CAS SCIFINDER DISCOVERY PLATFORM™
零基础入门

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2025 春季专题论坛

您在日常科研与研发工作中，是否会遇到如下问题?

- 如何检索并持续追踪跨学科融合的前沿最新进展?
- 各领域中特有的分子结构怎么画?
- 精心设计的分子有没有被他人报道过?
- 如何灵活绘制结构，分析目标化合物及相似结构在专利中的布局?
- 如何设计合成路线策略，优化绿色安全的制备工艺?
- 已制备的材料，如何实现应用上的突破?
- 如何高效管理和协作多个并行课题?

CAS SciFinder Discovery Platform 3 月至 5 月的六场专题论坛，直播时间为 周五 14:00 - 15:00。扫描二维码注册，观看直播有机会获得 CAS定制纪念品，欢迎在直播中提问互动。

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2025 春季专题论坛直播时间表

3 月 21 日 | 零基础入门

演讲人：刘子露 博士

3 月 28 日 | 解锁新功能

演讲人：杜德鑫 博士

4 月 18 日 | 助攻论文写作

演讲人：潘娜 博士

4 月 25 日 | 探索科研成果转化

演讲人：钱欣 博士

5 月 9 日 | 结构绘制面板及案例详解

演讲人：刘子露 博士

5 月 23 日 | 反应检索策略及典型案例

演讲人：陈开乾 博士

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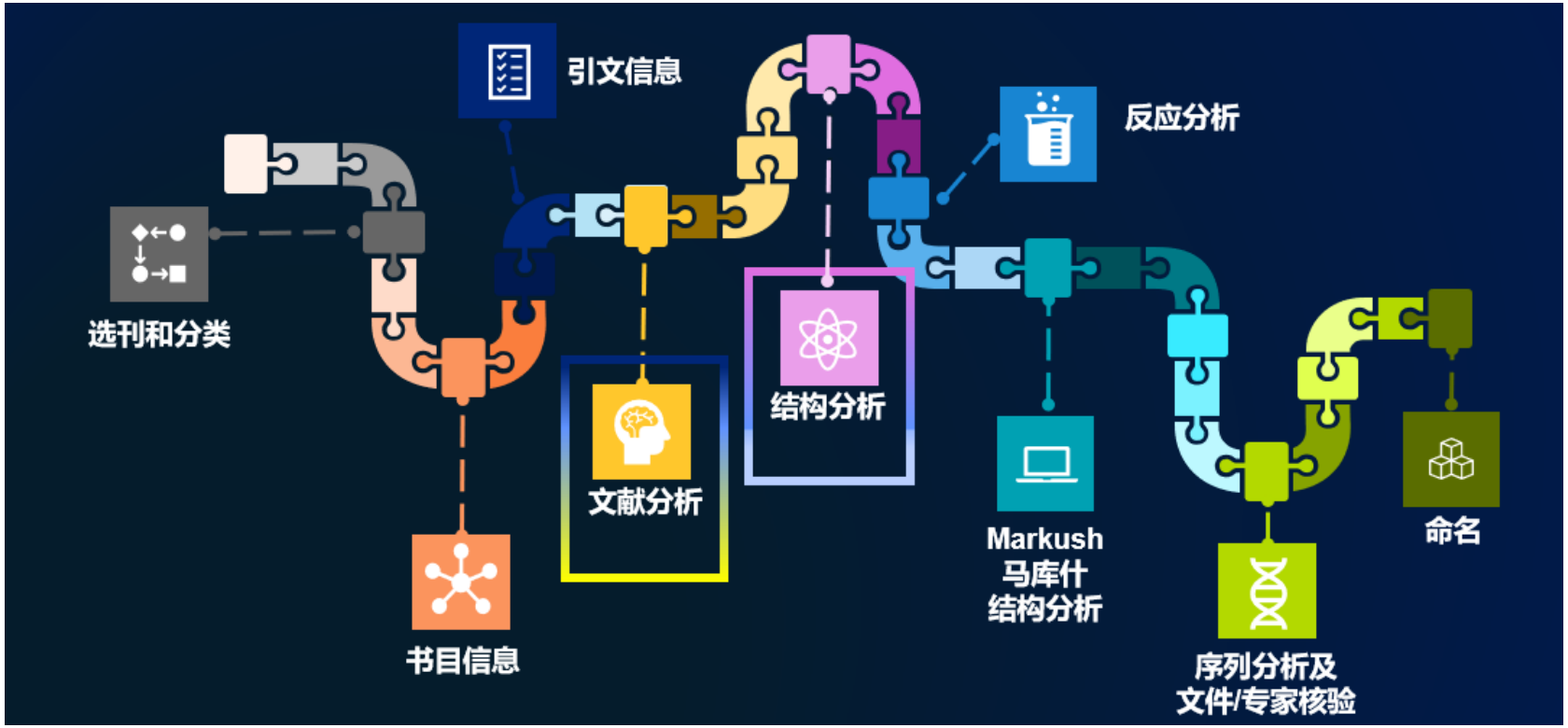
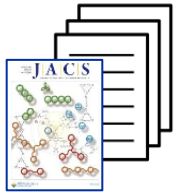
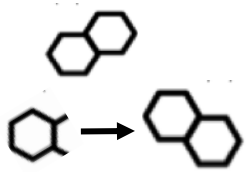
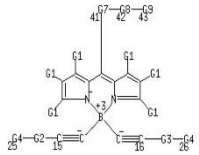
CAS 科学家的智力标引





1990
Smith, M.
anthracene





Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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CAS独特的内容合集

来源：
https://www.cas.org/cas-data
https://www.cas.org/about/cas-content

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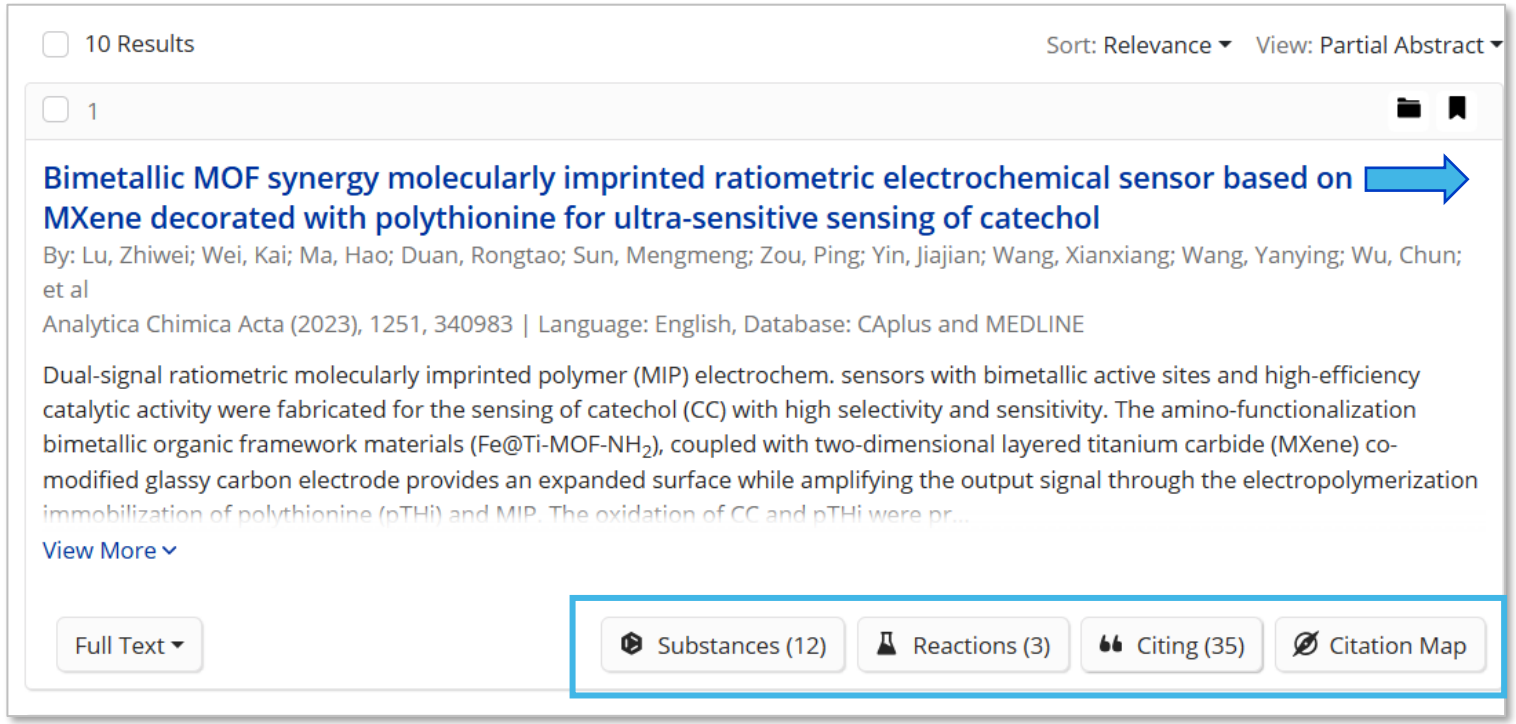
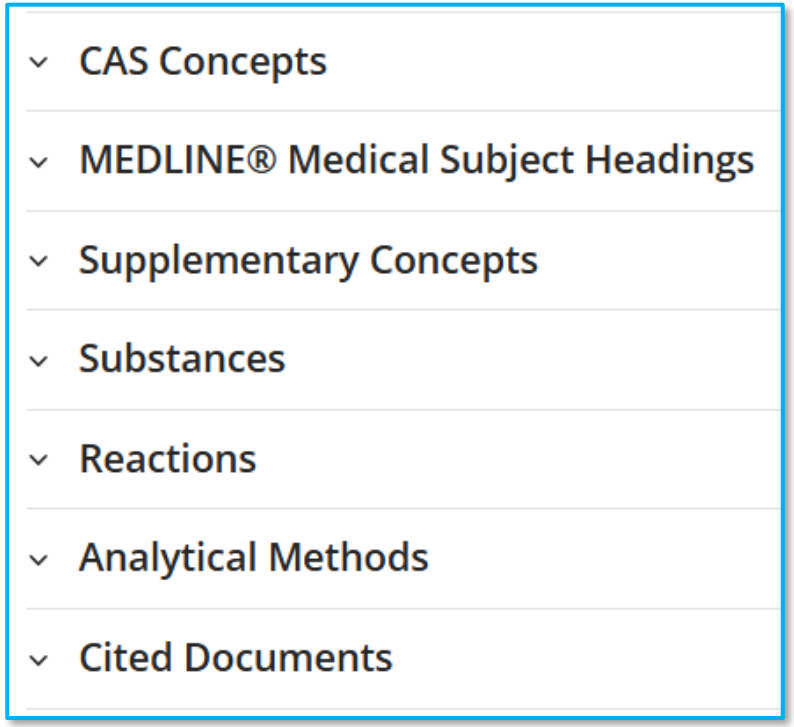
提纲

- 文献检索
- 物质检索
- 反应检索

高度互联的标引信息





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文献中重要的研究点、物质和反应

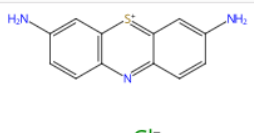
CAS Concepts

- Binding energy
- Crystallinity
- Electric current-potential relationship
- Electric impedance
- Electrochemical polymerization
- Electron transfer
- Faraday constant
- Glassy carbon electrodes

Substances

12

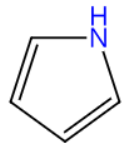
87257-37-2



$(C_{12}H_{10}N_3S.Cl)_x$
Phenothiazin-5-ium, 3,7-diamino-, chloride (1:1), homopolymer

Role: Analytical Reagent Use, Properties, Synthetic Preparation, Technical or Engineered Material Use, Analytical Study, Uses, Preparation

30604-81-0



$(C_4H_5N)_x$
1*H*-Pyrrole, homopolymer

Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

12070-08-5

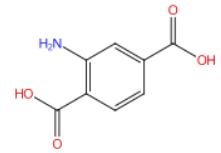
Image Not Available

CTi
Titanium carbide (TiC)

Role: Analytical Reagent Use, Properties, Synthetic Preparation, Analytical Study, Uses, Preparation

Notes: multilayerd

10312-55-7



$C_8H_7NO_4$
1,4-Benzenedicarboxylic acid, 2-amino-

Role: Analytical Reagent Use, Properties, Synthetic Preparation, Analytical Study, Uses, Preparation

Notes: titanium complexes

Reactions

3

31-614-CAS-35837877

View Experimental Protocols
Steps: 1

titanium complexes

1.1 Reagents: Titanium tetrabutoxide
Solvents: Methanol, Dimethylformamide; 48 h, 150 °C

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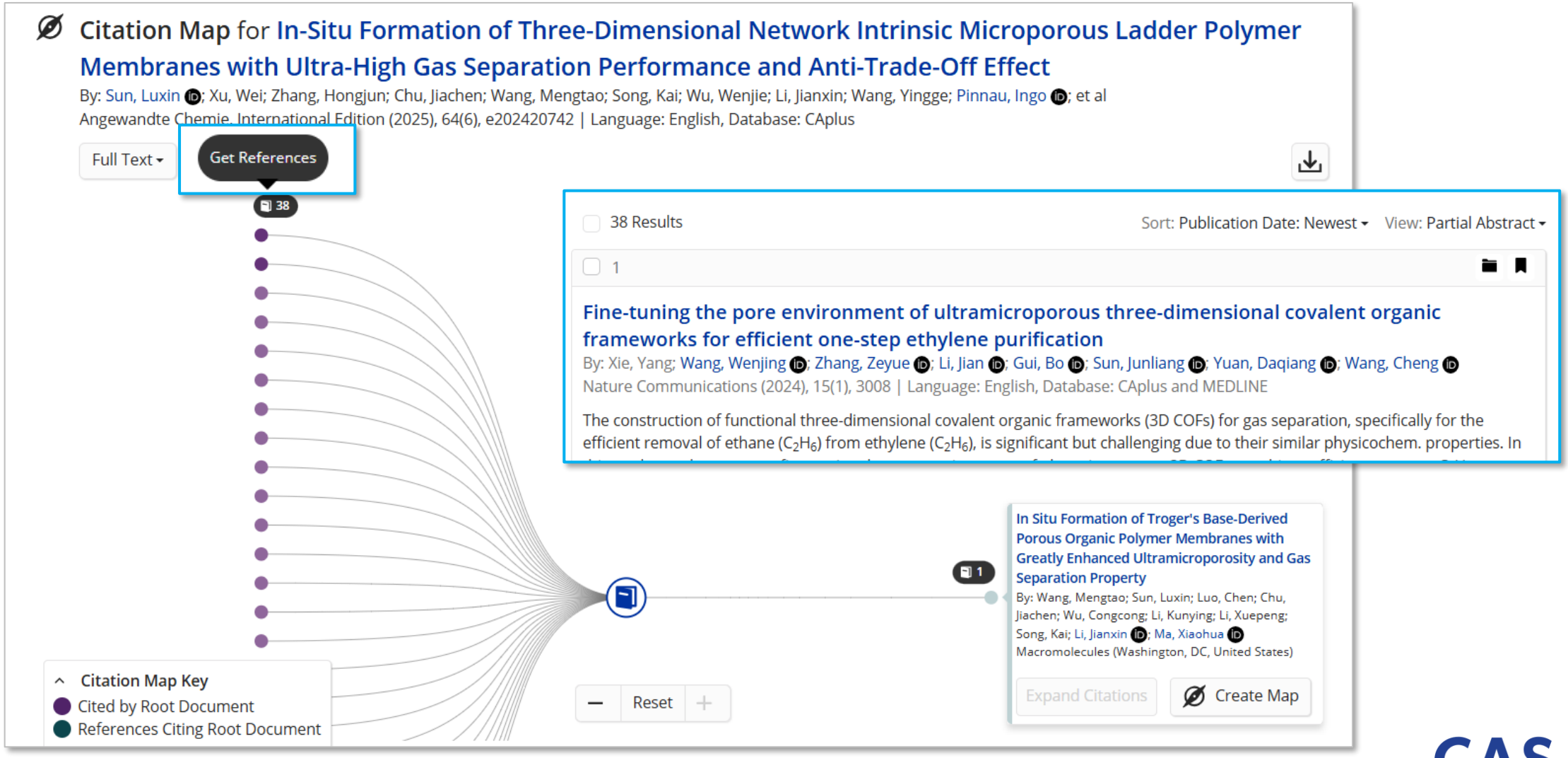
引文地图



