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

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美国化学文摘社中国代表处

2/25/2026

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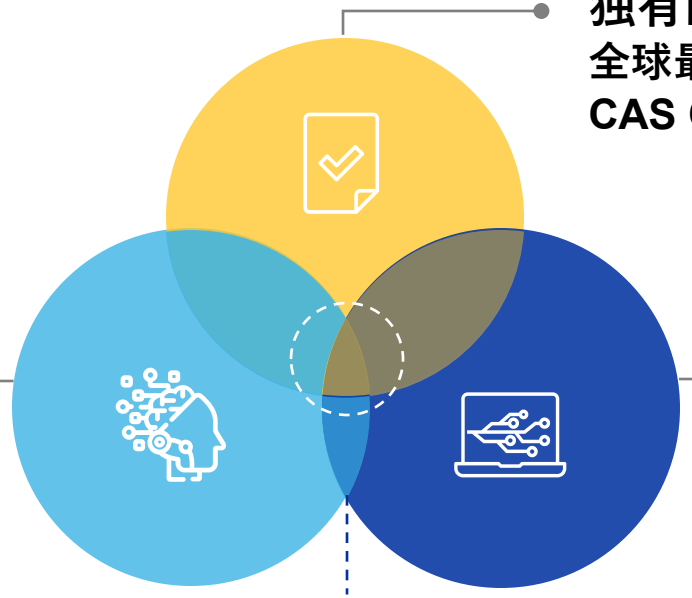

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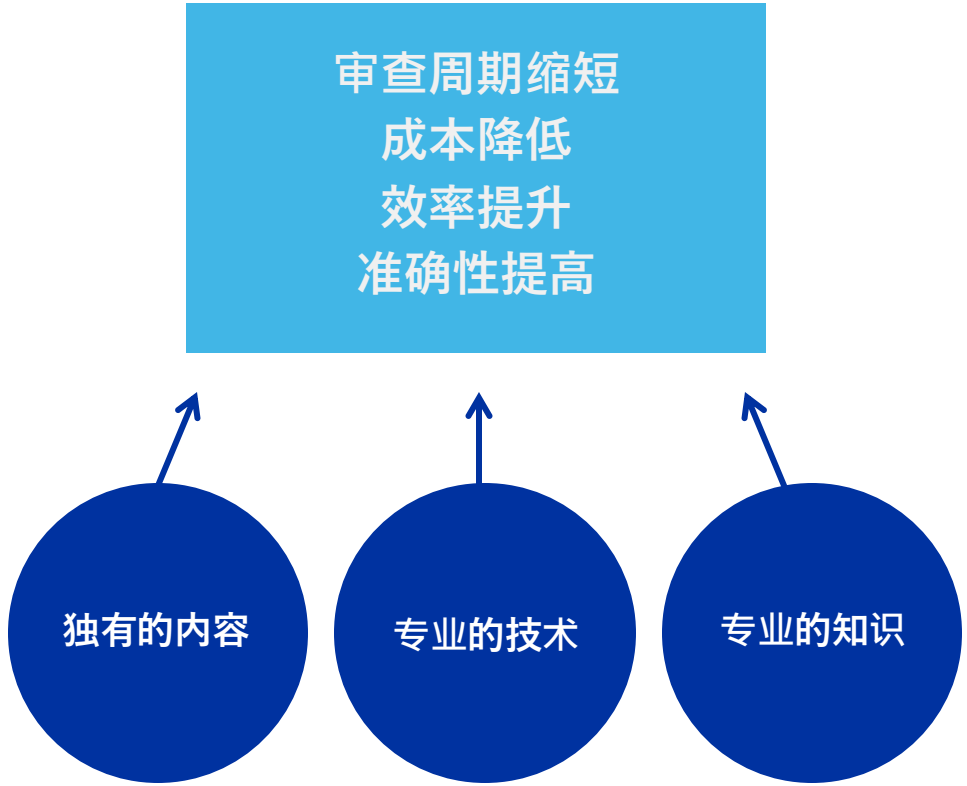

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- 用于现有技术检索的AI/ML算法
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- 跨学科的深厚科学/技术知识
- CAS检索专家预先筛选
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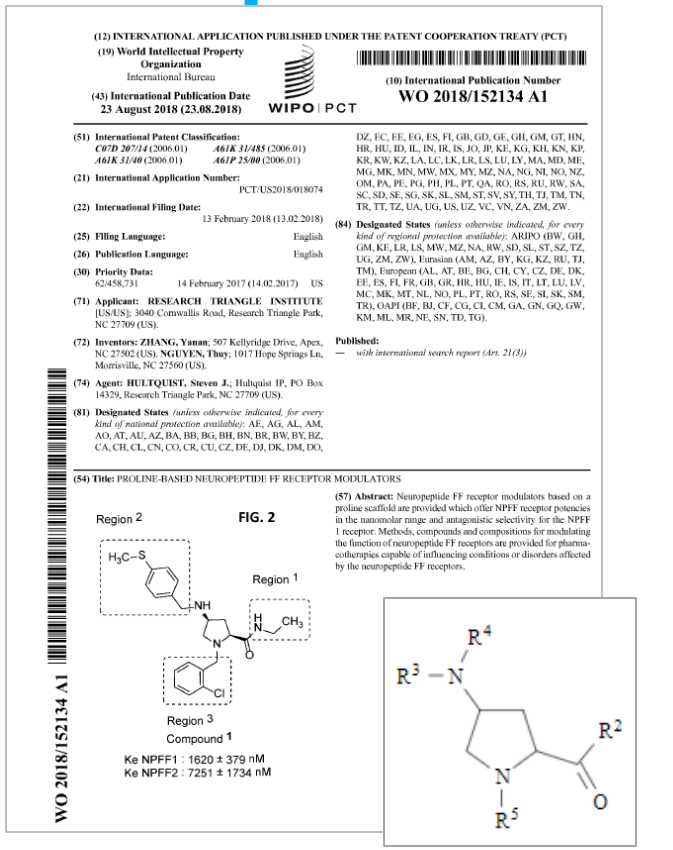
CAS结构化数据实现知识提取

以专利WO2018152134为例

改写的标准和摘要，尽可能揭示专利核心价值

丰富的增值标引信息：

- **19** Concepts
- **163** Substances
- **625** Reactions
- **15** Patent Family Members
- **3** Formulations
- **1** Markush structure
- **18** SAR data points
- **141** ADME data points



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WIPO | PCT

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Published:
— *with international search report (Art. 21(3))*

(54) Title: PROLINE-BASED NEUROPEPTIDE FF RECEPTOR MODULATORS

(57) Abstract: Neuropeptide FF receptor modulators based on a proline scaffold are provided which offer NPFF receptor potencies in the nanomolar range and antagonistic selectivity for the NPFF 1 receptor. Methods, compounds and compositions for modulating the function of neuropeptide FF receptors are provided for pharmacotherapies capable of influencing conditions or disorders affected by the neuropeptide FF receptors.

FIG. 2

Region 2 Region 1 Region 3

Compound 1

Ke NPFF1 : 1620 ± 379 nM
Ke NPFF2 : 7251 ± 1734 nM

WO 2018/152134 A1

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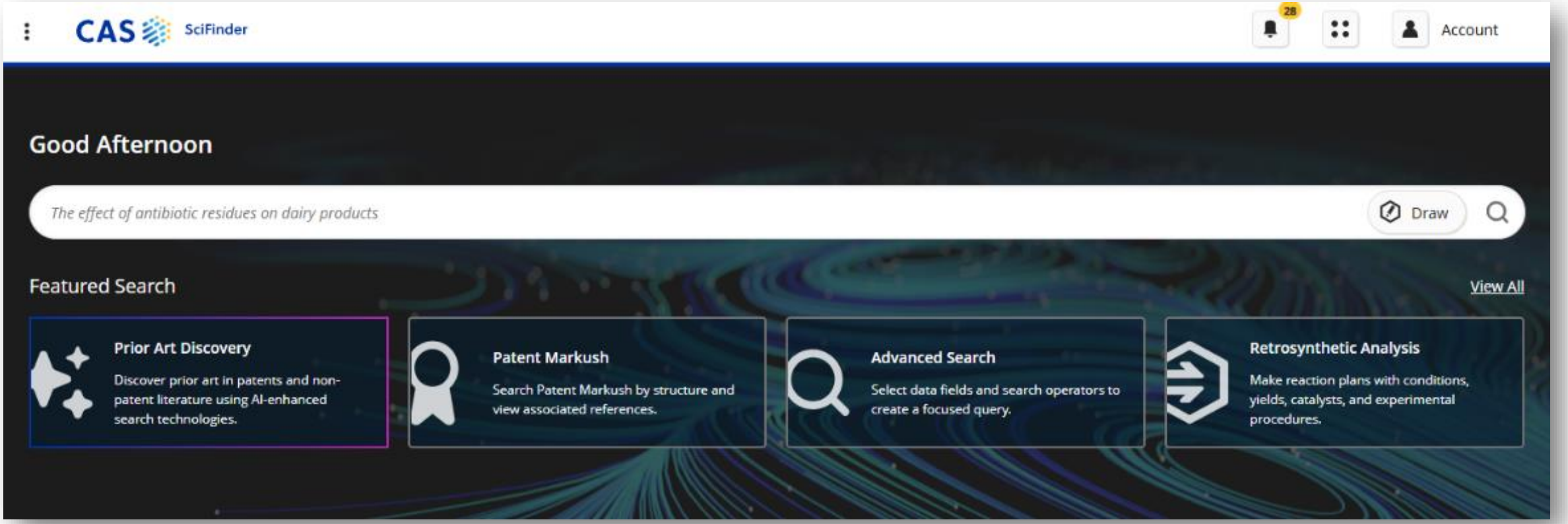
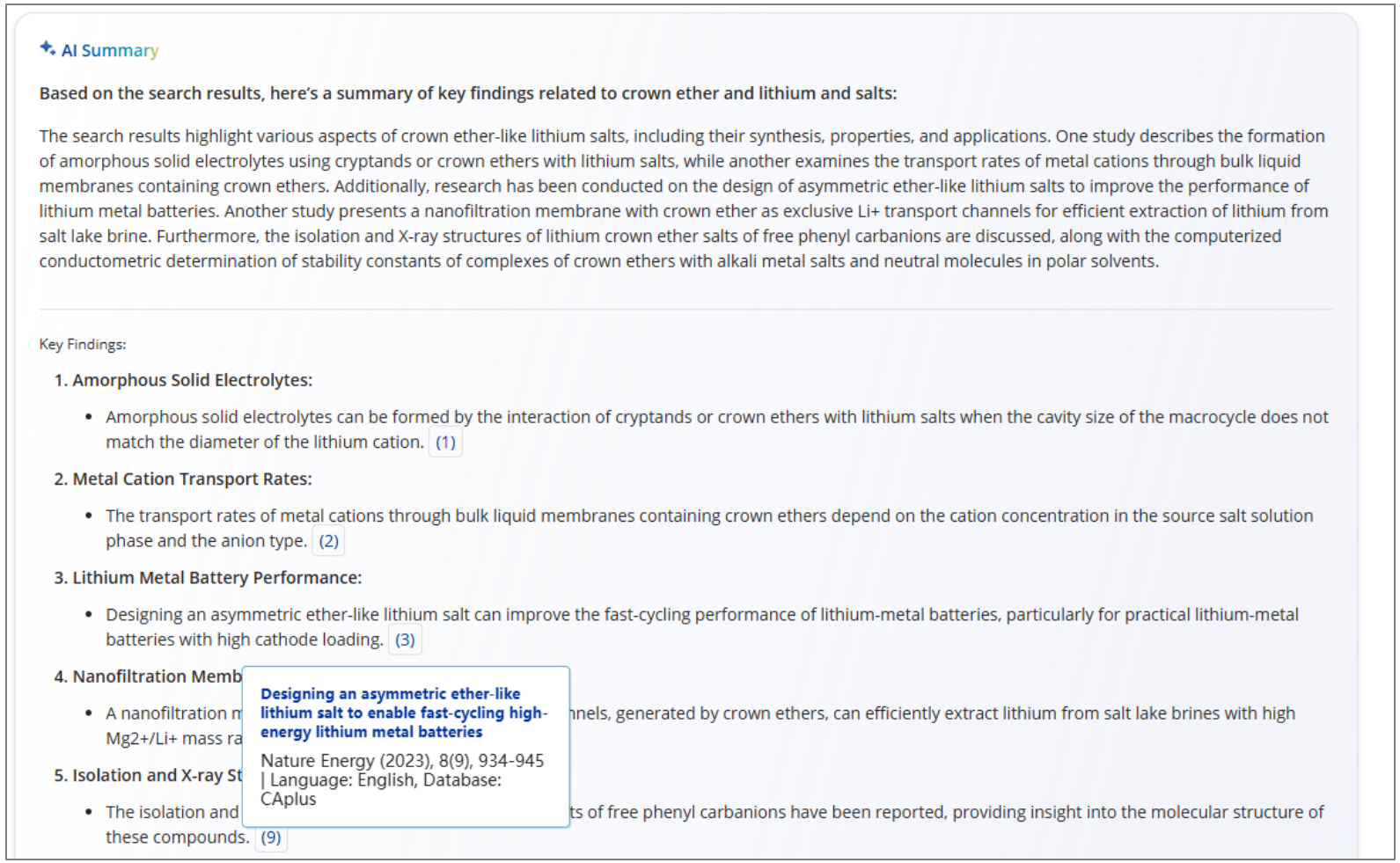
界面直观简洁，节省查找各选项时间



