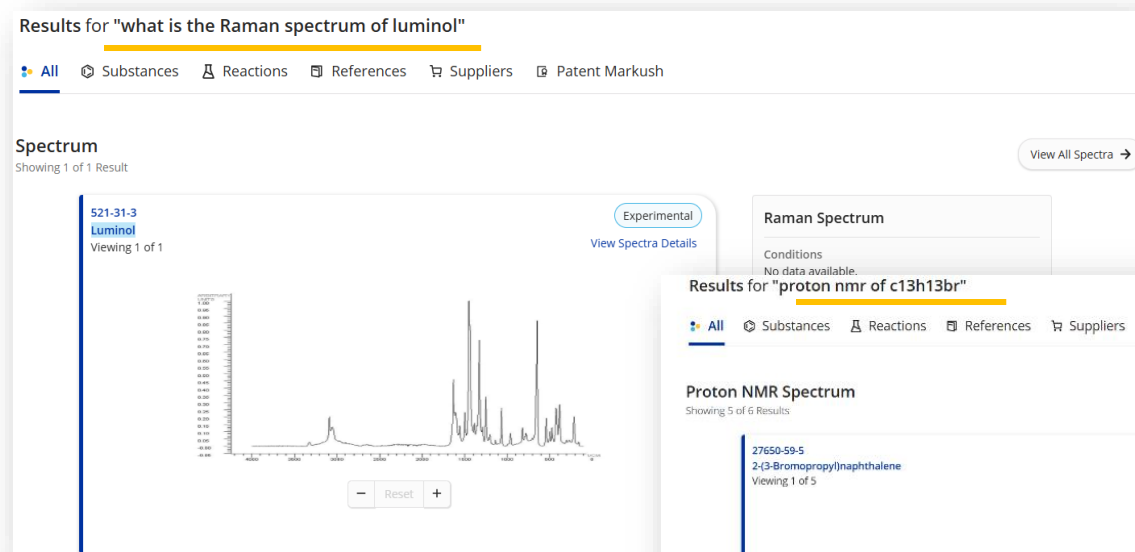
直接选择“物质”或“文献”入口，精准定位检索目标

更多角度精准筛选文献检索结果，省时高效

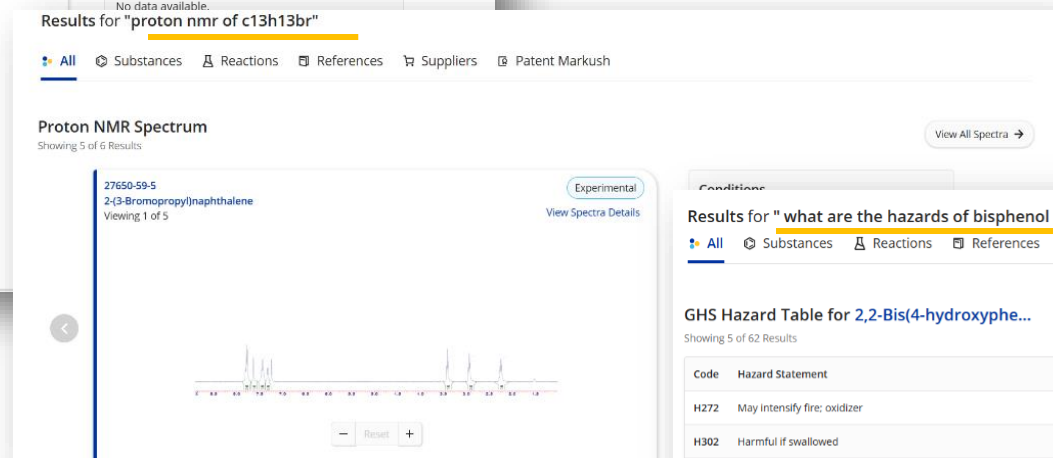
The screenshot displays the CAS SciFinder web interface. The search query 'previcox use in elderly dogs' is entered in the top search bar. The left sidebar contains several filter categories: Database, CAS Content, Life Science Data, Flags, and Patent Office. The 'Flags' section is highlighted with an orange box and includes the following options: Is Open Access (88K), Has DOI (781K), Has Claims (17K), Has PatentPak (37K), Has Related Substances (323K), and Has Related Reactions (2,803). The 'Patent Office' section includes: China (26K), United States (10K), World Intellectual Property Organization (9,401), Japan (7,549), and European Patent Organization (6,961). The central results pane shows two search results. The first result is titled 'The effects of firocoxib (Previcox) in geriatric dogs over a period of 90 days.' by Joubert, K E, published in the Journal of the South African Veterinary Association (2009), 80(3), 179-84. The second result is titled 'Use of trazodone to facilitate postsurgical confinement in dogs' by Gruen, Margaret E.; Roe, Simon C.; Griffith, Emily; Hamilton, Alexandra; Sherman, Barbara L., published in the Journal of the American Veterinary Medical Association (2014), 245(3), 296-301. The right pane, titled 'Analyze Results', shows a treemap visualization of document types: Journal (purple), Report (green), Review (orange), Patent (blue), and Clinical Trial (red). Below the treemap, the 'Top Assignees/Organizations' section shows a list of organizations with corresponding bar charts.

按文章是否开放获取、是否具备DOI、专利是否提供权利要求书、专利是否支持PatentPak浏览器、文献是否包含标引物质、文献是否包含标引反应筛选

扩展问答类型，快速聚焦物质谱图和安全信息



自然语言直接查阅Raman谱图



自然语言直接查阅NMR谱图

Results for "what are the hazards of bisphenol a?"

All Substances Reactions References Suppliers

GHS Hazard Table for 2,2-Bis(4-hydroxyphenyl)propane

Showing 5 of 62 Results

View Full Table →

Regulatory List

View in Detail Page →

Code	Hazard Statement
H272	May intensify fire; oxidizer
H302	Harmful if swallowed
H304	May be fatal if swallowed and enters airways
H313	May be harmful in contact with skin
H317	May cause allergic skin reaction

⚠️ ⚠️ ⚠️ ⚠️

Suggested based on your search

Regulatory List

AIIC, AEC, CANL, CLP, DSL, EECL, EINECS, ENCS, FDA, HAP, HHAZ, HTU, IECSC, INSQ, ITC, IUR, JDATA, NZIO, PICCS, PIL, PROP, REACH, RSTR, S313, SIDS, State_CA_PROP65, State_MA, State_MN, State_NJ, State_OR, State_PA, State_VT, State_WA, STOR, STY, TCSI, TDCA, TSCA, VNECI, VOC, WGK

Confidential Business Information: Public

Regulatory Synonyms (35)

Details by Country/International & Other Lists

自然语言直接查阅物质安全信息

支持自然语言直接检索物质理化性质，直观高效

Results for "what is the boiling point of ethanol"

All Substances Reactions References Suppliers Patent Markush

64-17-5
Ethanol

Boiling Point
78.5 °C

Source
"Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

Boiling Point Properties
Showing 5 of 415 Results

Value	Condition	Source
78.5 °C		
181.27 °C		
110 °C (approx)		
85 °C (approx)		
80 °C		

[View in Detail Page →](#)

自然语言直接查阅物质沸点

Results for "what is the pKa of benzene"

All Substances Reactions References Suppliers

71-43-2
Benzene

pKa
43

Source
CAS

pKa Properties
Showing 5 of 5 results

Value	Condition	Source
43		CAS

[View in Detail Page →](#)

自然语言直接查阅pKa值

Results for "melting point of mercury"

All Substances Reactions References Suppliers Patent Markush

7439-97-6
Mercury

Melting Point
-38.87 °C

Source
"Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

Melting Point Properties
Showing 5 of 30 Results

Value	Condition	Source
-38.87 °C	-	"Hazardous Substances Data Bank" data were obtained from the ...
>350 °C (decomp)	-	Niamnont, Nakorn; Organic Letters, (2009), 11(13), 2768-2771, CA...
39.25 °C	-	Connolly, James A. D.; Journal of Geophysical Research: Planets, (...)
38.8 °C	-	Vega, Cesar; Journal of Food Science, (2005), 70(3), E244-E251, CA...
-38.4 °C	-	Cicogna, Francesca; Reactive & Functional Polymers, (2012), 72(10...

[View in Detail Page →](#)

自然语言直接查阅熔点

支持自然语言查阅反应操作流程, 快速获取即时信息

Results for "how to make ibuprofen?"

[All](#) [Substances](#) [Reactions](#) [References](#) [Suppliers](#) [Patent Markush](#)

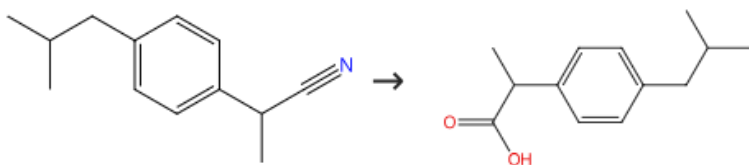
Reactions

Showing 1 of 1,084 Results

[View All Reactions →](#)

31-614-CAS-23979361

Steps: 1 Yield: 100%
[View Experimental Protocols](#)



- 1.1 Reagents: [Sodium hydroxide](#)
Solvents: [Methanol](#), [Water](#); 15 min, rt; 12 h, reflux
- 1.2 Reagents: [Hydrochloric...](#)
Solvents: [Water](#); pH 2, rt

[View Reaction Summary](#)

Procedure

[View in Detail Page](#)

Experimental Procedure

1. Add dialkylated phenylacetonitrile (1 equivalent), methanol (15 mL) and water (5 mL) to an oven dried 50 mL round bottomed flask charge with magnetic stirring bar at room temperature.
2. Stir the mixture for 15 minutes at room temperature.
3. Add sodium hydroxide (2 equivalents) to the mixture.
4. Stir the mixture under refluxing temperature for 12 hours (oil bath).
5. Allow the reaction mixture to cool down to room temperature.
6. Extract the reaction mixture with ethyl acetate (25 mL).
7. Acidify the separated aqueous layer with 15% hydrochloric acid to pH = 2.0.
8. Pour the separated aqueous layer into the crushed ice (for solid products)