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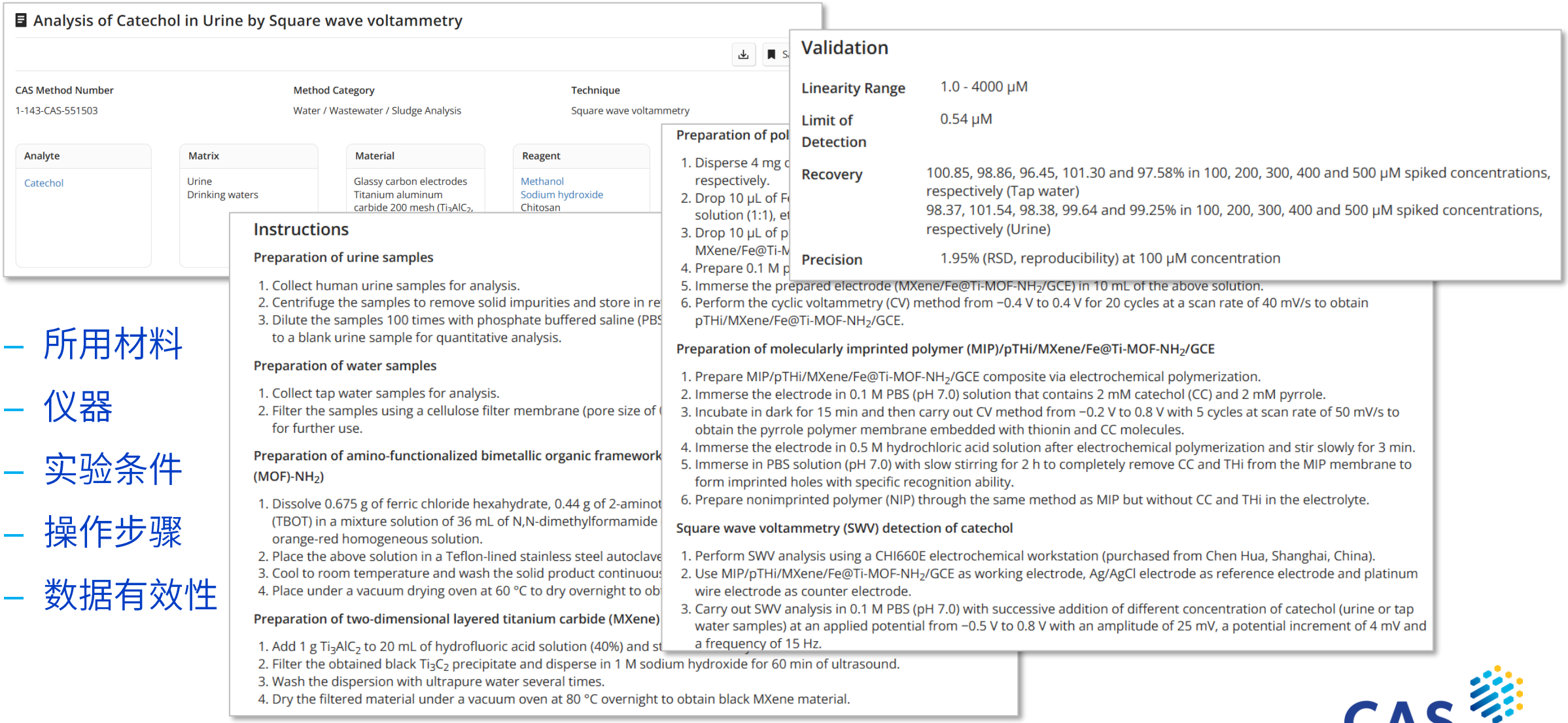
CAS标引的分析方法详情



Analysis of Catechol in Urine by Square wave voltammetry

CAS Method Number	Method Category	Technique
1-143-CAS-551503	Water / Wastewater / Sludge Analysis	Square wave voltammetry

Analyte	Matrix	Material	Reagent
Catechol	Urine Drinking waters	Glassy carbon electrodes Titanium aluminum carbide 200 mesh (Ti_3AlC_2,	Methanol Sodium hydroxide Chitosan

Validation

Linearity Range	1.0 - 4000 µM
Limit of Detection	0.54 µM
Recovery	100.85, 98.86, 96.45, 101.30 and 97.58% in 100, 200, 300, 400 and 500 µM spiked concentrations, respectively (Tap water) 98.37, 101.54, 98.38, 99.64 and 99.25% in 100, 200, 300, 400 and 500 µM spiked concentrations, respectively (Urine)
Precision	1.95% (RSD, reproducibility) at 100 µM concentration

Instructions

Preparation of urine samples

1. Collect human urine samples for analysis.
2. Centrifuge the samples to remove solid impurities and store in re
3. Dilute the samples 100 times with phosphate buffered saline (PBS to a blank urine sample for quantitative analysis.

Preparation of water samples

1. Collect tap water samples for analysis.
2. Filter the samples using a cellulose filter membrane (pore size of (for further use.

Preparation of amino-functionalized bimetallic organic framework (MOF)-NH_2)

1. Dissolve 0.675 g of ferric chloride hexahydrate, 0.44 g of 2-aminot (TBOT) in a mixture solution of 36 mL of N,N-dimethylformamide orange-red homogeneous solution.
2. Place the above solution in a Teflon-lined stainless steel autoclave
3. Cool to room temperature and wash the solid product continuous
4. Place under a vacuum drying oven at 60 °C to dry overnight to ob

Preparation of two-dimensional layered titanium carbide (MXene)

1. Add 1 g Ti_3AlC_2 to 20 mL of hydrofluoric acid solution (40%) and st
2. Filter the obtained black Ti_3C_2 precipitate and disperse in 1 M sodium hydroxide for 60 min of ultrasound.
3. Wash the dispersion with ultrapure water several times.
4. Dry the filtered material under a vacuum oven at 80 °C overnight to obtain black MXene material.

Preparation of pol

1. Disperse 4 mg c respectively.
2. Drop 10 µL of F solution (1:1), et
3. Drop 10 µL of p MXene/Fe@Ti-M
4. Prepare 0.1 M p
5. Immerse the prepared electrode (MXene/Fe@Ti-MOF-NH_2/GCE) in 10 mL of the above solution.
6. Perform the cyclic voltammetry (CV) method from −0.4 V to 0.4 V for 20 cycles at a scan rate of 40 mV/s to obtain pTHi/MXene/Fe@Ti-MOF-NH_2/GCE.

Preparation of molecularly imprinted polymer (MIP)/pTHi/MXene/Fe@Ti-MOF-NH_2/GCE

1. Prepare MIP/pTHi/MXene/Fe@Ti-MOF-NH_2/GCE composite via electrochemical polymerization.
2. Immerse the electrode in 0.1 M PBS (pH 7.0) solution that contains 2 mM catechol (CC) and 2 mM pyrrole.
3. Incubate in dark for 15 min and then carry out CV method from −0.2 V to 0.8 V with 5 cycles at scan rate of 50 mV/s to obtain the pyrrole polymer membrane embedded with thionin and CC molecules.
4. Immerse the electrode in 0.5 M hydrochloric acid solution after electrochemical polymerization and stir slowly for 3 min.
5. Immerse in PBS solution (pH 7.0) with slow stirring for 2 h to completely remove CC and THi from the MIP membrane to form imprinted holes with specific recognition ability.
6. Prepare nonimprinted polymer (NIP) through the same method as MIP but without CC and THi in the electrolyte.

Square wave voltammetry (SWV) detection of catechol

1. Perform SWV analysis using a CHI660E electrochemical workstation (purchased from Chen Hua, Shanghai, China).
2. Use MIP/pTHi/MXene/Fe@Ti-MOF-NH_2/GCE as working electrode, Ag/AgCl electrode as reference electrode and platinum wire electrode as counter electrode.
3. Carry out SWV analysis in 0.1 M PBS (pH 7.0) with successive addition of different concentration of catechol (urine or tap water samples) at an applied potential from −0.5 V to 0.8 V with an amplitude of 25 mV, a potential increment of 4 mV and a frequency of 15 Hz.

- 所用材料
- 仪器
- 实验条件
- 操作步骤
- 数据有效性

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CAS标引的配方工艺与实验数据

Paclitaxel-Piperine Pharmaceutical Nanoparticles: Drug Delivery Systems or Antitumor Agents

Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents, Drug delivery systems	paclitaxel, Homo sapiens, Mammary gland neoplasm, Ovary neoplasm, lungs cancer	Oral drug delivery systems	Particles	View

U.S. Pharmacopeia

Formulation Ingredients

Expand All Groups | Collapse All G

Component	Function	Amount Reported	Optionality
Group: paclitaxel nanoparticles	-	-	Mandatory
Paclitaxel	Antitumor agents	0.5 mg	Mandatory
Acrylic polymers	-	0.1 g	Mandatory
Water	Solvents, Pharmaceutical carriers	90 mL	Mandatory
Poly(vinyl alcohol)	Surfactants		
Piperine	bioenhancers		

Experimental Activity

Descriptor	Notes	Details
area under curve(0-infinite)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-infinite).	12315.2 ± 916.3
area under curve(0-t)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-t).	10335.3 ng. h/mL ± 983.2 ng. h/mL
clearance rate of drug	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of clearance rate of drug (CL).	6.9 L/h ± 1.8 L/h
cytotoxicity test	the cytotoxic action of cell lines was determined by high throughput MTT assay and the cell growth was measured by calorimetric assay.	cell apoptosis and better anticancer activity.
drug diffusion	the drug diffusion of the composition was evaluated at 0.5 hours.	9.15 %
drug diffusion	the drug diffusion of the composition was evaluated at 1 hours.	9.55 %

More Formulations like this...

Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
Purpose: improving oral bioavailability...
Target: Homo sapiens, paclitaxel
Delivery Route: Oral drug delivery syst...
Physical Form: Powders, nanosuspensi...

Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
Purpose: improving oral bioavailability...
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Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
Purpose: improving oral bioavailability...
Target: Homo sapiens, paclitaxel
Delivery Route: Oral drug delivery syst...
Physical Form: Powders, nanosuspensi...

Process

the paclitaxel-piperine pharmaceutical nanoparticles is prepared by: adding the Eudragit and drug which contain paclitaxel is dissolved in acetone to obtain the organic phase; pouring it into the aqueous phase having surfactant which is composed of polyvinyl alcohol and distilled water to produce the oil in water type emulsion; crushing it into the nanoparticles using sonicator-driven external energy; the organic solvent is evaporated during magnetic stirrer for 2 hours at 300 rpm under the atmospheric conditions to the obtain paclitaxel nanoparticles is prepared; the obtained paclitaxel nanoparticles are combined with piperine.

提纲

- 文献检索
- 物质检索
- 反应检索

✓ 获取关键词

✓ 灵活缩放检索式

✓ 高效筛选和追踪文献

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关键词从哪里来?

1. 初步确定的关键词：根据课题的研究方向和学科知识，提炼基本关键词进行初步检索
2. 积累文献中的关键词：在初步检索的文献中积累相关的关键词

   例如：来自标题、摘要、Keywords、Concept、物质标引信息、全文
3. CAS Lexicon：浏览CAS科学家标引的不同层级概念词和物质，拓展检索词
4. 精炼或扩展关键词：基于初步检索到的文献，结合自己对课题本身的理解，锁定多个关键词，

   进行组合检索

   例如：专业术语、同义词/近义词、上下位概念词

一篇文献中的关键词

Highly Selective Inhibition of Tyrosine Kinase 2 (TYK2) for the Treatment of Autoimmune Diseases: Discovery of the Allosteric Inhibitor BMS-986165

97 | 234 | 230 | Citation Map

In this Reference

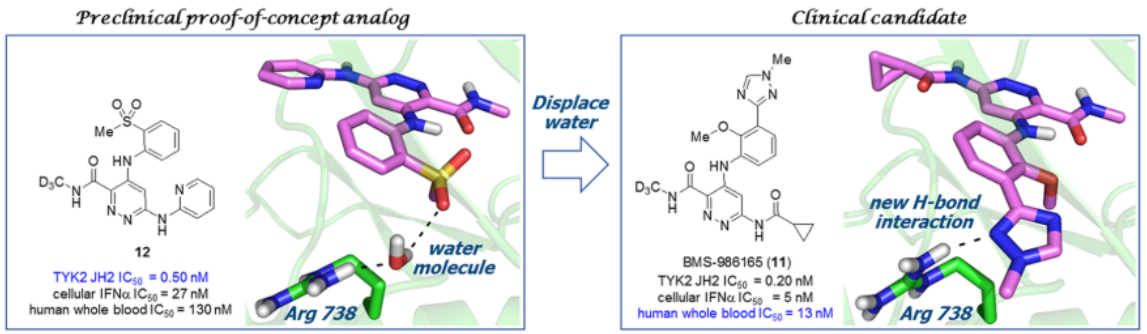
- Concepts
  - CAS Concepts
  - MEDLINE MeSH
  - Supplementary Concepts
- Substances
- Reactions
- Life Science Data
- Cited Documents

By: Wrobleski, Stephen T.; Moslin, Ryan; Lin, Shuqun; Zhang, Yanlei; Spergel, Steven; Kempson, James; Tokarski, John S.; Strnad, Joann; Zupa-Fernandez, Adriana; Cheng, Lihong; et al

View All

DOI: 10.1021/acs.jmedchem.9b00444

Small mol. JAK inhibitors have emerged as a major therapeutic advancement in treating autoimmune diseases. The discovery of isoform selective JAK inhibitors that traditionally target the catalytically active site of this kinase family has been a formidable challenge. Our strategy to achieve high selectivity for TYK2 relies on targeting the TYK2 pseudokinase (JH2) domain. Herein we report the late stage optimization efforts including a structure-guided design and water displacement strategy that led to the discovery of BMS-986165 (11, **I**) as a high affinity JH2 ligand and potent allosteric inhibitor of TYK2. In addition to unprecedented JAK isoform and kinome selectivity, **I** shows excellent pharmacokinetic properties with minimal profiling liabilities and is efficacious in several murine models of autoimmune disease. On the basis of these findings, **I** appears differentiated from all other reported JAK inhibitors and has been advanced as the first pseudokinase-directed therapeutic in clin. development as an oral treatment for autoimmune diseases.