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 Memb**
   - A nanofiltration m nnels, generated by crown ethers, can efficiently extract lithium from salt lake brines with high Mg2+/Li+ mass ra
5. **Isolation and X-ray St**
   - The isolation and ts 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

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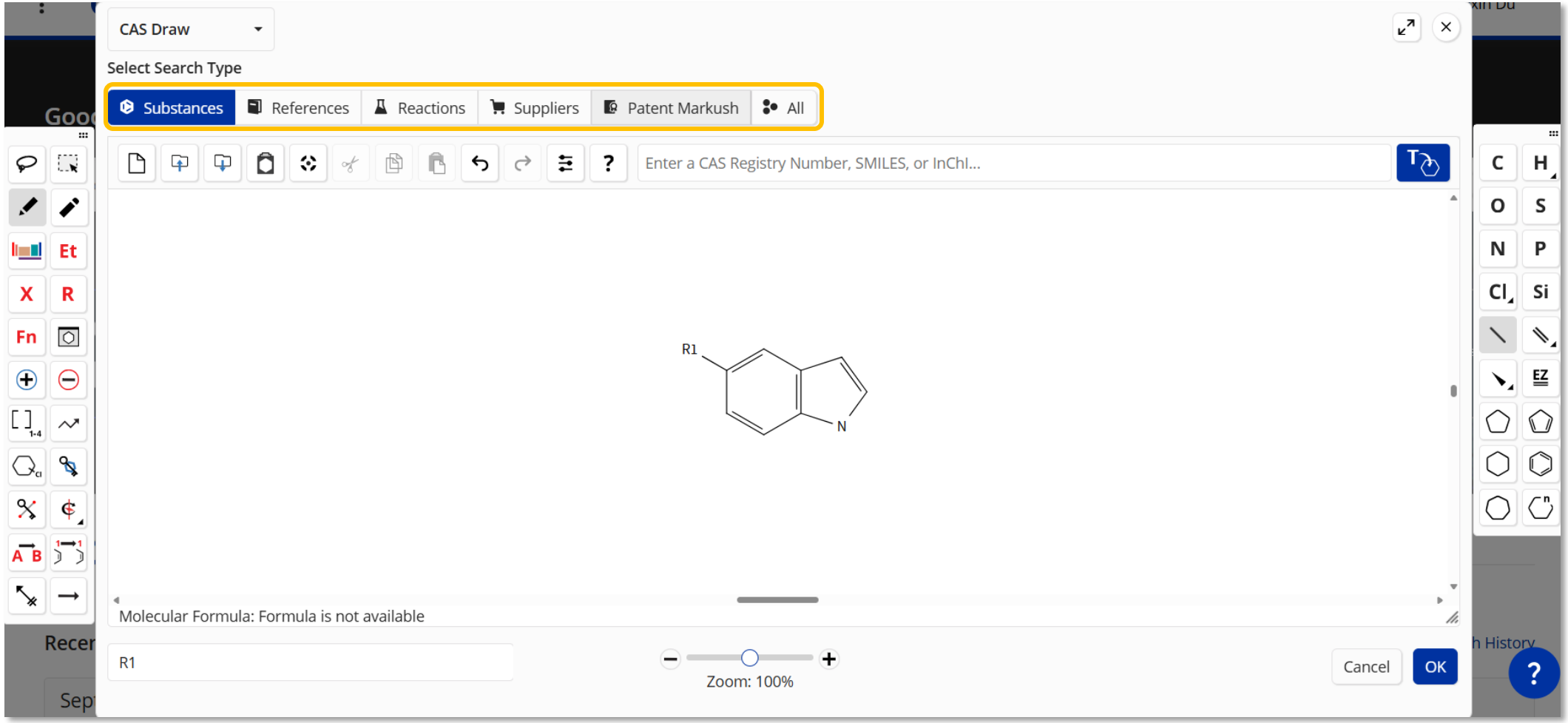

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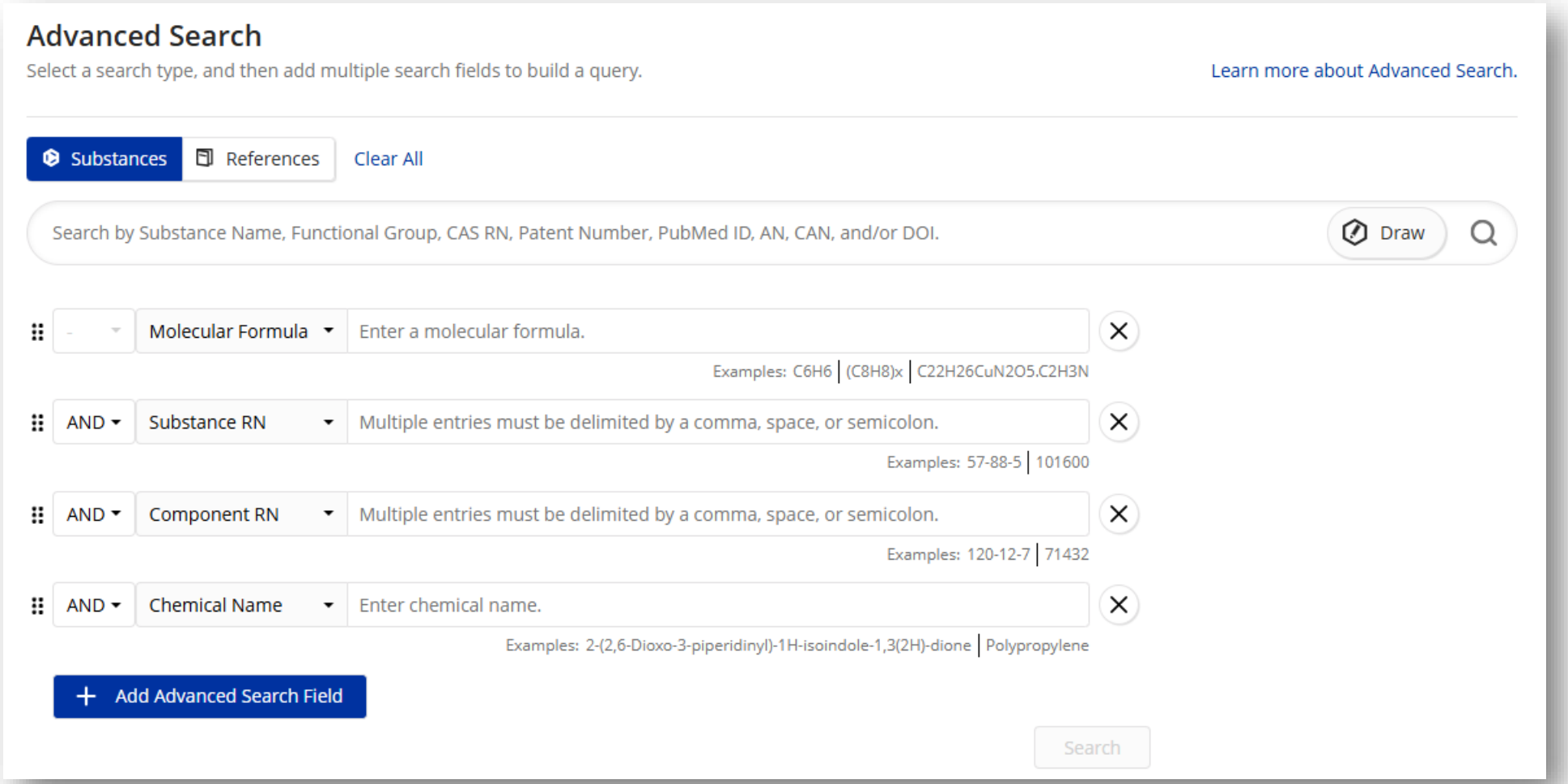

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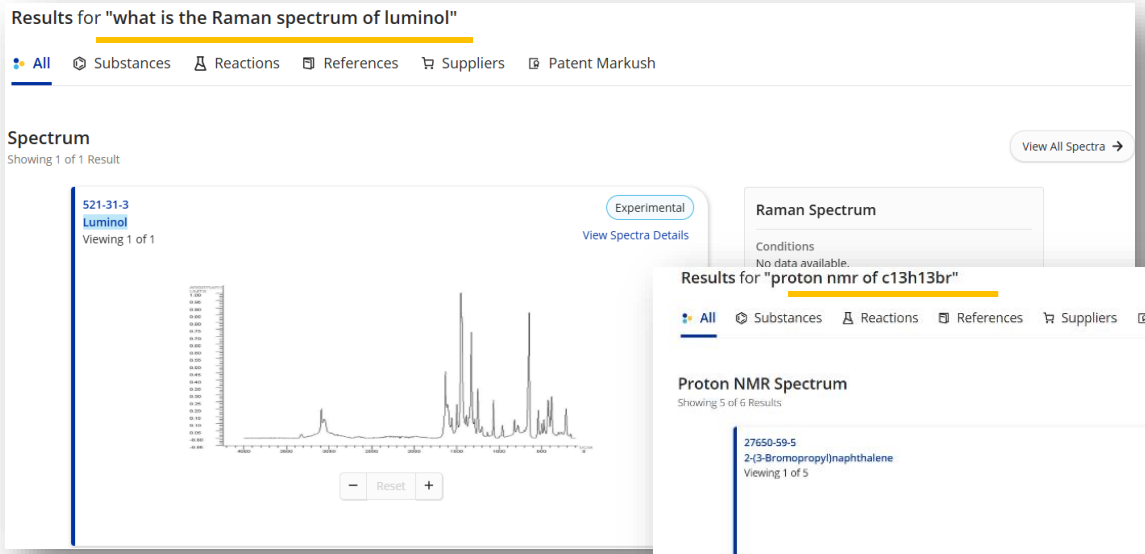
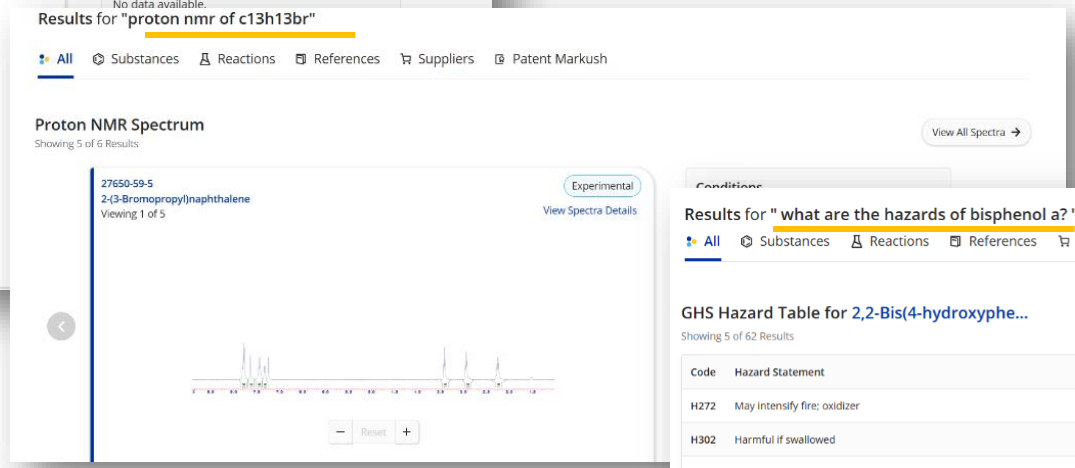
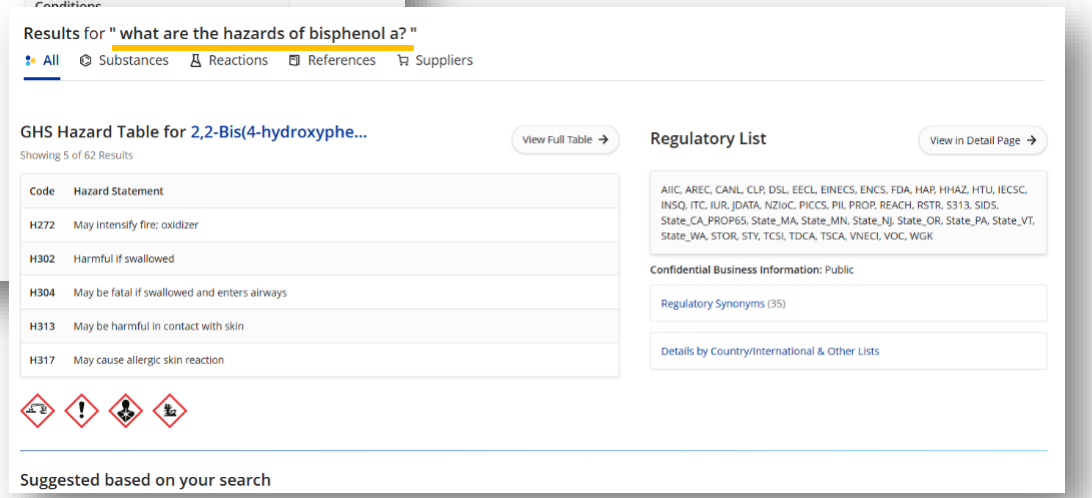
扩展问答类型，快速聚焦物质谱图和安全信息