[View All](#) ▾

通过自然语言查询特定收率或收率区间的反应

CAS SciFinder

synthesis of ibuprofen with 80-86% yield with pdcl2 catalyst

← Return to Home

Results for "synthesis of ibuprofen with 80-86% yield with pdcl2 catalyst"

All Substances Reactions References Suppliers

Reactions

Showing 1 of 1 Result

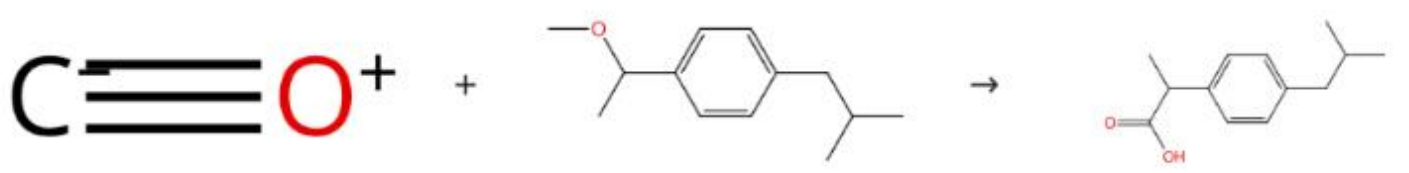
31-614-CAS-26935461

View All Reactions →

Steps: 1 Yield: 85%

1.1 Reagents: Hydrochloric acid
Catalysts: Triphenylphosphine, Cupric chloride, Palladium chloride
Solvents: Methyl ethyl ketone, Water

View Reaction Summary



更快获取实验方案与反应数据

自然语言检索反应识别多种反应角色，降低检索难度

Reactions search for "synthesis of aspirin from sodium bicarbonate in water"

🔍 All 📦 Substances **🧪 Reactions** 📖 References 🛒 Suppliers 📄 Patent Markush

View Related Results ▾

Filter Results <

Behavior

Filter by **Exclude**

▼ Search Within Results

^ Non-Participating Functional Groups

☐ Carboxylic acid (12)

☐ Carboxylic ester (7)

☐ Amide (4)

☐ Imine (4)

^ Experimental Protocols

☐ Synthetic Methods (1)

☐ Experimental Procedure (1)

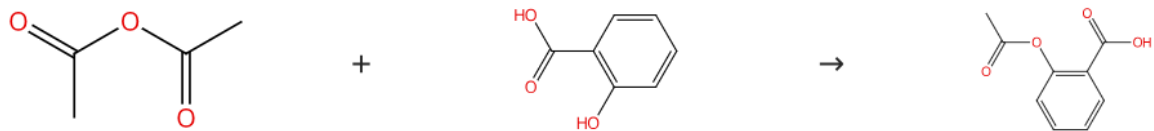
^ Number of Steps

☐ 1 (14)

☐ 14 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

Scheme 1 (6 Reactions) Steps: 1 Yield: 83-95% ...



 Suppliers (85)

 Suppliers (158)

 Suppliers (122)

☐ 31-355-CAS-15059619 Steps: 1 Yield: 95% ...

1.1 Catalysts: [Zinc acetate](#); 3 h, rt

1.2 Reagents: [Sodium bicarbonate](#)

Solvents: [Water](#); 1 h, rt

[Acetylation of hydroxy radical catalyzed by Zn\(AcO\)₂ using acetic anhydride as solvent](#)

By: Xu, Shao-hong; et al

Huaxue Shiji (2009), 31(9), 761-763

Full Text ▾

☐ 31-355-CAS-10881517 Steps: 1 Yield: 88% ...

1.1 Catalysts: [Titania](#)

Solvents: [Dichloromethane](#); 18 h, rt

1.2 Reagents: [Sodium bicarbonate](#)

Solvents: [Water](#); rt

[Oxidative, photo-activated TiO₂ nanoparticles in the catalytic acetylation of primary alcohols](#)

By: Chen, Chien-Tien; et al

Catalysis Science & Technology (2011), 1(1), 54-57

Full Text ▾

1. synthesis/preparation of... 指定目标反应产物
2. “from”连接物质指定反应物或试剂
3. “in”连接物质指定溶剂

自然语言检索反应识别指定催化剂

Reactions search for "synthesis of paclitaxel catalyzed by triphenylphosphine"

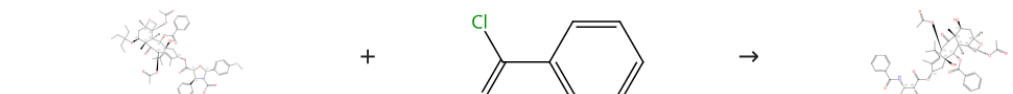
☞ All ☞ Substances **Reactions** ☞ References ☞ Suppliers ☞ Patent Markush

View Related Results ▾

7,007 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 60% ...



Absolute stereochemistry shown, Rotation (-)

1. “catalyzed by” 连接物质指定催化剂
2. “mediated by” 连接物质指定试剂

Reactions search for "synthesis of paclitaxel mediated by triethylamine"

☞ All ☞ Substances **Reactions** ☞ References ☞ Suppliers ☞ Patent Markush

View Related Results ▾

8,823 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 99% ...



Absolute stereochemistry shown, Rotation (-)

Suppliers (139)

31-049-CAS-18450406

1.1 Reagents: [Hydrochloric acid](#)
Solvants: [Ethanol](#), [Tetrahydrofuran](#)
1.2 Reagents: [Formic acid](#), [Triethylamine](#)
Catalysts: [Triphenylphosphine](#)
Solvants: [Tetrahydrofuran](#)
1.3 Reagents: [Pyridinium p-toluenesulfonate](#)
Solvants: [Methanol](#); 24 h, r
1.4 Reagents: [Sodium bicarbonate](#)
Solvants: [Ethyl acetate](#), [Water](#)

Collapse Scheme ▴

31-614-CAS-29999091

Steps: 1 Yield: 99% ...

1.1 Reagents: [Hydrogen](#)
Catalysts: [Palladium](#)
Solvants: [Ethanol](#)
1.2 Reagents: [Trifluoroacetic acid](#)
Solvants: [Acetic acid](#), [Water](#)
1.3 Reagents: [Triethylamine](#)

Synthesis of paclitaxel by protecting the 7-hydroxyl of baccatin III using a strong base and an electrophile
Assignee: Bristol-Myers Squibb Co.
World Intellectual Property Organization, WO9945001 A1 1999-09-10

PatentPak ▾ Full Text ▾

自然语言高效检索人名反应

Reactions search for "suzuki coupling reactions"

🔍 All 📦 Substances 🧪 Reactions 📄 References 🏪 Suppliers 📜 Patent Markush

View Related Results ▾

Filter Results <

Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

Number of Steps

Reaction Scale

Yield

Reaction Type

Catalyst

Reaction Mapping

Stereochemistry

Reagent

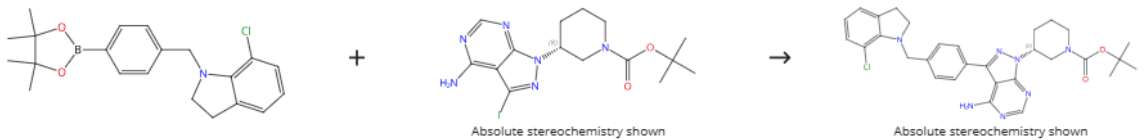
Solvent

Commercial Availability

1,473,931 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 100% ...



Supplier (1) Suppliers (50)

31-179-CAS-11123183 Steps: 1 Yield: 100% ...

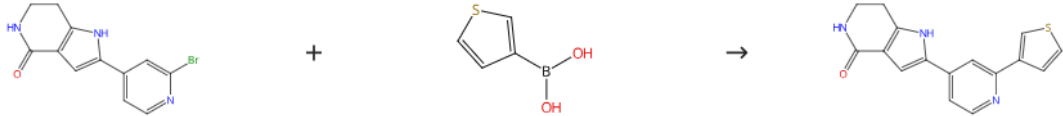
1.1 Reagents: [Potassium carbonate](#)
Catalysts: [Dichloro\[1,1'-bis\(diphenylphosphino\)ferrocene\]pal...](#)
Solvents: [1,4-Dioxane](#), [Water](#); 60 - 90 min, 120 - 140 °C

Preparation of pyrazolo[3,4-d]pyrimidine derivatives useful as inhibitors of Bruton's tyrosine kinase
Assignee: Redx Pharma Limited
World Intellectual Property Organization, WO2014188173 A1 2014-11-27

PatentPak ▾ Full Text ▾

Collapse Scheme ▴

Scheme 2 (1 Reaction) Steps: 1 Yield: 100% ...



^ Catalyst

☐ Tetrakis(triphenylphosphine) palladium (647K)

☐ [1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium (214K)

☐ Palladium diacetate (128K)

☐ Dichloro[1,1'-bis(diphenylphosphino)ferrocene] palladium(II) dichloro methane adduct (119K)

☐ Dichlorobis(triphenyl phosphine)palladium (89K)

[View All](#)

^ Reagent

☐ Potassium carbonate (582K)

☐ Sodium carbonate (378K)

☐ Tripotassium phosphate (187K)

☐ Cesium carbonate (157K)

☐ Hydrochloric acid (124K)

[View All](#)

^ Solvent

☐ Water (1.1M)

☐ 1,4-Dioxane (525K)

☐ Tetrahydrofuran (339K)

☐ Toluene (328K)