- 标题
- 摘要
- Keywords
- Concepts

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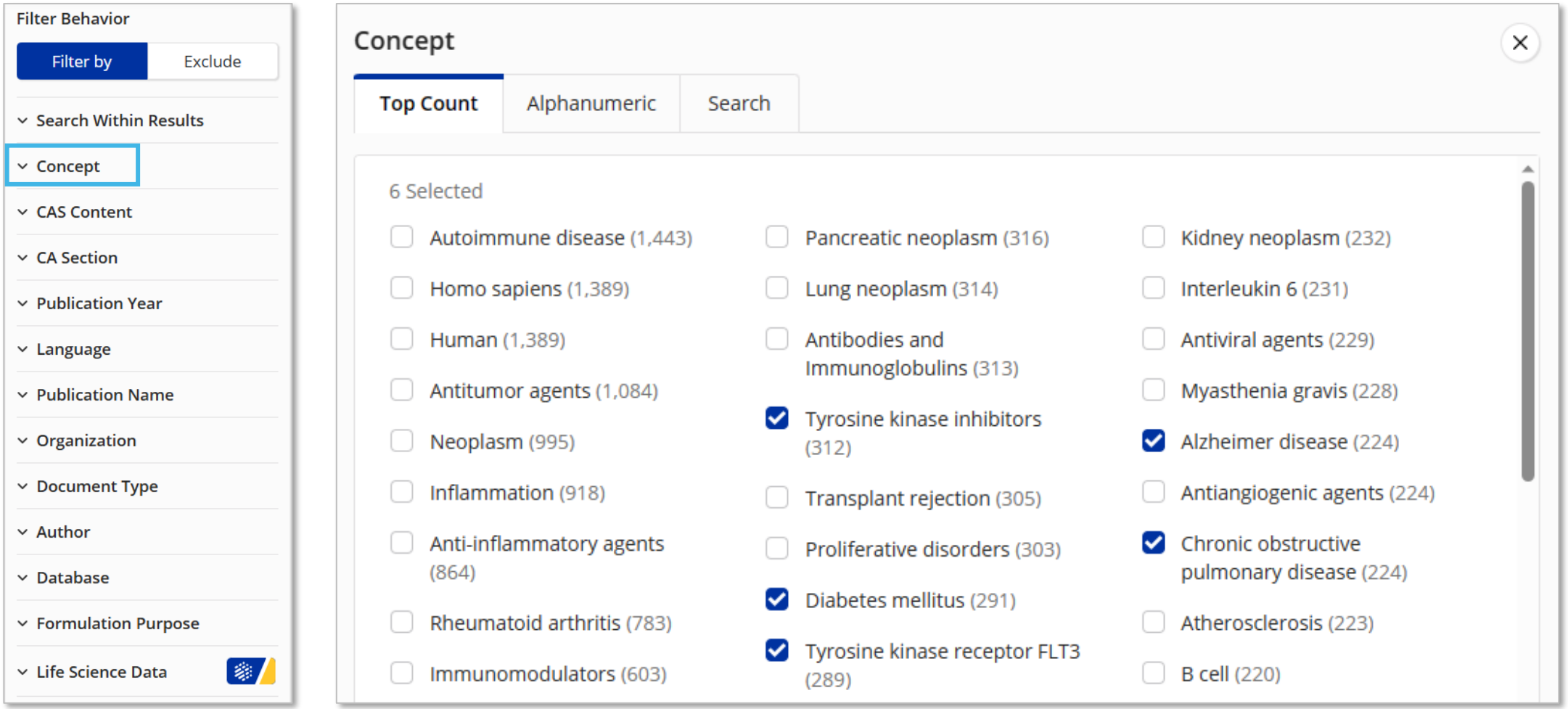
从文献结果集中获得概念词



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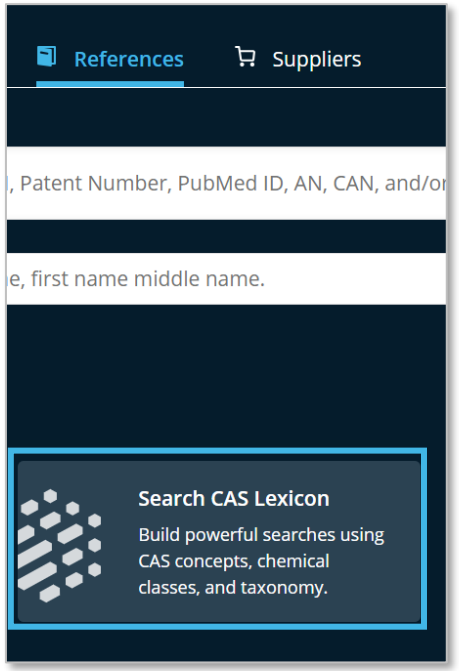
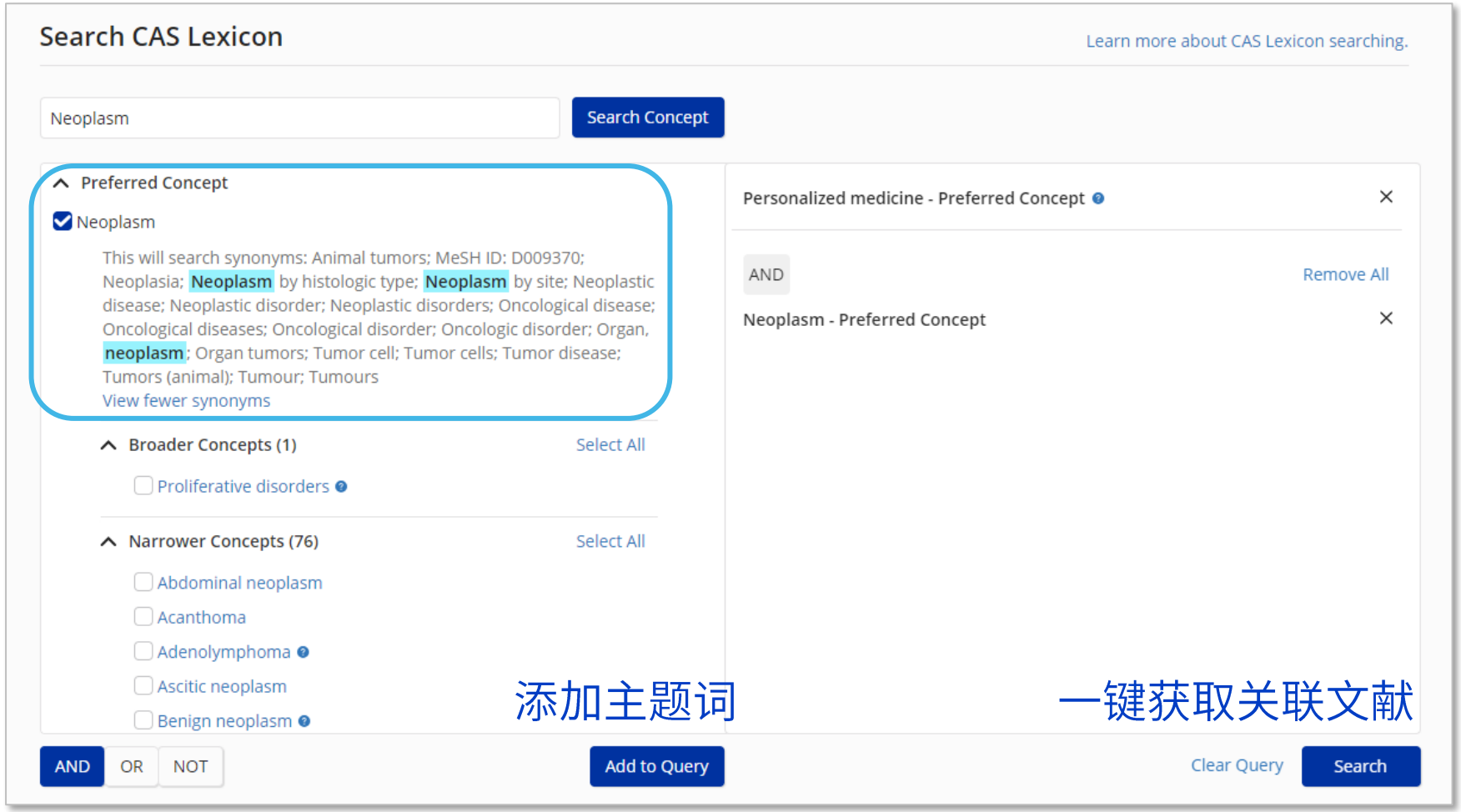
利用CAS Lexicon拓展检索词





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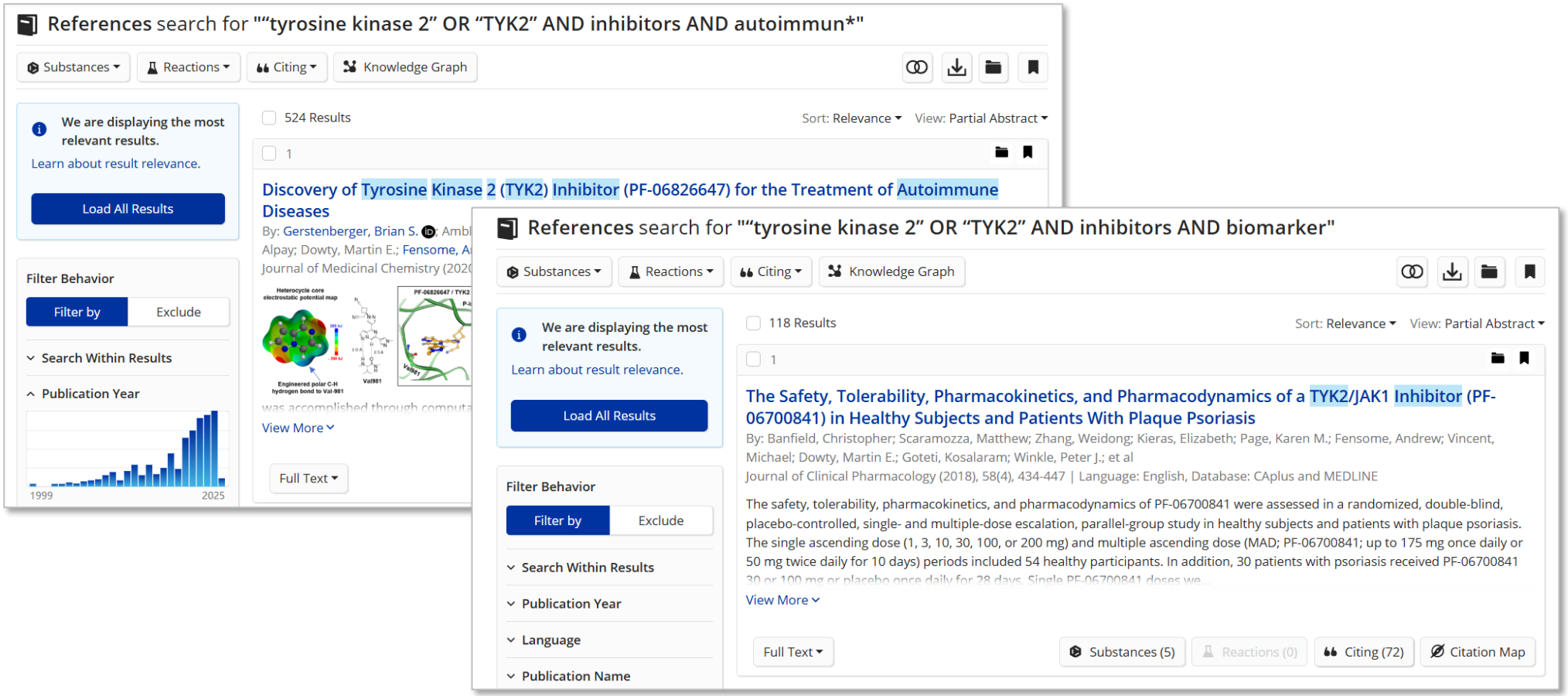
灵活缩放检索式——逻辑算符和通配符的使用

示例：

“tyrosine kinase 2” OR “TYK2” AND inhibitors AND autoimmun* （524）

“tyrosine kinase 2” OR “TYK2” AND inhibitors AND biomarker（118）



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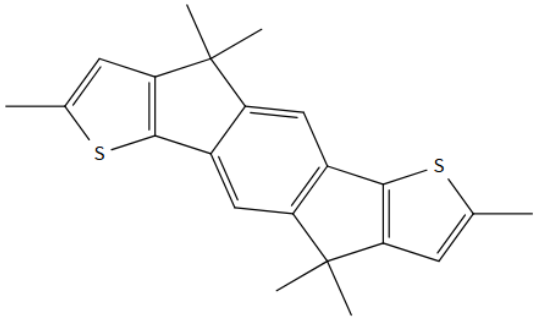
锁定研究了目标结构的文献

同时识别关键词与结构式



CAS SciFinder | References | Organic photovoltaic cell | Edit

References search for "Organic photovoltaic cell" + drawn structur

Substances | Reactions | Citing | Knowledge Graph

Structure Match

As Drawn (0)

Substructure (1,877)

Filter Behavior

Filter by | Exclude

Search Within Results

Publication Year

Language

Publication Name

1,877 Results

1

Fused-Ring Acceptors with Asymmetric Side Chains for High-
Solar Cells

By: Feng, Shiyu; Zhang, Cai-e; Liu, Yahui; Bi, Zhaozhao; Zhang, Zhe; Xu, Xinjun;
Advanced Materials (Weinheim, Germany) (2017), 29(42), n/a | Language: English

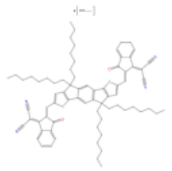
A kind of new fused-ring electron acceptor, IDT-OB, bearing asym. side chains, is
solar cells. The introduction of asym. side chains can increase the solubility of ac
closely in a dislocated way, and form favorable phase separation when blended w
devices exhibit high and balanced hole and electron mobility and give a high pow
importantly, the IDT-OB-based devices are not very sensitive to the film thickness

View More

Full Text | Substances (17) | Re

Edit Draw

2213434-11-6

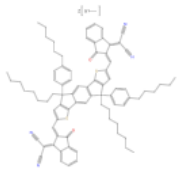


$C_{76}H_{86}N_4O_2S_2$

Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

Notes: electron acceptor with asym. fused ring side chain

2213434-10-5



$C_{84}H_{86}N_4O_2S_2$

Propanedinitrile, 2,2'-[[4,9-bis(4-hexylphenyl)-4,9-dihydro-4,9-dioctyl-s-indace...

Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

Notes: electron acceptor with asym. fused ring side chain

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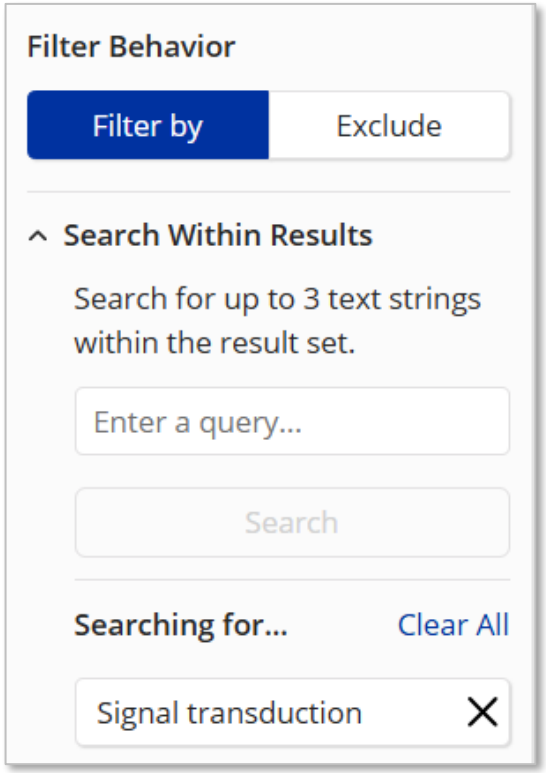
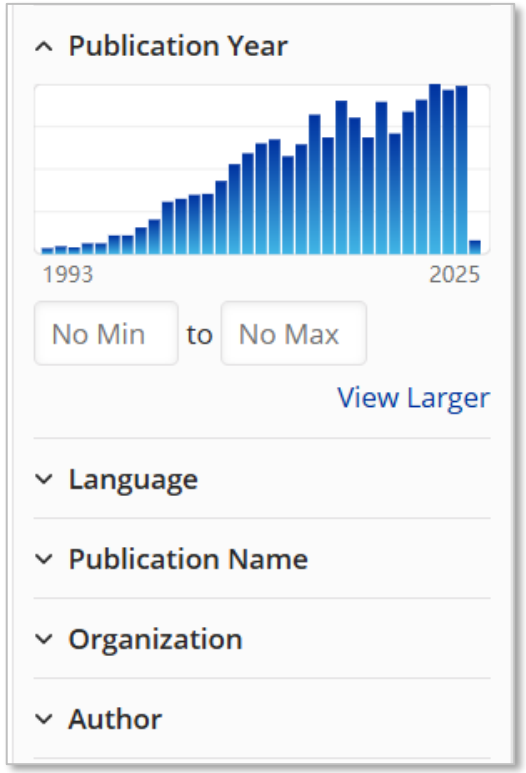
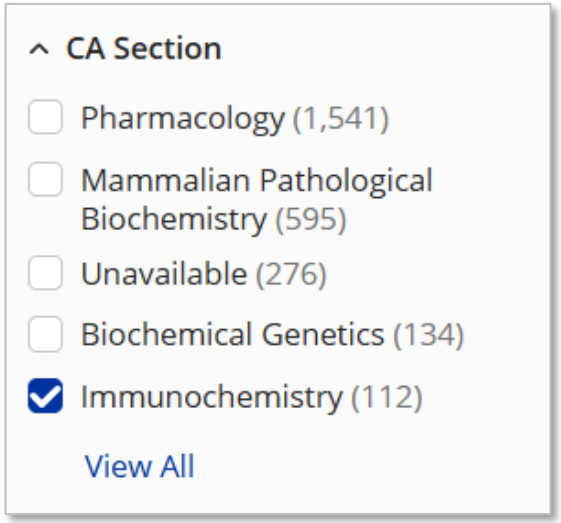
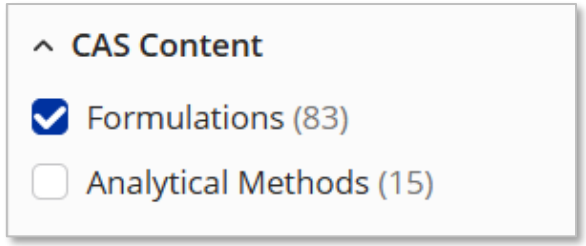
丰富的筛选工具

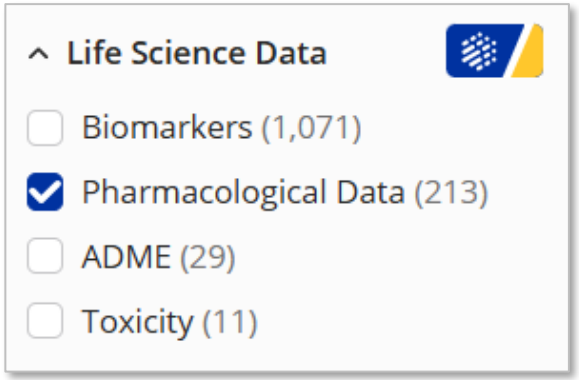
文献类型、语言、作者、发表机构、发表年份、CAS标引的技术术语、CAS标引的学科研究方向、二次检索、下载数据分析报告…











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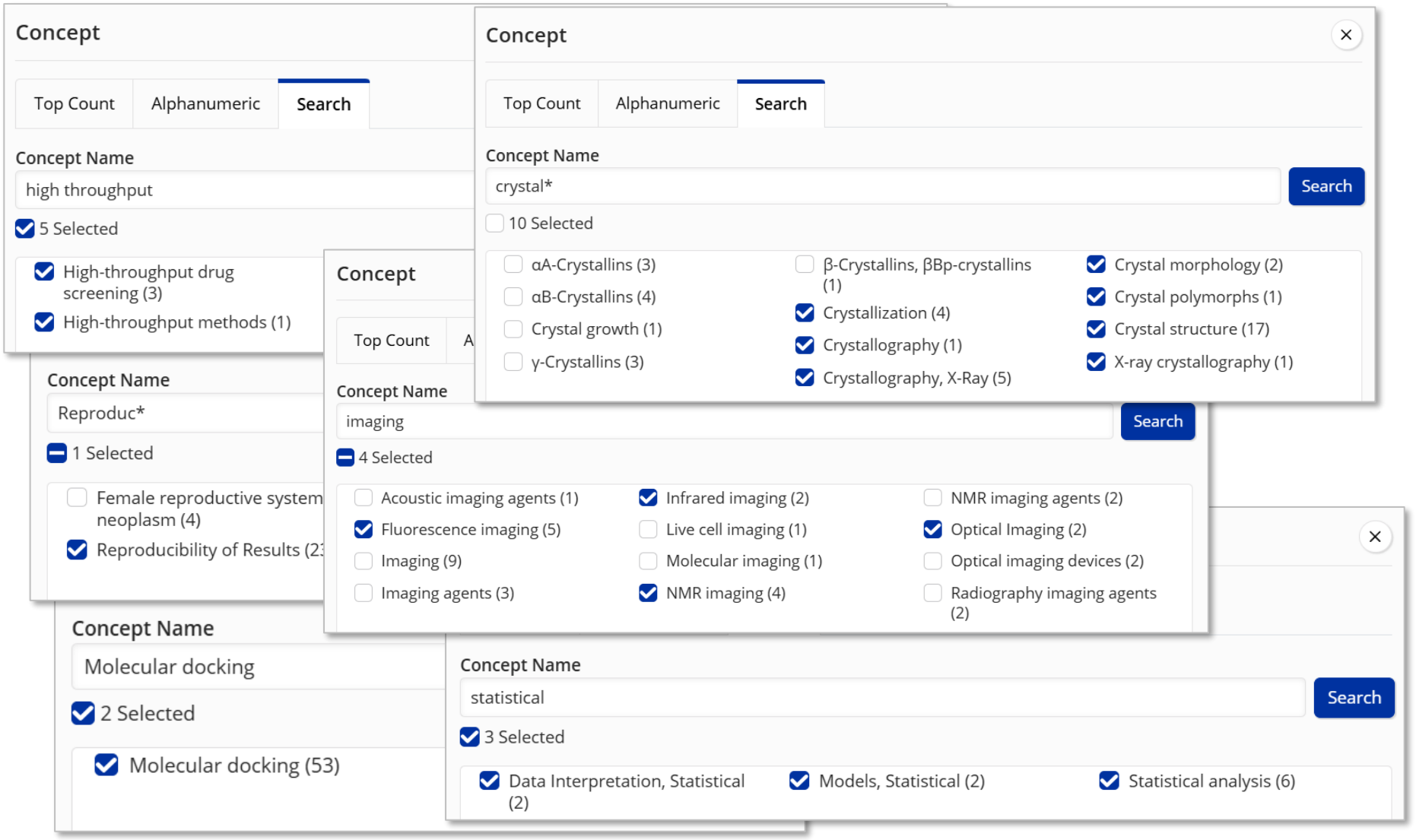
筛选与目标研究点相关的文献：Concept



- 实验设计/方法
- 测试表征
- 结果重复性
- 统计分析
- 理论计算与模拟
- 研究应用

…

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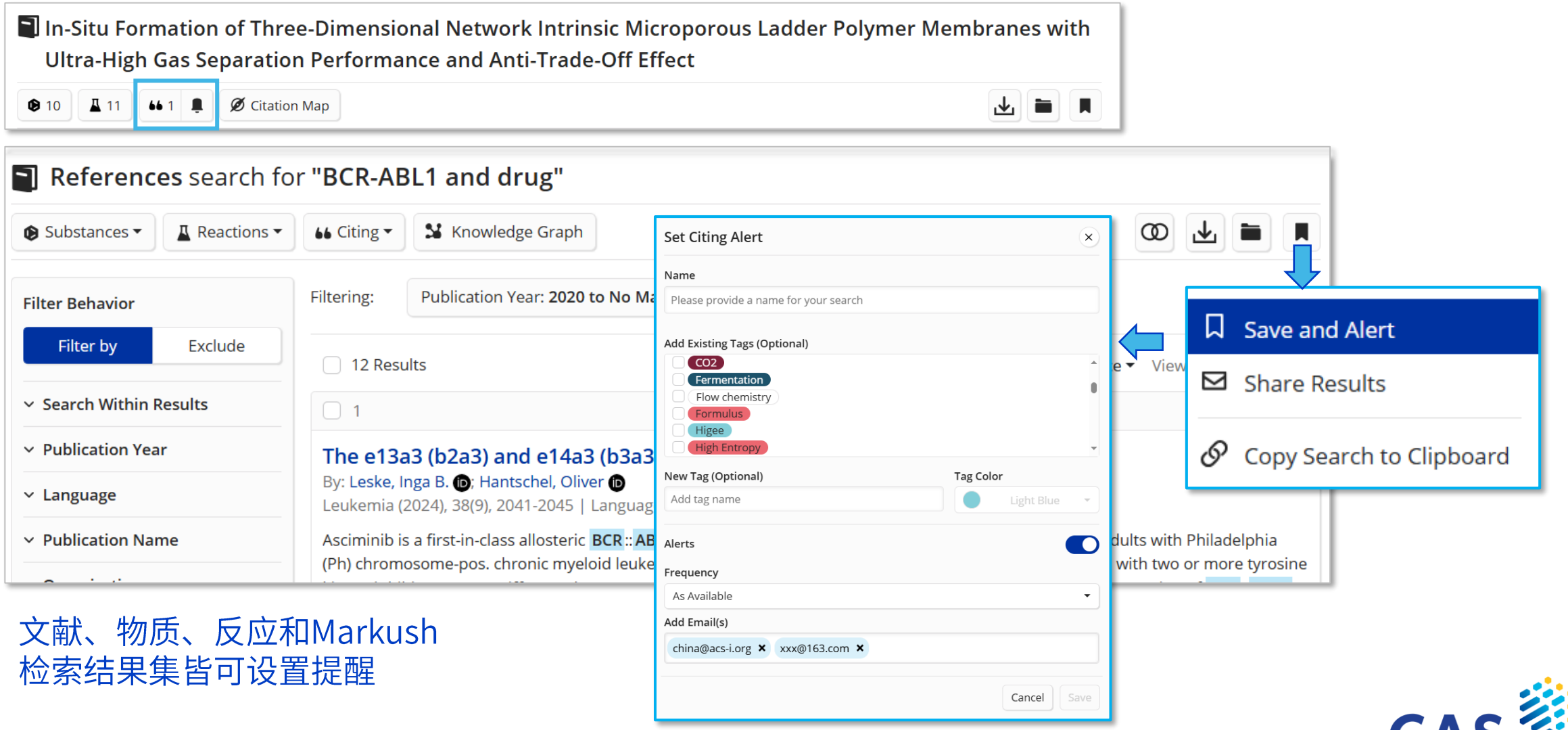
定题追踪：研究领域中的最新进展



文献、物质、反应和Markush
检索结果集皆可设置提醒

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提纲

物质

- 物质详情
- 检索方法

- ✓ 属性
- ✓ 谱学信息
- ✓ 生物学数据

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属性信息

声学、化学、密度、电学、电子、界面、磁学、机械、光学、结构、热学等实验属性

1

12244-10-9

Component	Ratio
O_5Si_2	1.45-1.50
Al	1-1.10
Na	0.90-1
O	0-0.50
Ca	0-0.10

$Al.Ca.Na.O_5Si_2.O$

Components: 5

Albite $((Si_{2.9\text{-}3}Al_{1\text{-}1.1})(Na_{0.9\text{-}1}Ca_{0\text{-}0.1})O_8)$

12K References | 5 Reactions | 0 Suppliers

Experimental Properties

Chemical | Density | Flow and Diffusion | Interface | Mechanical | Optical and Scattering | Structure Related | Thermal

Property	Value	Condition	Source
Entropy	208.20 J/mol·K (approx)	Temp: 298 K; Press: 1 x 10^5 Pa	(1) CAS
Formation Enthalpy	-3935.0 kJ/mol	Temp: 298 K	(2) CAS
Formation Enthalpy	-3936.476 kJ/mol (approx)	Temp: 298 K; Press: 1 x 10^5 Pa	(1) CAS
Free Energy of Formation	-3711.6 kJ/mol	Temp: 298 K	(2) CAS
Free Energy of Formation	-3713.038 kJ/mol (approx)	Temp: 298 K; Press: 1 x 10^5 Pa	(1) CAS
Melting Point	1118 °C	-	(3) CAS
Melting Point	795-810 °C	-	(4) CAS
Thermal Conductivity	2.349 W/m·K (solid)	Temp: 300 K	(5) CAS
Thermal Conductivity	2.30-2.32 W/m·K	-	(6) CAS
Enthalpy - 1 Source	See Full Text		(7) CAS
Entropy - 1 Source	See Full Text		(8) CAS
Fusion Enthalpy - 1 Source	See Full Text		(9) CAS
Gibbs Free Energy - 1 Source	See Full Text		(10) CAS

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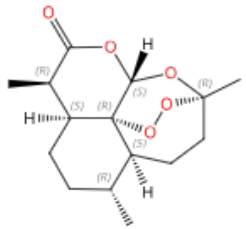
谱图信息

1

63968-64-9



Absolute stereochemistry shown

$C_{15}H_{22}O_5$

3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trime...