自然语言直接查阅Raman谱图



自然语言直接查阅NMR谱图



自然语言直接查阅物质安全信息

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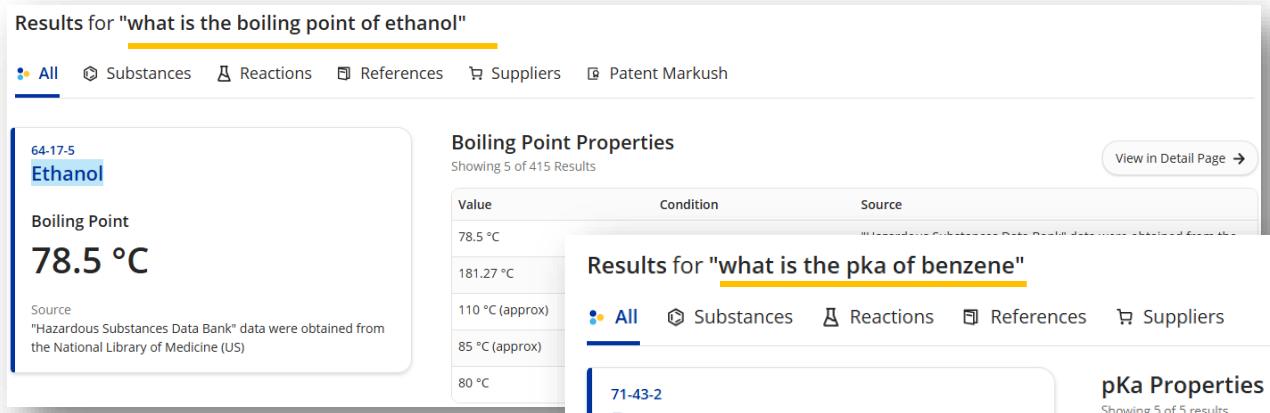
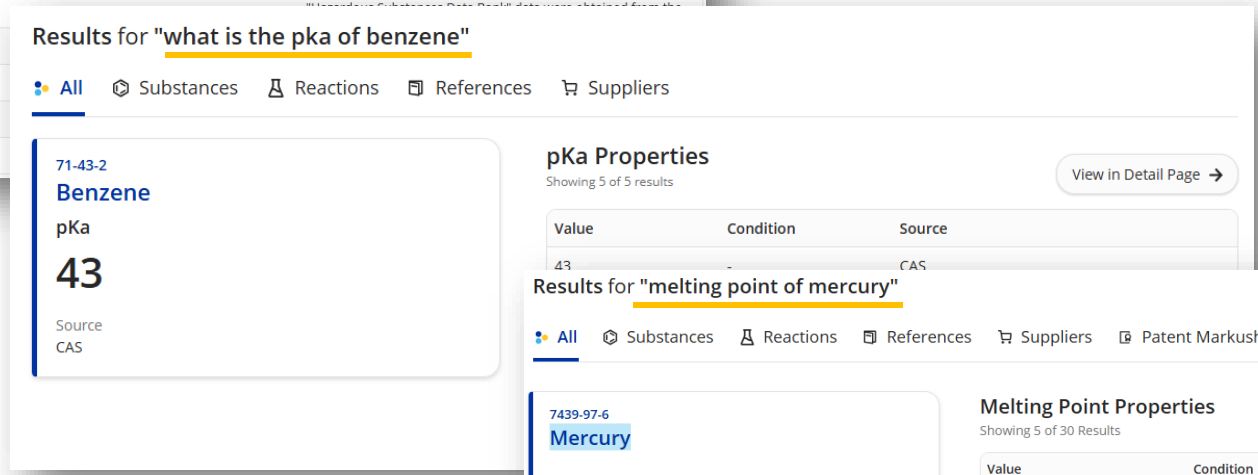
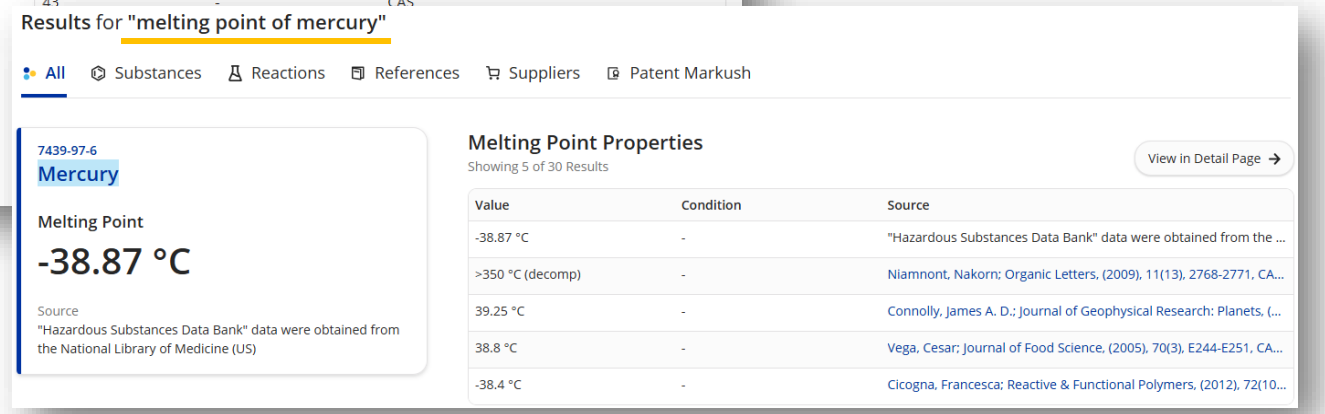
支持自然语言直接检索物质理化性质，直观高效



自然语言直接查阅物质沸点



自然语言直接查阅pKa值



自然语言直接查阅熔点

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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

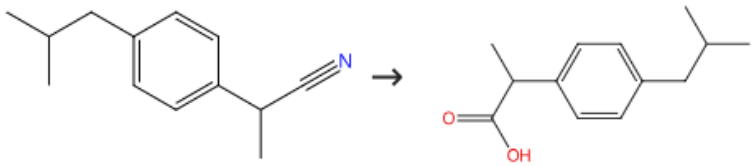
Showing 1 of 1,084 Results

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

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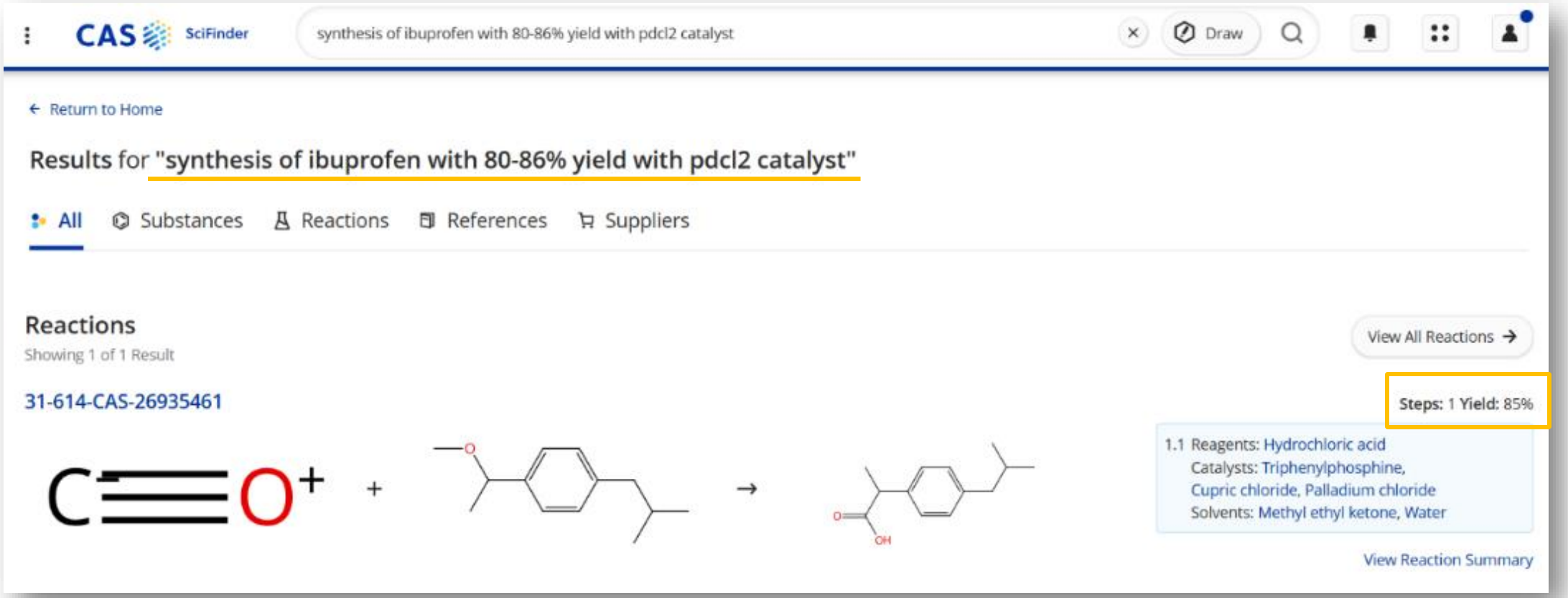
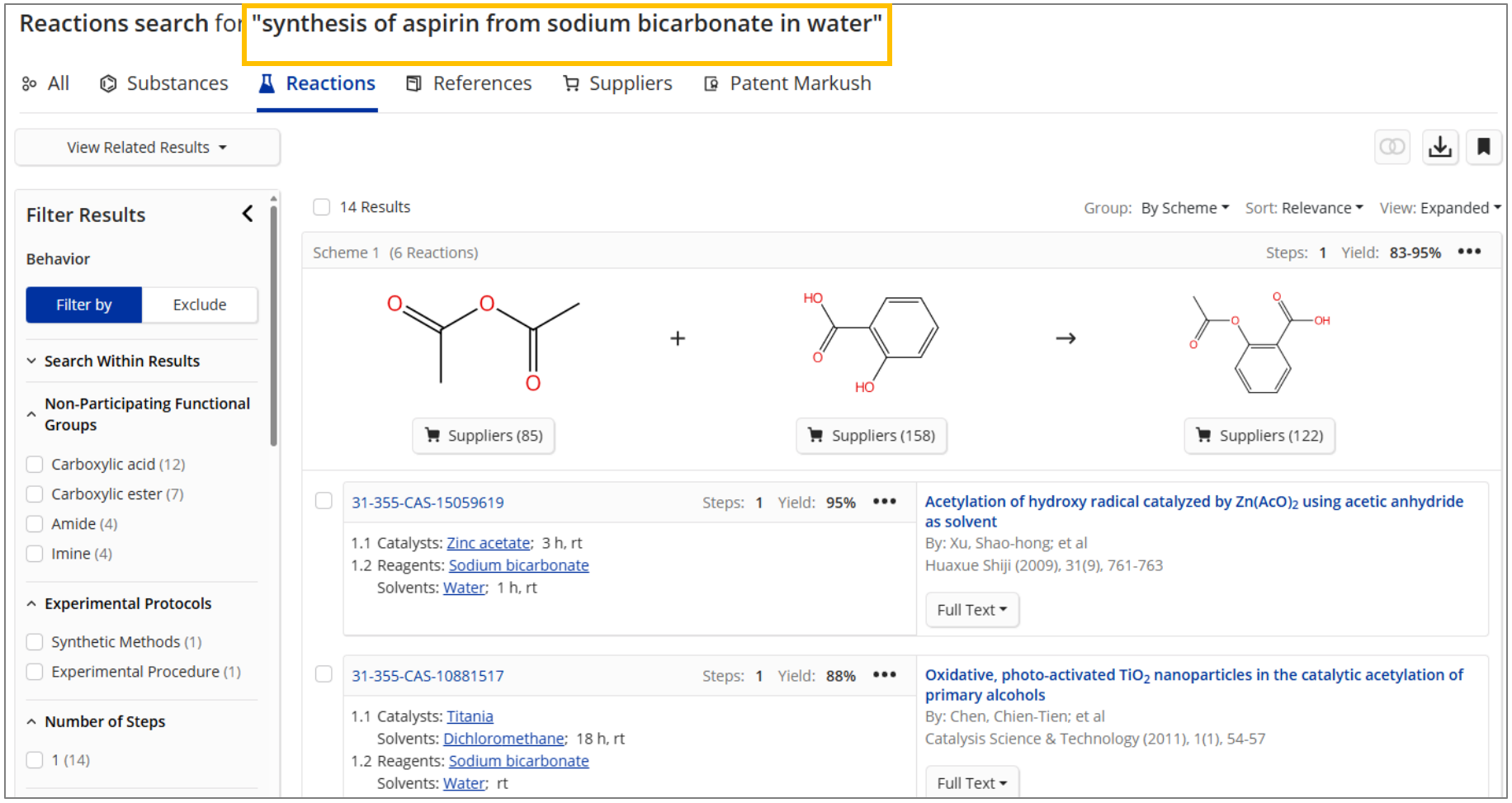


