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4/18/2025

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提纲

- CAS 简介
- CAS SciFinder Discovery Platform 助攻论文写作
  - 研究背景：研究现状和发展趋势的全面调研
  - 实验设计：课题的创新性及已有相关实验报道
  - 结果分析：数据的比对及关联研究检索拓展
- Q&A

关于 CAS

CAS 从专业知识、内容和技术三方面为全球创新保驾护航

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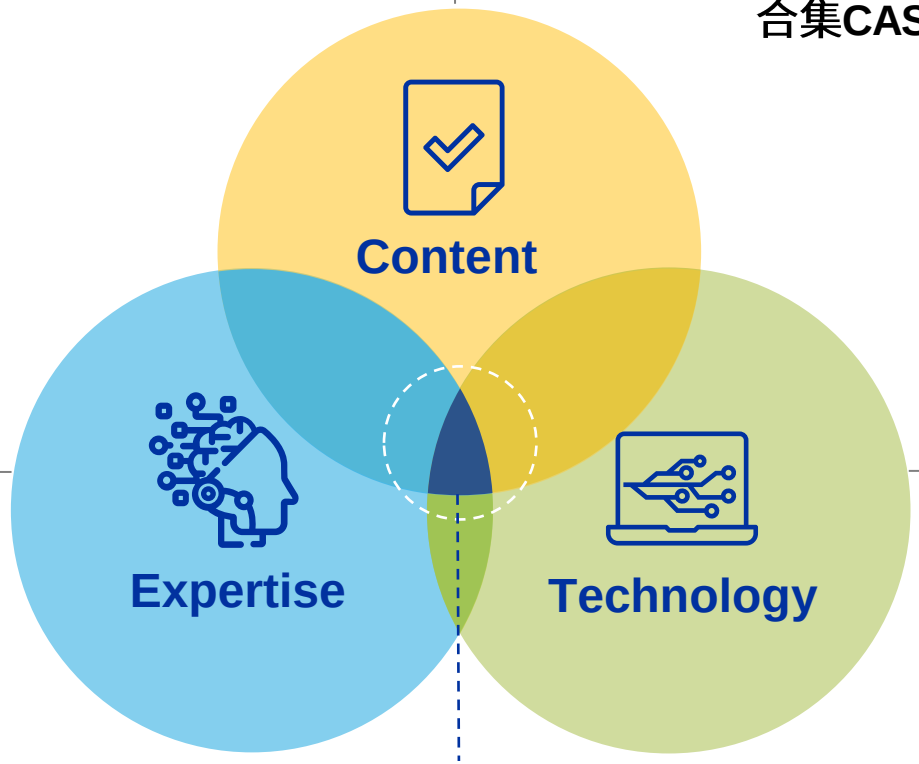

专业知识 | 多学科背景的科学家和技术专家，精通50多国语言

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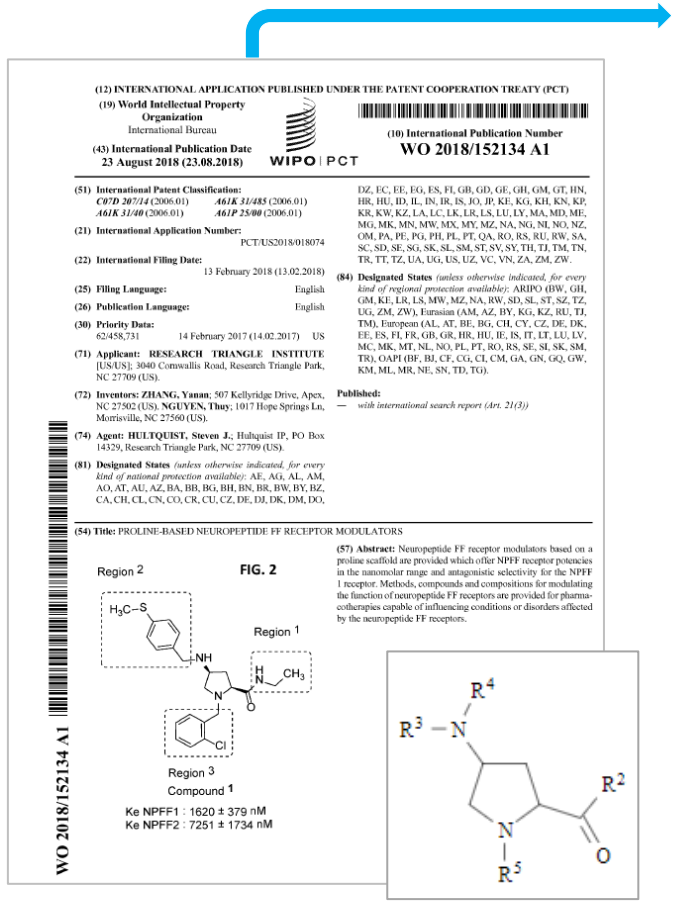
CAS 对文献的独特解读

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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23 August 2018 (23.08.2018)

WIPO | PCT

(10) International Publication Number
WO 2018/152134 A1

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A61K 31/40 (2006.01) *A61P 25/00* (2006.01)

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(74) Agent: HULTQUIST, Steven J.; Hultquist IP, PO Box 14329, Research Triangle Park, NC 27709 (US).

(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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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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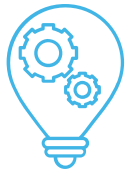

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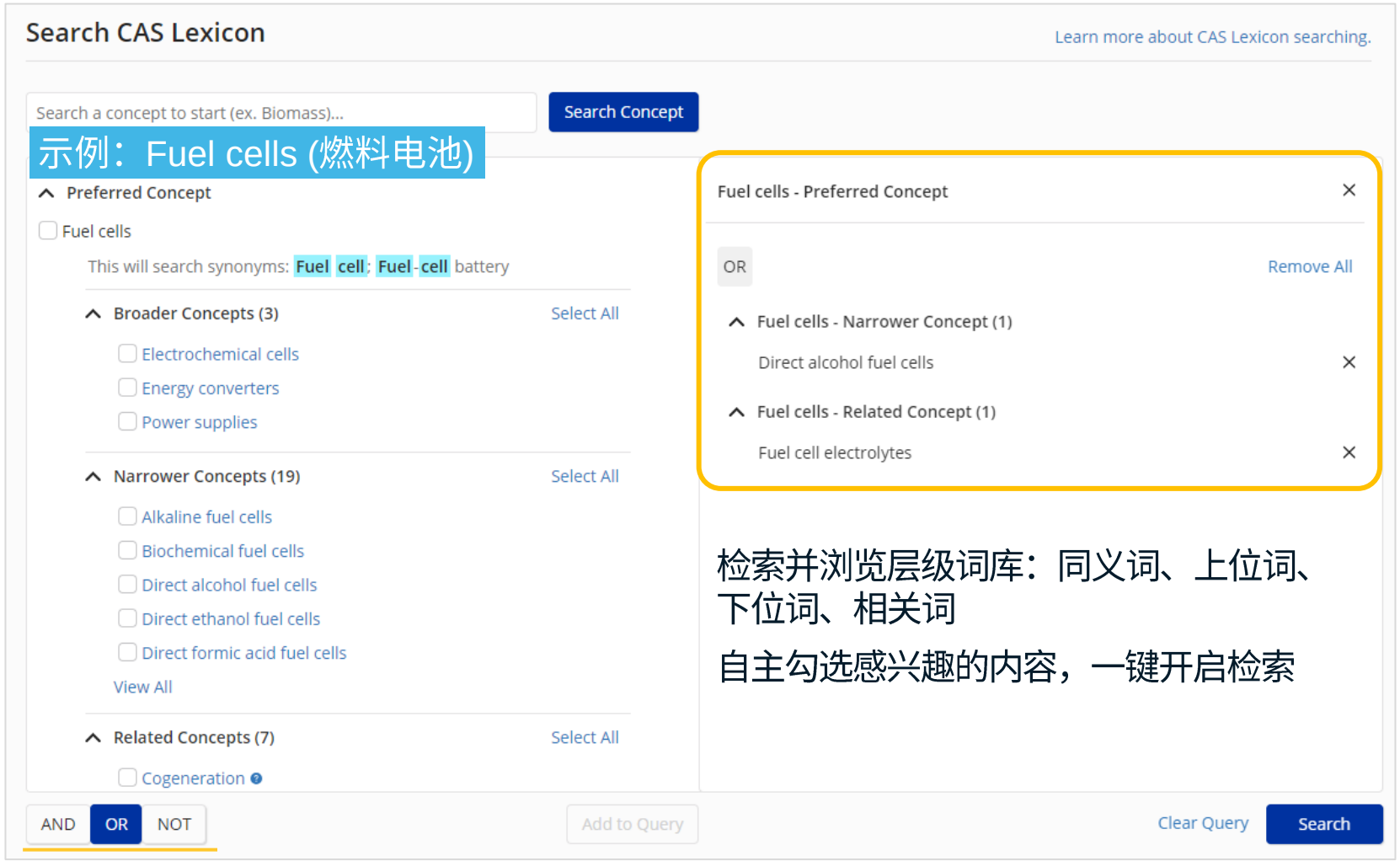
- Q&A

纵览关注领域的相关研究文献

想要快速开启新研究方向的检索？CAS Lexicon词库来帮忙



检索并浏览层级词库：同义词、上位词、下位词、相关词

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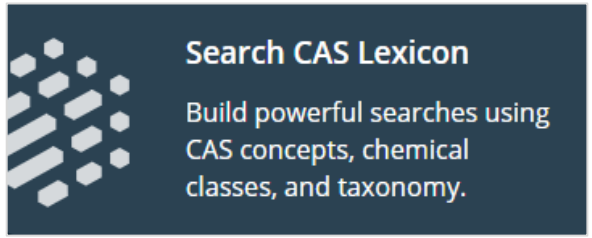

- 提供标准技术词
- 启发获取信息的新思路

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根据研究需求，灵活构建检索主题

优化主题词可细化文献检索结果，更加精准定位文献

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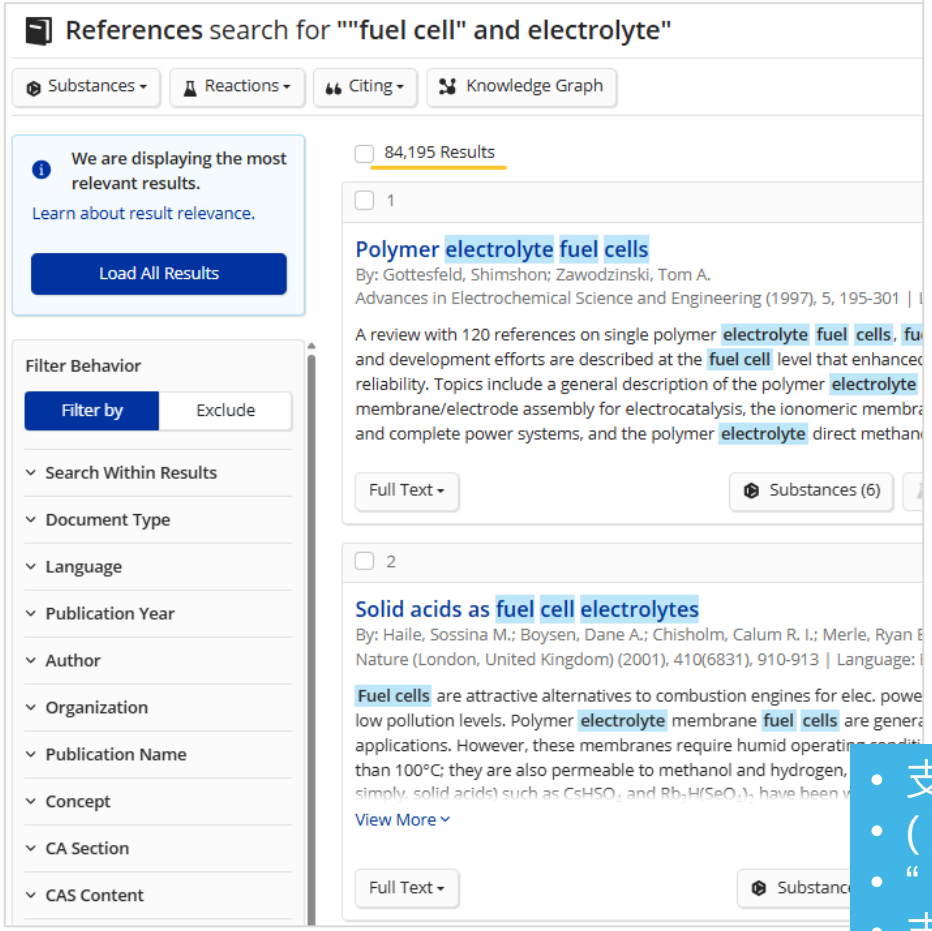
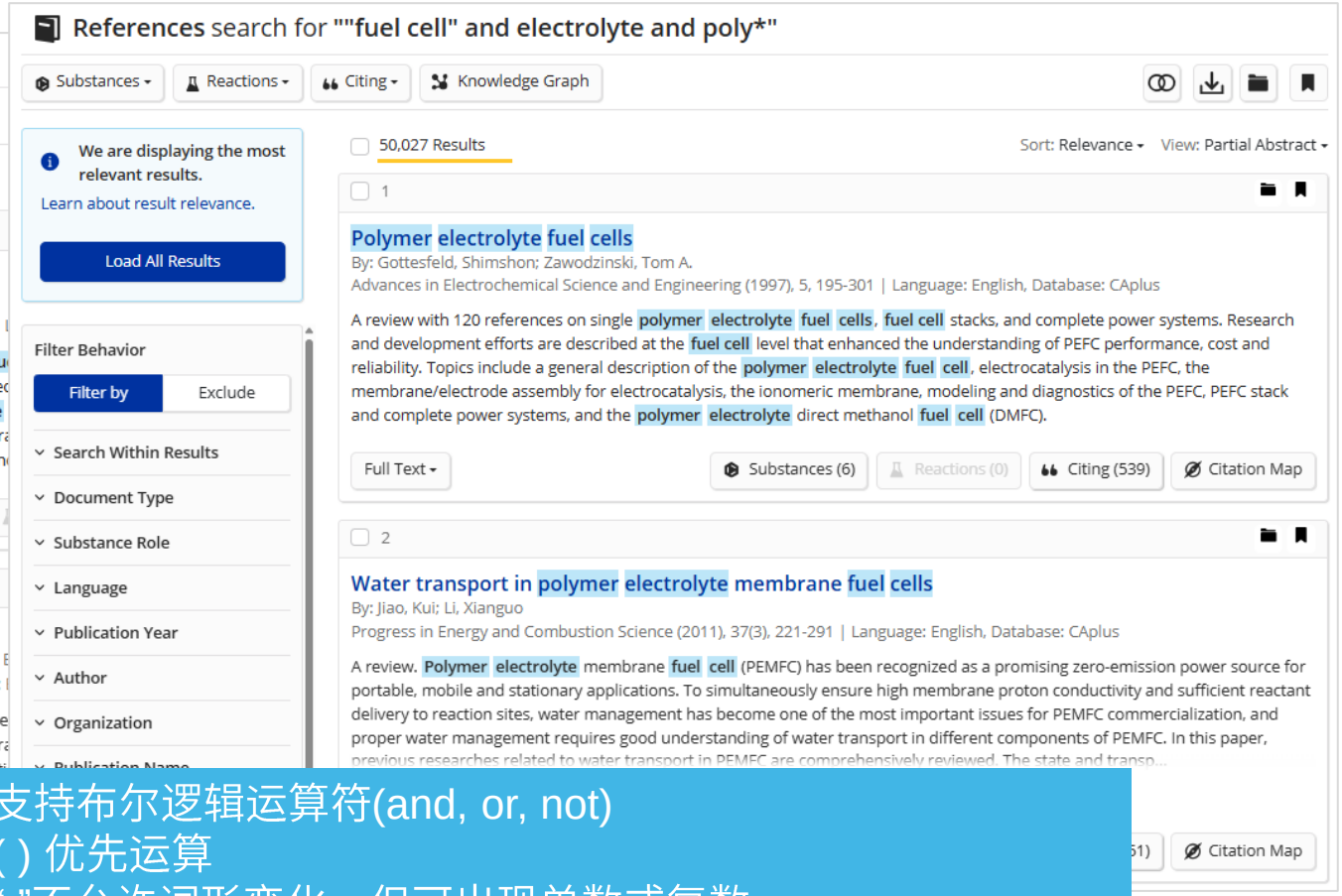