9,268 References

3,039 Reactions

101 Suppliers

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Pharmacological Data — CAS LIFE SCIENCES
- ADME — CAS LIFE SCIENCES
- Toxicity — CAS LIFE SCIENCES
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

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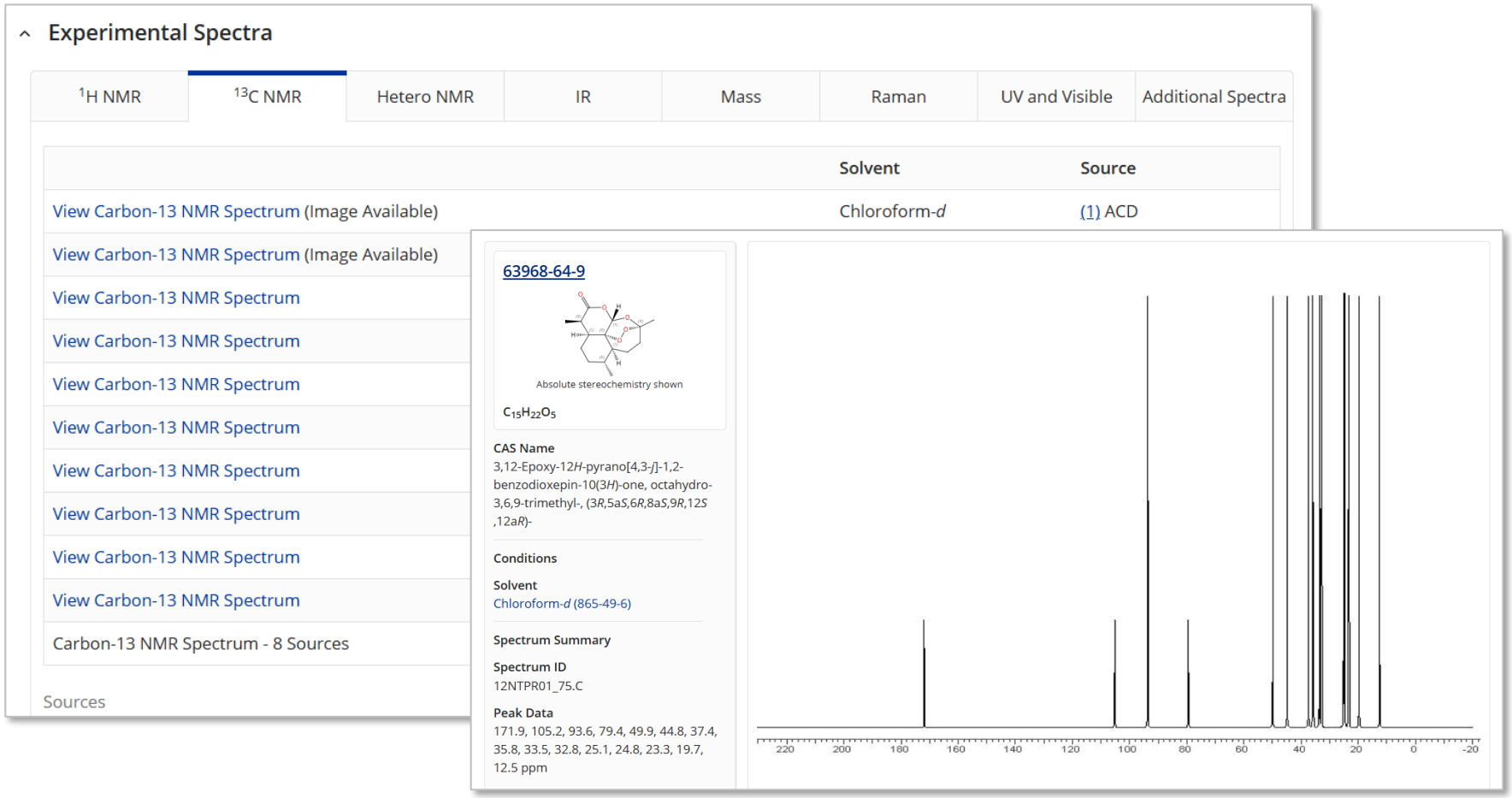
谱图信息

核磁、红外、质谱、拉曼、红外、UV-vis、X-Ray等



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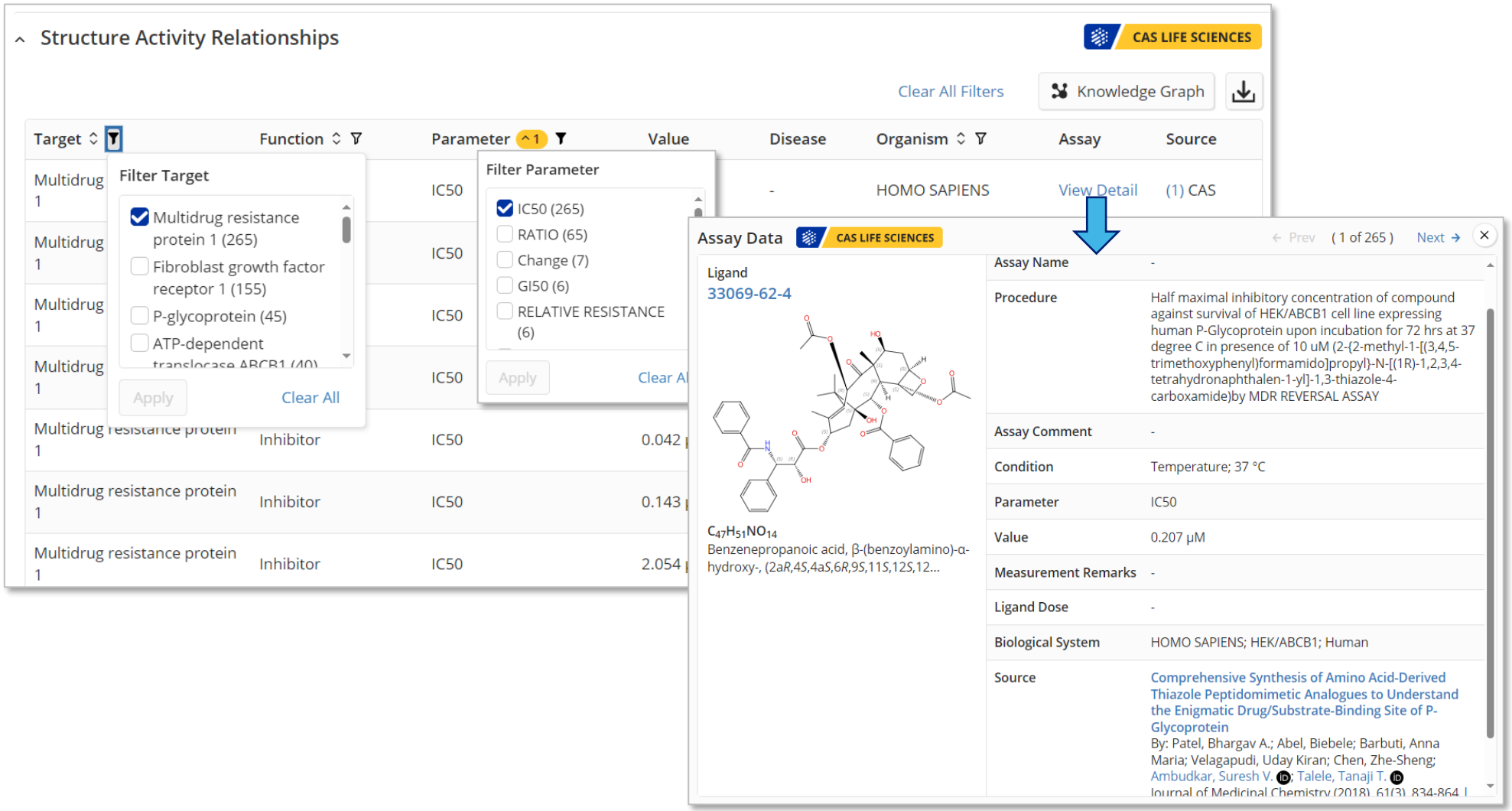
生物学数据信息



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提纲

物质

- 物质详情
- 检索方法

- ✓ 标识符、分子式
- ✓ 属性值、谱图数值
- ✓ 结构检索
- ✓ 序列检索

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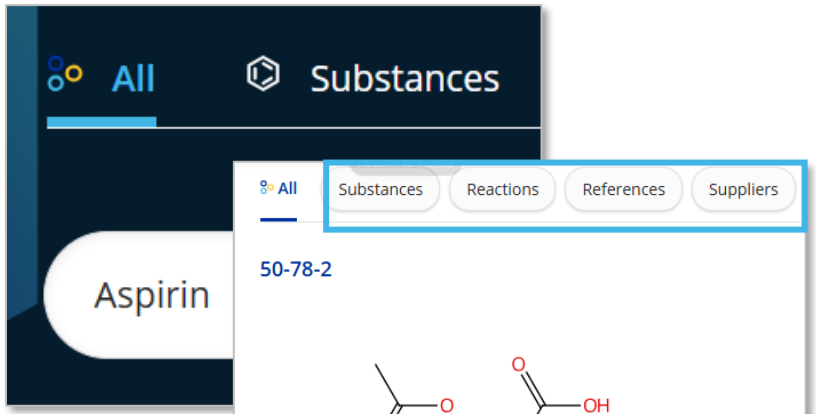
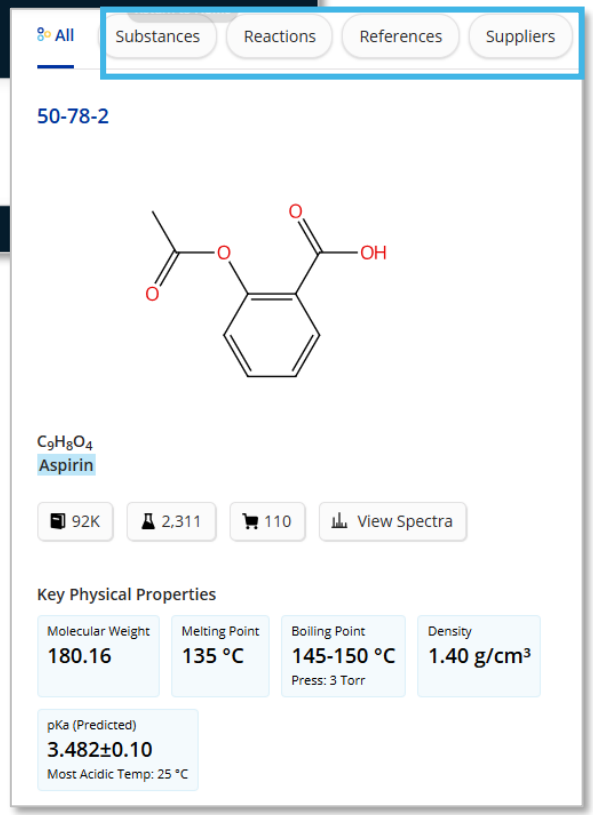
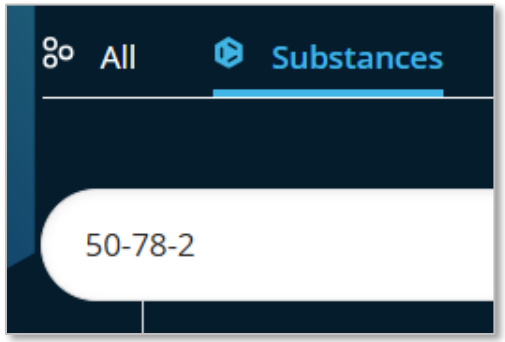
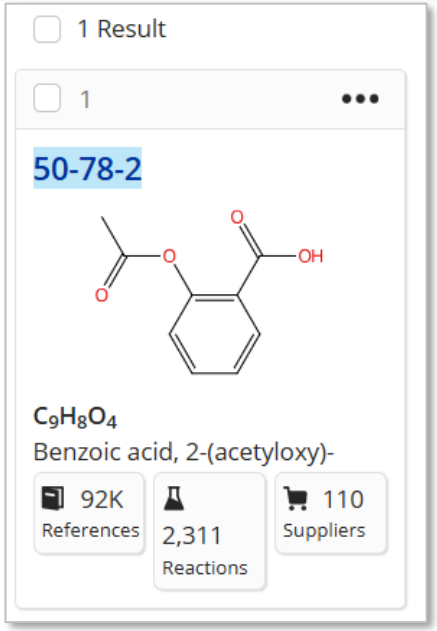
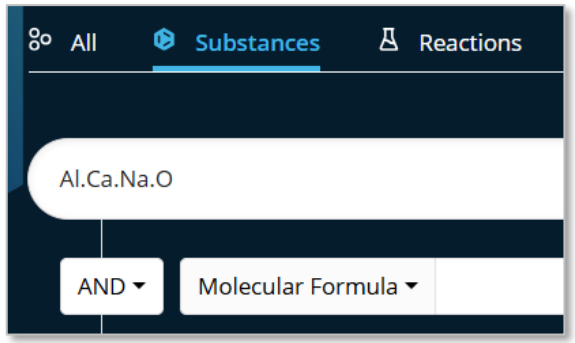
物质的检索策略

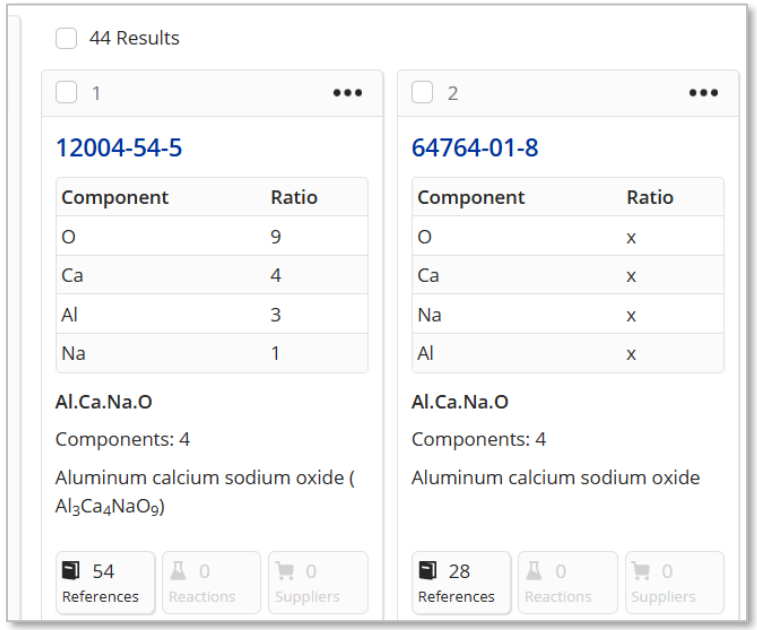












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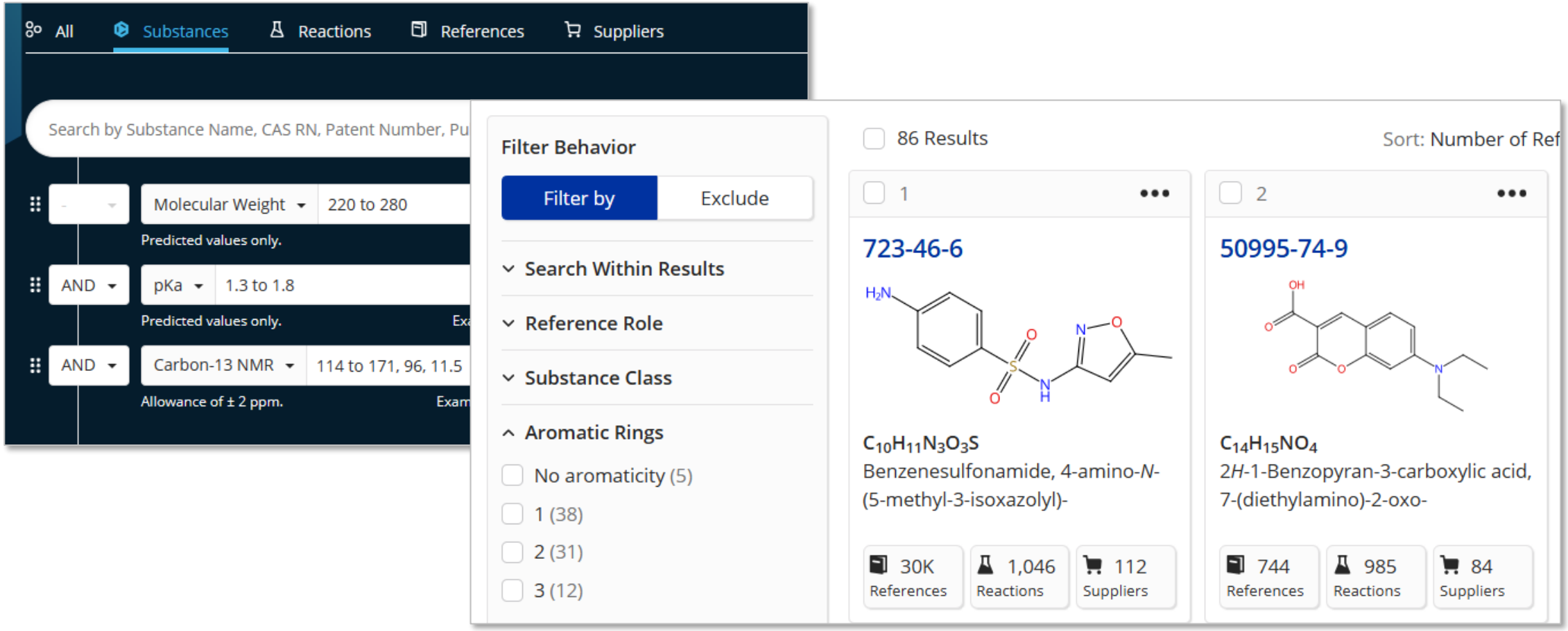
利用属性值、谱图数值检索物质