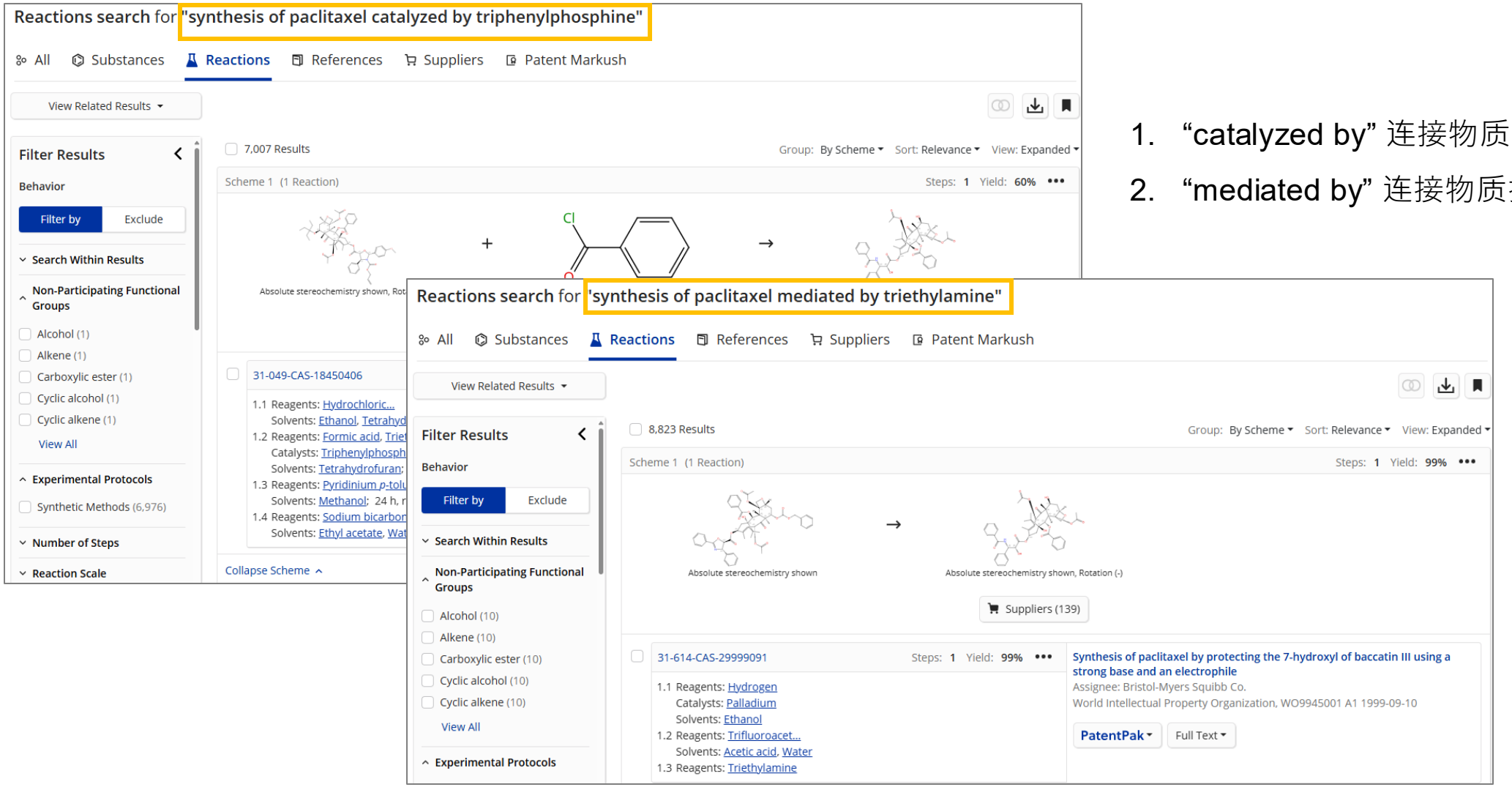
更快获取实验方案与反应数据

自然语言检索反应识别多种反应角色，降低检索难度



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



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

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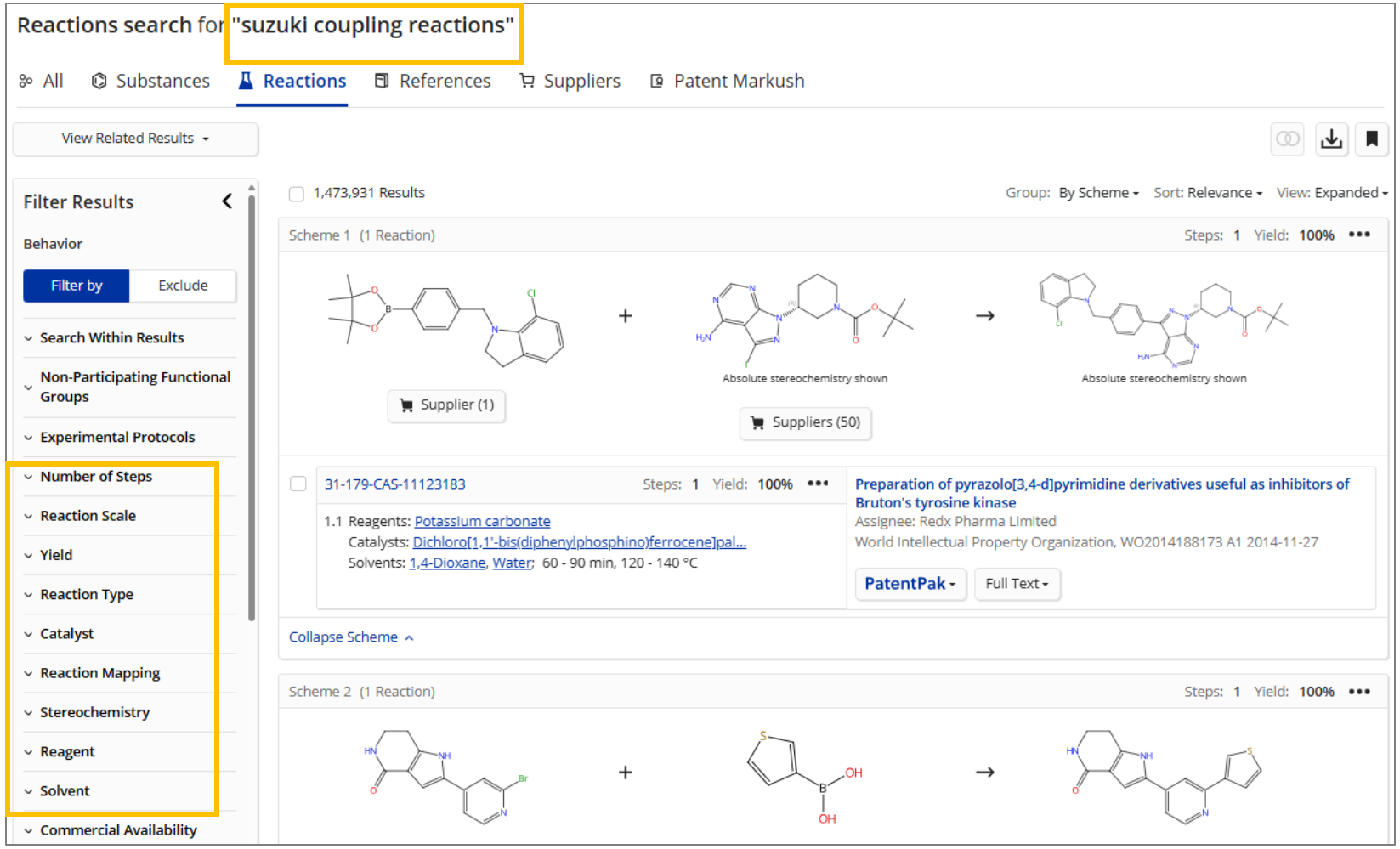
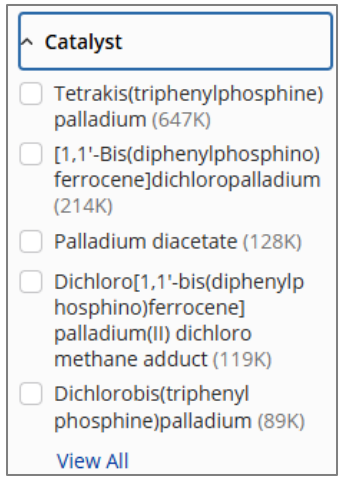
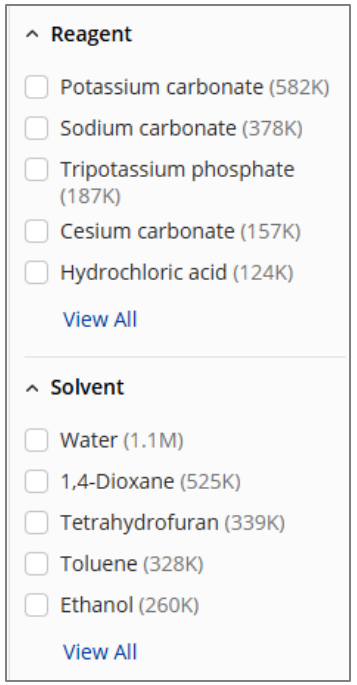
自然语言高效检索人名反应







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

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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。

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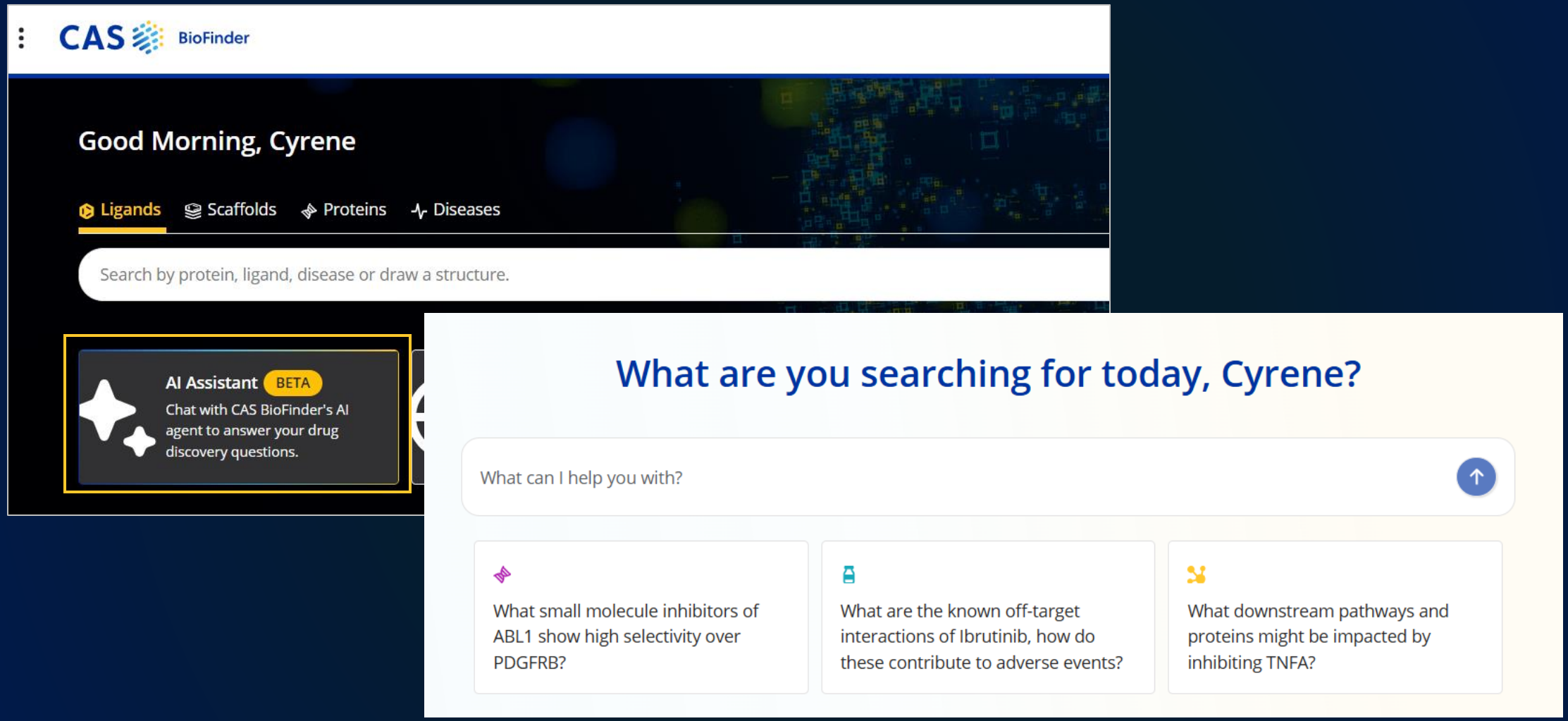
检索式问答回答药物研发问题



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] (Ki 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

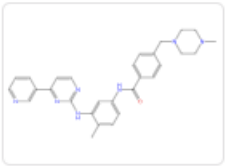
2. Pyrido[2,3-d]pyrimidin-7(8H)-one Derivative

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

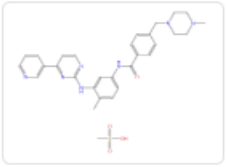
Sources

7 Results

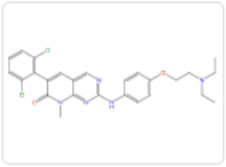
[1] Imatinib
CAS Registry Number: 152459-95-5