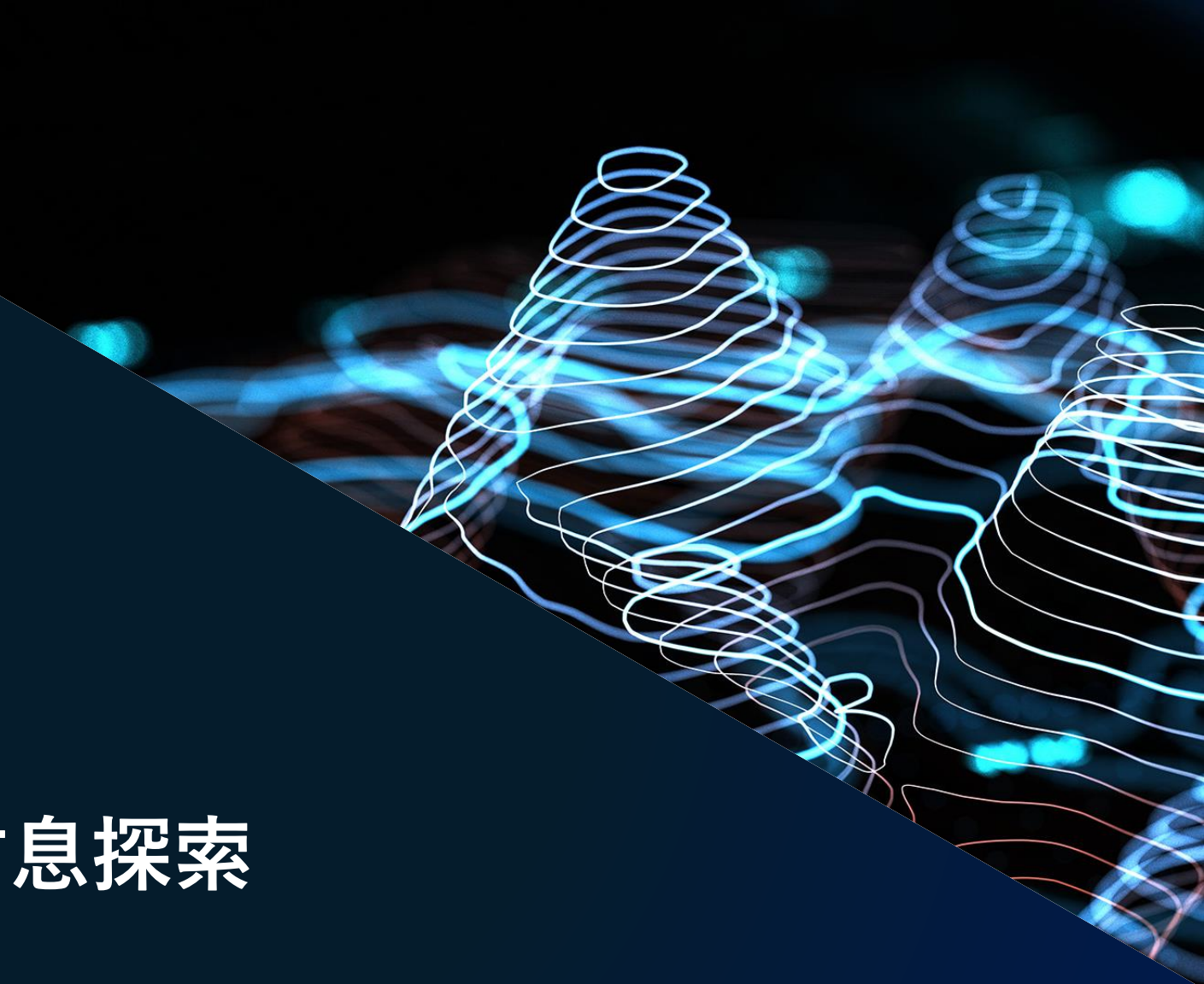
☐ Ethanol (260K)

[View All](#)

利用 CAS 科学家标引的催化剂、试剂和溶剂等信息，高效对比评估反应条件

重点回顾

自然语言快速便捷获取物质理化性质、实验谱图与安全信息，加速表征判断；
高效聚焦反应操作流程与产率，直观查阅实验方案与反应数据，节省关键信息的查阅时间；优化交互界面，新增一键筛选开放获取文献、含有物质与反应标引、权利要求和 **PatentPak** 等选项，高效定位目标文献。



CAS BIOFINDER[®]

人工智能助手助力药化信息探索

检索式问答回答药物研发问题



Good Morning, Cyrene

Ligands

Scaffolds

Proteins

Diseases

Search by protein, ligand, disease or draw a structure.



AI Assistant

BETA

Chat with CAS BioFinder's AI agent to answer your drug discovery questions.

What are you searching for today, Cyrene?

What can I help you with?



What small molecule inhibitors of ABL1 show high selectivity over PDGFRB?



What are the known off-target interactions of Ibrutinib, how do these contribute to adverse events?



What downstream pathways and proteins might be impacted by inhibiting TNFA?

CAS BioFinder 全面整合药物研发信息, 获取可靠答案



Based on the comprehensive analysis of bioactivity data in the BioFinder database, several small molecule inhibitors demonstrate high selectivity for ABL1 over PDGFRB. Here are the most selective compounds:

Top Selective ABL1 Inhibitors

1. Imatinib and Imatinib Mesylate

- [Imatinib](#) [1] (IC₅₀ vs ABL1: 0.038 nM)
- [Imatinib mesylate](#) [2] (K_i vs ABL1: 0.05 nM)
- Selectivity ratios : 200,000-480,000x over PDGFRB
- SMILES :
O=C(NC1=CC=C(C(=C1)NC=2N=CC=C(N2)C3=CN=CC=C3)C)C4=CC=C(C(=C4)CN5CCN(C)CC5

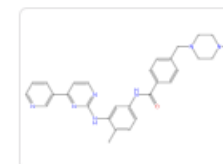
2. Pyrido[2,3-d]pyrimidin-7(8H)-one Derivative

- [Compound](#) [3] (pK_i vs ABL1: 0.50 nM)

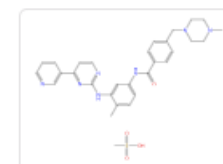
Sources

7 Results

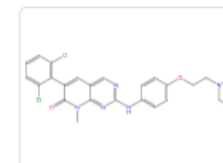
- [1] [Imatinib](#)
CAS Registry Number: 152459-95-5

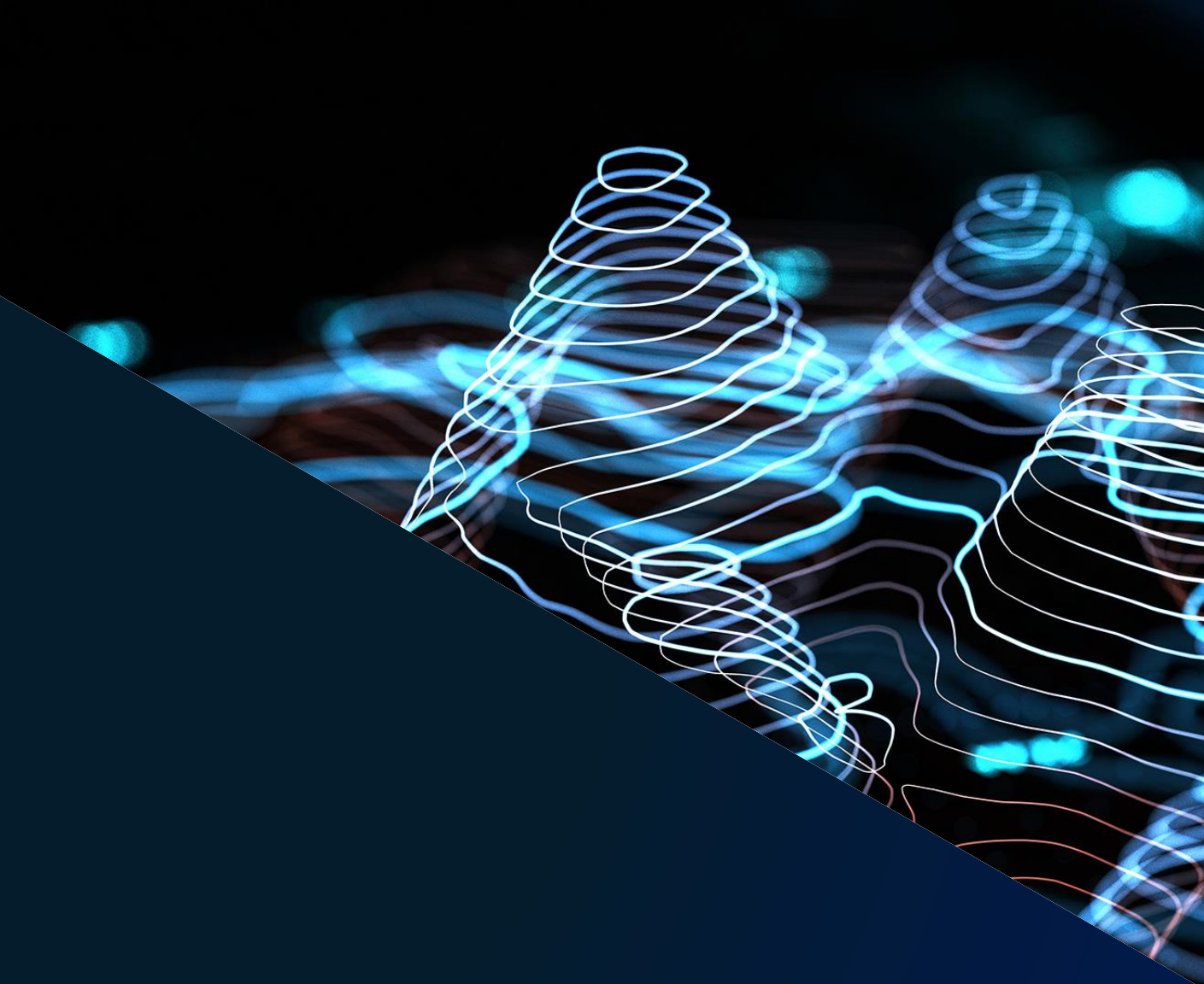


- [2] [Imatinib mesylate](#)
CAS Registry Number: 220127-57-1



- [3] [6-\(2,6-Dichlorophenyl\)-2-\[\[4-...](#)
CAS Registry Number: 185039-89-8

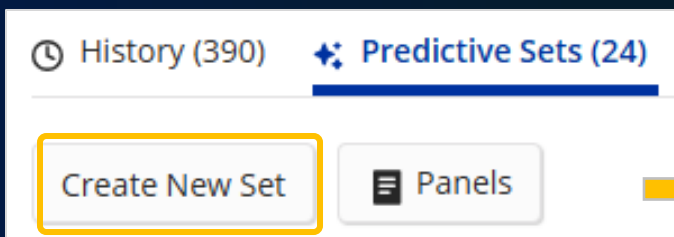
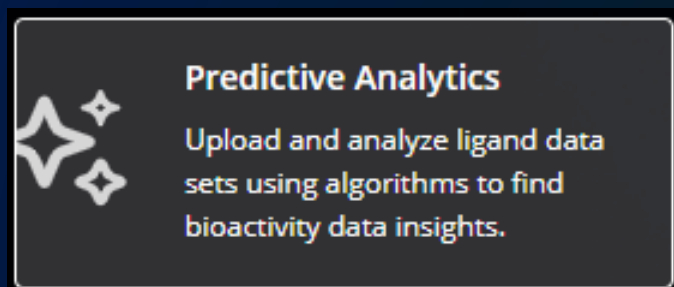




CAS BIOFINDER

药物靶点活性预测示例

哪些关注的分子可能和目标靶点有相互作用？



Create Predictive Analytics Set

Name your set
Predictive_Set_08_29_2025_1324

Select Color
Light Blue

Select Panel
PARP

Upload a predefined set (Optional)

Select a file (.sdf) or drag and drop here.