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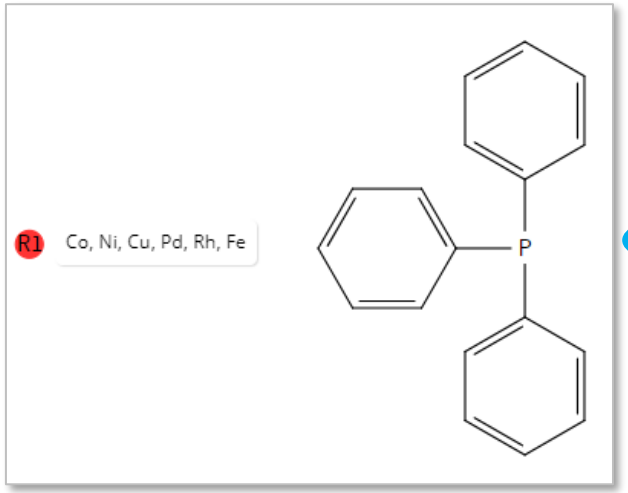
结构检索



Filter Behavior

Filter by | Exclude

- Search Within Results
- Substance Class
  - Coordination Compound (32)
  - Salt and Compound With (1)
- Reference Role
- Reaction Role
  - Product (60)
  - Reactant (32)
  - Reagent (11)
  - Catalyst (32)
  - Solvent (1)
- Aromatic Rings
- Functional Group
- Element

4

33991-60-5

$C_{36}H_{30}NiP_2$
Bis(triphenylphosphine)nickel

47 References | 24 Reactions | 0 Suppliers

5

33775-59-6

$C_{36}H_{30}NiP_2$
Bis(triphenylphosphine)nickel(2+)

3 References | 1 Reaction | 0 Suppliers

7

24355-89-3

$C_{36}H_{30}CuP_2.I$

8

69878-70-2

$C_{36}H_{30}P_2Pd_2$

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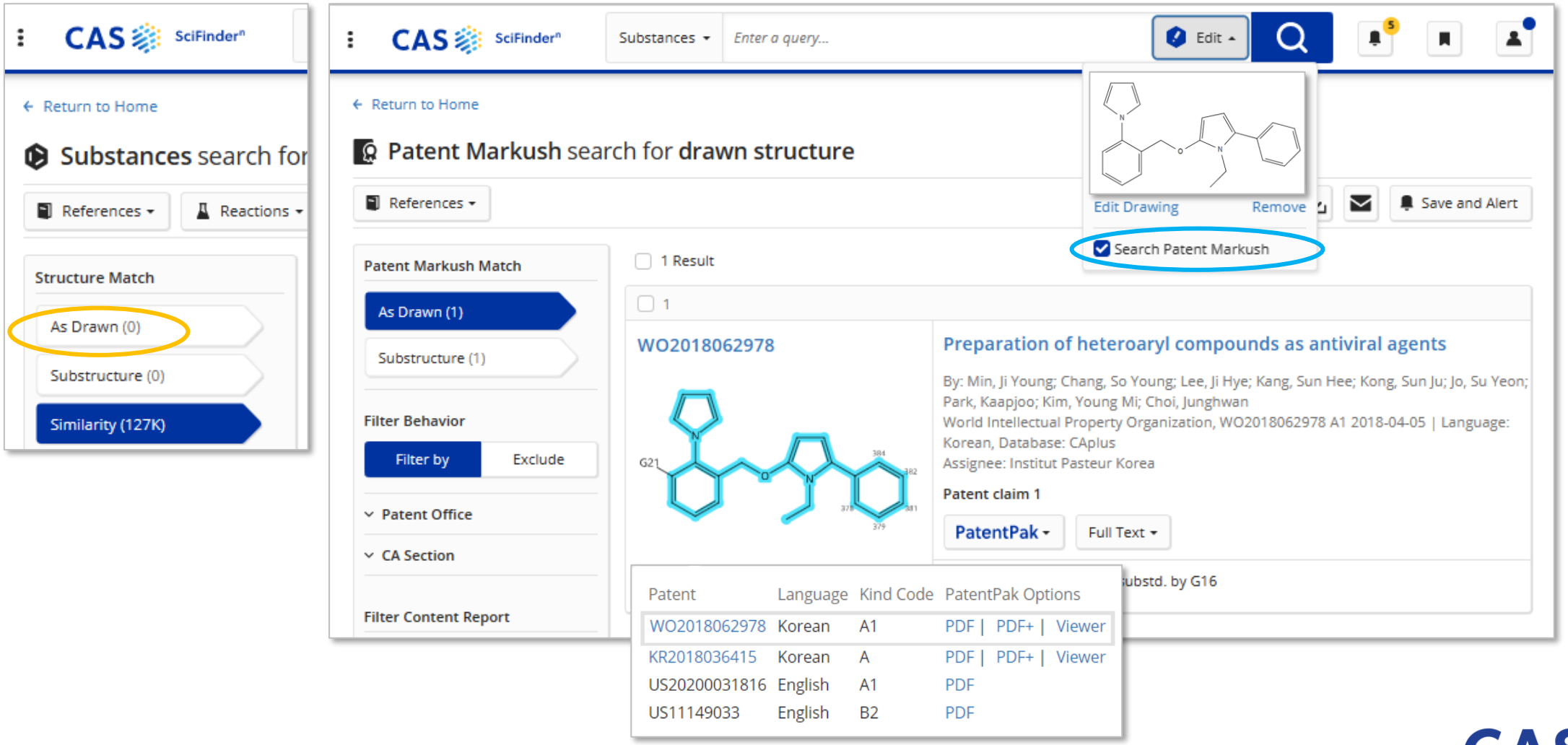
Markush検索



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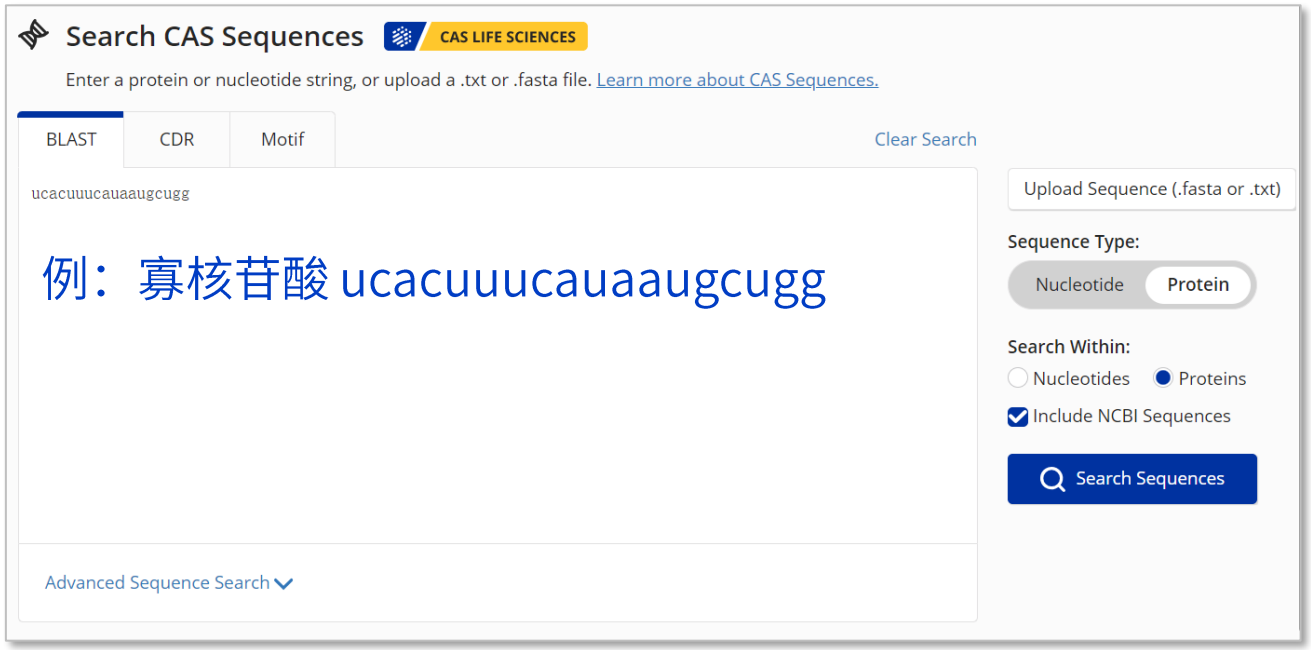
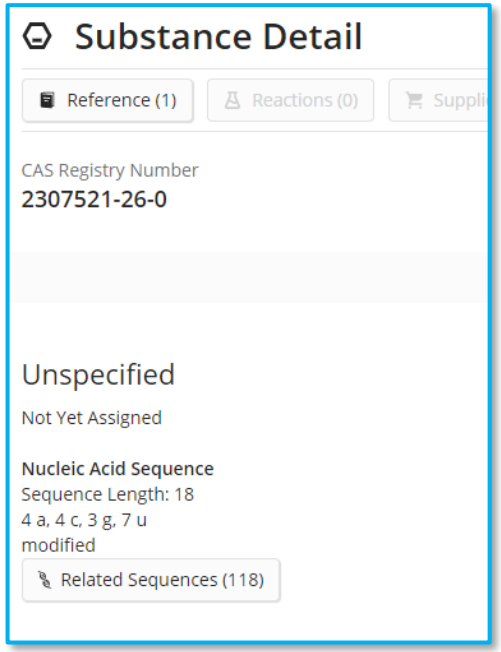
序列检索





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提纲

反应
- 检索方法
- 逆合成设计

合成反应操作详情

CAS Reaction Number: 31-289-CAS-15718311

Get Similar Reactions

Save

Suppliers (46)

Experimental Protocols

Synthetic Methods (7)

Procedure

1. Suspend 3-(pyrimidine-2-yl)phenanthro[9,10-e]-1,2,4-triazin
2. Add isoamyl nitrite (0.47 ml, 3.5 mmol) to the mixture.
3. Stir the resulting mixture under reflux.
4. Add a solution of corresponding anthranilic acid (3.5 mmol)
   dropping funnel for 30 minutes.
5. Heat the reaction mixture under reflux for 1 hour.
6. Cool the reaction mixture to room temperature.
7. Wash the reaction mixture with potassium hydroxide soluti
8. Dry the reaction mixture with anhydrous sodium sulfate.
9. Concentrate the crude product under reduced pressure.
10. Dry the crude product under vacuum.
11. Separate the crude product by column chromatography (Si
    (1:2) as eluent.

Characterization Data

1*H*-Phenanthro[9,10-*d*]-1,2,3-triazole, 1-pyrimido[1,2-*a*]indol-10-yl-

Proton NMR Spectrum	δ, ppm ($CDCl_3$): 6.70 (dd, 1H, *J* 7.1, 3.7 Hz, H-3 (pyrimidoindole)), 7.19 (m, 1H), 7.42-7.61 (m, 5H), 7.72 (m, 1H), 7.80 (m, 1H), 8.04 (m, 1H), 8.35 (dd, 1H, *J* 3.7, 2.0 Hz, H-4 (pyrimidoindole)), 8.67 (m, 1H), 8.71 (m, 1H), 8.79 (dd, 1H, *J* 7.1, 2.0 Hz, H-2 (pyrimidoindole)), 8.97 (dd, 1H, *J* 8.1, 0.9 Hz).
Carbon-13 NMR	δ, ppm ($CDCl_3$): 101.9, 105.6, 110.9, 118.4, 120.8, 122.5, 122.7, 123.1, 123.4, 124.0, 125.0, 125.4, 125.7, 125.9, 126.9, 127.0, 127.6, 128.1, 129.1, 130.5, 131.2, 131.9, 138.1, 141.4, 151.8.
Elemental Analysis	Calcd for $C_{25}H_{15}N_5$: C 77.91; H 3.92; N 18.17. Found: C 77.80; H 3.81; N 17.98.
Mass Spectrum	ESI-MS, m/z: found 386.14, calculate 386.14 $(M+H)^+$.
Melting Point	181-183°C.
R_f	0.8.