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



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



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药物靶点活性预测示例

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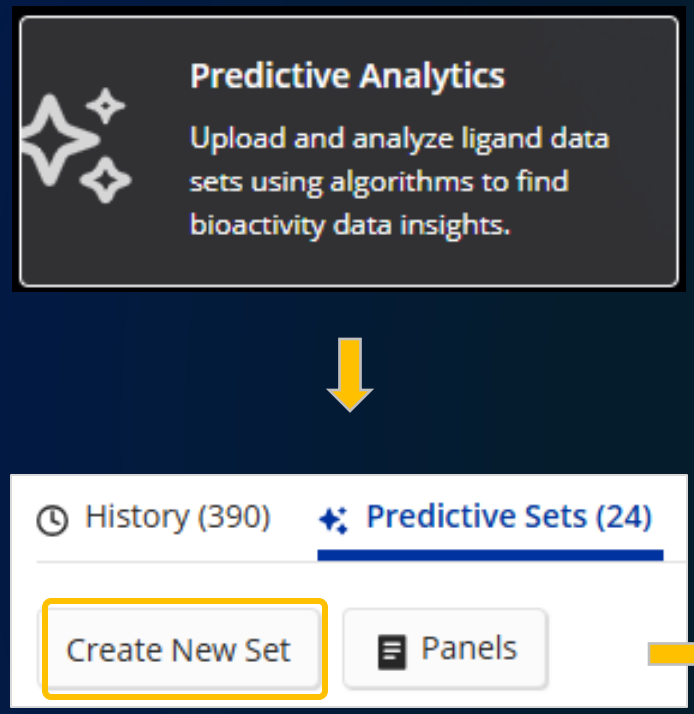
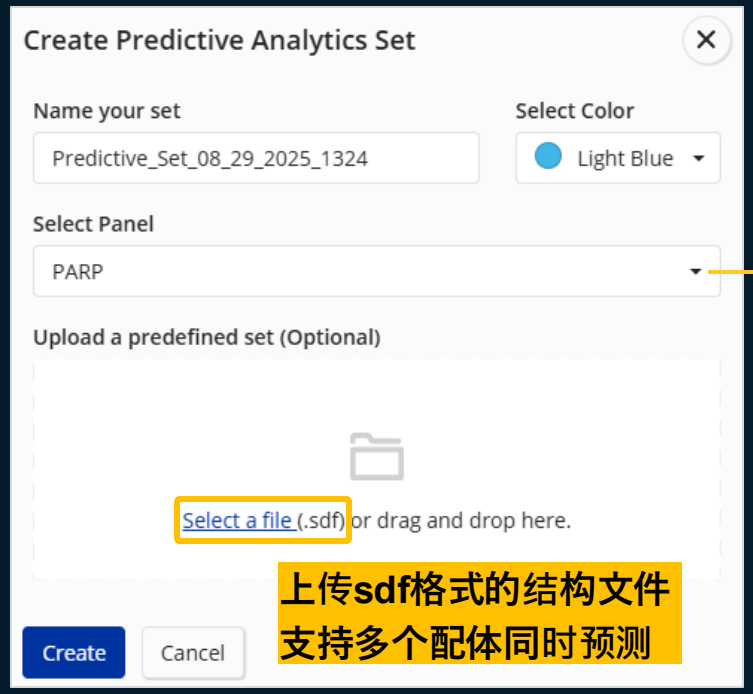
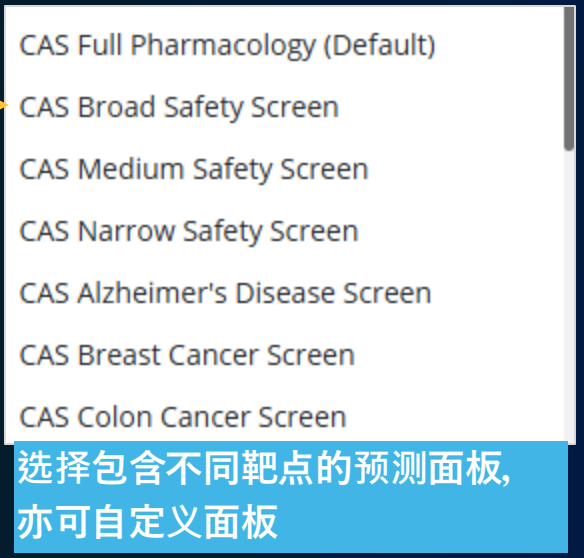
哪些关注的分子可能和目标靶点有相互作用？



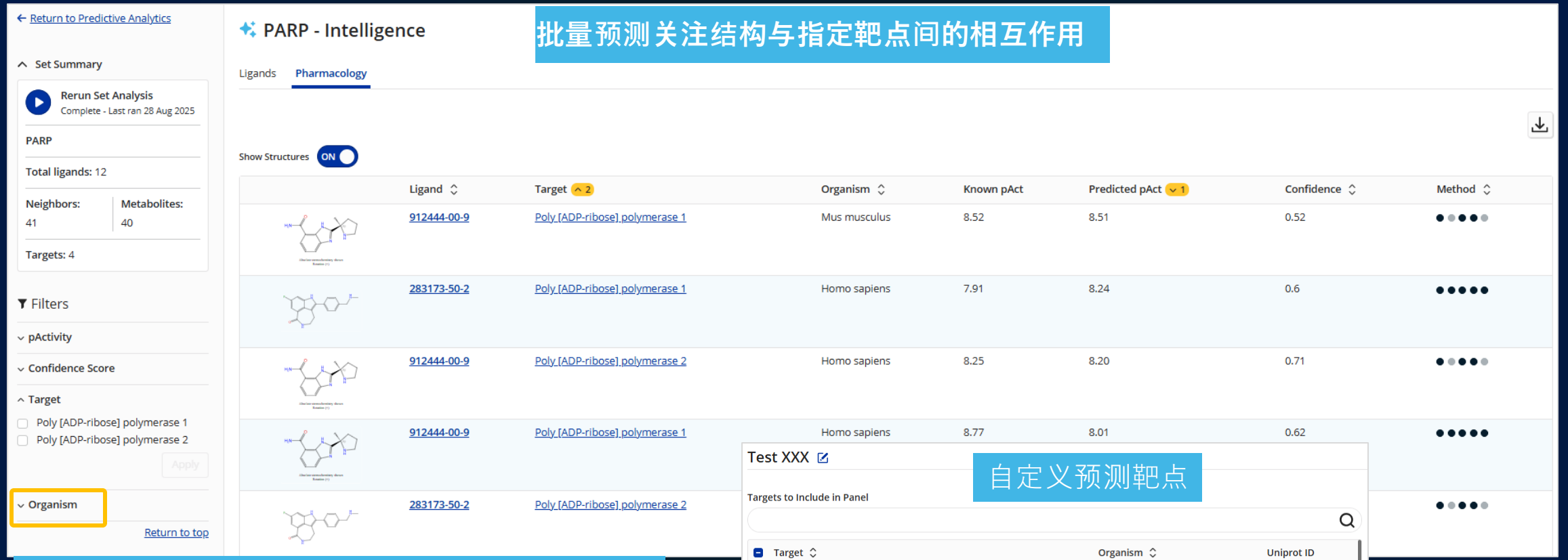


Predictive Analytics Description



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？



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

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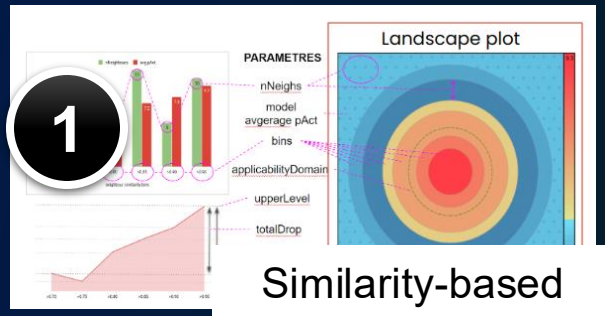
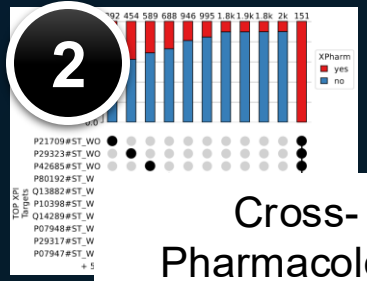
药物靶点活性预测

预测配体对蛋白质靶点的活性

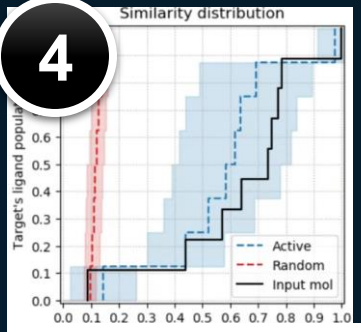


1 Similarity-based method (**SIM**)



2 Cross-Pharmacology Index (**XPI**)

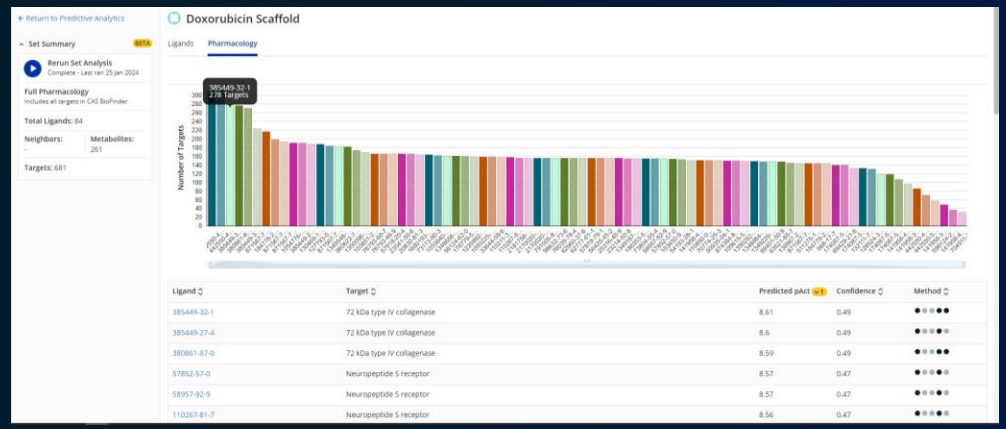
3 Machine Learning Method (**MLM**)



4 Similarity ensemble approach (**SEA**)

5 Simplest Active Substructure (**SAS**)

配体对靶点的活性预测：
多模型集成共识值



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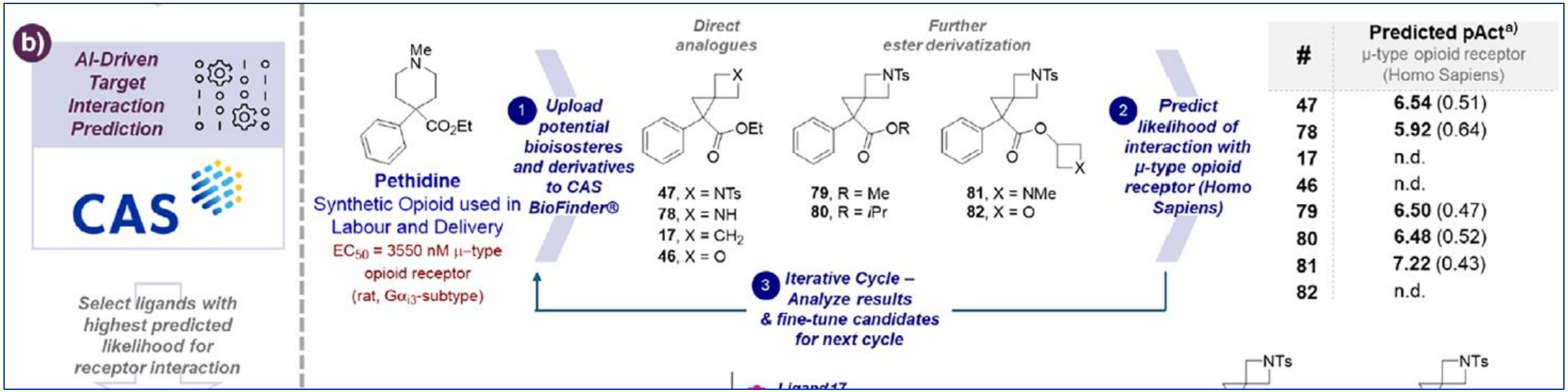
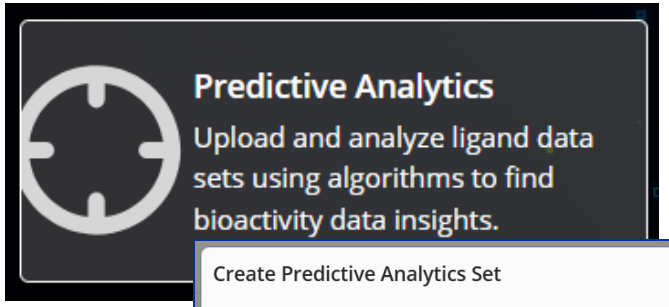
CAS BioFinder 加速“合成→评估→优化”药物发现流程，尤其适用于缺乏历史活性数据的全新骨架