Create Cancel

上传sdf格式的结构文件
支持多个配体同时预测

[Predictive Analytics Description](#)

CAS Full Pharmacology (Default)
CAS Broad Safety Screen
CAS Medium Safety Screen
CAS Narrow Safety Screen
CAS Alzheimer's Disease Screen
CAS Breast Cancer Screen
CAS Colon Cancer Screen

选择包含不同靶点的预测面板,
亦可自定义面板

哪些关注的分子可能和目标靶点有相互作用？

[Return to Predictive Analytics](#)

Set Summary

Rerun Set Analysis

Complete - Last ran 28 Aug 2025

PARP

Total ligands: 12

Neighbors: 41

Metabolites: 40

Targets: 4

Filters

pActivity

Confidence Score

Target

☐ Poly [ADP-ribose] polymerase 1

☐ Poly [ADP-ribose] polymerase 2

Organism

Apply

Return to top

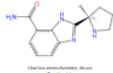
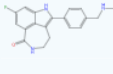
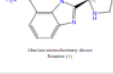
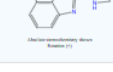
PARP - Intelligence

批量预测 关注结构与指定靶点间的相互作用

Ligands Pharmacology

Show Structures

ON

Ligand	Target	Organism	Known pAct	Predicted pAct	Confidence	Method
 912444-00-9	Poly [ADP-ribose] polymerase 1	Mus musculus	8.52	8.51	0.52	● ● ● ● ●
 283173-50-2	Poly [ADP-ribose] polymerase 1	Homo sapiens	7.91	8.24	0.6	● ● ● ● ●
 912444-00-9	Poly [ADP-ribose] polymerase 2	Homo sapiens	8.25	8.20	0.71	● ● ● ● ●
 912444-00-9	Poly [ADP-ribose] polymerase 1	Homo sapiens	8.77	8.01	0.62	● ● ● ● ●
 283173-50-2	Poly [ADP-ribose] polymerase 2					● ● ● ● ●

Test XXX

自定义预测靶点

Targets to Include in Panel

Target	Organism	Uniprot ID
☒ Prostaglandin F2-alpha receptor	Felis catus	6L9K4
☒ Gag-pol polyprotein	Escherichia coli	A0A0A0F4Y0
☒ Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	Rattus norvegicus	A0A0G2K344
☒ Dihydroorotate dehydrogenase (quinone)	Plasmodium falciparum Dd2	A0A0L7M6L3
☐ Bifunctional dihydrofolate reductase-thymidylate synthase	Cryptosporidium hominis	A0A0S4TER9
☐ Dihydrofolate reductase	Cryptosporidium hominis	A0A0W0CF37

结构、靶点、有机体、活性数据(实验和预测值)、可信度分数助力评估最佳预测信息

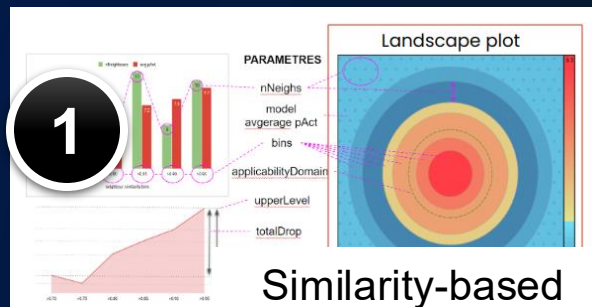
26

© 2025 American Chemical Society. All rights reserved.

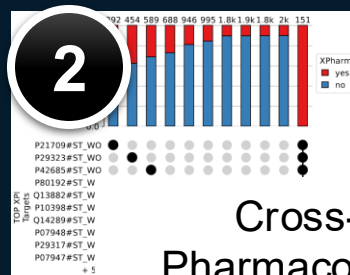
CAS
A division of the
American Chemical Society

药物靶点活性预测

预测配体对蛋白质靶点的活性



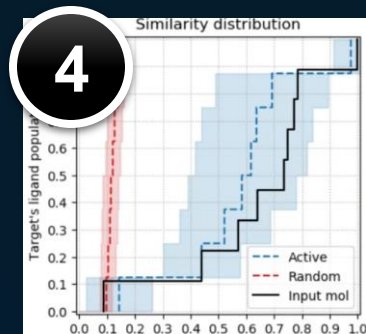
Similarity-based method (SIM)



Cross-Pharmacology Index (XPI)



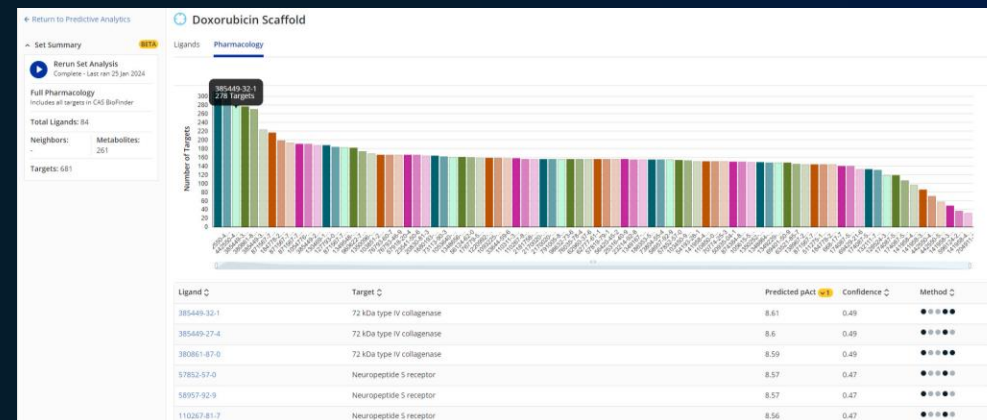
Machine Learning Method (MLM)



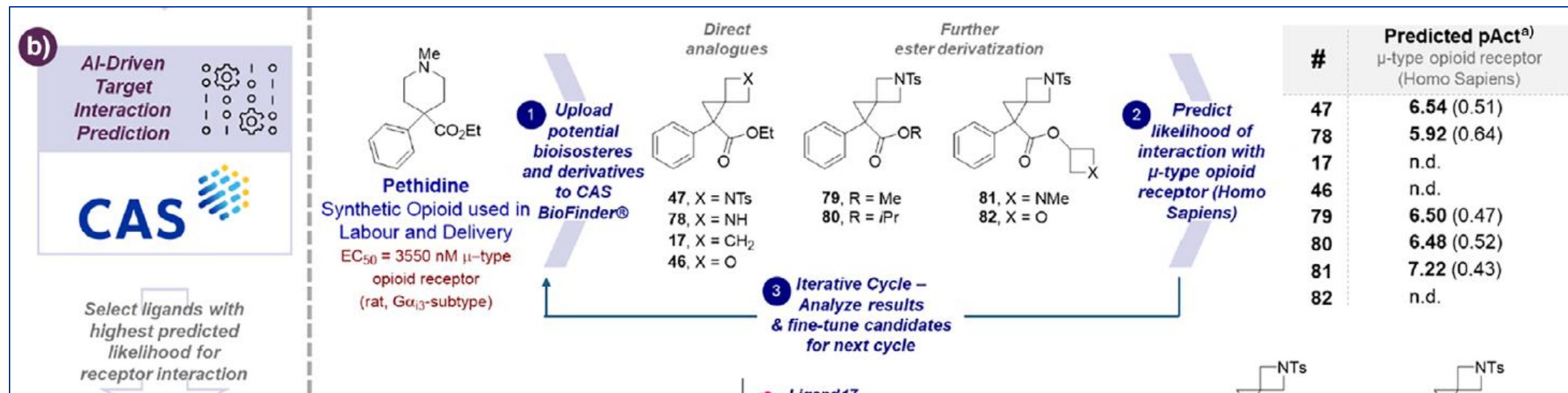
Similarity ensemble approach (SEA)



配体对靶点的活性预测：
多模型集成共识值



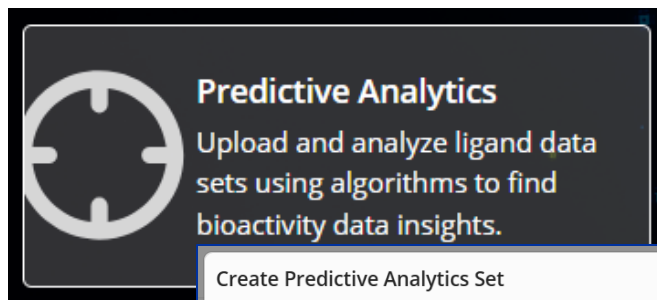
CAS BioFinder 加速“合成→评估→优化”药物发现流程，尤其适用于缺乏历史活性数据的全新骨架



- AI增强的靶点活性预测：
确定5-氮杂螺[2.3]己烷可以模拟哌啶后，作者利用CAS BioFinder的AI预测功能，对一系列哌替啶类似物与 μ -阿片受体的相互作用进行打分（pAct值）和置信度评估（图4b）。实现了：
 - 快速筛选高潜力候选分子（如化合物**47**、**78**、**81**）；
 - 指导结构优化（如酯基替换为氮杂环丁基显著提升预测活性）；
 - 大幅缩小体外实验范围，提高研发效率。
- 验证预测可靠性：体外实验结果与BioFinder预测高度一致（高pAct值对应实测微摩尔活性），证明了该工具在新型骨架生物活性初筛中的实用价值。

doi.org/10.1002/anie.202521633

CAS BioFinder 靶点活性预测功能大幅降低体外实验范围，提高研发效率



Create Predictive Analytics Set

Name: Predictive_Set_12_16_2025_1535

Color: Light Blue

Panel: opioid receptor

Upload a predefined set (Optional)

Select a file (.sdf) or drag and drop here.