"fuel cell" and electrolyte and poly*



- 支持布尔逻辑运算符(and, or, not)
- ( ) 优先运算
- “ ”不允许词形变化，但可出现单数或复数
- 支持通配符*或？ （*代表0或多个字符；？ 代表0或1个字符）

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快速概览关注的研究方向

多维度的筛选、排序方式

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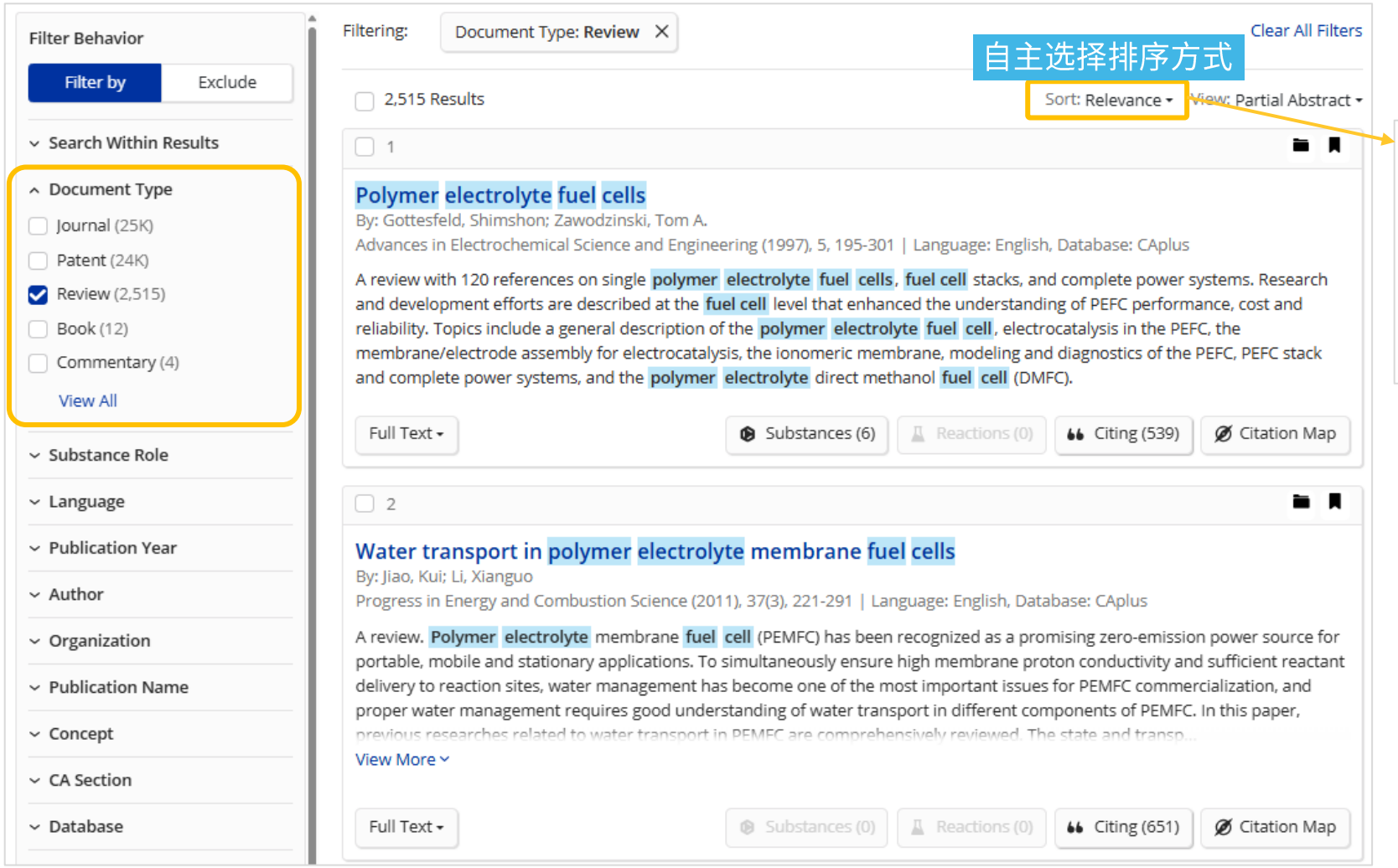

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参考相关文献中的用词

文献的标题、摘要、Keywords、核心研究点、物质及研究角色等

Transition metal nitrides: Essential and potential use in low-temperature fuel cells

5 | 0 | 0 | Citation Map

In this Reference
- CAS Concepts
- Substances
- Cited Documents

内容导航速览

By: Antolini, Ermete

DOI: 10.1016/j.jelechem.2024.118926

A review. Transition metal nitrides (TMNs) and TMN-containing compounds can play different roles in low-temperature fuel cells. They can be used as bipolar plate coatings, catalyst support and catalysts. Titanium nitride (TiN) is the most used TMN as bipolar plate coating and catalyst support, while molybdenum nitrides (MoN and Mo_2N) and cobalt nitrides (Co_xN) are the most used TMN as catalyst for oxygen reduction, and nickel nitride (Ni_3N) as catalyst for hydrogen oxidation In this work the essential and potential use of TMNs and TMN-containing materials in polymer electrolyte membrane fuel cells is overviewed and discussed.

Keywords: review transition metal nitride polymer electrolyte membrane fuel cell

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Publication Information • **Journal** View Less

Source	Database Information	Company/Organization	Publisher	Language
Journal of Electroanalytical Chemistry Volume: 979 Pages: 118926 Journal; General Review 2025 DOI: 10.1016/j.jelechem.2024.118926 CODEN: JECHES ISSN: 1873-2569	AN: 2025:46673 CAplus	Scuola di Scienza dei Materiali, Via 25 aprile 22 Cogoleto Genova 16016 Italy		

Substances

25583-20-4

N≡Ti

NTi
Titanium mononitride

Role: Catalyst Use, Properties, Technical or Engineered Material Use, Uses

12033-45-3

Component	Ratio
Ni	3
N	1

N.Ni
Nickel nitride (Ni_3N)

Role: Catalyst Use, Properties, Technical or Engineered Material Use, Uses

物质研究角色

CAS Concepts 核心研究点

Catalyst supports	Low temperature
Coating materials	Polymer electrolyte fuel cells
Electrochemical reduction catalysts	Transition metal nitrides Role: Catalyst Use; Properties; Technical or Engineered Material Use

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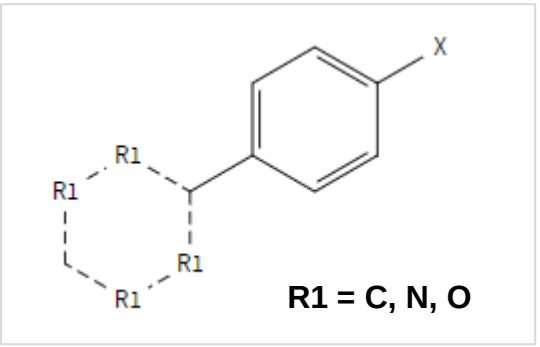
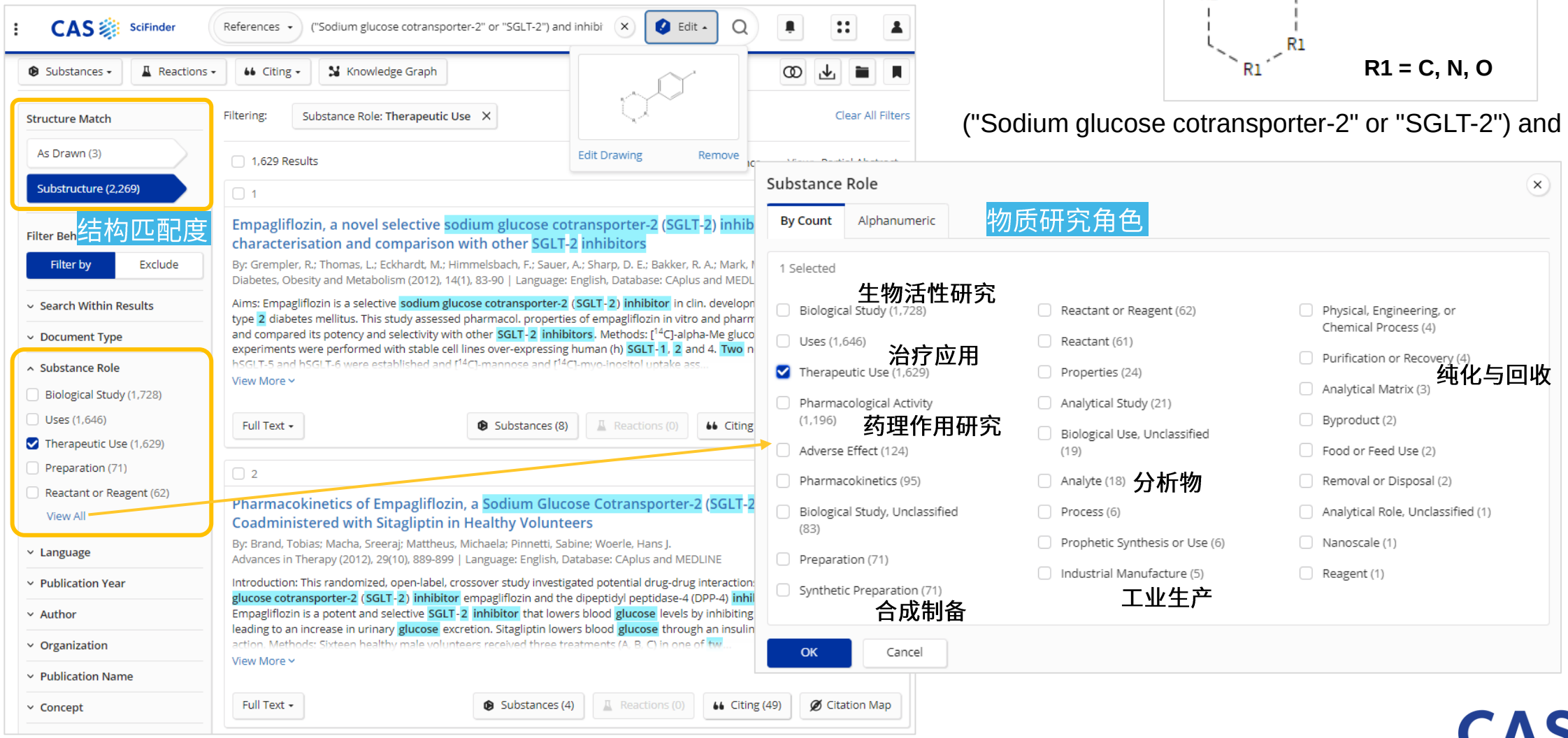
获取与特定结构相关的研究

关键词+结构绘制联合检索



("Sodium glucose cotransporter-2" or "SGLT-2") and inhibitor



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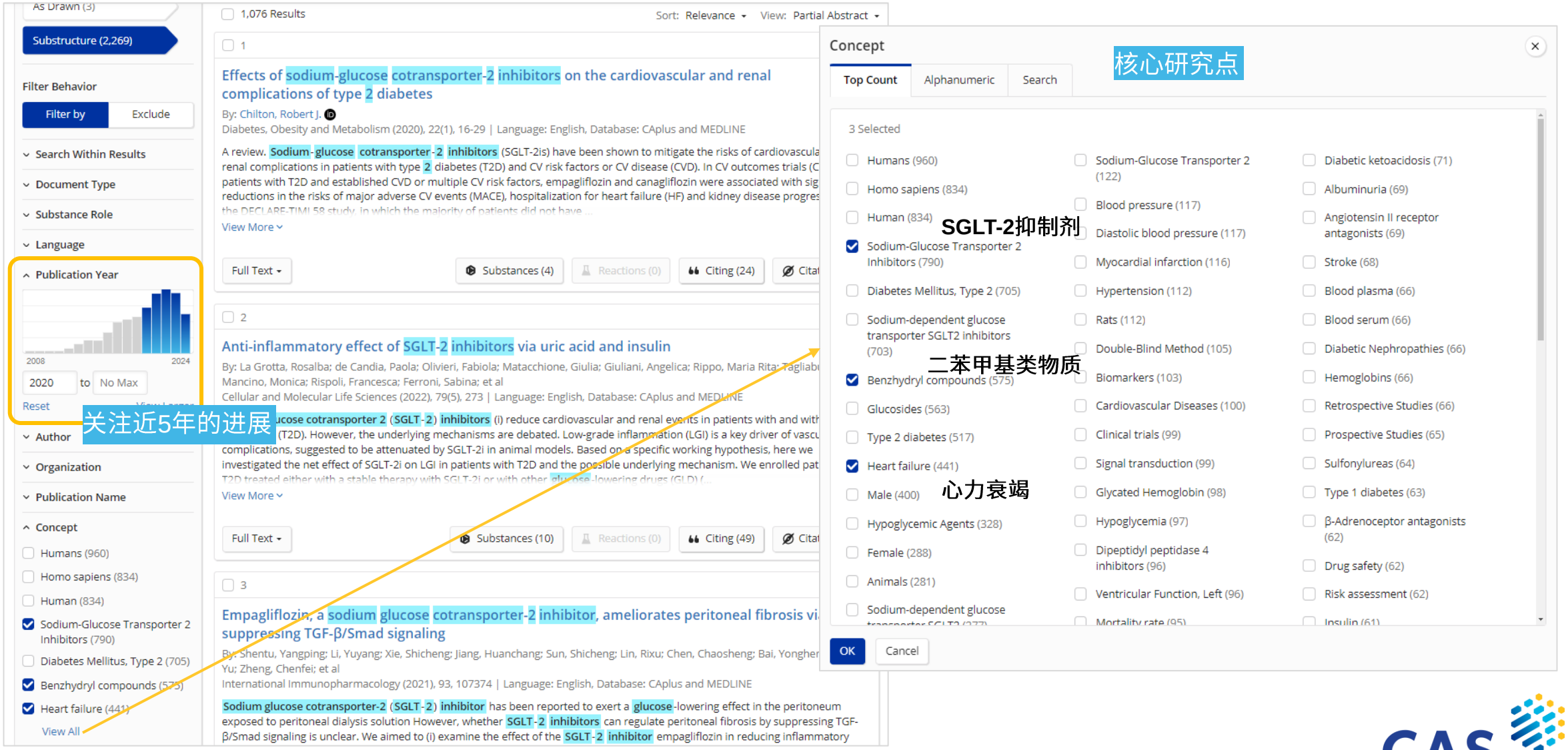