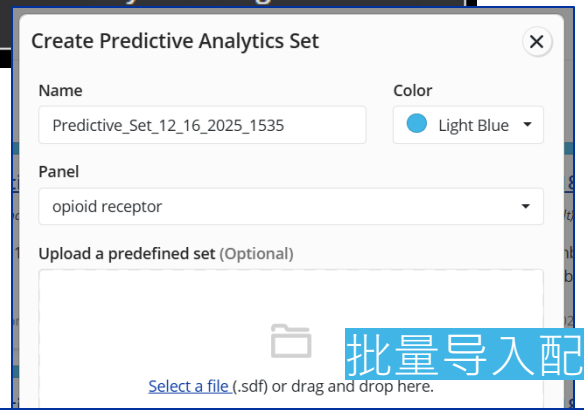


- AI增强的靶点活性预测：
  确定5-氮杂螺[2.3]己烷可以模拟哌啶后，作者利用CAS BioFinder的AI预测功能，对一系列哌替啶类似物与μ-阿片受体的相互作用进行打分（pAct值）和置信度评估（图4b）。实现了：
  - 快速筛选高潜力候选分子（如化合物**47、78、81**）；
  - 指导结构优化（如酯基替换为氮杂环丁基显著提升预测活性）；
  - 大幅缩小体外实验范围，提高研发效率。
- 验证预测可靠性：体外实验结果与BioFinder预测高度一致（高pAct值对应实测微摩尔活性），证明了该工具在新型骨架生物活性初筛中的实用价值。

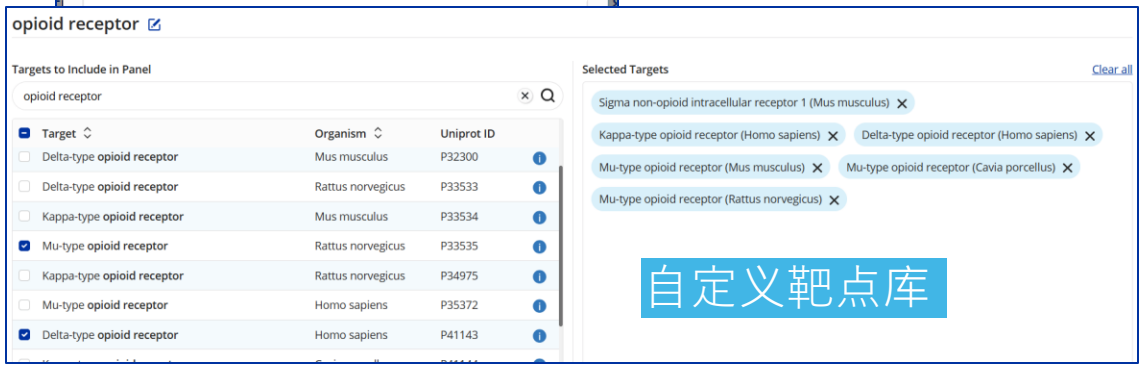
doi.org/10.1002/anie.202521633

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





批量导入配体结构sdf文件



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.	
47	Delta-type opioid receptor (Homo sapiens)	7.	
79	Delta-type opioid receptor (Homo sapiens)	7.	
81	Mu-type opioid receptor (Homo sapiens)	7.	
81	Delta-type opioid receptor (Homo sapiens)	6.	
79	Kappa-type opioid receptor (Homo sapiens)	6.	
80	Kappa-type opioid receptor (Homo sapiens)	6.	

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	-	-

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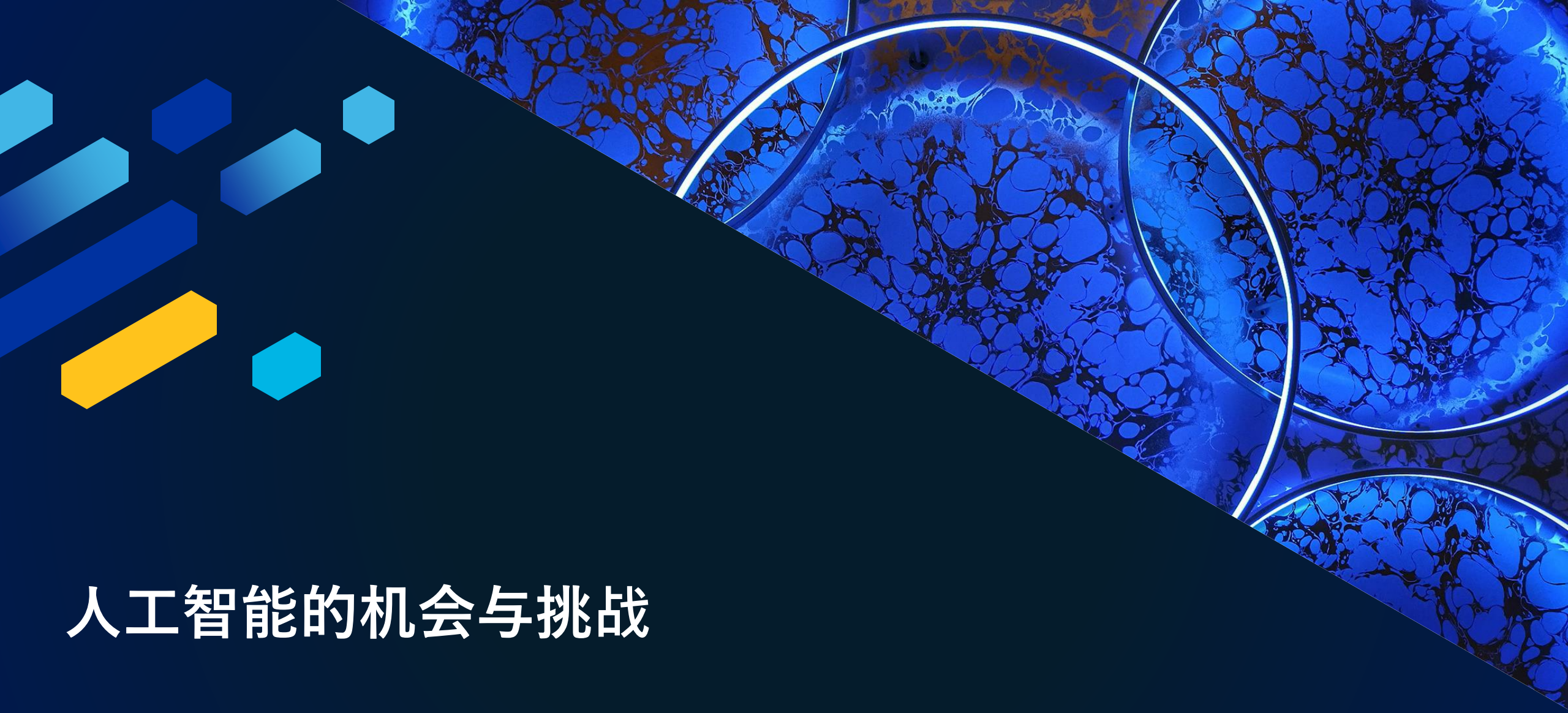

人工智能的机会与挑战

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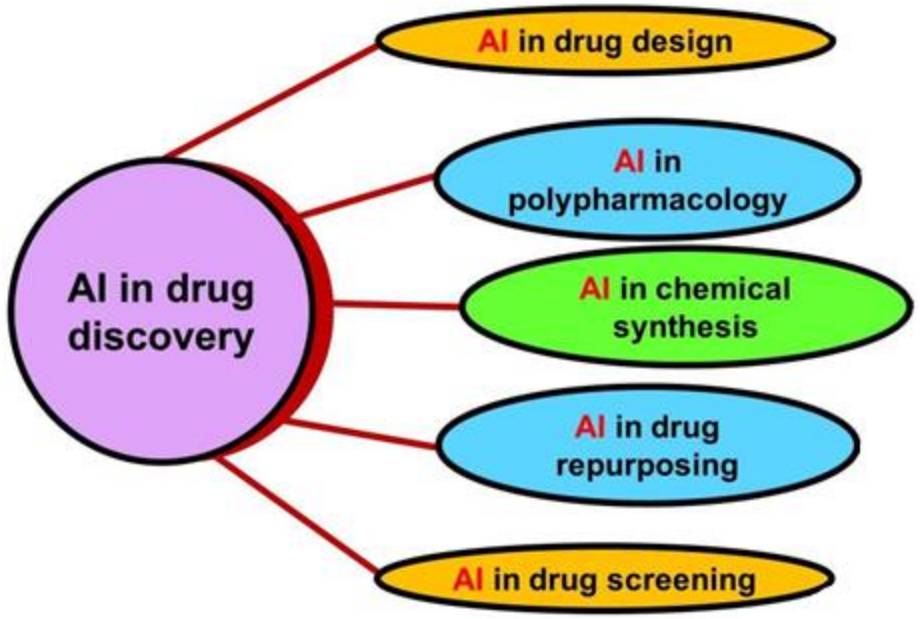
AI 在药物发现中的应用

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

ENDPOINTS *in* FOCUS

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

Andrew Dunn
Senior Biopharma Correspondent

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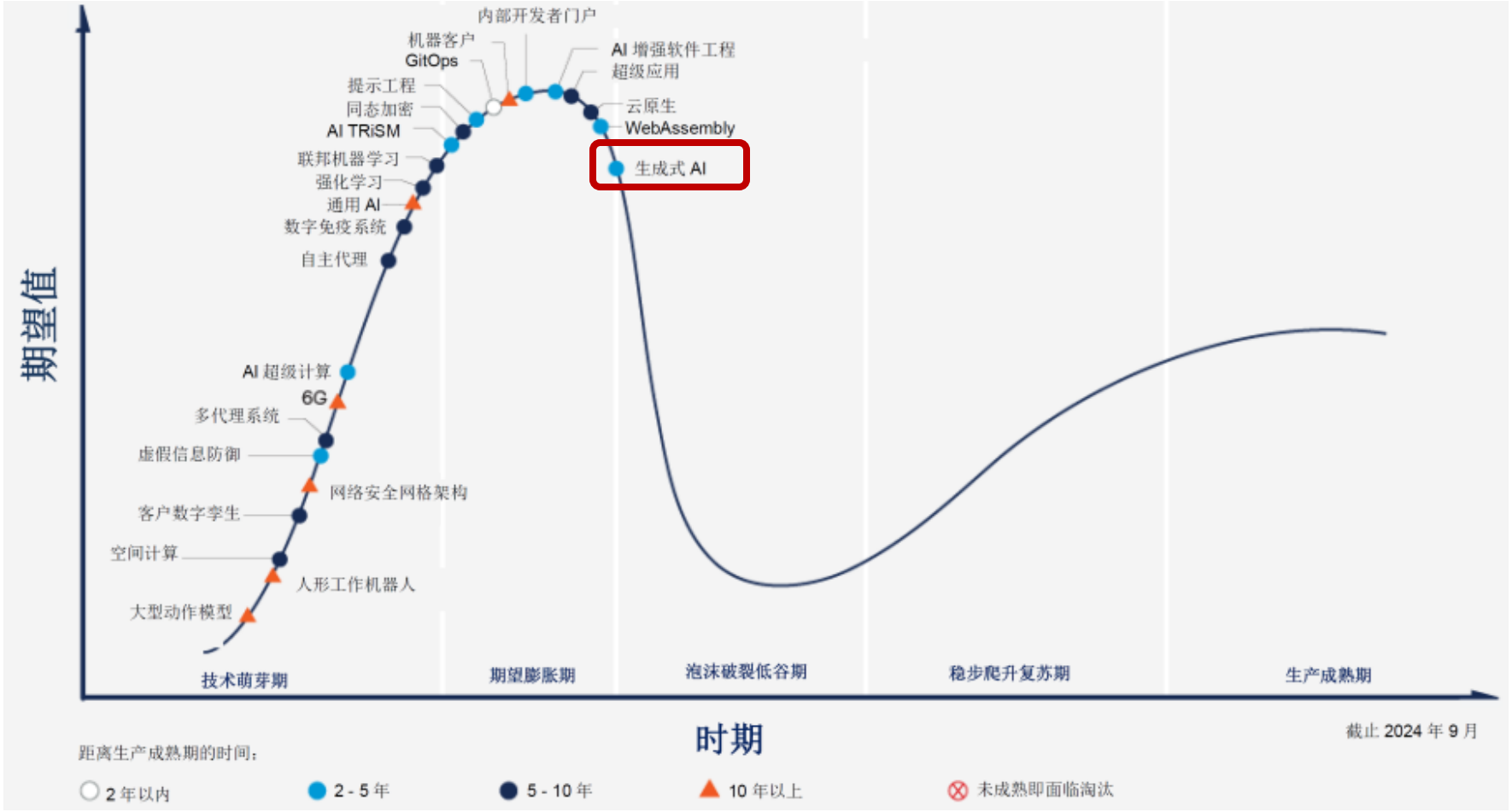
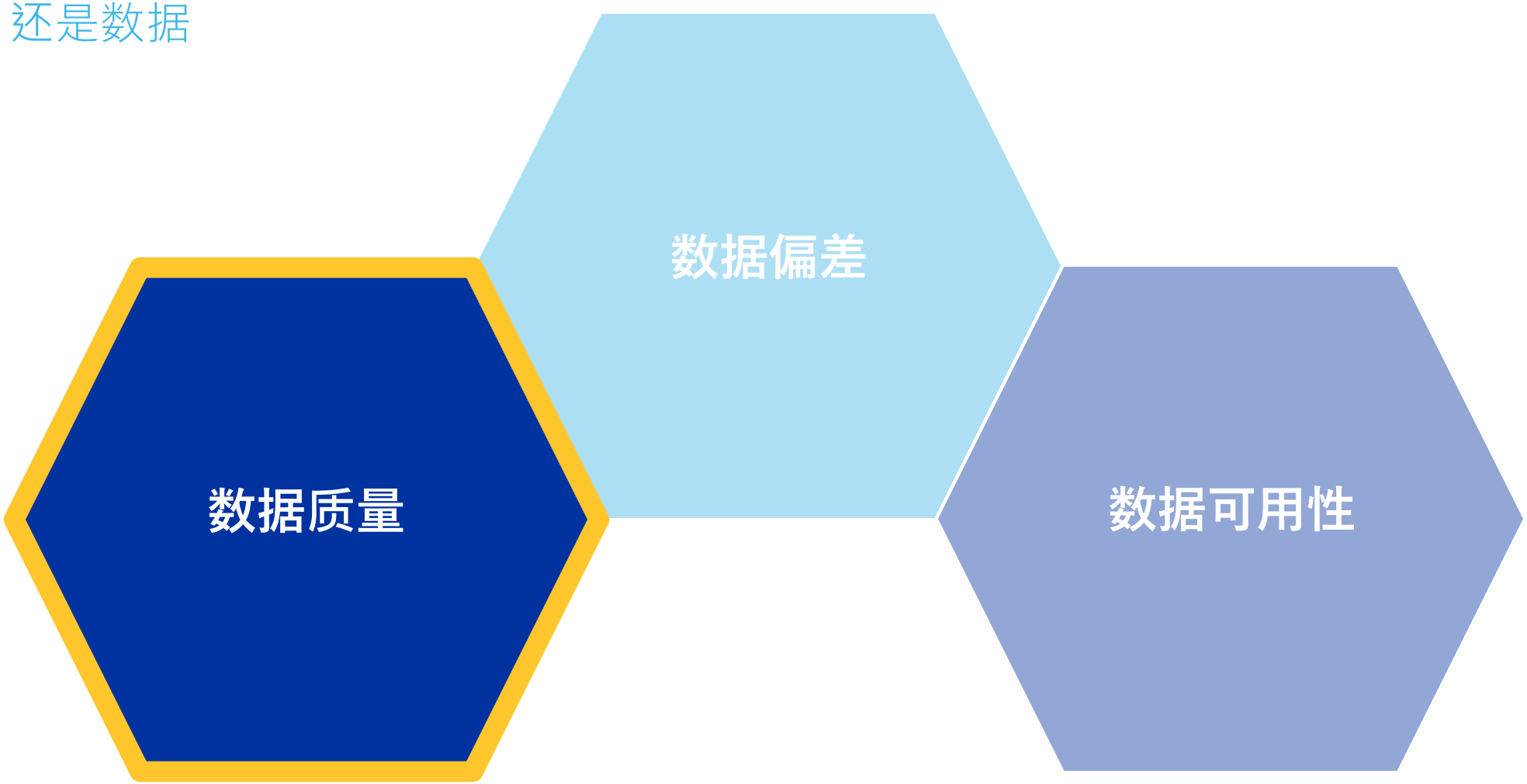
新兴技术成熟度曲线