批量导入配体结构sdf文件

opioid receptor

Targets to Include in Panel

opioid receptor

Target	Organism	Uniprot ID
☐ Delta-type opioid receptor	Mus musculus	P32300
☐ Delta-type opioid receptor	Rattus norvegicus	P33533
☐ Kappa-type opioid receptor	Mus musculus	P33534
☒ Mu-type opioid receptor	Rattus norvegicus	P33535
☐ Kappa-type opioid receptor	Rattus norvegicus	P34975
☐ Mu-type opioid receptor	Homo sapiens	P35372
☒ Delta-type opioid receptor	Homo sapiens	P41143

Selected Targets

Sigma non-opioid intracellular receptor 1 (Mus musculus)

Kappa-type opioid receptor (Homo sapiens)

Delta-type opioid receptor (Homo sapiens)

Mu-type opioid receptor (Mus musculus)

Mu-type opioid receptor (Cavia porcellus)

Mu-type opioid receptor (Rattus norvegicus)

自定义靶点库

Ligand	Target	Predicted pAct	Confidence
78	Sigma non-opioid intracellular receptor 1 (Rattus norvegicus)	8.53	0.36
81	Kappa-type opioid receptor (Homo sapiens)	7.68	0.39
80	Delta-type opioid receptor (Homo sapiens)	7.1	
47	Delta-type opioid receptor (Homo sapiens)	7.1	
79	Delta-type opioid receptor (Homo sapiens)	7.1	
81	Mu-type opioid receptor (Homo sapiens)	7.1	
81	Delta-type opioid receptor (Homo sapiens)	6.1	
79	Kappa-type opioid receptor (Homo sapiens)	6.1	
80	Kappa-type opioid receptor (Homo sapiens)	6.1	

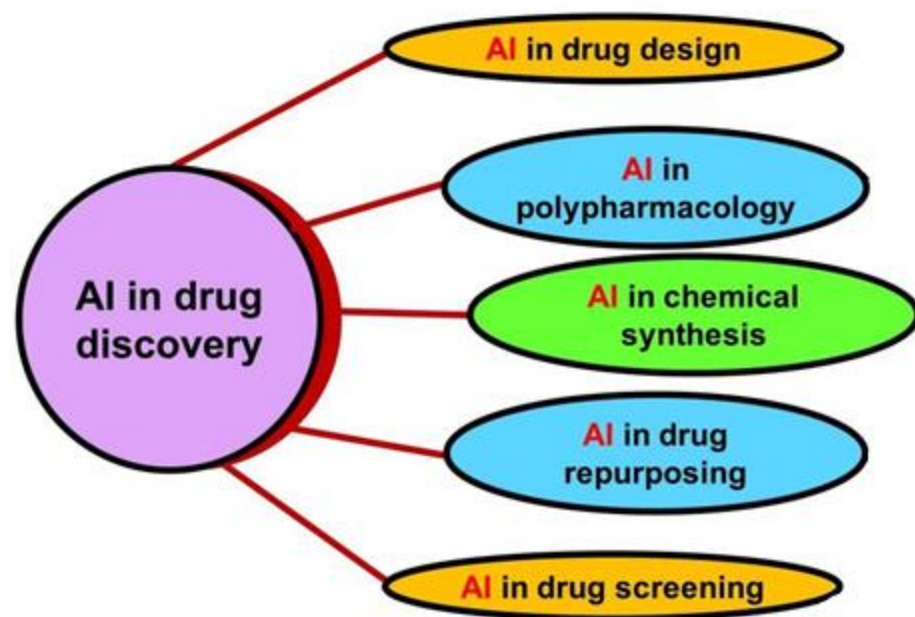
CAS BioFinder预测配体和靶点作用分值与置信度评估

47	Kappa-type opioid receptor (Homo sapiens)	6.62	0.46
47	Mu-type opioid receptor (Homo sapiens)	6.54	0.51
79	Mu-type opioid receptor (Homo sapiens)	6.50	0.47
80	Mu-type opioid receptor (Homo sapiens)	6.48	0.52
78	Mu-type opioid receptor (Cavia porcellus)	6.35	0.44
78	Sigma non-opioid intracellular receptor 1 (Cavia porcellus)	6.10	0.36
78	Mu-type opioid receptor (Homo sapiens)	5.92	0.64
78	Kappa-type opioid receptor (Homo sapiens)	5.63	0.60
17	Sigma non-opioid intracellular receptor 1 (Cavia porcellus)	5.05	0.53
78	Delta-type opioid receptor (Homo sapiens)	5.00	0.70
78	Mu-type opioid receptor (Rattus norvegicus)	4.95	0.52
82	No predicted activity for this ligand against panel targets	-	-
46	No predicted activity for this ligand against panel targets	-	-

人工智能的机会与挑战

AI 在药物发现中的应用

机会



Paul D et al. Artificial intelligence in drug discovery and development. Drug Discov Today. 2021

挑战

October 19, 2023 09:37 AM EDT Updated 11:05 AM | AI, In Focus

[in](#) [X](#)

ENDPOINTS *in* FOCUS

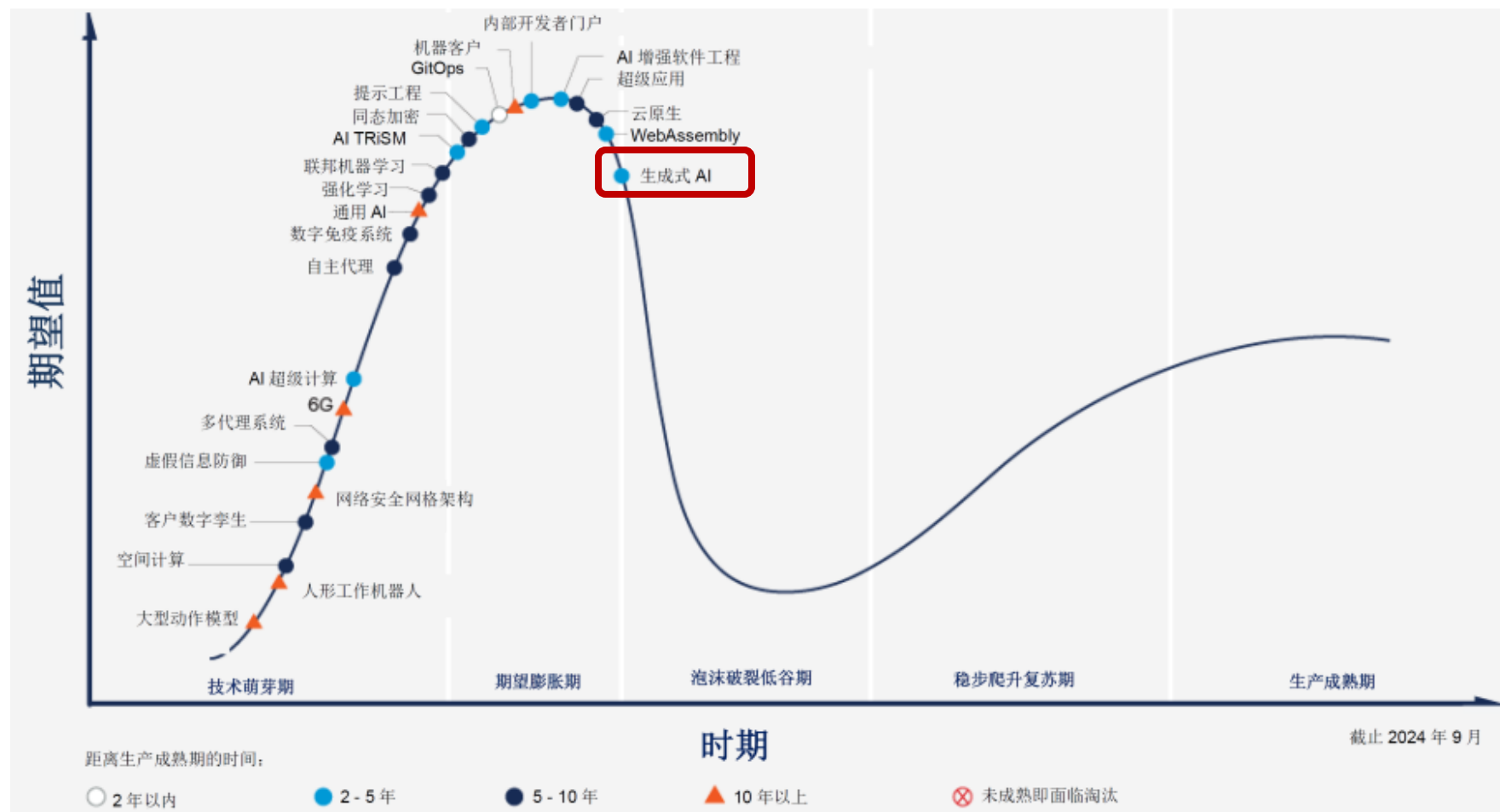
After years of hype, the first AI-designed drugs fall short in the clinic