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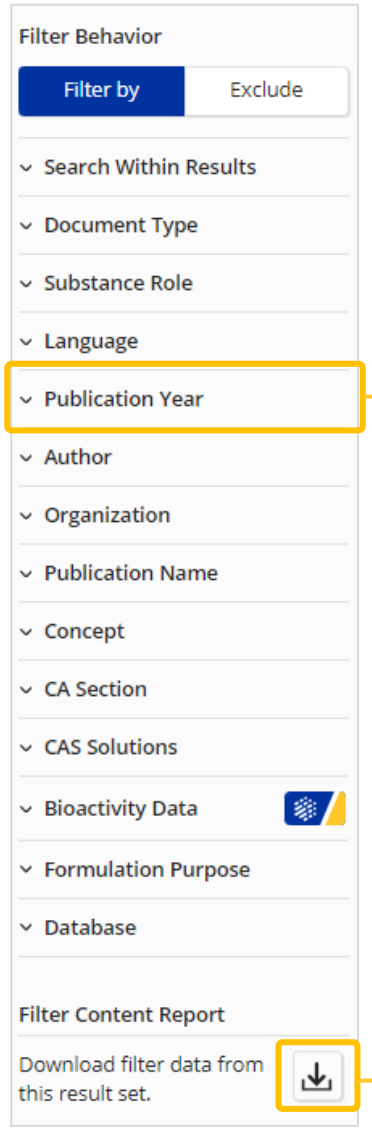

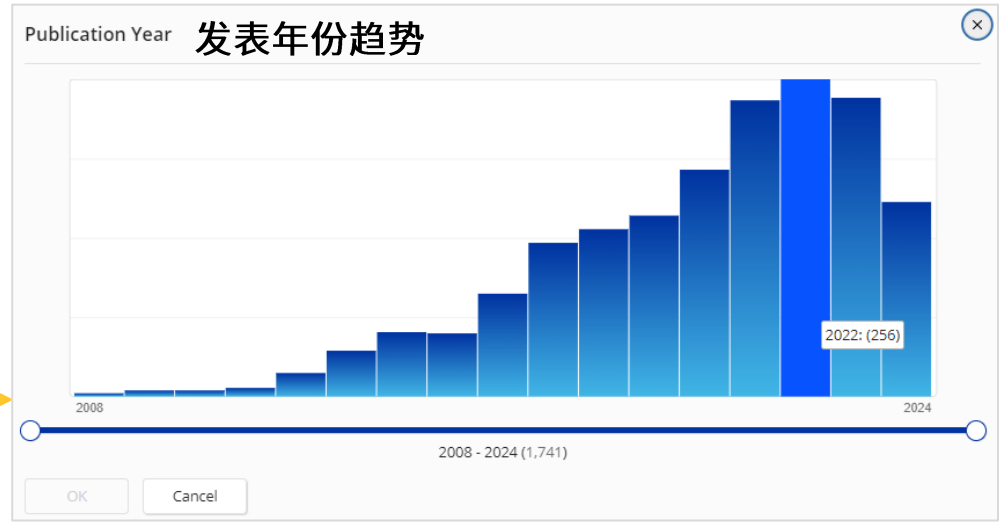

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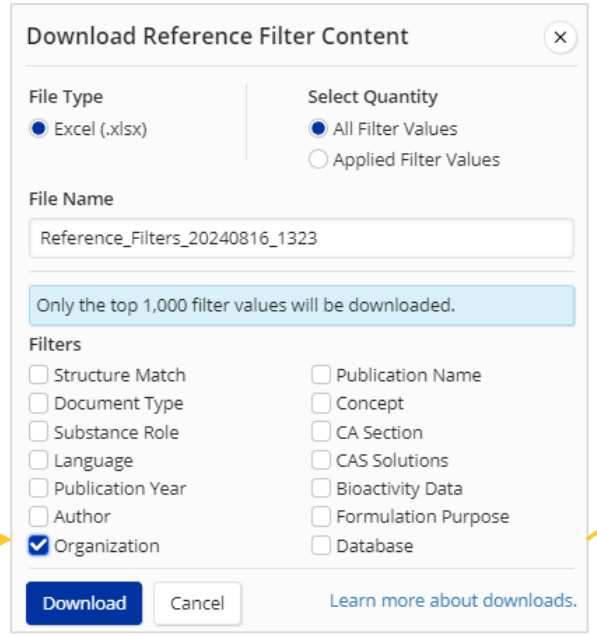

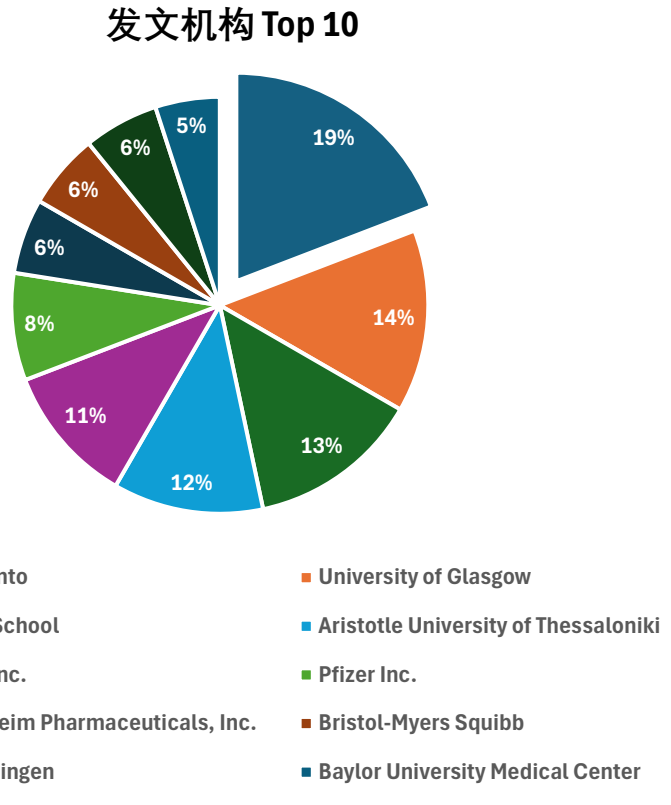

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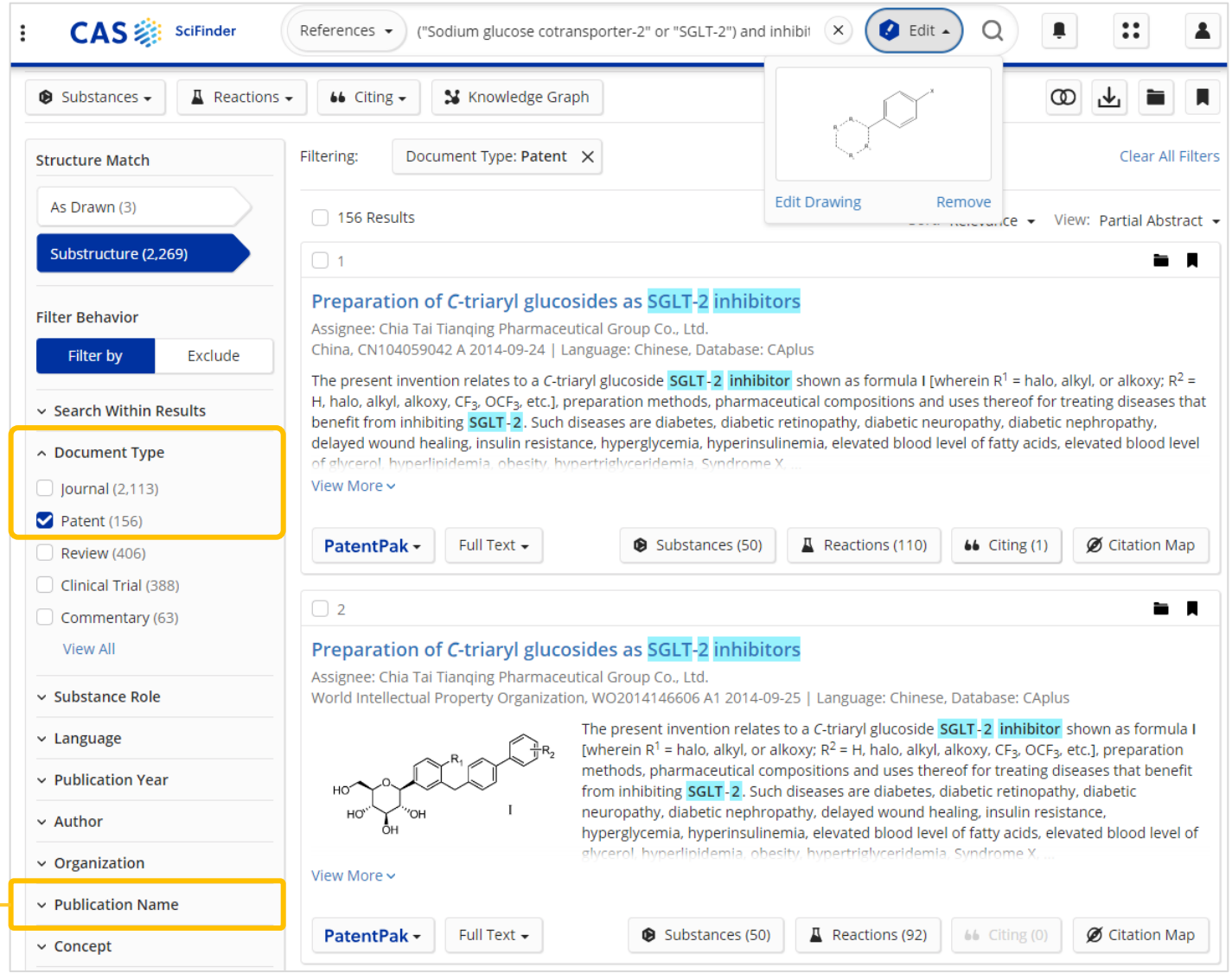

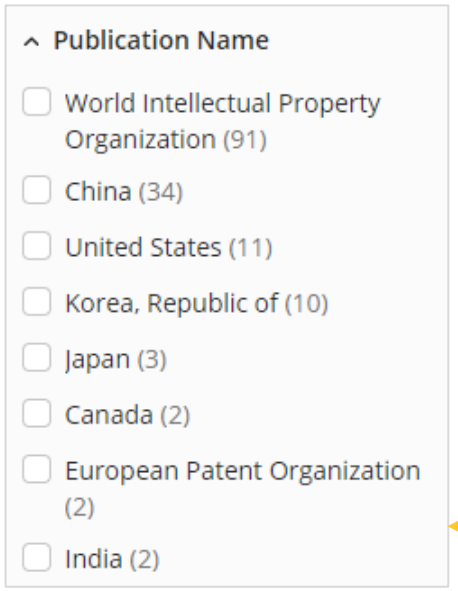

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针对专利文献的现有技术分析，拓展对行业发展的了解

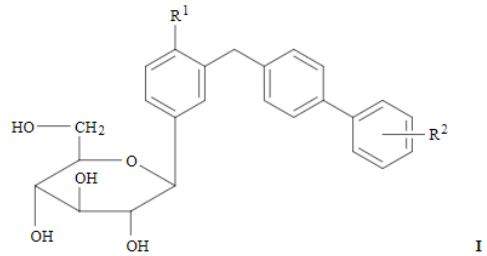
Preparation of *C*-triaryl glucosides as SGLT-2 inhibitors

50 | 110 | 1 | Citation Map

In this Reference
- IPC Data
- CAS Concepts
- Substances
- Reactions

By: Zhao, Junling; Hu, Wenhui; Xu, Dengfeng; Ding, Yuyang; Yang, Ling; Xu, Hongjiang

The present invention relates to a *C*-triaryl glucoside SGLT-2 inhibitor shown as formula I [wherein R^1 = halo, halo, alkyl, alkoxy, CF_3, OCF_3, etc.], preparation methods, pharmaceutical compositions and uses thereof for tre from inhibiting SGLT-2. Such diseases are diabetes, diabetic retinopathy, diabetic neuropathy, diabetic nephro healing, insulin resistance, hyperglycemia, hyperinsulinemia, elevated blood level of fatty acids, elevated blood l hyperlipidemia, obesity, hypertriglyceridemia, Syndrome X, atherosclerosis, or hypertension. The title compoun activity against SGLT-2, higher selectivity, improved drug metabolism properties in oral treatment, etc.



I

Keywords: preparation triaryl glucoside SGLT2 inhibitor treatment human diabetes

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Recent Search History

References
2:23 PM

Prior Art Analysis (191)
Preparation of *C*-triaryl glucosides as SGLT-2 inhibitors

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References from Prior Art Analysis for "Preparation of C-triaryl glucosides as SGLT-2 inhibitor...