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



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数据不一致

导致下游问题

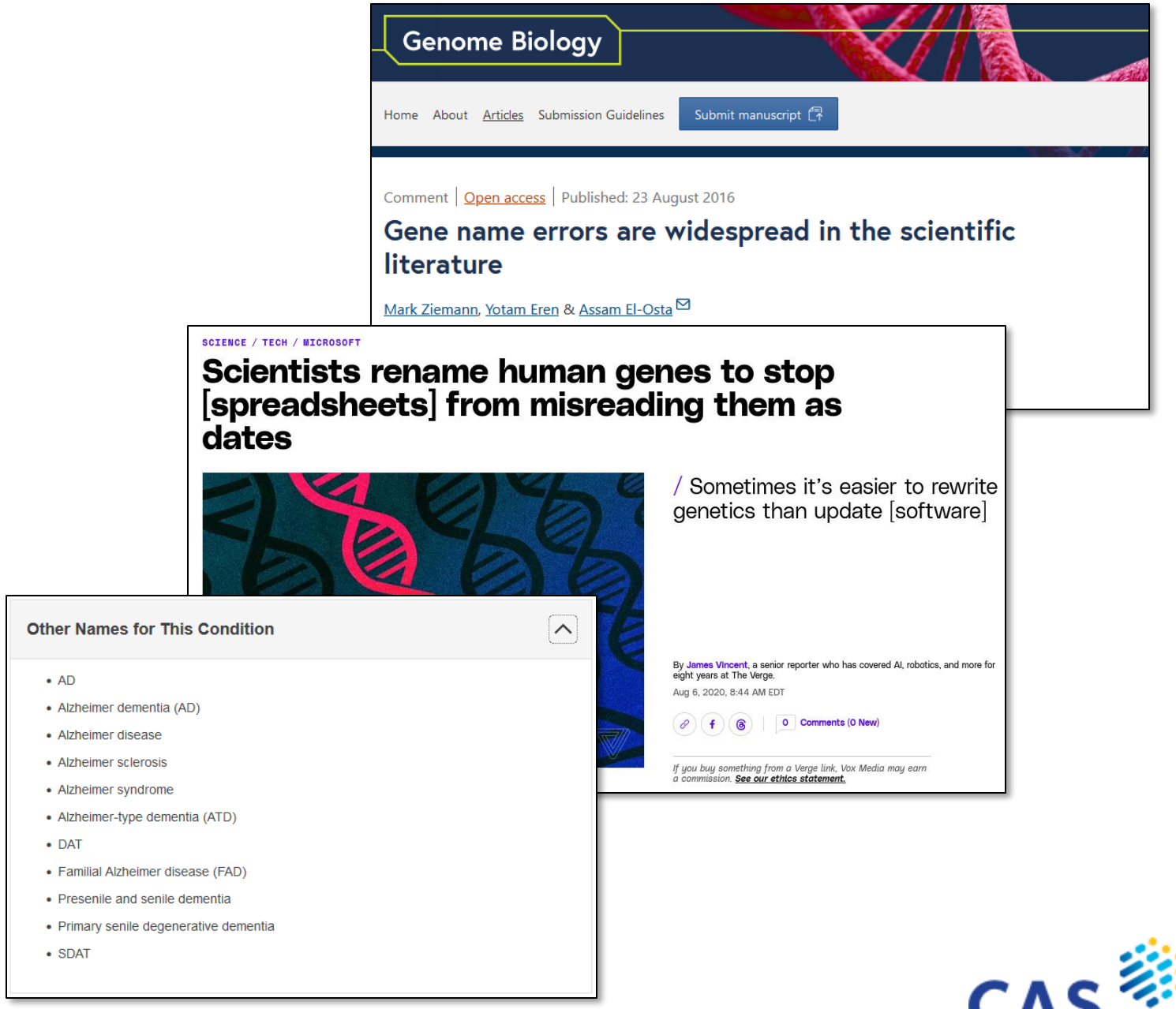
同一实体存在多个名称

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



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协调实现一致性

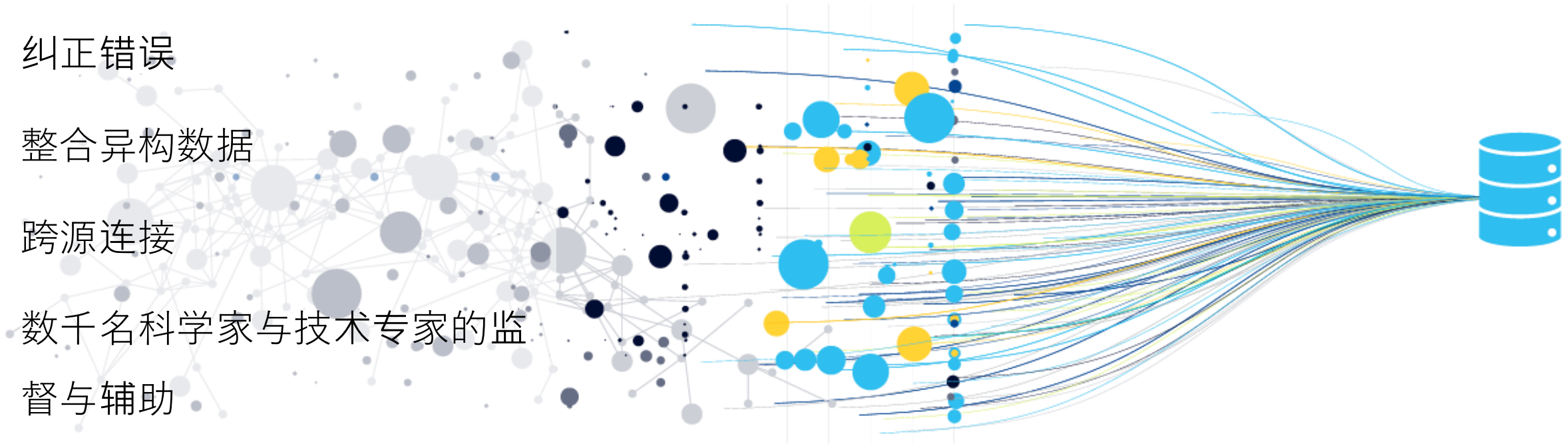
人工策展是提升AI效率的基石

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



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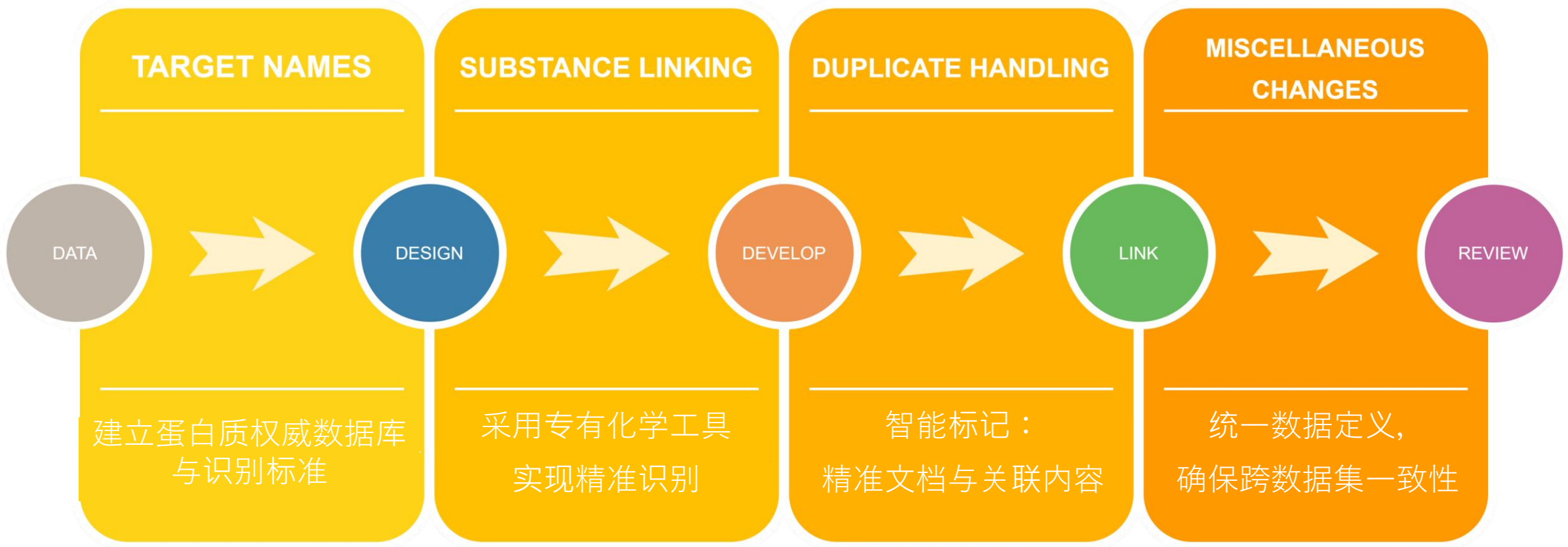
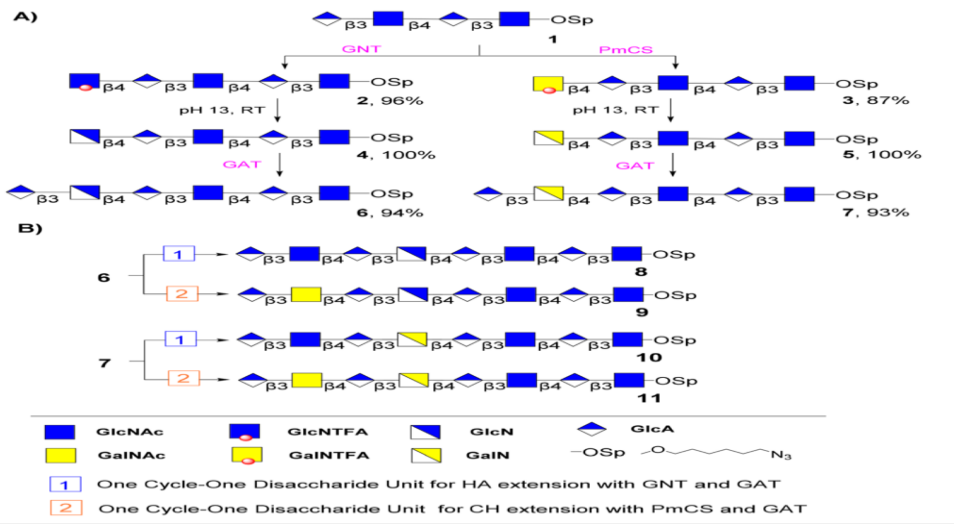
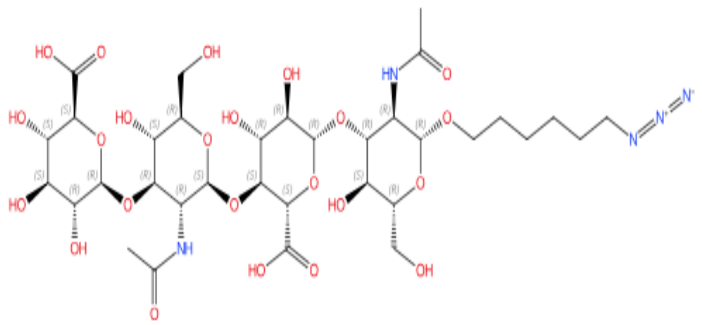
数据协调的流程