Andrew Dunn
Senior Biopharma Correspondent

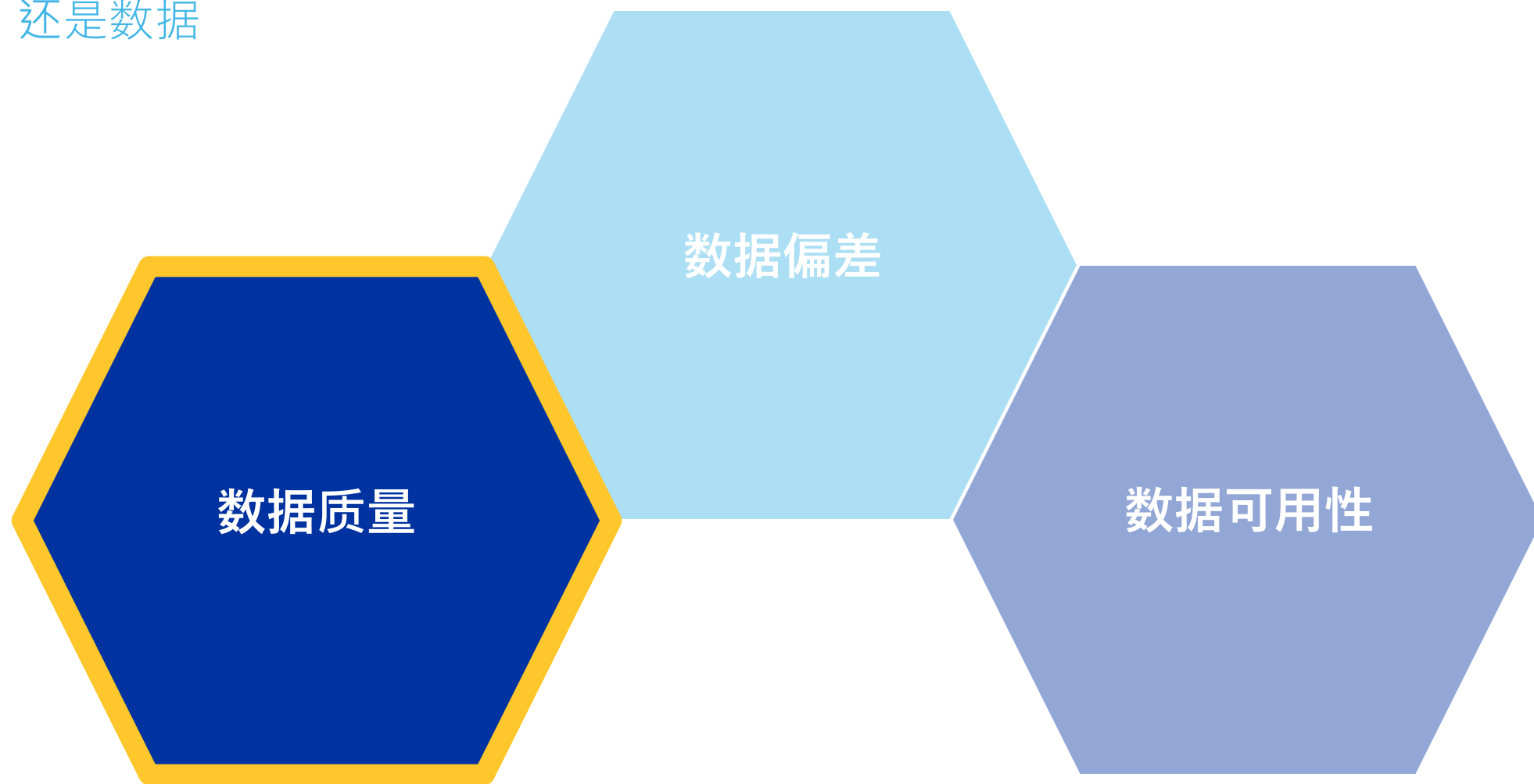
新兴技术成熟度曲线

Gartner Hype Cycle™, 2024



是什么原因导致了这些挑战的出现？

数据，还是数据



数据不一致

导致下游问题

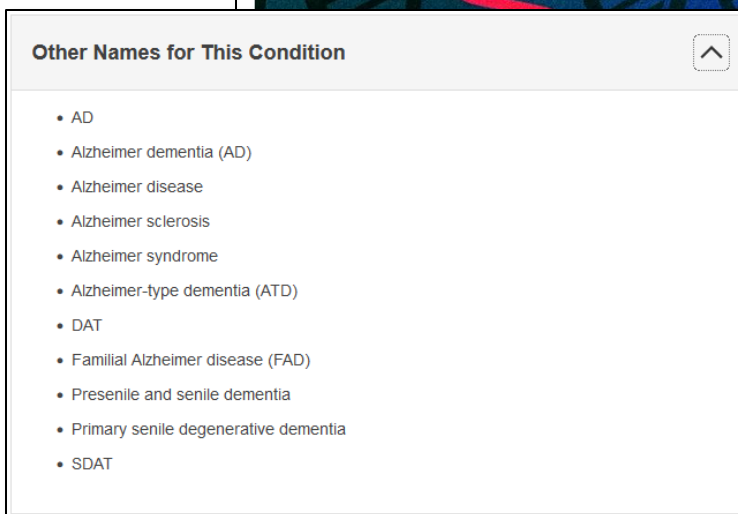
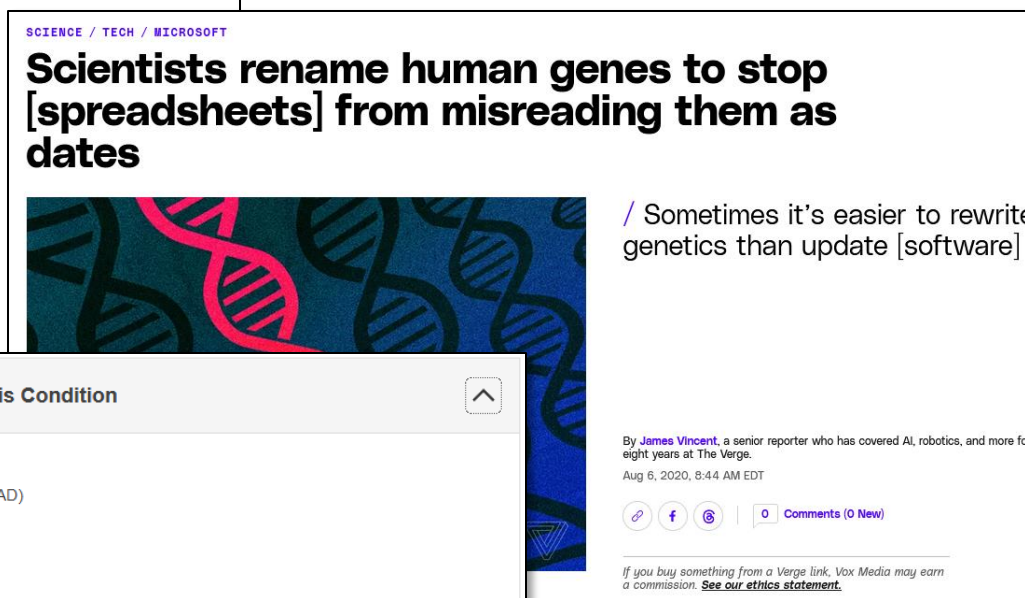
同一实体存在多个名称