Substances | Reactions | Citing | Knowledge Graph

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  - Journal (99)
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- Concept
- CA Section
- CAS Solutions
- Bioactivity Data
- Formulation Purpose

191 Results | Sort: Relevance | View: Partial Abstract

1

Preparation of antidiabetic agents C-aryl glucoside as human SGLT2 inhibitors

Assignee: Bristol-Myers Squibb Company
United States, US20020137903 A1 2002-09-26 | Language: English, Database: CAplus

A SGLT2-inhibiting compound is provided having the formula I method is also provided for treating diabetes and related diseases employing a SGLT2-inhibiting amount of the above compound alone or in combination with another antidiabetic agent or other therapeutic agent (no data). 1A pharmaceutical combination comprising a SGLT2 inhibitor compound and an antidiabetic agent other than a SGLT2 inhibitor, for treating the complications of diabetes, an antiobesity agent, an antihypertensive agent, an antiplatelet agent, an antiatherosclerotic agent, and/or a lipid-lowering agent (no data). A method

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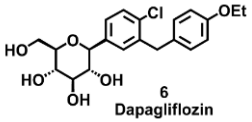
PatentPak | Full Text | Substances (78) | Reactions (40) | Citing (11) | Citation Map

2

Discovery of Dapagliflozin: A Potent, Selective Renal Sodium-Dependent Glucose Cotransporter 2 (SGLT2) Inhibitor for the Treatment of Type 2 Diabetes

By: Meng, Wei; Ellsworth, Bruce A.; Nirschl, Alexandra A.; McCann, Peggy J.; Patel, Manorama; Girotra, Ravindar N.; Wu, Gang; Sher, Philip M.; Morrison, Eamonn P.; Biller, Scott A.; et al
Journal of Medicinal Chemistry (2008), 51(5), 1145-1149 | Language: English, Database: CAplus and MEDLINE



6
Dapagliflozin

The C-aryl glucoside 6 (dapagliflozin) was identified as a potent and selective hSGLT2 inhibitor which reduced blood glucose levels in a dose-dependent manner by as much as 55% in hyperglycemic streptozotocin (STZ) rats. These findings, combined with a favorable ADME profile, have prompted clin. evaluation of dapagliflozin for the treatment of type 2 diabetes.

Full Text | Substances (17) | Reactions (21) | Citing (480) | Citation Map

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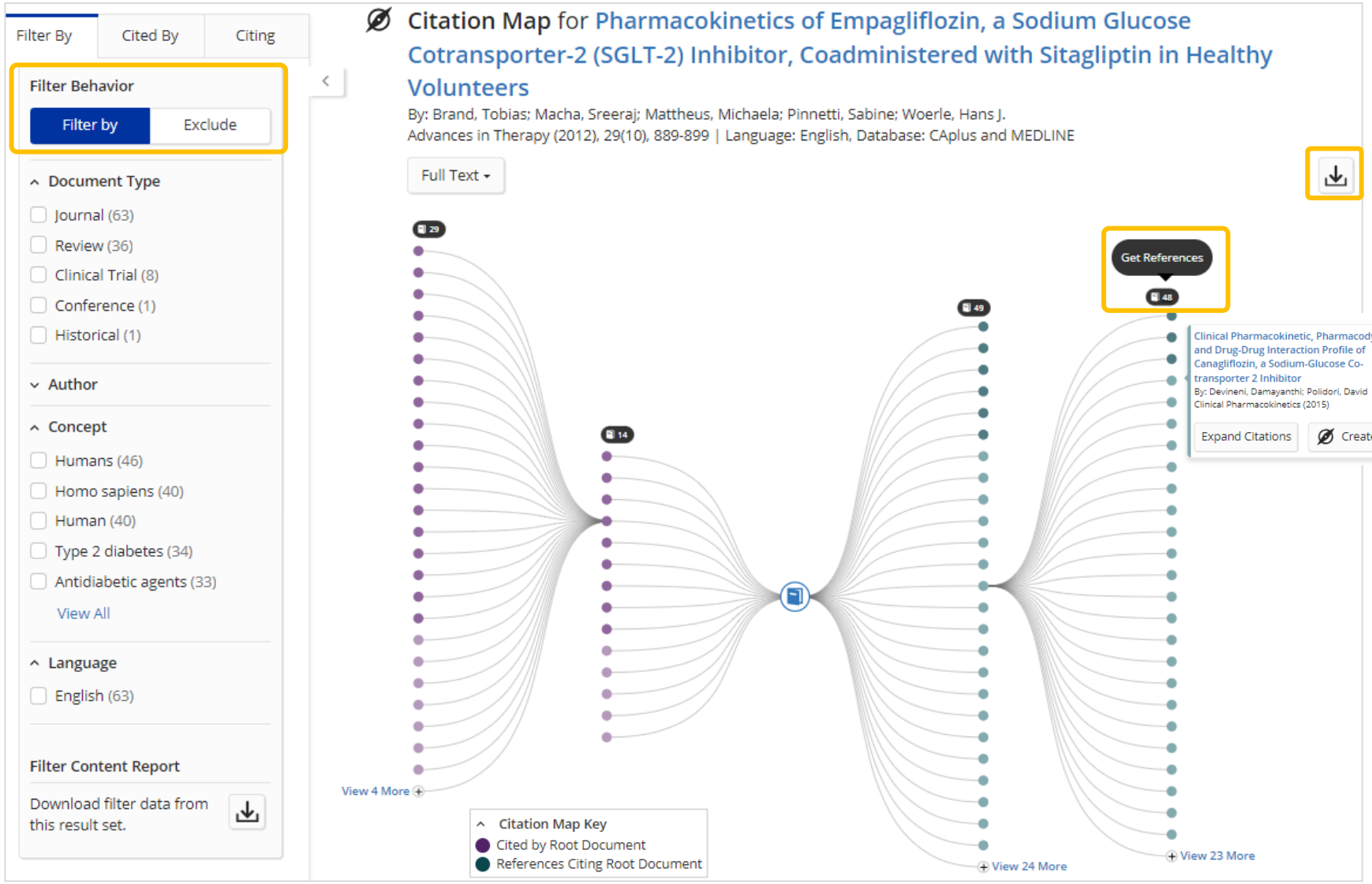
通过引文，了解关联的研究趋势和方向



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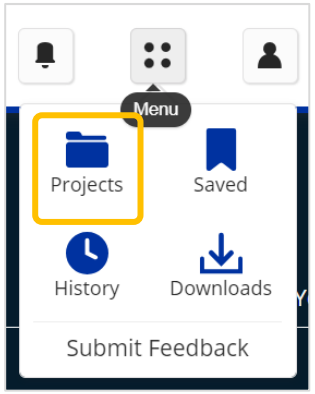
Projects——便捷管理与分享文献、物质



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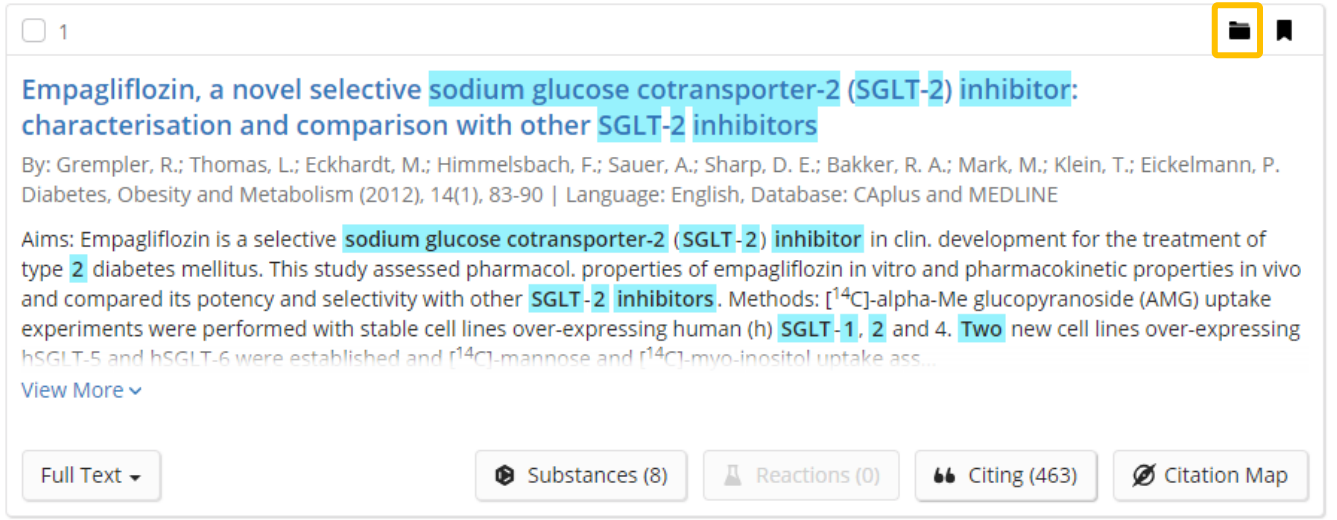

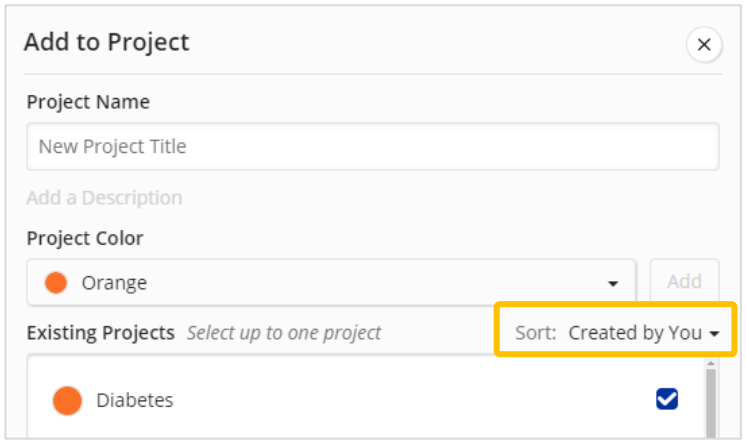

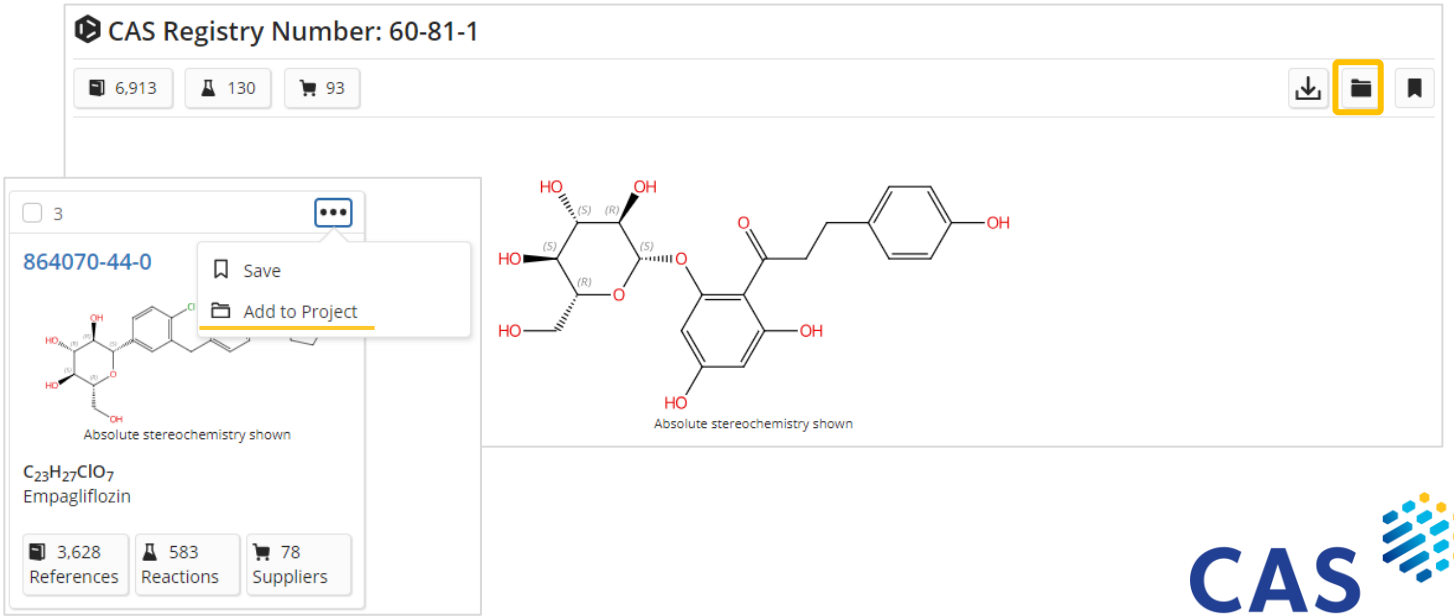

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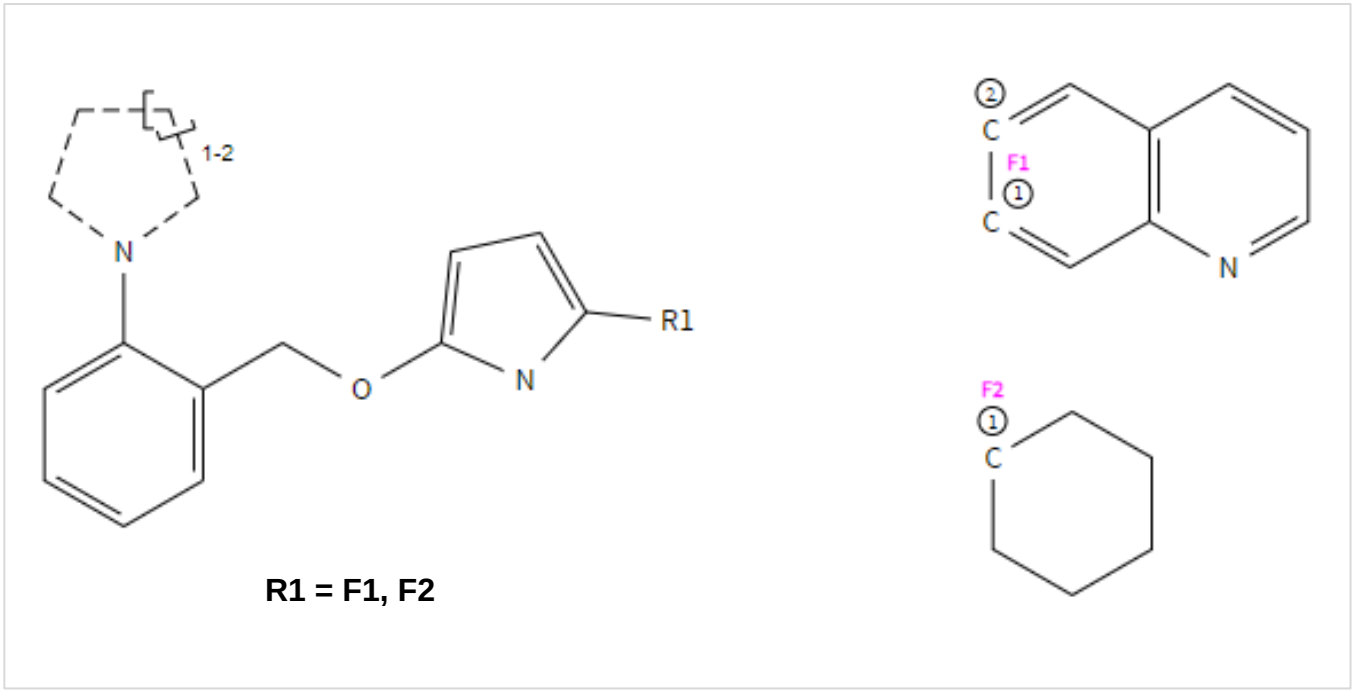
  - 实验设计：课题的创新性及已有相关实验报道
  - 结果分析：数据的比对及关联研究检索拓展
- Q&A

聚焦物质/材料结构层面的查新

我设计的结构是否有公开报道?