人工策展的必要性

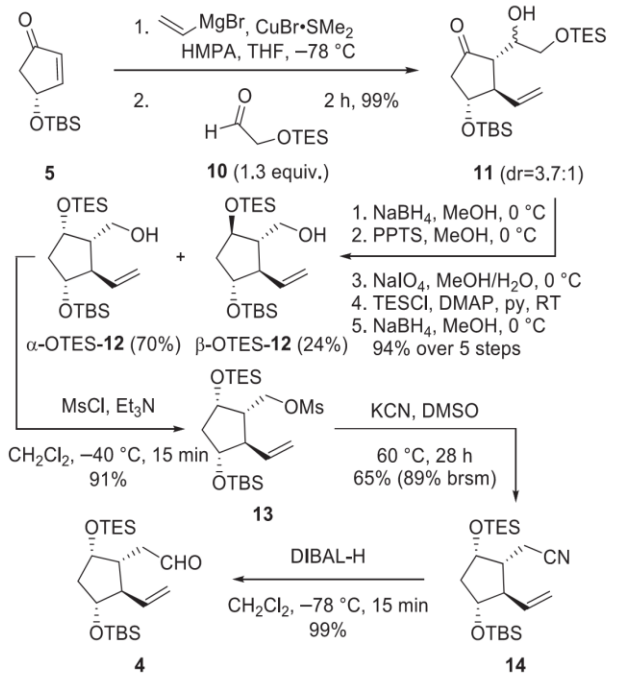


10.1039/d2gc04071a



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

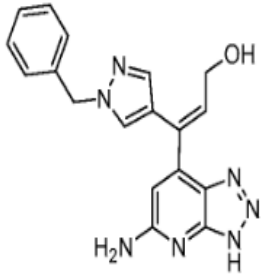
RNs 2378367-14-5 and 2378367-15-6

*4.6. ((1S,2R,3R,5S)-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 NH_4Cl 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 Na_2SO_4 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 NH_4Cl 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 Na_2SO_4 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 Na_2SO_4 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 Na_2SO_4 and concentrated *in vacuo*. Without any purification, sodium borohydride (819 mg, 21.6 mmol, 3.9 equiv) was added to crude mixture in methyl alcohol (50 mL) at 0 °C. After 30 min, the reaction mixture was quenched with saturated NH_4Cl 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 Na_2SO_4 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); $[\alpha]_D^{25} = +18.6$ (c = 1.0, $CHCl_3$); IR(neat) υ_{max} 2956, 2930, 2878, 1471, 1362, 1251, 1131, 1073, 1006, 894, 836, 776, 744, 670 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) 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:



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), K_2CO_3 (109 mg, 0.792 mmol) and $PdCl_2(dppf)$-CH_2Cl_2 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 diluted with water and EtOAc. The aq. phase was extracted 3x with EtOAc. The combined organic phases were washed with brine, dried with Na_2SO_4, 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).

结构和名称不匹配

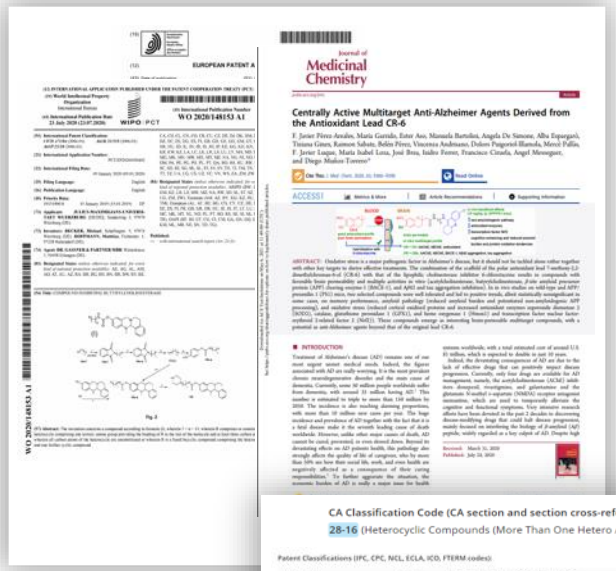
- Stereochemistry is inconsistent between name and structure
- Name indicates trityl protecting groups, but none are shown

CAS 专家解决不一致性问题

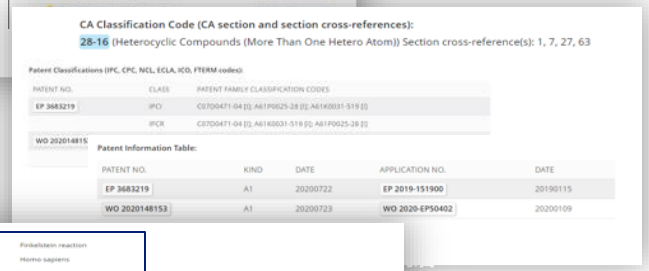
- Examine the starting materials and molecular mass
- The structure is correct as named

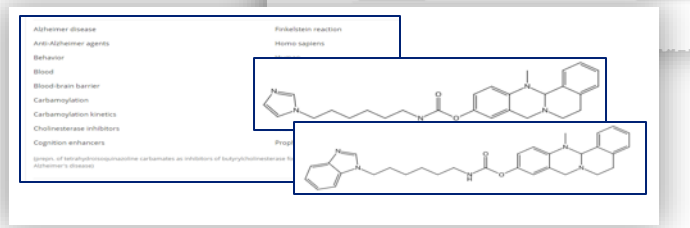
专业技术的独特应用

使用连接的结构化数据更快地生成更相关的结果



专利和期刊





专利族、IPC分类、CAS分类

精选数据结果

受控词汇
标引物质

CAS集成AI方法

- 深度学习
- TF-IDF文档相似性
- 物质结构相似性
- 图数据库

AI

智能集成器

更准确的预测

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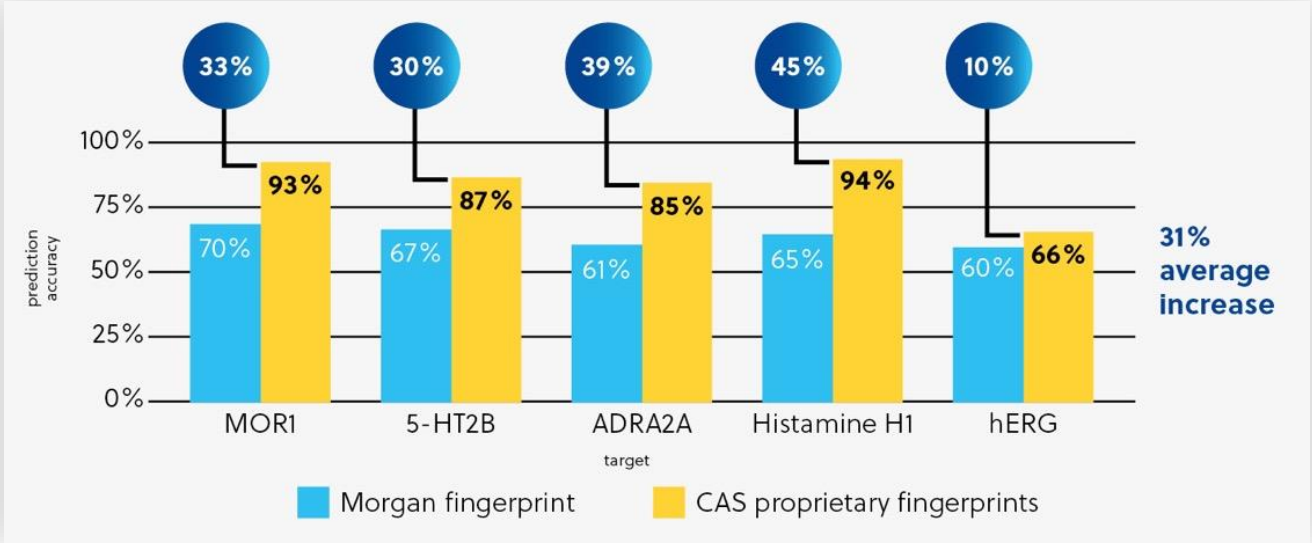
预测精度显著提高

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

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协调数据的价值

高质量数据产生更优结果

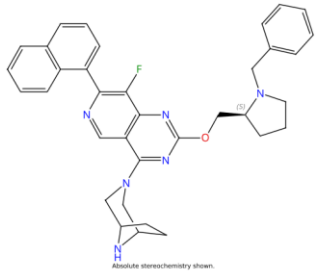
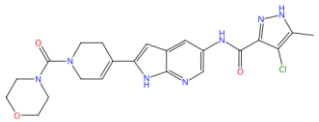
- CAS拥有全面的标准化生物活性数据
- 用于重新训练现有模型

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

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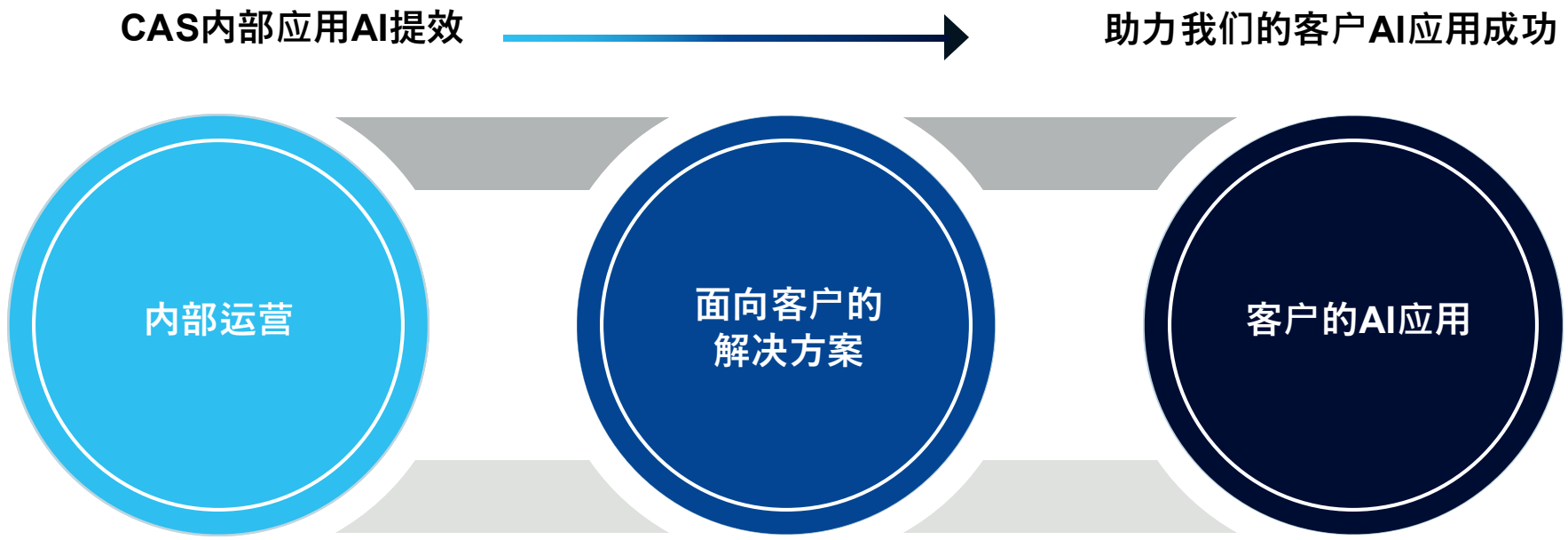
CAS 在 AI 领域的持续投入

优化运营，推动解决方案，助力客户AI应用落地



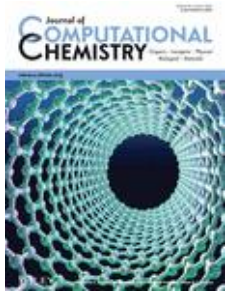
CAS高质量数据助力人工智能模型结果提升

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

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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

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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

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问卷调研及抽奖

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