各实验室命名标准不一

作者输入错误

技术处理误差

数据库与ID系统差异



协调实现一致性

人工策展是提升AI效率的基石

纠正错误

整合异构数据

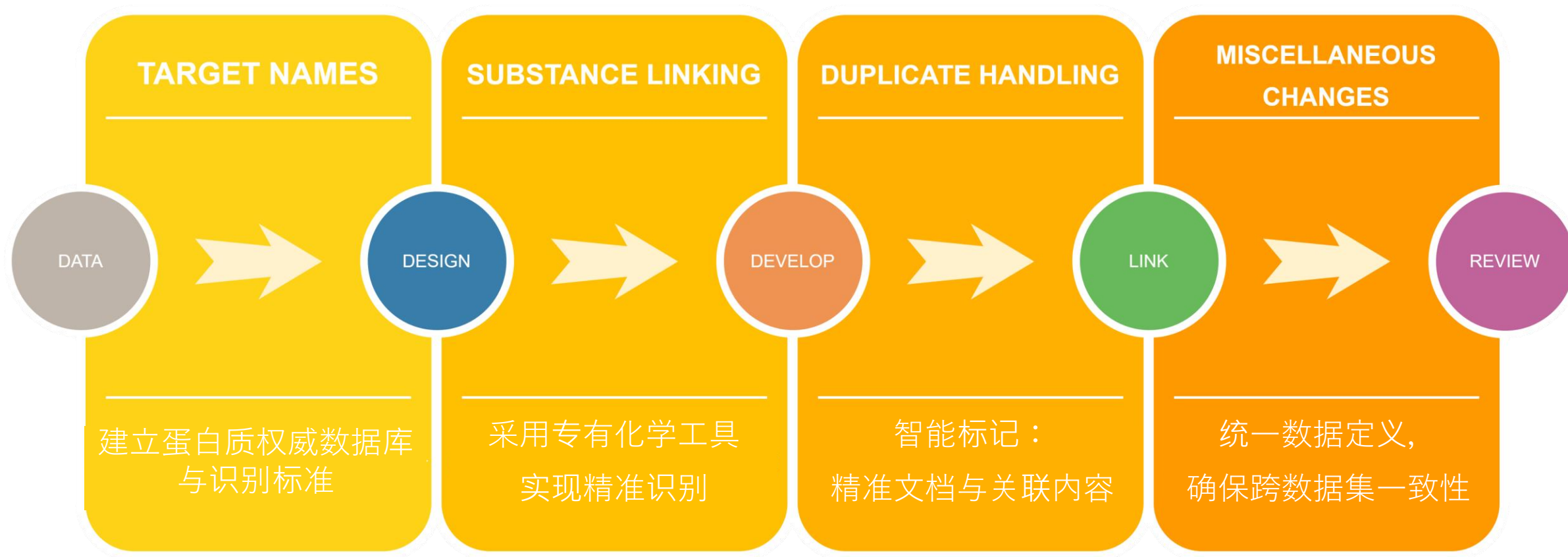
跨源连接

数千名科学家与技术专家的监

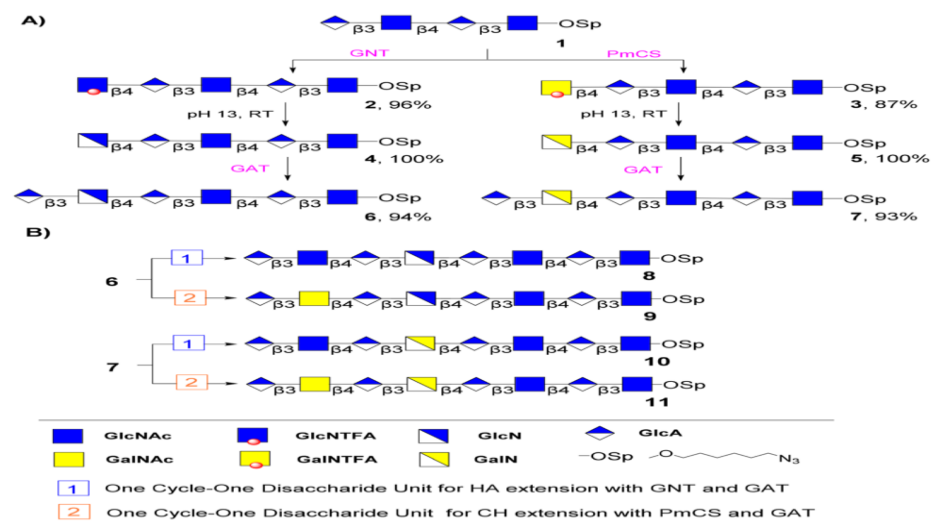
督与辅助



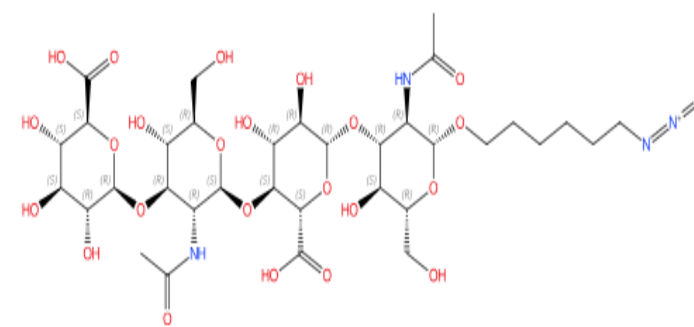
数据协调的流程



人工策展的必要性

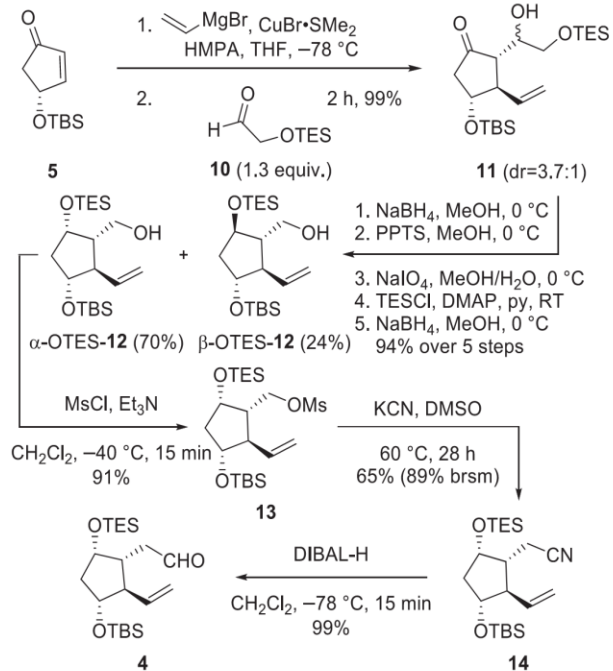


10.1039/d2gc04071a



Compound 1

人工策展的必要性



Scheme 3. Synthesis of the key intermediate 4.

RN 2378367-10-1

RN 2378367-11-2

RNs 2378367-12-3
and 2378367-13-4

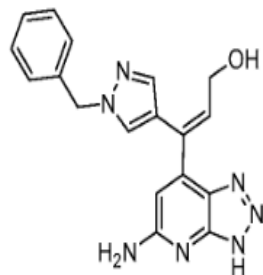
RNs 2378367-14-5
and 2378367-15-6

4.6. ((1*S*,2*R*,3*R*,5*S*)-3-(*tert*-Butyldimethylsilyloxy)-5-(triethylsilyloxy)-2-vinylcyclopentyl)methanol (α -OTES-12)

To a stirred solution of **11** (2.3 g, 5.56 mmol, 1.0 equiv) in methyl alcohol (50 mL) at 0 °C was added sodium borohydride (1.05 g, 27.8 mmol, 5.0 equiv). After 30 min, the reaction mixture was quenched with saturated NH₄Cl solution (10 mL) at 0 °C. The aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated *in vacuo*. Without any purification, pyridinium *p*-toluenesulfonate (419 mg, 1.67 mmol, 0.3 equiv) was added to **crude mixture** in methyl alcohol (50 mL) at 0 °C. After 70 min, the reaction mixture was quenched with saturated NH₄Cl solution (10 mL) at 0 °C. The aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated *in vacuo*. Without any purification, sodium periodate (2.38 g, 11.12 mmol, 2.0 equiv) was added to **crude mixture** in methyl alcohol (25 mL) and water (25 mL) at 0 °C. After 30 min, water (10 mL) was added to the reaction mixture. The aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated *in vacuo*. Without any purification, chlorotriethylsilane (1.87 mL, 11.12 mmol, 2.0 equiv) and 4-dimethylaminopyridine (34 mg, 0.278 mmol, 0.05 equiv) were added to **crude mixture** in pyridine (25 mL) at room temperature. After 20 min, water (10 mL) was added to the reaction mixture. The aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated *in vacuo*. The residue was purified by column chromatography (Ethyl acetate:*n*-Hexane = 1:30) on silica gel to obtain the product α -OTES-12 (1.5 g, 70% isolated yield) as colorless oil and its diastereomer 24% isolated yield: TLC *R*_f = 0.39 (α -OTES-12), 0.3 (β -OTES-12, silica gel, Ethyl acetate:*n*-Hexane = 1:9); [α]_D²⁵ = +18.6 (*c* = 1.0, CHCl₃); IR(neat) ν _{max} 2956, 2930, 2878, 1471, 1362, 1251, 1131, 1073, 1006, 894, 836, 776, 744, 670 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 5.60 (ddd, *J*_{AB} = 16.8 Hz, *J*_{AC} = 10.2 Hz, *J*_{AD} = 8.4 Hz, 1H),

人工策展的必要性

16A. (E)-3-(1-Benzyl-1*H*-pyrazol-4-yl)-3-(3-trityl-5-(tritylamino)-3*H*-[1,2,3]triazolo[4,5-*b*]pyridin-7-yl)prop-2-en-1-ol:



结构和名称不匹配

- Stereochemistry is inconsistent between name and structure
- Name indicates trityl protecting groups, but none are shown

CAS 专家解决不一致性问题

- Examine the starting materials and molecular mass
- The structure is correct as named

- 5 A mixture of Intermediate 2 (127 mg, 0.158 mmol), 1-benzyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-pyrazole (54.0 mg, 0.190 mmol), K₂CO₃ (109 mg, 0.792 mmol) and PdCl₂(dppf)-CH₂Cl₂ adduct (12.9 mg, 0.016 mmol) was dissolved in 1:1 THF /water in a pressure-rated vial. The vial was evacuated and backfilled 3x with Ar, then heated behind a blast shield at 80 °C for 2 hours. The reaction mixture was
- 10 diluted with water and EtOAc. The aq. phase was extracted 3x with EtOAc. The combined organic phases were washed with brine, dried with Na₂SO₄, filtered and concentrated. The product was the purified by silica gel chromatography to provide 16A. (97 mg , 74 %), as a yellow oil. MS (ESI): *m/z* 832.5 (M+H).

专业技术的独特应用

使用连接的结构化数据更快地生成更相关的结果

精选数据结果

专利和期刊

**受控词汇
标引物质**

CA Classification Code (CA section and section cross-references):
28-16 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 1, 7, 27, 63

Patent Classifications (IPC, CPC, NCL, ECLA, ICD, FTERM codes):

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 3683219	IPC	C07D0471-04 [1]; A61P0025-28 [1]; A61K0031-519 [1]
	IPC	C07D0471-04 [1]; A61K0031-519 [1]; A61P0025-28 [1]

Patent Information Table:

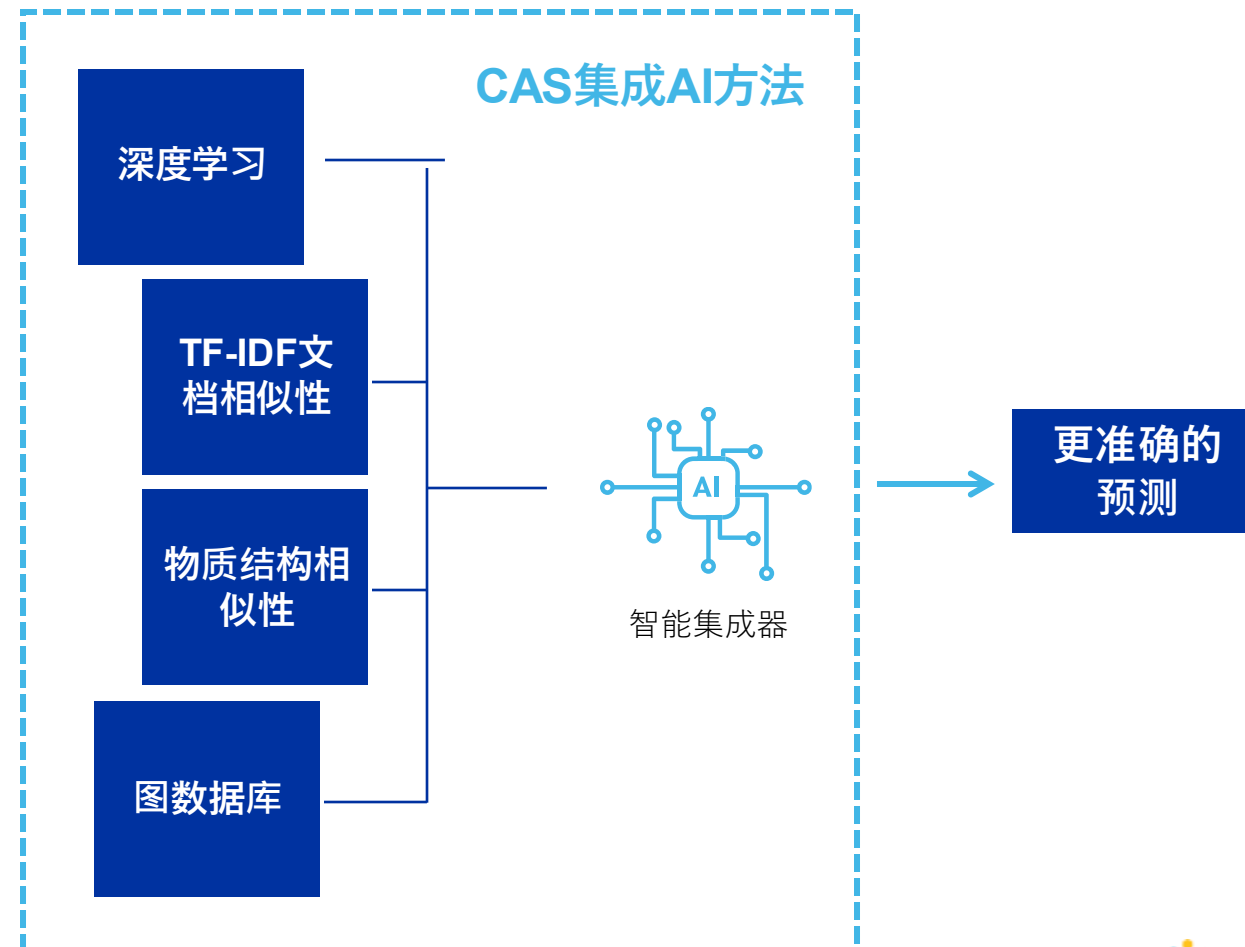
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 3683219	A1	20200722	EP 2019-151900	20190115
WO 2020148153	A1	20200723	WO 2020-EP0402	20200109