R 自定义R基团

Fn 片段结构

[ ] 1-4 重复工具

不确定键级

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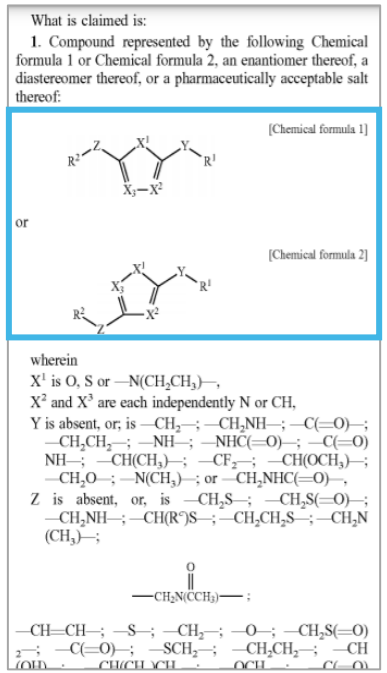
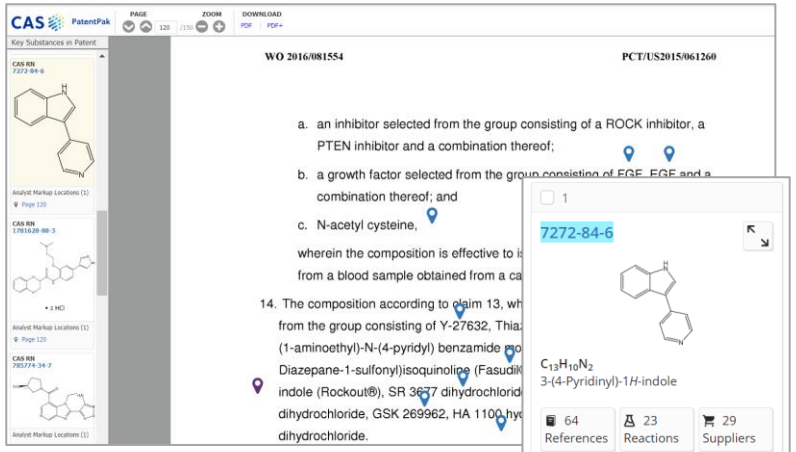
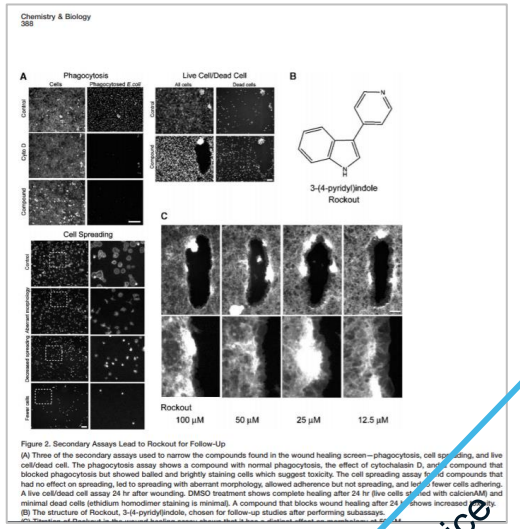
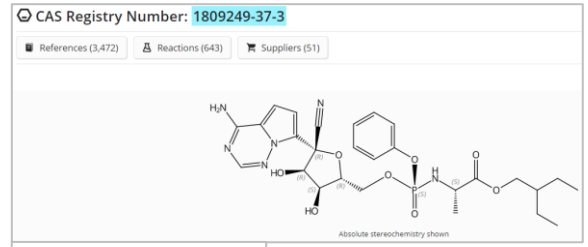
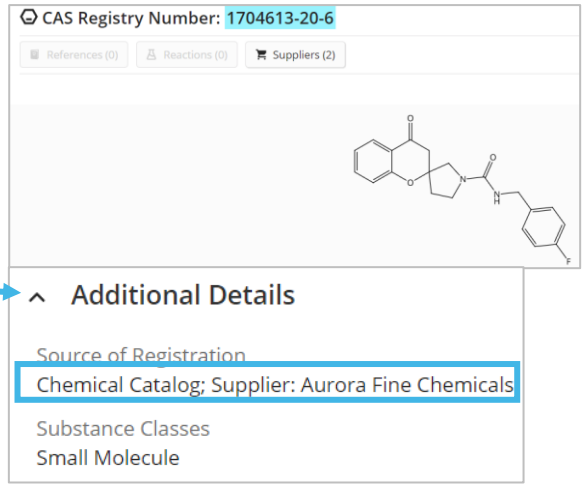
物质结构的数据来源

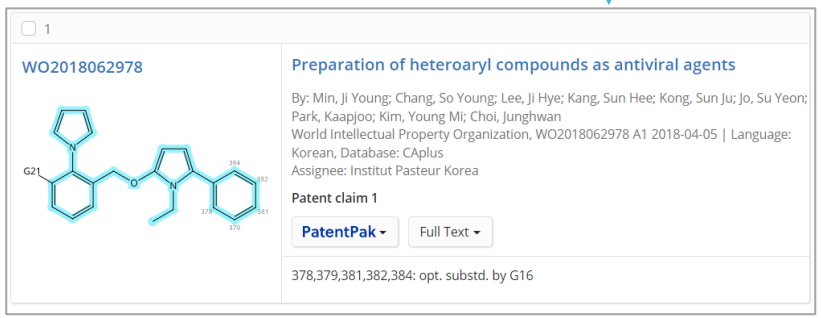












CAS Markush

Patent

Patent

Journal

CAS Client Service

CAS REGISTRY

Chemical catalog/library

Other web sources

CAS
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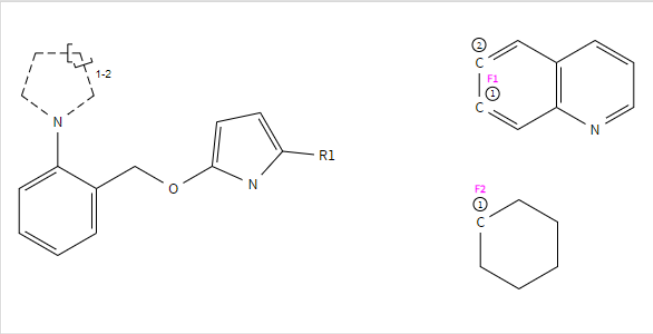
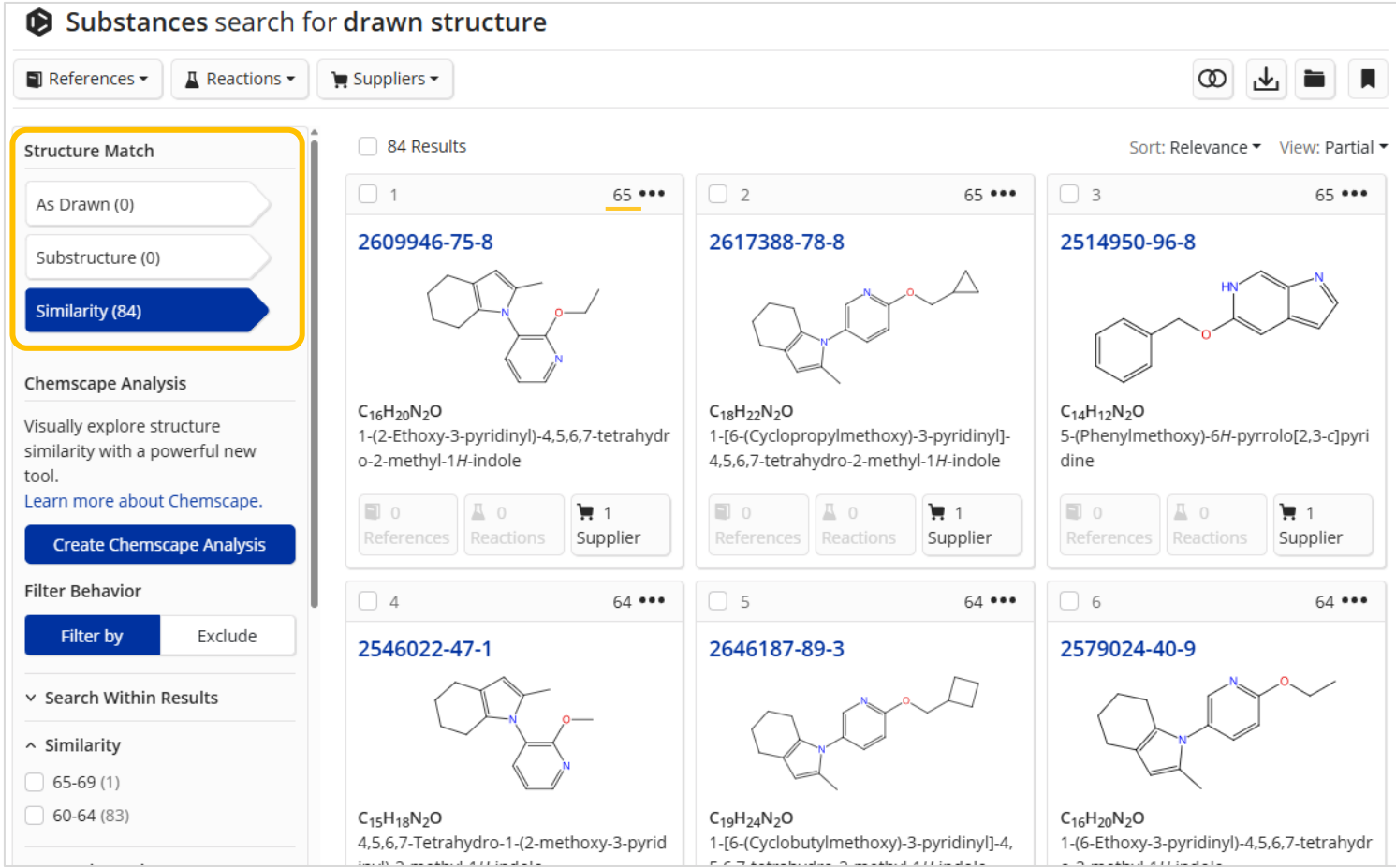
示例：片段结构组合查新

CAS 物质数据集 CAS REGISTRY® 是专利审查员进行新颖性判断的重要依据



- CAS Registry中As Drawn为0，初步判断此结构比较新
- 可辅以查看相似结构，参考相似度评分



Structure Match的说明： https://cas-product-help.zendesk.com/hc/en-us/articles/9945764238477-Filter-Substances-by-Structure-Match
相似度评分： https://cas-product-help.zendesk.com/hc/en-us/articles/11112258474125-What-are-similarity-scores

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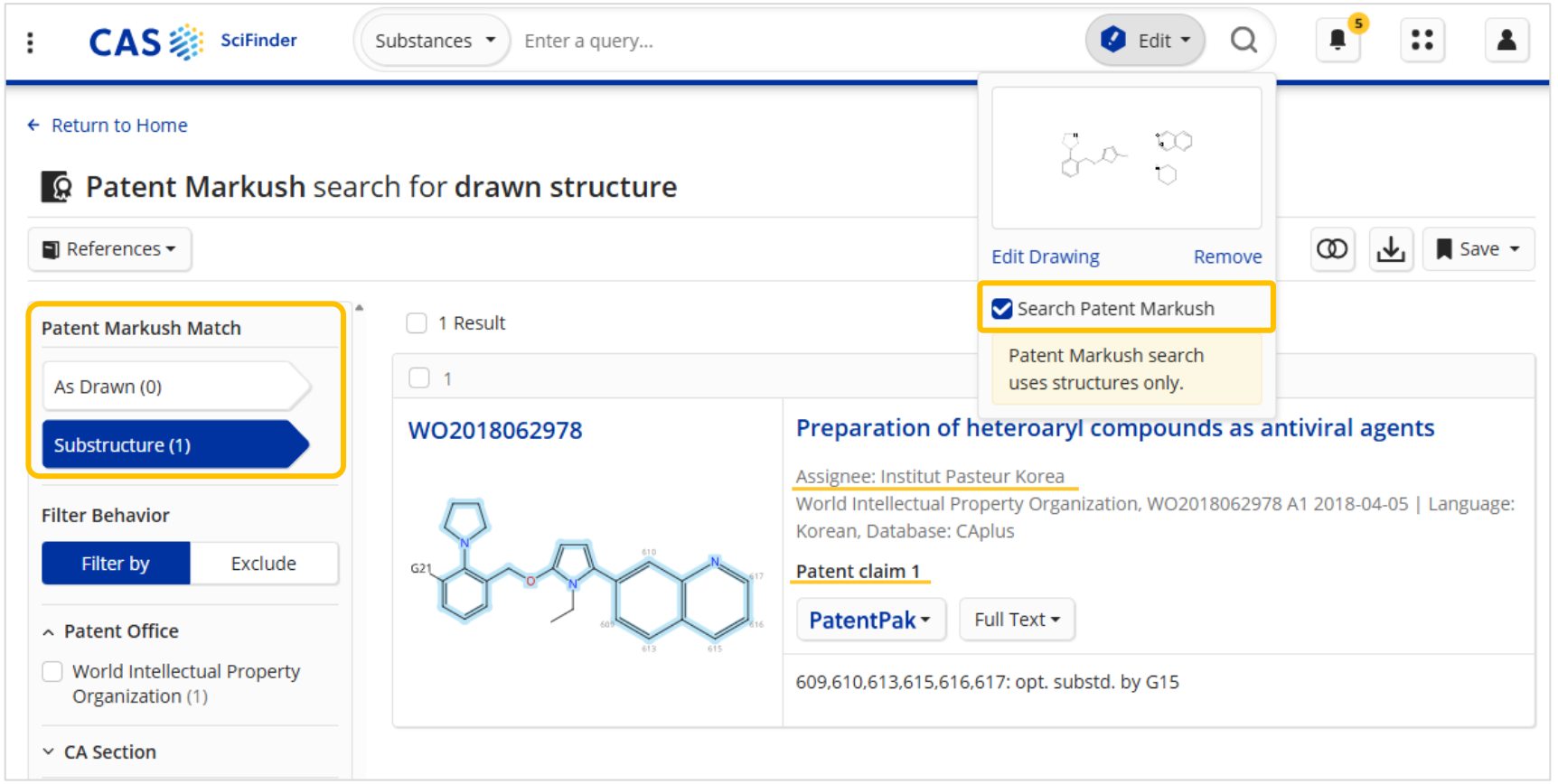
示例：片段结构组合查新