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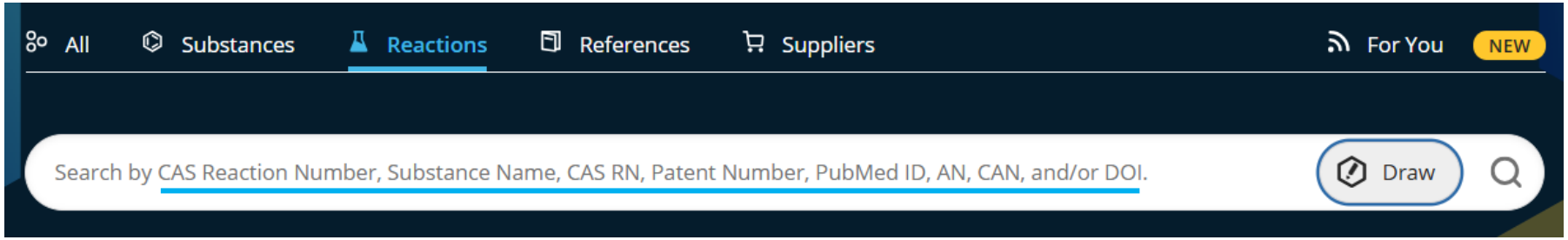
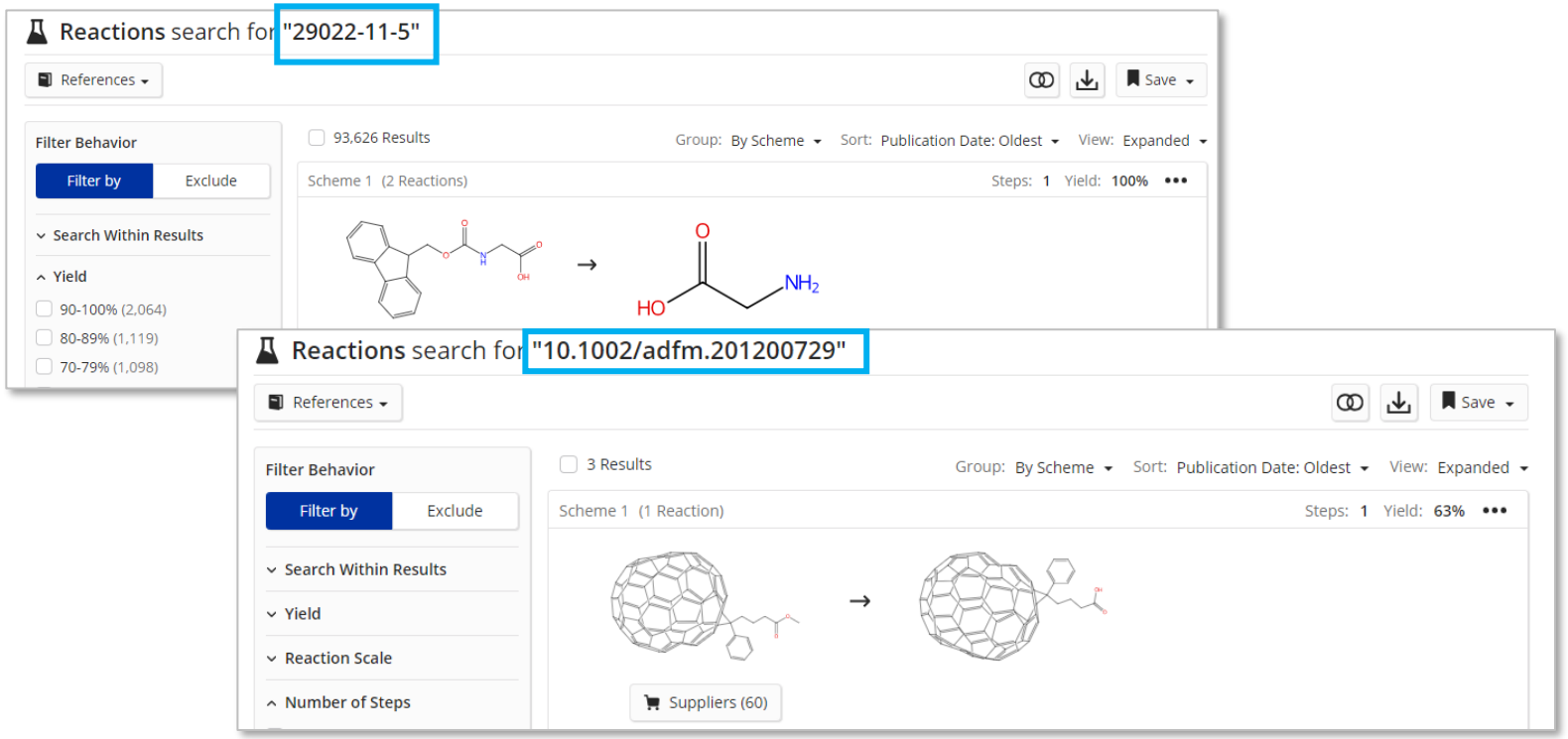
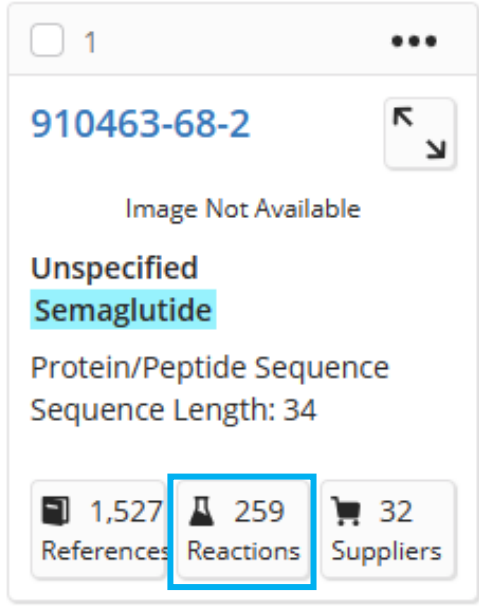
反应检索方法







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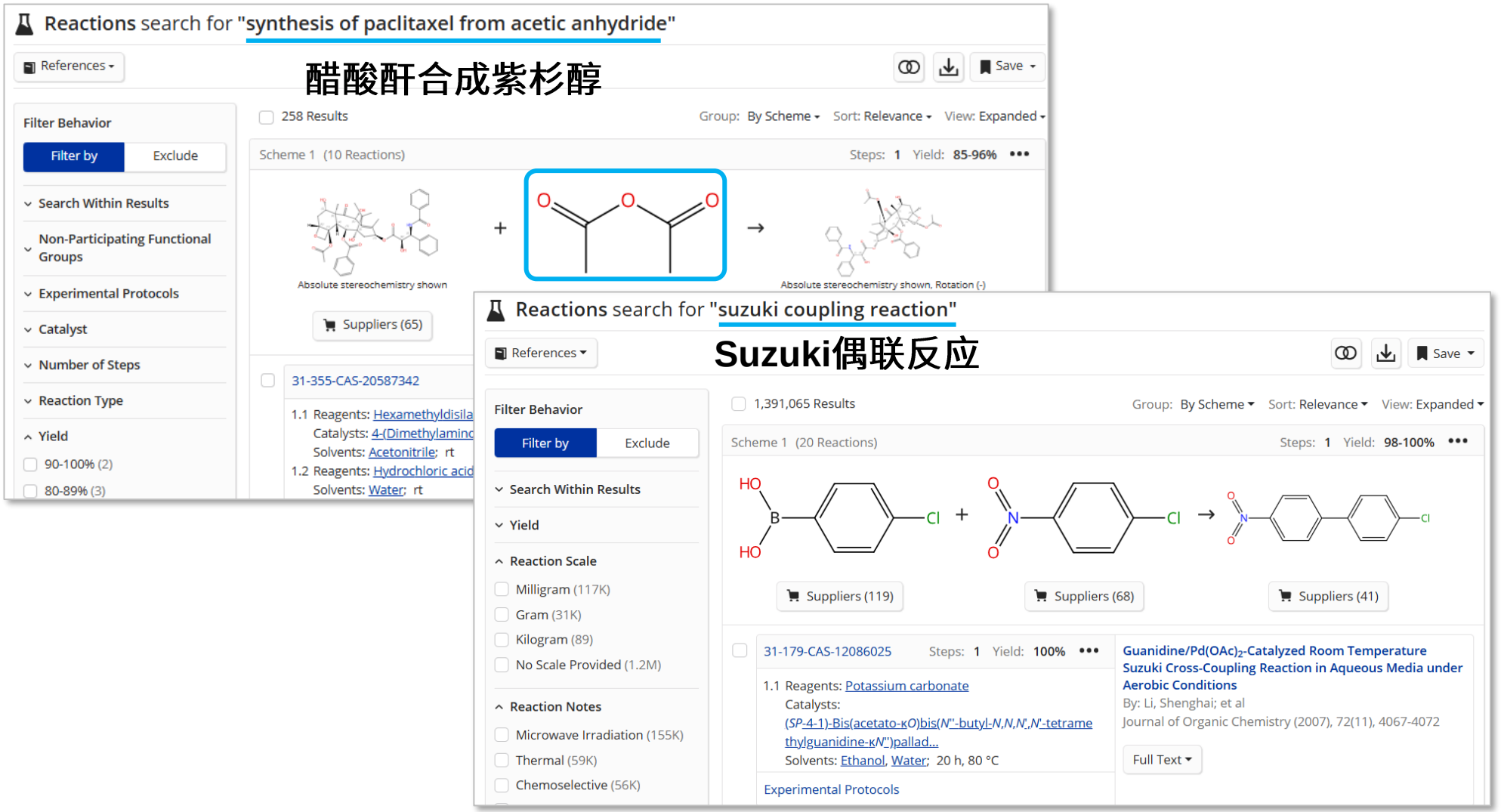
利用自然语言便捷检索反应



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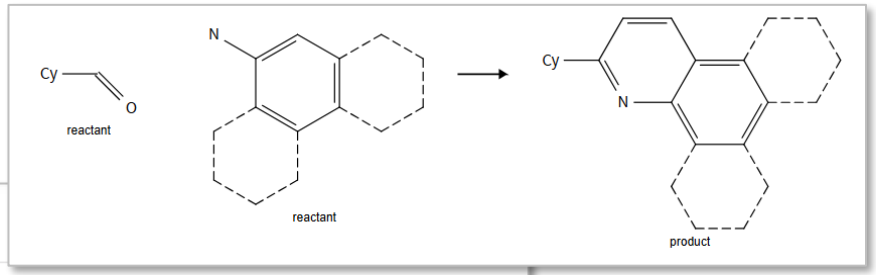
结构式检索



Reactions search for drawn structure

References

Save

Structure Match

As Drawn (0)

Substructure (472)

Similarity (0)

Filter Behavior

Filter by | Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Catalyst

472 Results

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 91%

31-087-CAS-17090818

Steps: 1 Yield: 91%

1.1 Reagents: Phosphorus oxychloride
Solvents: Nitrobenzene; 4 h, reflux

Preparation benzothiophene-fused heterocyclic compound for organic light emitting device

Assignees: Heesung Material Ltd.; LT Materials Co., Ltd.

Korea, Republic of, KR2016051212 A 2016-05-11

PatentPak | Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 91%

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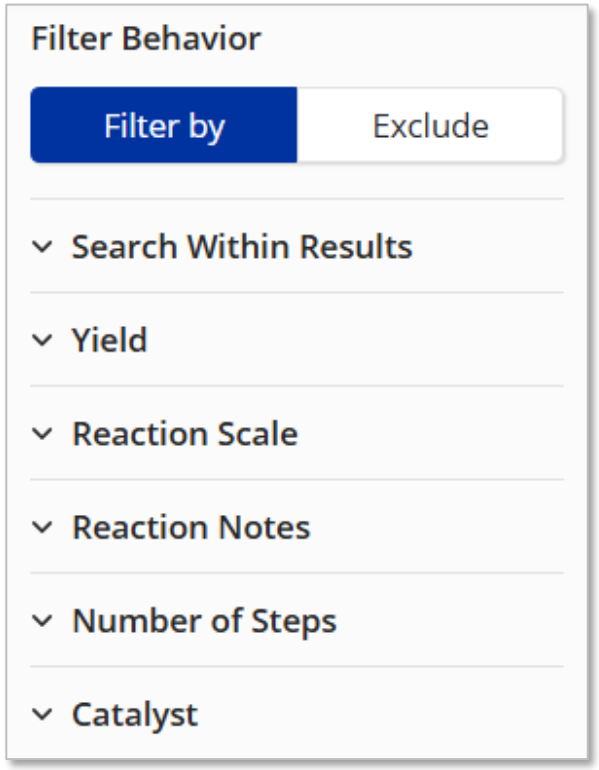
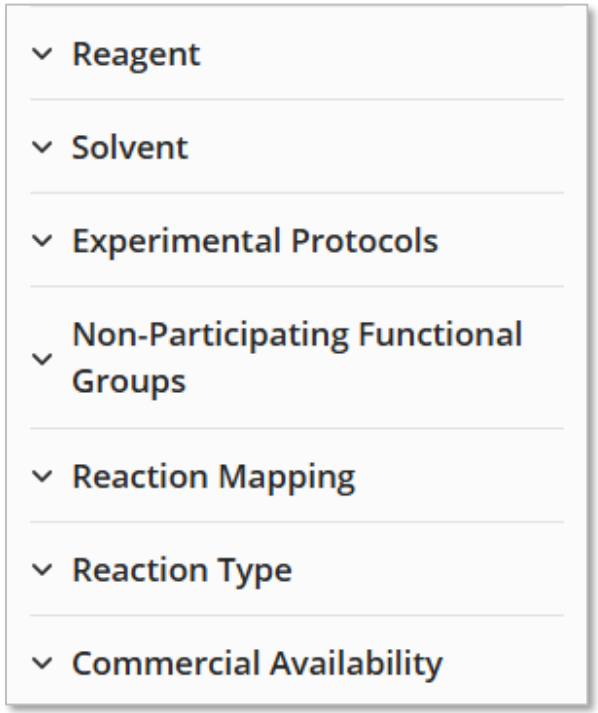
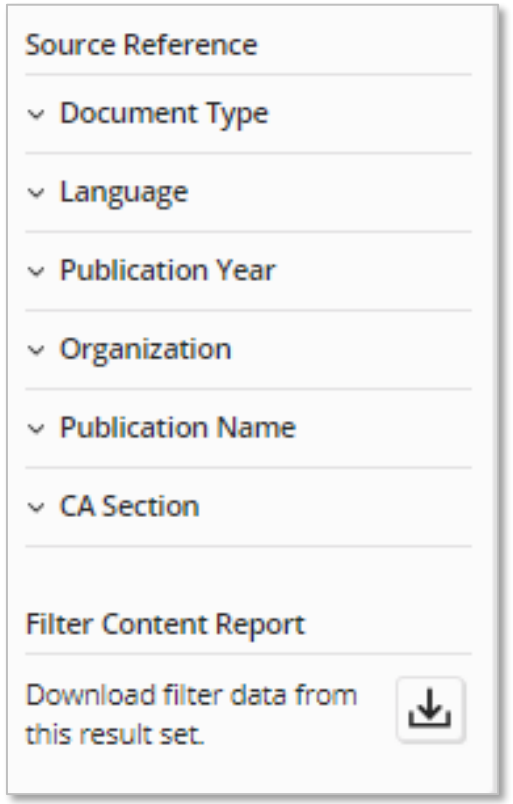
高效筛选目标反应