Chemical Structure and Classification:

Alzheimer disease
Anti-Alzheimer agents
Behavior
Blood
Blood-brain barrier
Carbamoylation
Carbamoylation kinetics
Cholinesterase inhibitors
Cognition enhancers

Propr...

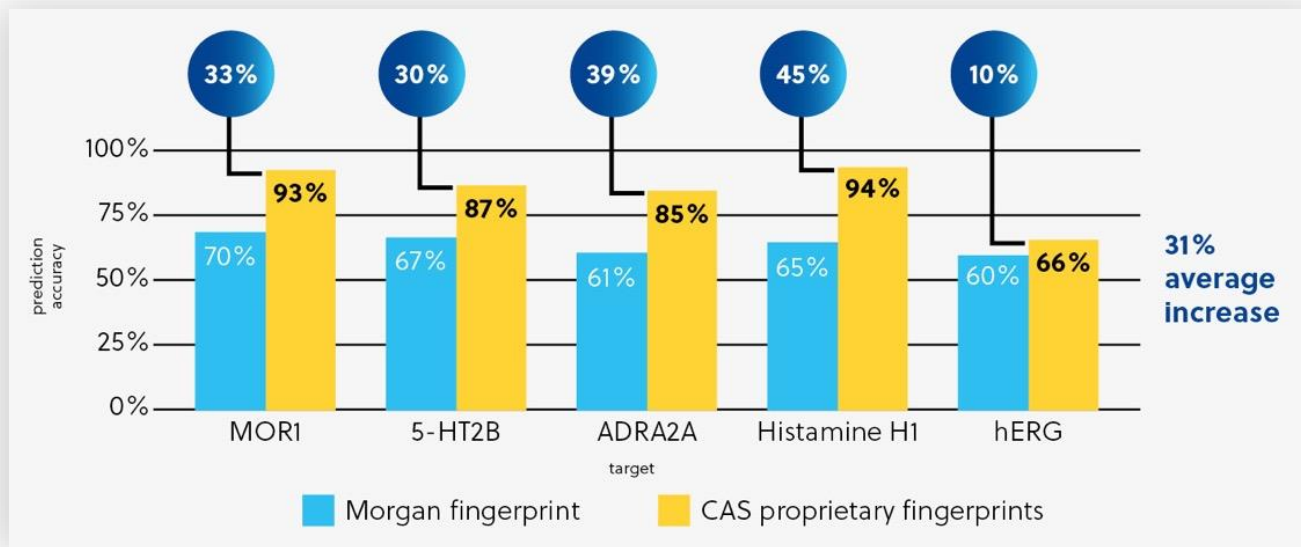
Chemical structure diagram showing a complex molecule with a carbamate group and a cholinesterase inhibitor moiety.



专利族、IPC分类、CAS分类

预测精度显著提高

当人工智能在科学家策划的内容上接受训练时



更高质量的化学描述符（分子指纹）改善了人工智能算法寻找生物活性化合物的预测结果

来源：知识产权组织

协调数据的价值

高质量数据产生更优结果

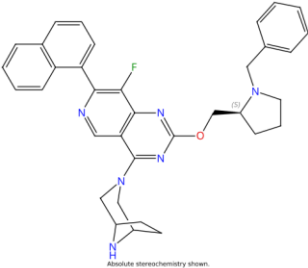
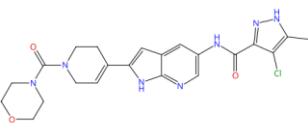
- CAS拥有全面的标准化生物活性数据
- 用于重新训练现有模型

预测值
与实验值
差异减少

56%

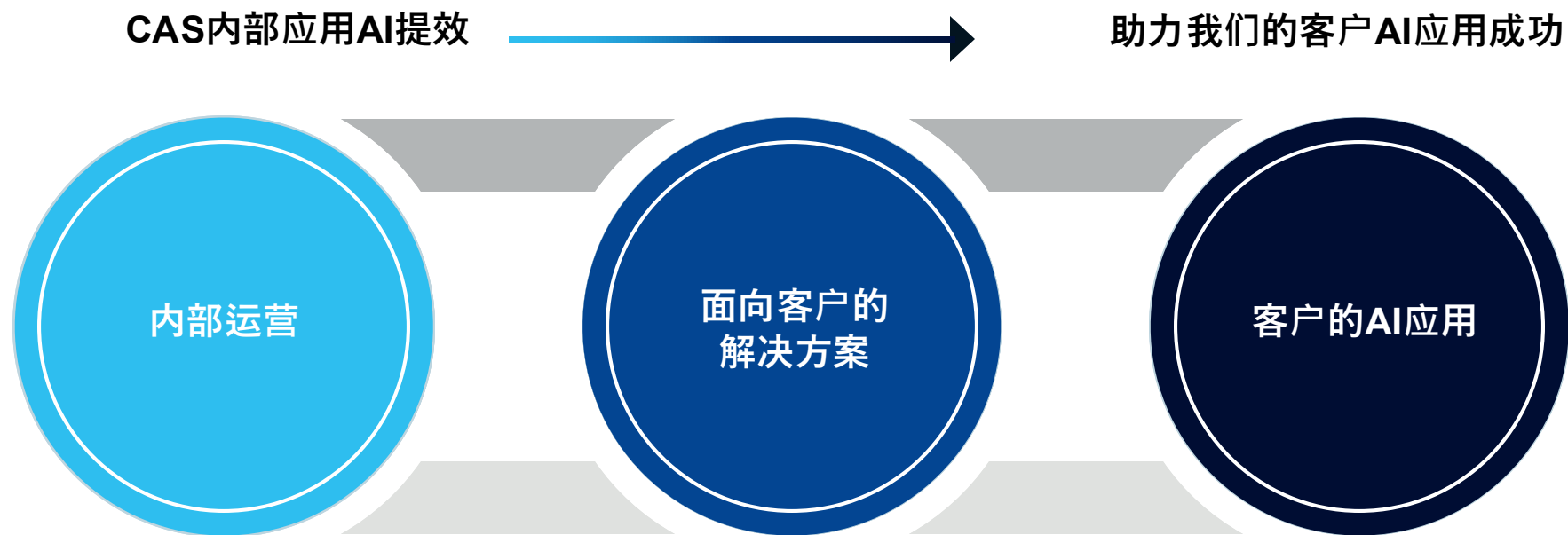
预测值
与实验值
标准差降低

23%

配体	靶点	p值 (实验值)	原始 模型	重训练 模型
	KRas	4.2	11.1	4.8
	KIT	10.0	4.4	9.9

CAS 在 AI 领域的持续投入

优化运营，推动解决方案，助力客户AI应用落地



CAS高质量数据助力人工智能模型结果提升

案例分享



Regio-MPNN: predicting regioselectivity for general metal-catalyzed cross-coupling reactions using a chemical knowledge informed message passing neural network

“After adding [high-quality data from the CAS Content Collection](#), there is an increase in the data portion of Heck, Hiyama, Negishi and Kumada coupling reactions.”

The model achieved [>96% accuracy](#)



Learning organo-transition metal catalyzed reactions by graph neural networks

- “[CAS reaction data](#) has the advantage that it is [essentially error-free because of human curation](#). In addition, we can refer to the original papers to examine the reaction mechanism.”
- The model achieved [97% accuracy](#)

Pharma Company

Leveraged curated reaction data from CAS

- Suzuki and amide coupling reactions
- Reduced AI preprocessing time
- Incorporated into synthetic reaction workflow

“We would not have attempted to build these predictive models without CAS data.”



In Silico Insights: QSAR Modeling of TBK1 Kinase Inhibitors for Enhanced Drug Discovery

- Published by CAS
- QSAR modeling based on multiple ML techniques and molecular descriptors
- All data from the [CAS Content Collection](#)

线上学习资源



扫码访问 CAS SciFinder 学习中心
便捷查阅视频课程、专题论坛和检索技巧等资源

微信公众号：ACS美国化学会



本次论坛口令：

数据与AI

微信公众号回复论坛口令
获得PPT分享链接

问卷调研及抽奖

您的意见对我们非常重要！

欢迎微信**视频号观众**扫码留言，

小鹅通观众可直接在直播窗口填写问卷，

我们将选取**5**位幸运观众，

送出**CAS**定制咖啡杯！

*幸运观众名单将会收到我们的邮件通知。



感谢关注！

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@CASchemistry