CAS 专利马库什数据集是专利审查员进行可专利性评估的重要参考依据

- 马库什检索可以使用具体结构、骨架结构和通式结构来进行迭代检索，确保获得完整的公开结构信息
- 可以根据必要性使用 CAS 文献数据集 CAplus 进行文本检索补充



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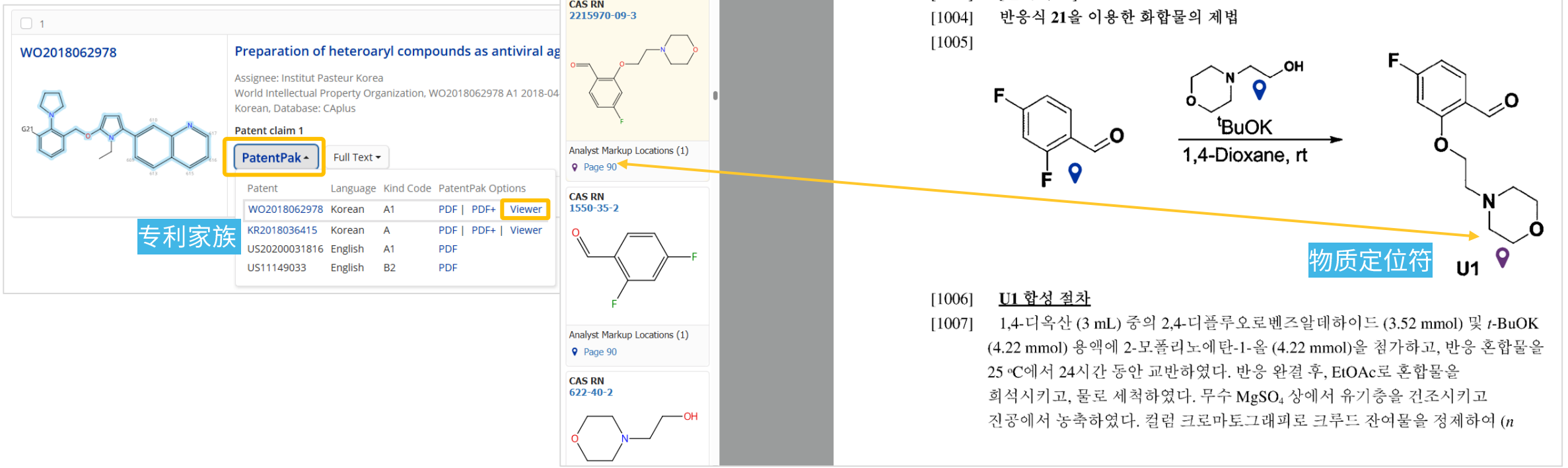
借助CAS科学家的智慧，快速在专利中发现关键物质

CAS PatentPak 模式浏览专利原文



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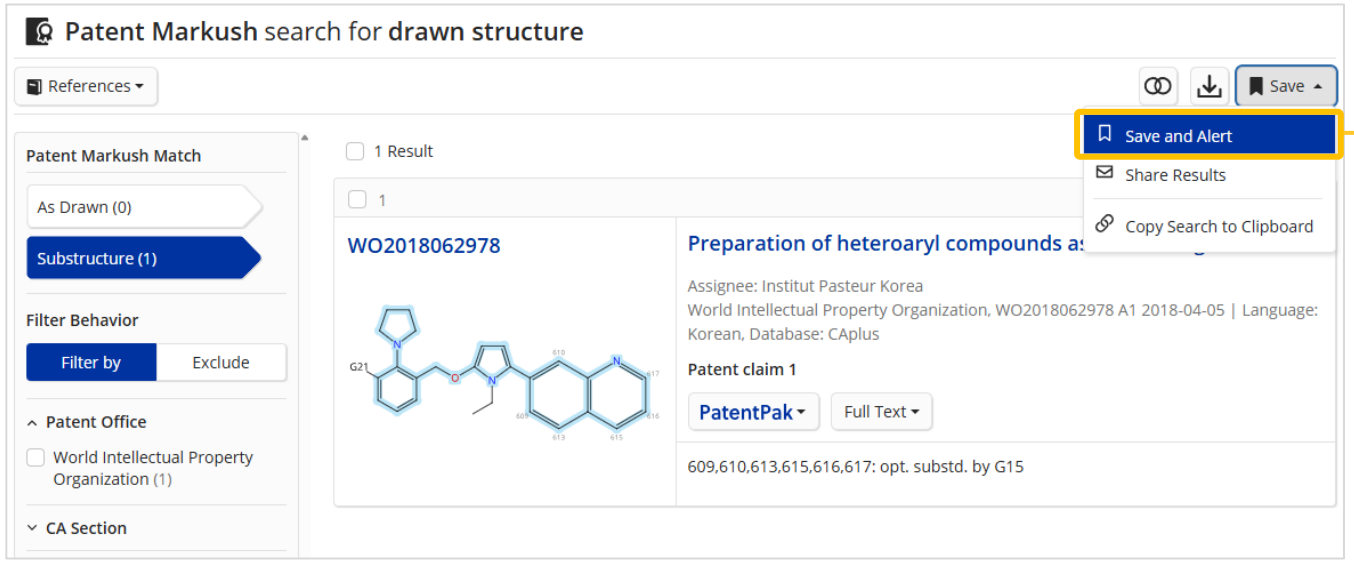
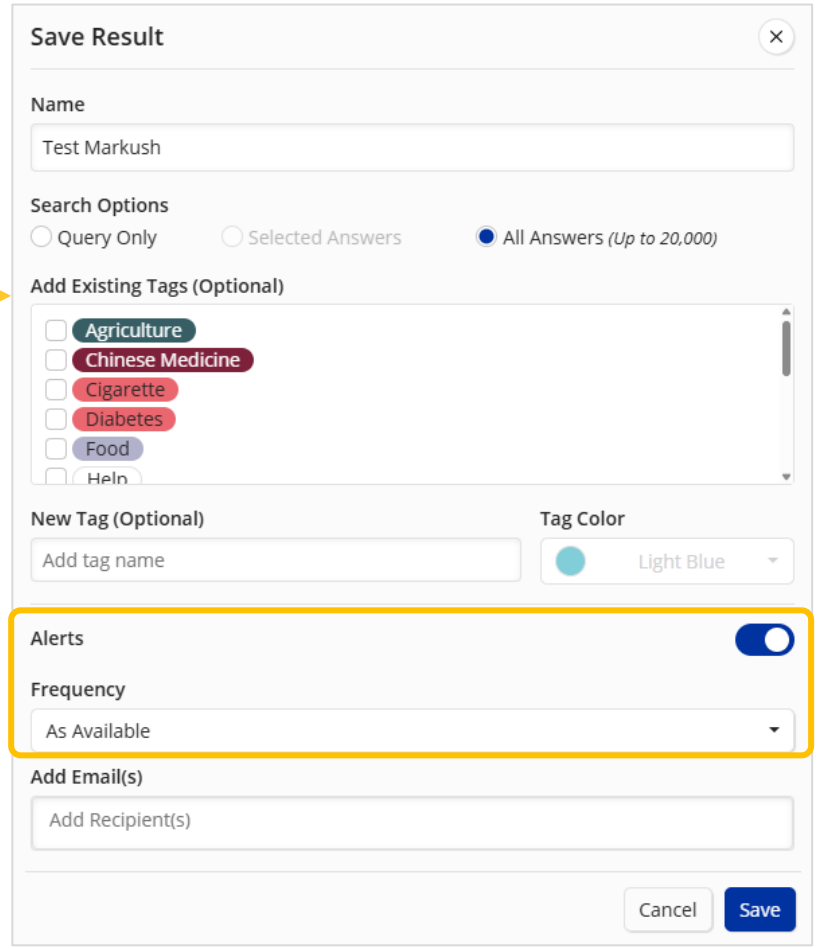
持续关注研究前沿信息，设置定题追踪

文献、物质、反应、专利马库什检索结果均可设置提醒





提醒频率：

- 即时提醒
- 每周提醒
- 每月提醒

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参考已有的合成制备方法

Structure Match
As Drawn (0)
Substructure (2,603)
Similarity (67K)

Filter Behavior
Filter by | Exclude

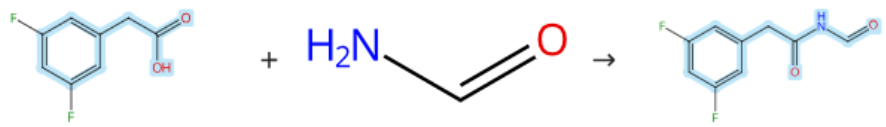
Search Within Results
Yield
Number of Steps
Non-Participating Functional Groups
不参与反应官能团
Ether (402)
Halide (402)
Phenyl halide (300)
Carbamate (291)
Alkene (116)
View All
Reaction Mapping
Reaction Scale
反应规模
Milligram (45)
Gram (20)
Kilogram (1)
No Scale Provided (336)
Experimental Protocols
Synthetic Methods (133)
Experimental Procedure (85)

Filtering: Non-Participating Functional Groups: Halide ×
Clear All Filters

402 Results
Group: By Scheme
Sort: Relevance
View: Expanded

By Scheme
By Document
By Transformation

Scheme 1 (1 Reaction) Steps: 1



Suppliers (87) Suppliers (128) Supplier (1)

31-367-CAS-9914102 Steps: 1

1.1 Reagents: Oxalyl chloride
Solvents: Toluene; 2 h, 110 °C
1.2 Reagents: Pyridine
Solvents: Acetone; cooled; 30 min, 5 °C; overnight, rt

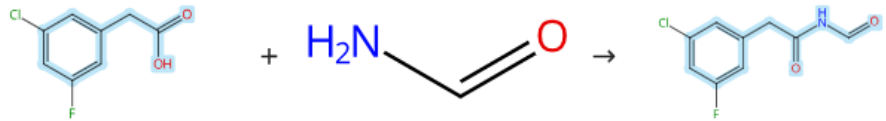
Experimental Protocols

Preparation of 2-aminopyridine as kinase inhibitors
Assignee: OSI Pharmaceuticals, Inc.
United States, US20090197862 A1 2009-08-06

PatentPak Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1



Suppliers (65) Suppliers (128) Supplier (1)

31-367-CAS-5023742 Steps: 1

1.1 Reagents: Oxalyl chloride
Solvents: Toluene; 2 h, 110 °C
1.2 Reagents: Pyridine
Solvents: Acetone; cooled; 30 min, 5 °C; overnight, rt

Preparation of 2-aminopyridine as kinase inhibitors
Assignee: OSI Pharmaceuticals, Inc.
United States, US20090197862 A1 2009-08-06

PatentPak Full Text

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参考Synthetic Methods中CAS科学家对合成实验的描述

Experimental Protocols

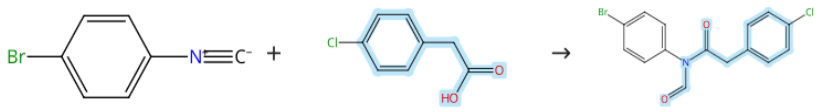
Synthetic Methods (133)

Experimental Procedure (85)

CAS Reaction Number: 31-367-CAS-9910920

Get Similar Reactions

Save



Suppliers (48)

Suppliers (101)

70%

Reaction Overview

Steps: 1 Yield: 70%

JOURNAL

On the reaction of carboxylic acids and isonitriles with conventional heating

By: Polisar, Jason G.; et al

View All

Tetrahedron (2012), 68(49), 10236-10240

View Source | Full Text

Company/Organization

Department of Chemistry
Columbia University
New York, New York 10027

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Toluene	18 - 24 h, 110 °C

Alternative Steps (0)

Experimental Protocols

Synthetic Methods

Products	*N*-(4-Bromophenyl)-4-chloro-*N*-formylbenzeneacetamide, Yield: 70%
Reactants	(4-Chlorophenyl)acetic acid 1-Bromo-4-isocyanobenzene
Solvents	Toluene

Transformations

1. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
2. Addition of Water to Isocyanides

反应转化类型

Reaction Notes

chemoselective, sealed tube used

反应注释

Procedure	1. Filter the two equivalent of the isonitrile in 1 mL dry toluene through a short plug (approximately 0.5 cm in a 5 inch glass pipette) of silica gel into a flame dry 50 mL round bottom flask containing the carboxylic acid. 2. Flush the plug with an additional milliliter of toluene. 3. Add the remainder of the toluene (0.02 M final acid concentration) to the mixture. 4. Seal the reaction vessel with a wire secured septum. 5. Blanket the reaction vessel under argon. 6. Heat the reaction vessel as a sealed tube in a 110 °C oil bath overnight (18-24 hours). 7. Remove the volatile residues in vacuo. 8. Purify the product by silica gel flash chromatography in 4:1 hexanes:ethyl acetate.
Transformation	Acylation of Nitrogen Nucleophiles by Carboxylic Acids Addition of Water to Isocyanides
Scale	milligram

清晰的操作流程

Characterization Data

N-(4-Bromophenyl)-4-chloro-*N*-formylbenzeneacetamide

产物表征

Proton NMR Spectrum	^{1}H NMR (300 MHz, $CDCl_3$): δ= 3.59 (s, 2H, Ar-CH_2), 6.94-7.0 (m, 4H, Ar), 7.25-7.28 (m, 2H, Ar), 7.59-7.63 (m, 2H, Ar), 9.53 (s, 1H, CHO) ppm.
Carbon-13 NMR	^{13}C NMR (75 MHz, $CDCl_3$): δ= 42.33, 124.03, 129.07, 130.58, 130.67, 130.77, 133.34, 133.97, 162.38, 172.68 ppm.
IR Absorption Spectrum	IR (cm^{-1}): 1724, 1701.
Mass Spectrum	MS: 351.76/352.76/353.76/354.76/355.76 (M+1).
State	Pale yellow oil.