反应筛选类别：产率、规模、步数、不参与反应的官能团、实验步骤、反应类型、立体化学、试剂、催化剂、溶剂、商品信息

文献筛选类别：文献类型、语言、出版年份、刊物名







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提纲

反应

- 检索方法
- 逆合成设计

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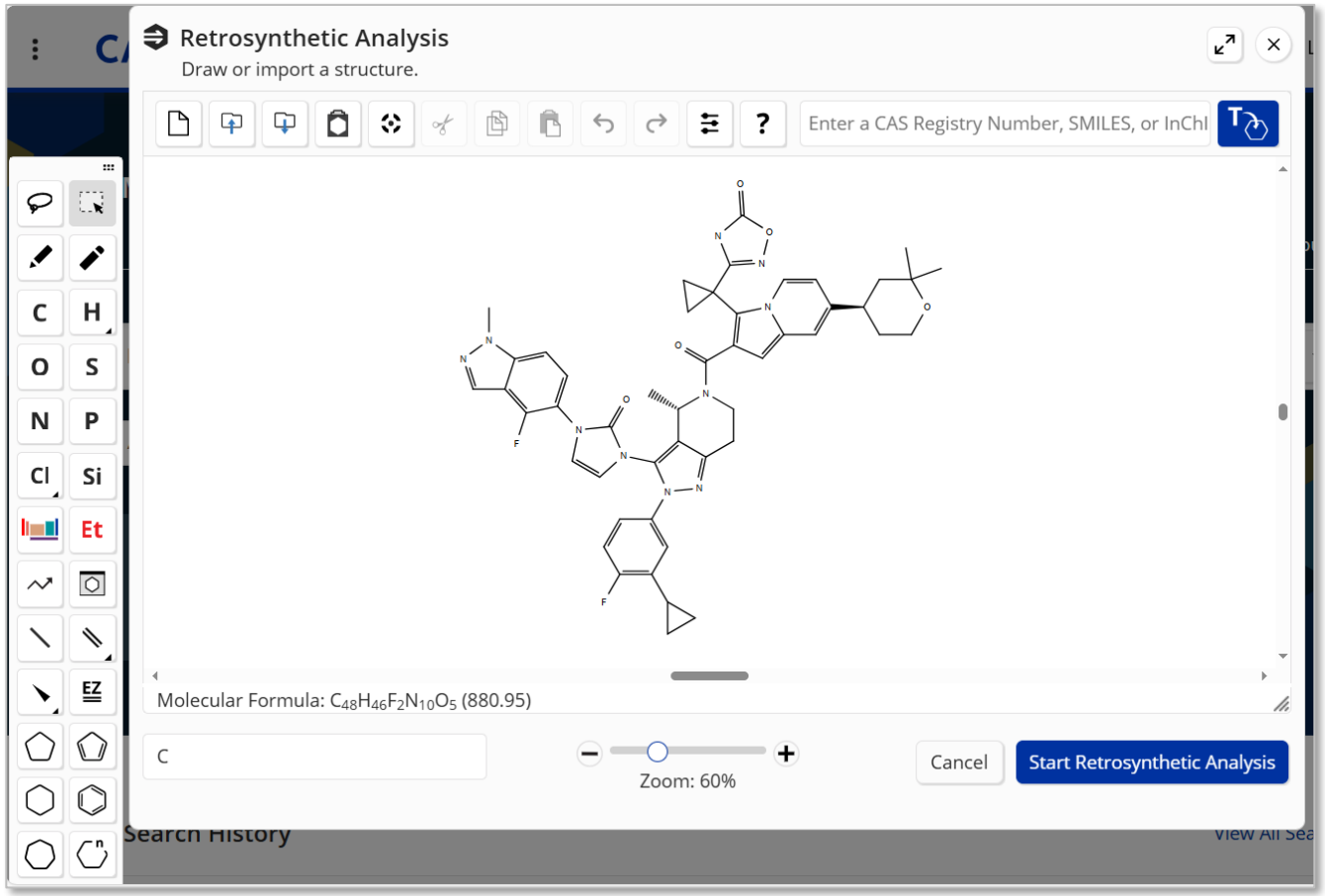
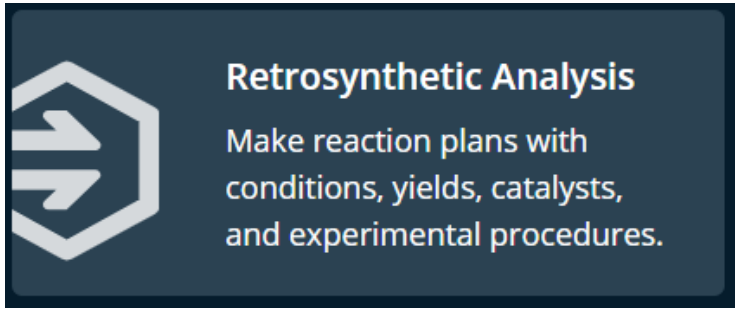
启发逆合成路线的设计

可用于未知化合物或已知化合物和的逆合成路线设计





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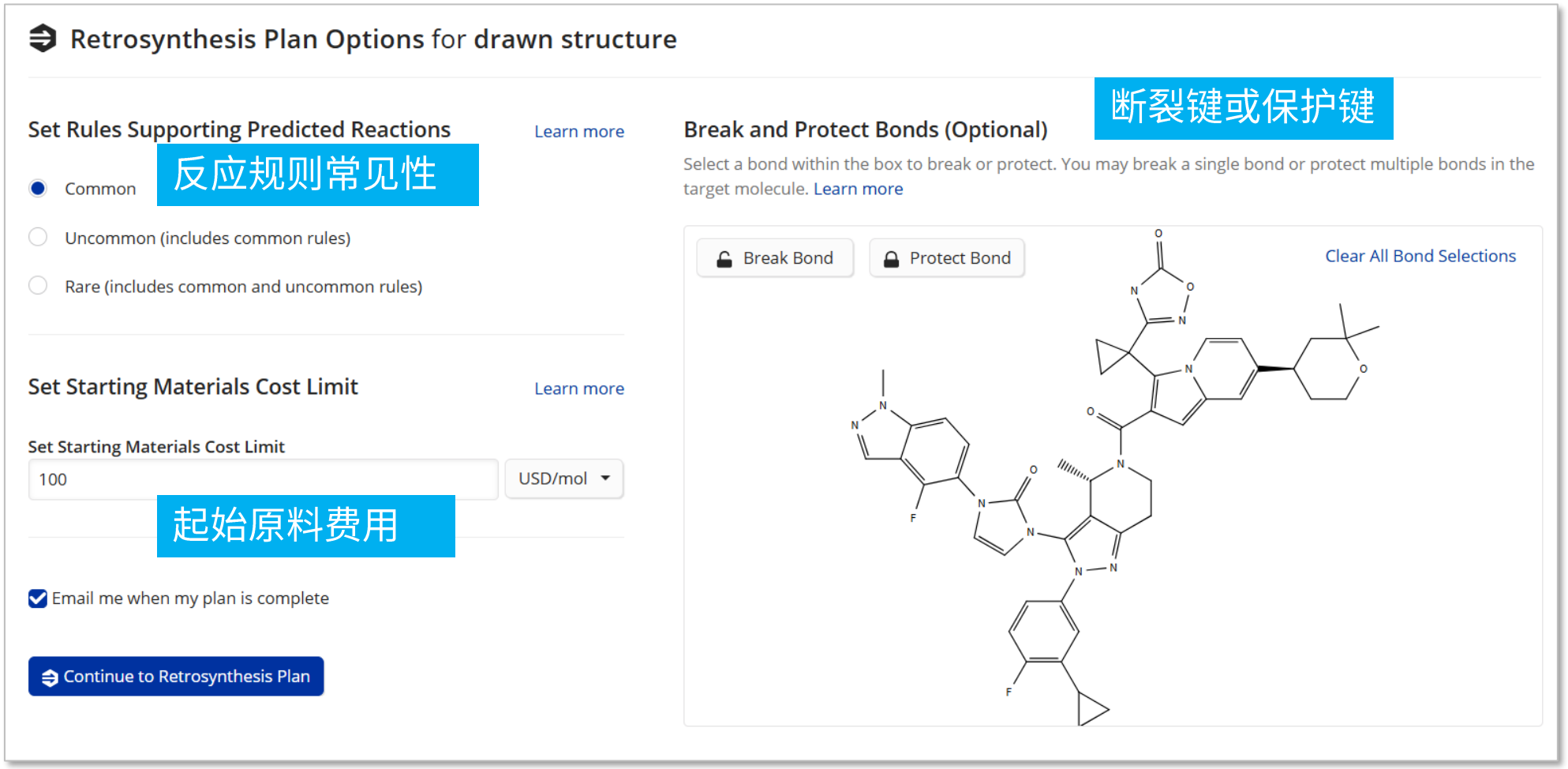
预设合成参数



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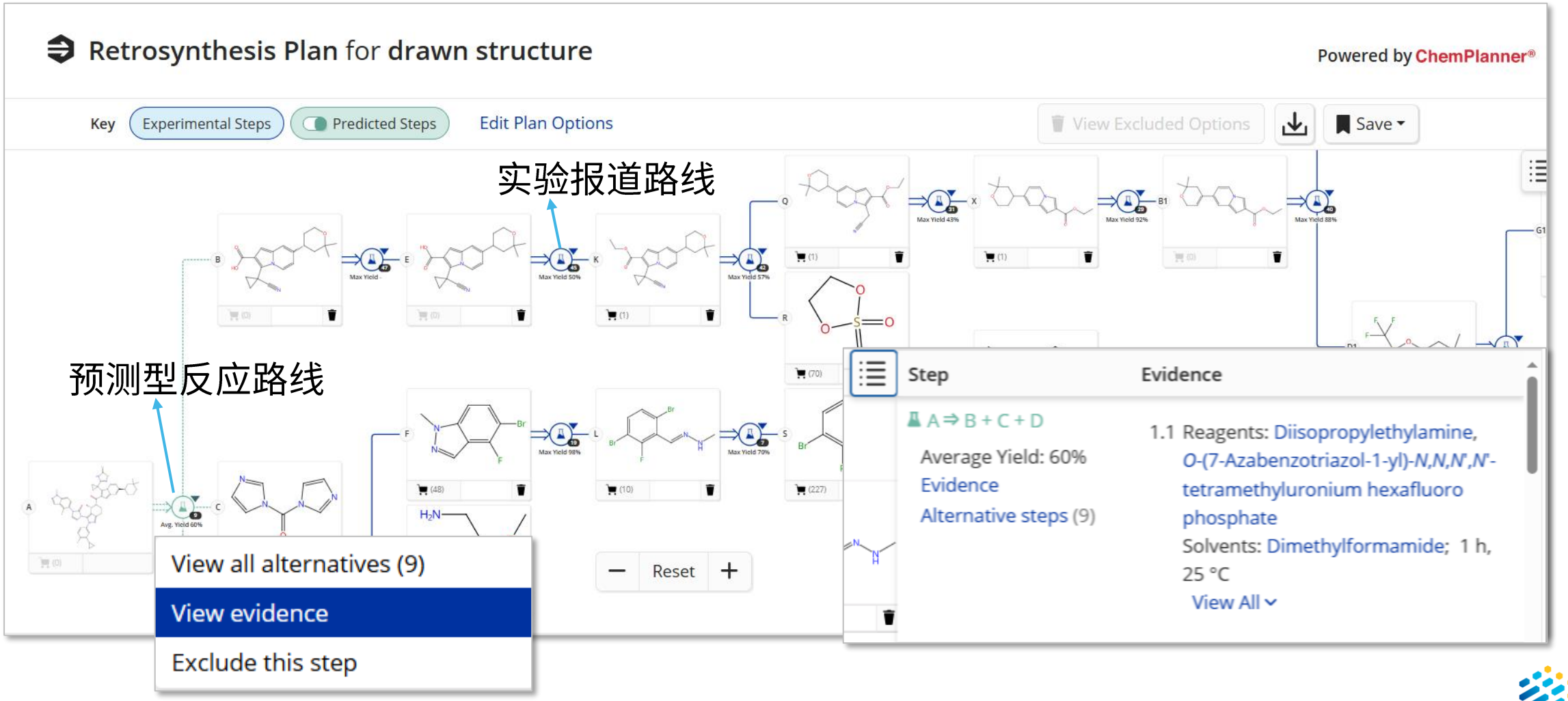
获得逆合成反应路线



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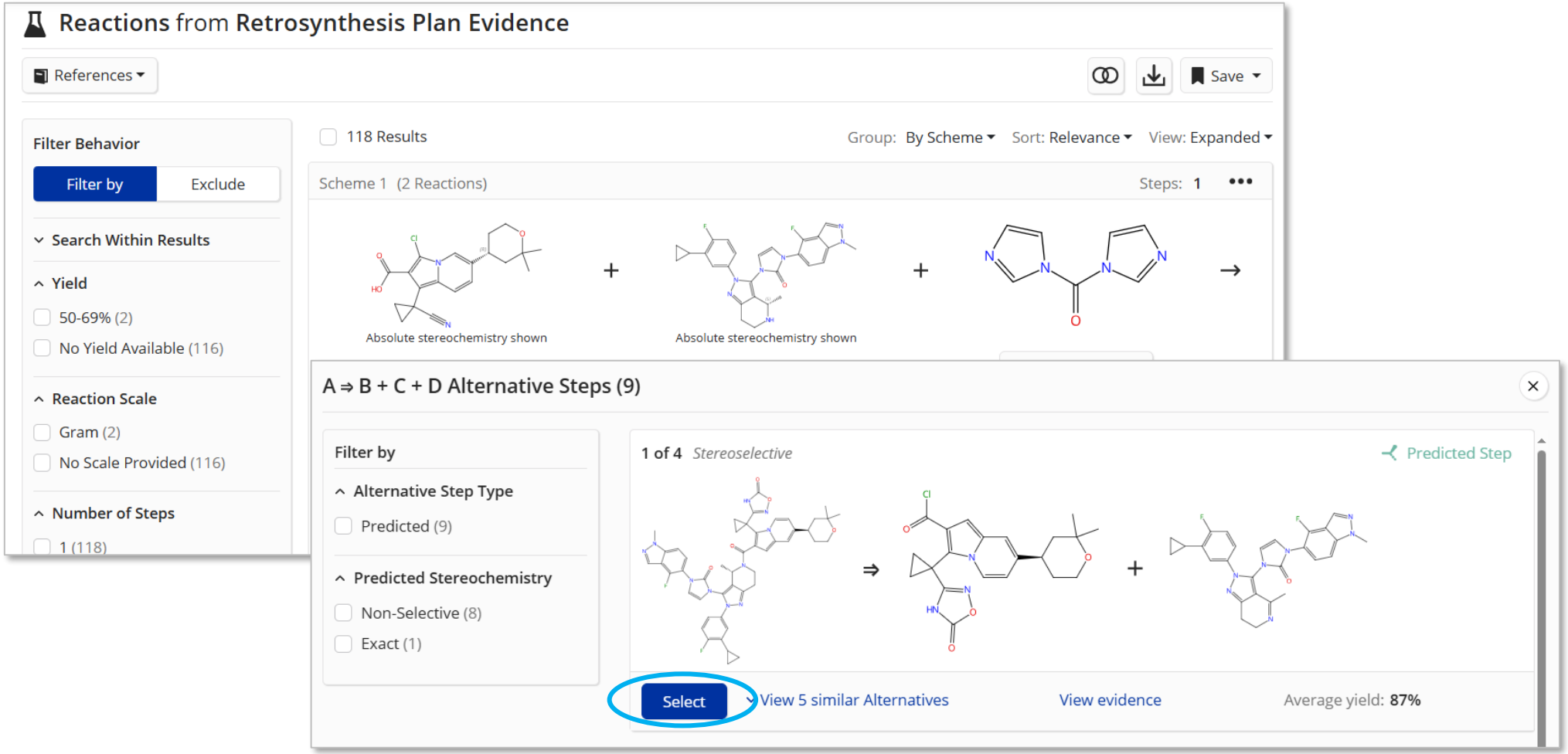
查看文献支持与替换路线



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总结

文献检索

- 基于数据关联，高效查看文献中的核心研究点、物质、反应、分析方法及配方信息
- 利用Concept、Lexicon辅助关键词的积累，灵活构建检索式，利用丰富的筛选工具高效筛选

物质检索

- 基于数据关联，高效获取物质的属性、谱学、生物学数据、GHS危险说明等信息
- 利用物质/文献标识符、分子式、属性值/谱图数值、结构检索物质

反应检索

- 利用物质或文献标识符、自然语言或结构式灵活检索，高效筛选目标反应，利用Synthetic Methods高效查看合成反应详情
- Retrosynthetic Analysis获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

Between problems and progress are connections that matter

谢谢！

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