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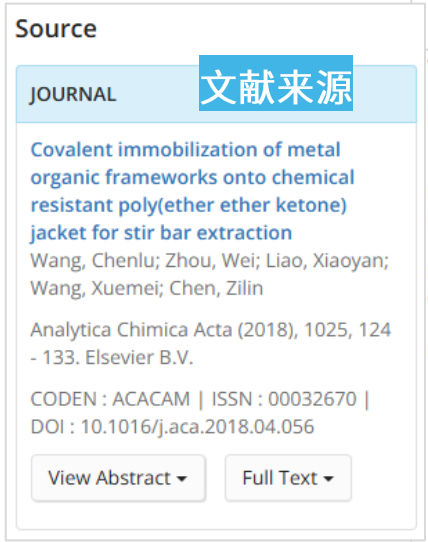
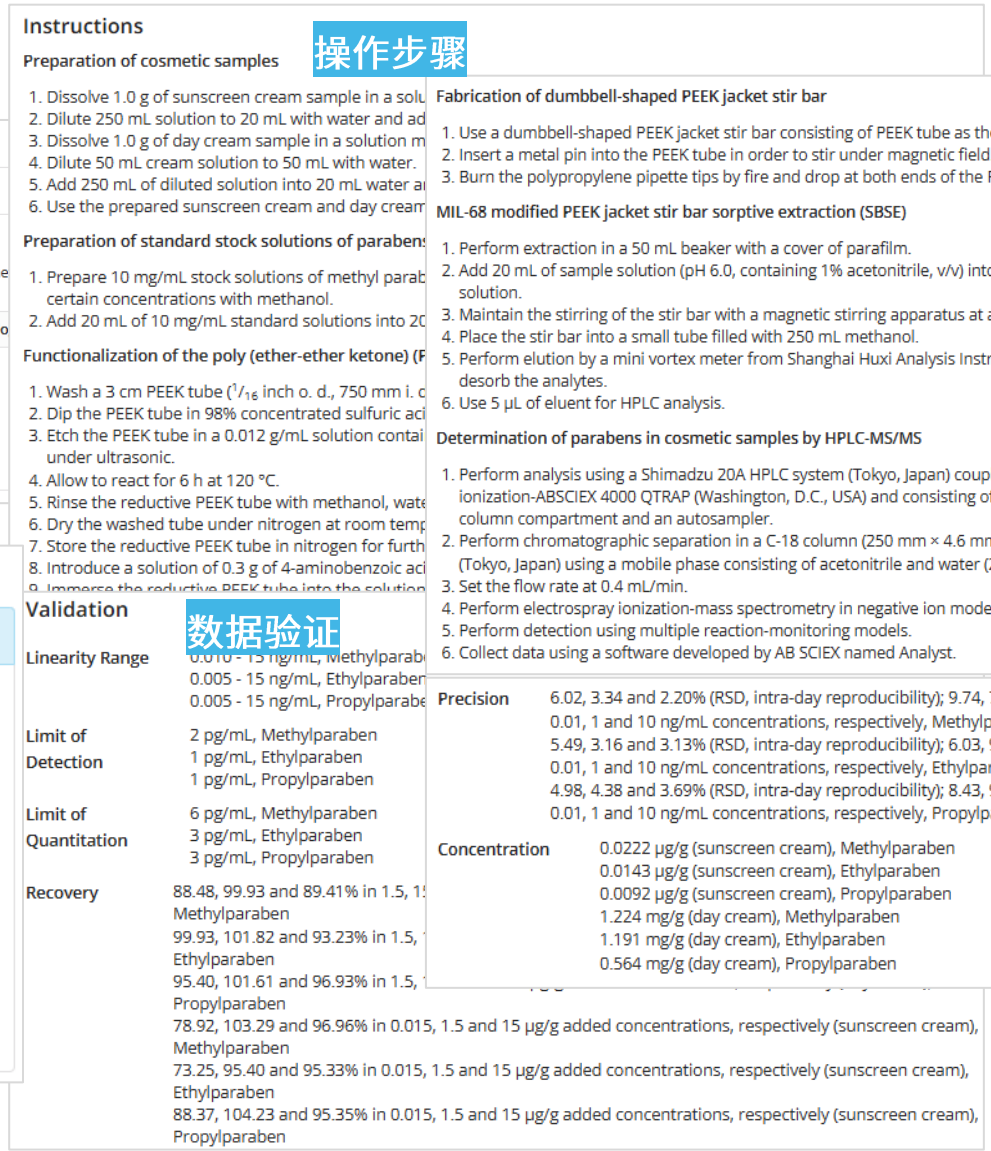
参考CAS Analytical Methods中分析方法详情的描述

https://methods.cas.org/





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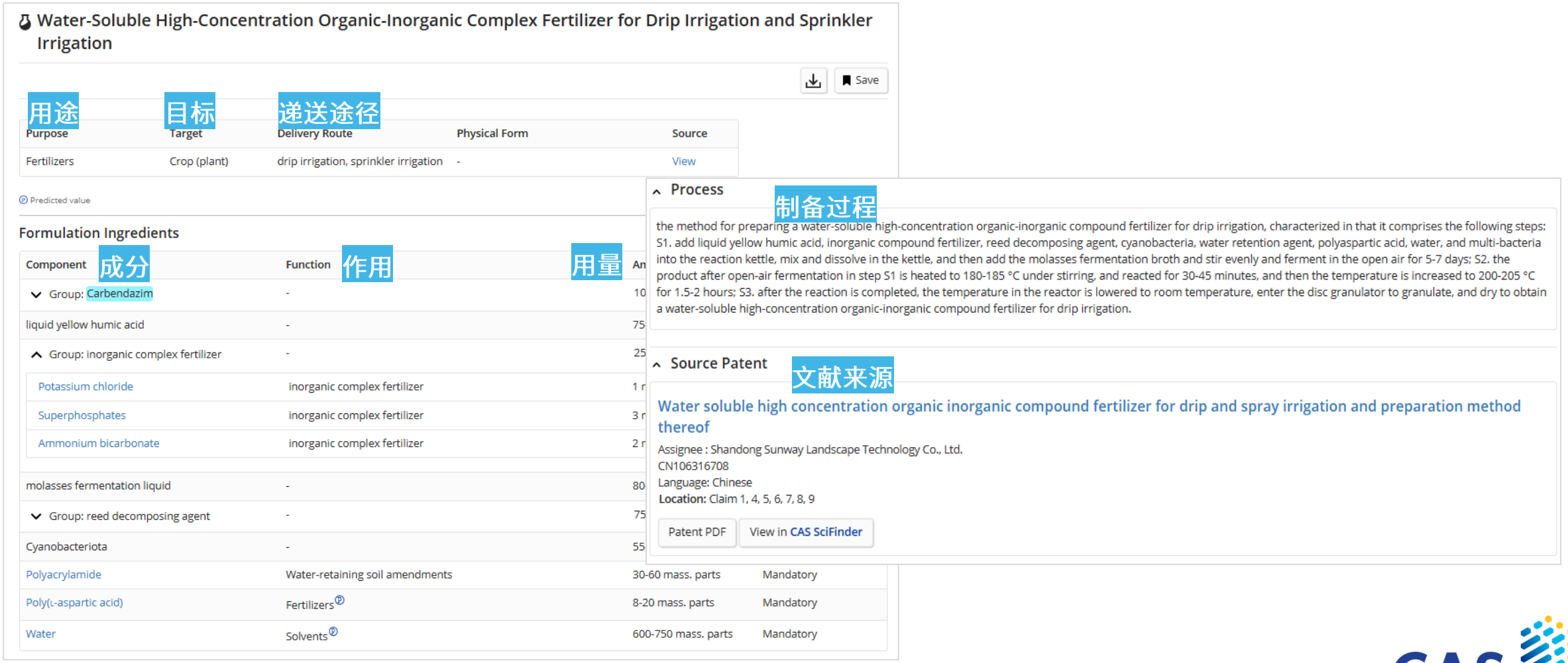
参考CAS Formulus中制剂/配方详情的描述

https://formulus.cas.org/



Water-Soluble High-Concentration Organic-Inorganic Complex Fertilizer for Drip Irrigation and Sprinkler Irrigation

Save

用途 目标 递送途径

Purpose	Target	Delivery Route	Physical Form	Source
Fertilizers	Crop (plant)	drip irrigation, sprinkler irrigation	-	View

Predicted value

Formulation Ingredients

成分 作用 用量

Component	Function	Amount	
Group: Carbendazim	-	10	
liquid yellow humic acid	-	75	
Group: inorganic complex fertilizer	-	25	
Potassium chloride	inorganic complex fertilizer	1 r	
Superphosphates	inorganic complex fertilizer	3 r	
Ammonium bicarbonate	inorganic complex fertilizer	2 r	
molasses fermentation liquid	-	80	
Group: reed decomposing agent	-	75	
Cyanobacteriota	-	55	
Polyacrylamide	Water-retaining soil amendments	30-60 mass. parts	Mandatory
Poly(L-aspartic acid)	Fertilizers	8-20 mass. parts	Mandatory
Water	Solvents	600-750 mass. parts	Mandatory

Process

制备过程

the method for preparing a water-soluble high-concentration organic-inorganic compound fertilizer for drip irrigation, characterized in that it comprises the following steps: S1. add liquid yellow humic acid, inorganic compound fertilizer, reed decomposing agent, cyanobacteria, water retention agent, polyaspartic acid, water, and multi-bacteria into the reaction kettle, mix and dissolve in the kettle, and then add the molasses fermentation broth and stir evenly and ferment in the open air for 5-7 days; S2. the product after open-air fermentation in step S1 is heated to 180-185 °C under stirring, and reacted for 30-45 minutes, and then the temperature is increased to 200-205 °C for 1.5-2 hours; S3. after the reaction is completed, the temperature in the reactor is lowered to room temperature, enter the disc granulator to granulate, and dry to obtain a water-soluble high-concentration organic-inorganic compound fertilizer for drip irrigation.

Source Patent

文献来源

Water soluble high concentration organic inorganic compound fertilizer for drip and spray irrigation and preparation method thereof

Assignee : Shandong Sunway Landscape Technology Co., Ltd.
CN106316708
Language: Chinese
Location: Claim 1, 4, 5, 6, 7, 8, 9

Patent PDF View in CAS SciFinder

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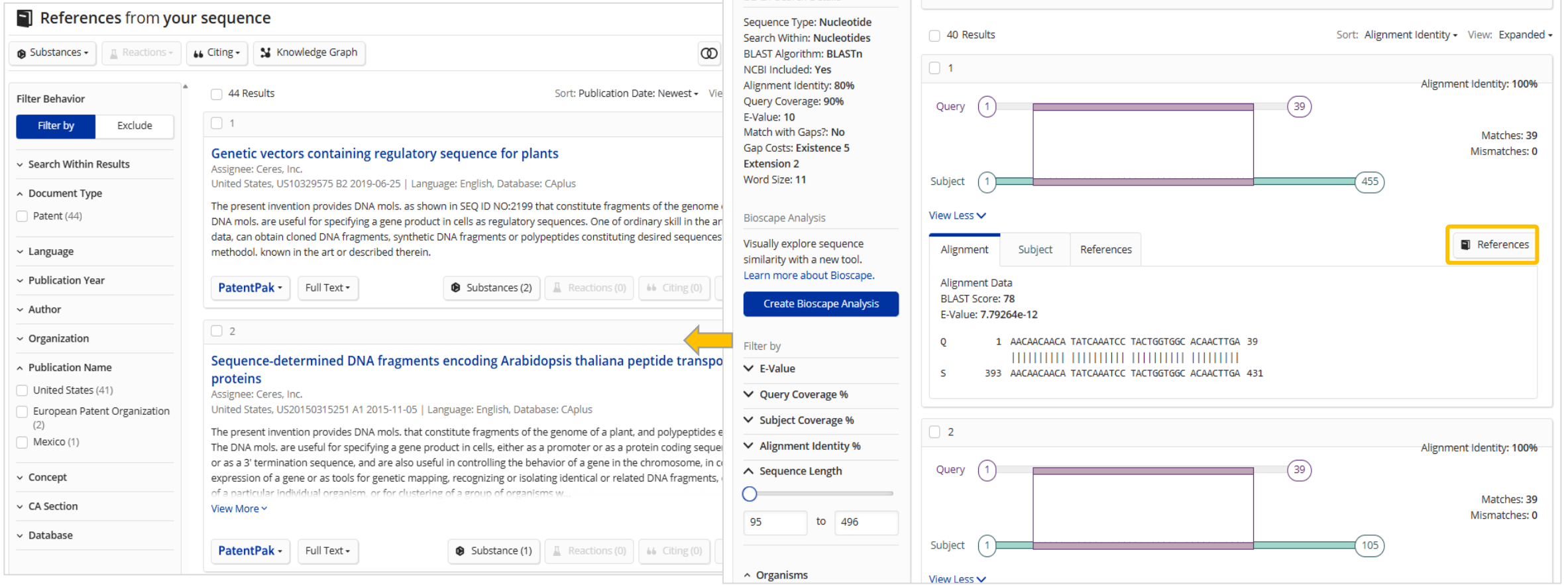
提纲

- CAS 简介
- CAS SciFinder Discovery Platform 助攻论文写作
  - 研究背景：研究现状和发展趋势的全面调研
  - 实验设计：课题的创新性及已有相关实验报道
  - 结果分析：数据的比对及关联研究检索拓展
- Q&A

生物序列一致性的比对

支持BLAST，CDR，Motif检索



通过底层数据的密切关联，可直接获取报道文献。

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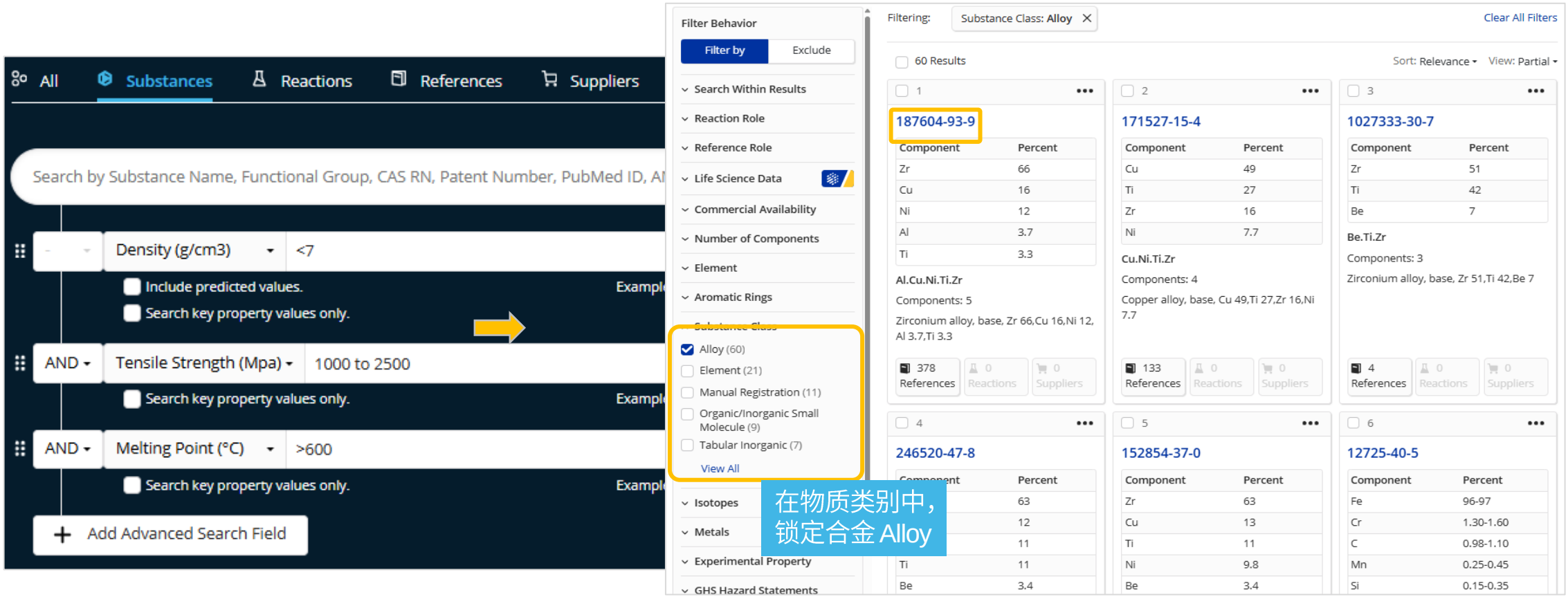
通过属性需求，获取相似材料

灵活联用物质高级检索选项

检索示例：满足多属性值要求的轻质合金，密度<7g/cm3、拉伸强度>1000MPa、熔点>600℃



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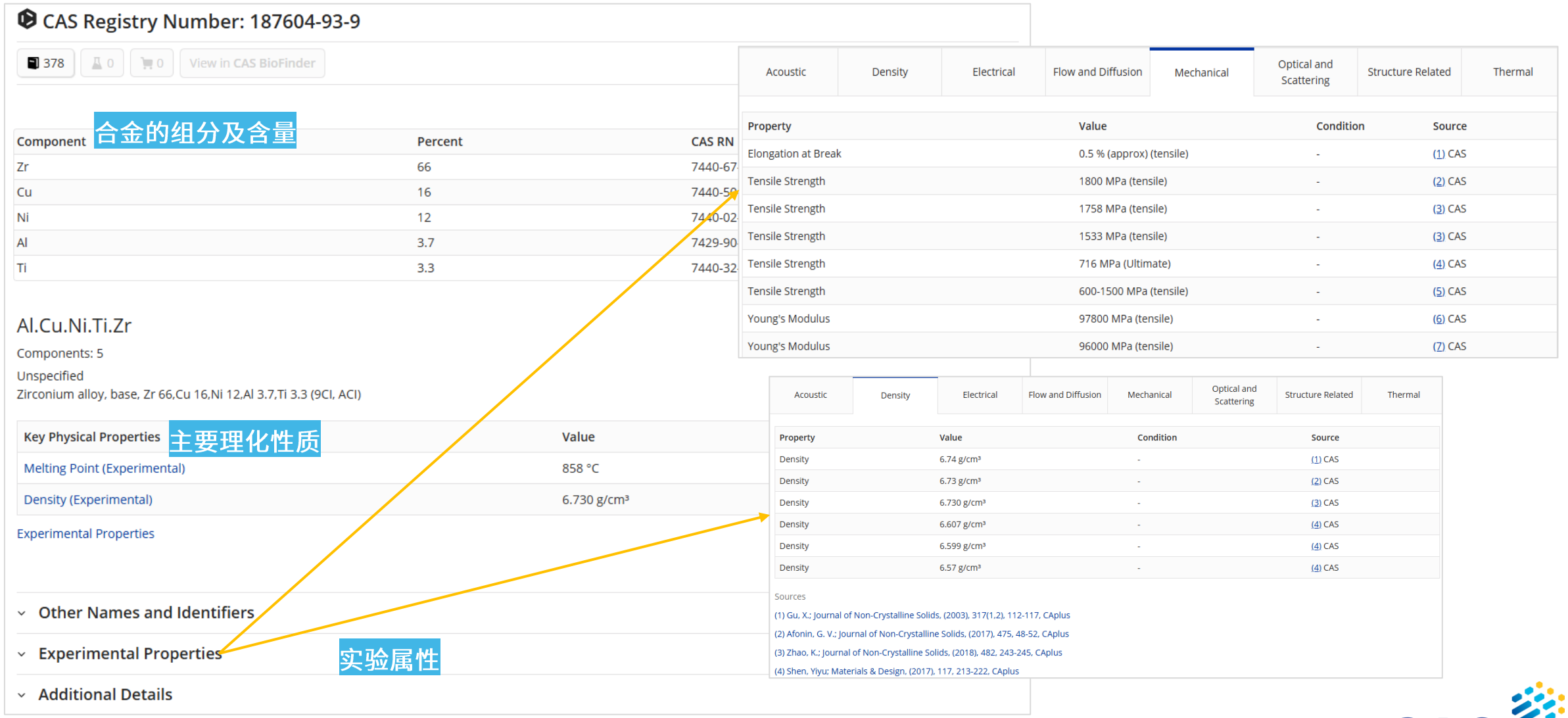
材料详情页中的详细信息



CAS Registry Number: 187604-93-9

378 | 0 | 0 | View in CAS BioFinder

合金的组分及含量

Component	Percent	CAS RN
Zr	66	7440-67
Cu	16	7440-5
Ni	12	7440-02
Al	3.7	7429-90
Ti	3.3	7440-32

Al.Cu.Ni.Ti.Zr

Components: 5

Unspecified

Zirconium alloy, base, Zr 66,Cu 16,Ni 12,Al 3.7,Ti 3.3 (9CI, ACI)

Key Physical Properties 主要理化性质	Value
Melting Point (Experimental)	858 °C
Density (Experimental)	6.730 g/cm³

Experimental Properties

Other Names and Identifiers

Experimental Properties 实验属性

Additional Details

Acoustic | Density | Electrical | Flow and Diffusion | Mechanical | Optical and Scattering | Structure Related | Thermal

Property	Value	Condition	Source
Elongation at Break	0.5 % (approx) (tensile)	-	(1) CAS
Tensile Strength	1800 MPa (tensile)	-	(2) CAS
Tensile Strength	1758 MPa (tensile)	-	(3) CAS
Tensile Strength	1533 MPa (tensile)	-	(3) CAS
Tensile Strength	716 MPa (Ultimate)	-	(4) CAS
Tensile Strength	600-1500 MPa (tensile)	-	(5) CAS
Young's Modulus	97800 MPa (tensile)	-	(6) CAS
Young's Modulus	96000 MPa (tensile)	-	(7) CAS

Acoustic | Density | Electrical | Flow and Diffusion | Mechanical | Optical and Scattering | Structure Related | Thermal

Property	Value	Condition	Source
Density	6.74 g/cm³	-	(1) CAS
Density	6.73 g/cm³	-	(2) CAS
Density	6.730 g/cm³	-	(3) CAS
Density	6.607 g/cm³	-	(4) CAS
Density	6.599 g/cm³	-	(4) CAS
Density	6.57 g/cm³	-	(4) CAS

Sources

(1) Gu, X.; Journal of Non-Crystalline Solids, (2003), 317(1,2), 112-117, CAplus

(2) Afonin, G. V.; Journal of Non-Crystalline Solids, (2017), 475, 48-52, CAplus

(3) Zhao, K.; Journal of Non-Crystalline Solids, (2018), 482, 243-245, CAplus

(4) Shen, Yiyu; Materials & Design, (2017), 117, 213-222, CAplus

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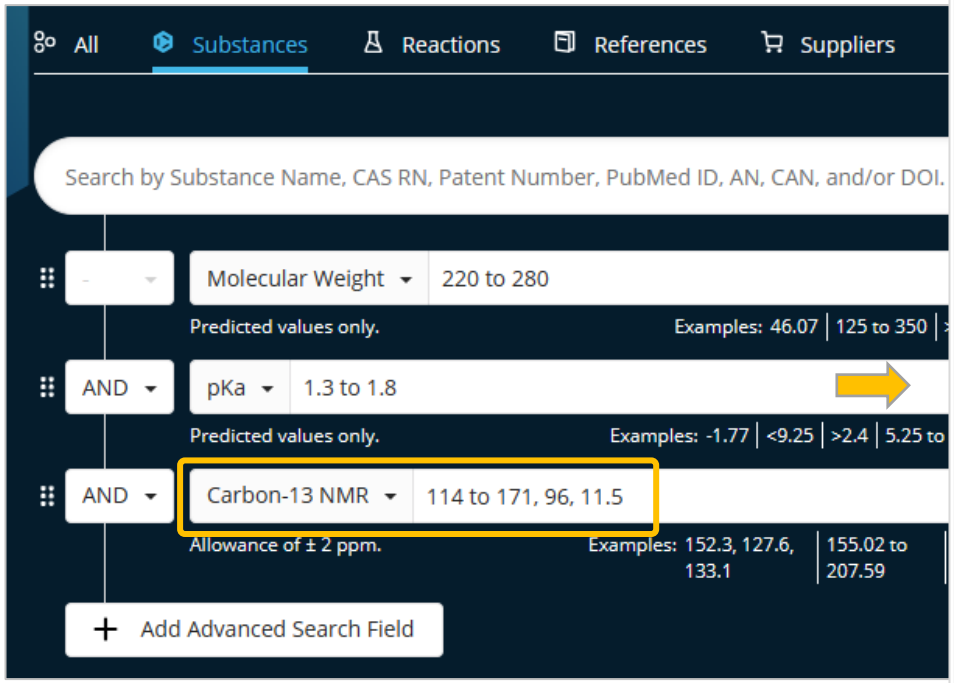
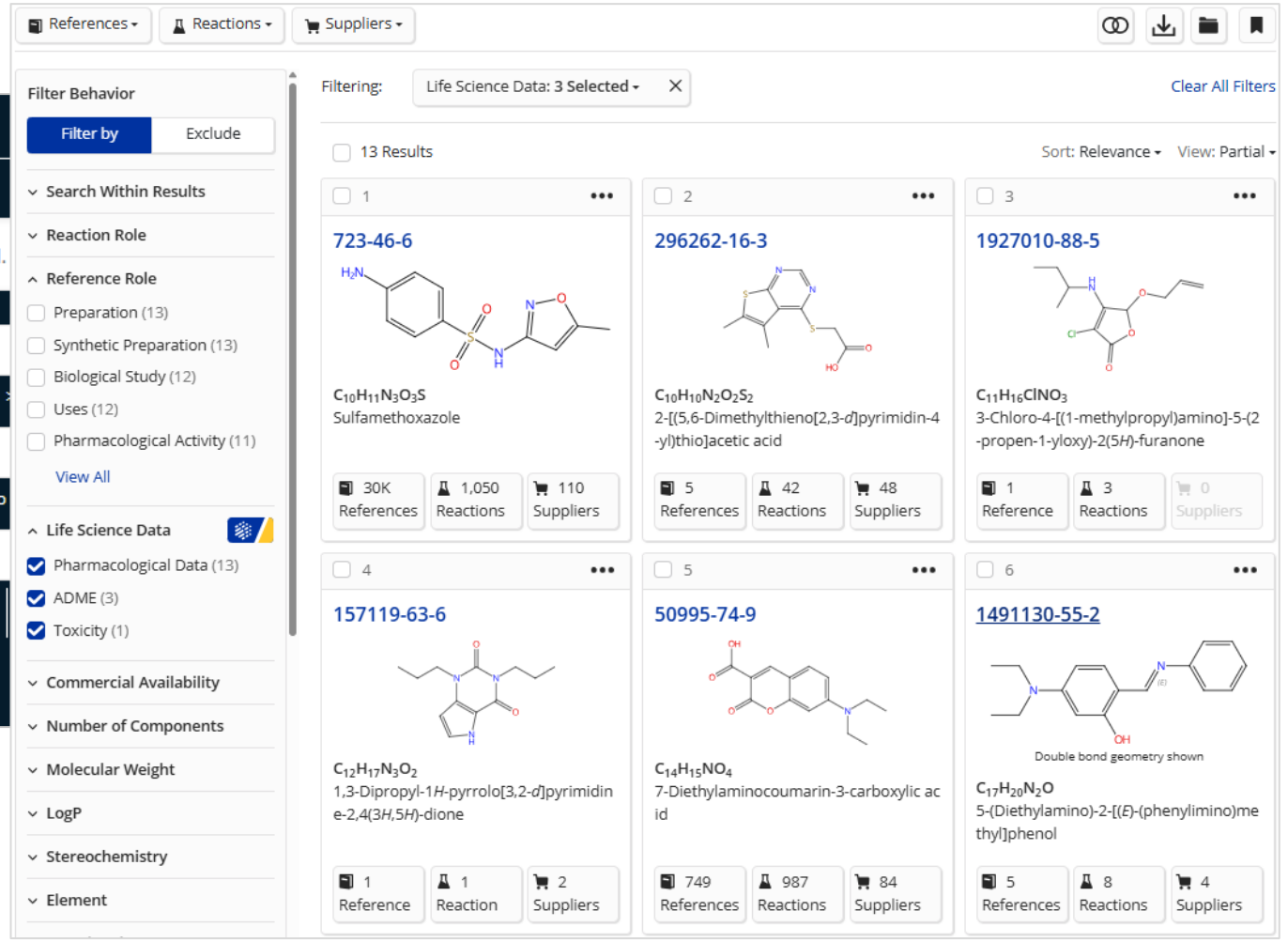
参考已有结构的核磁数据信息



- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5



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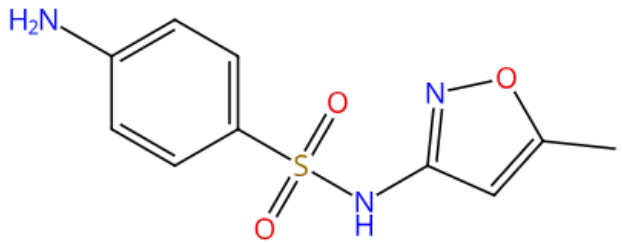
物质详情页中的表征信息

CAS Registry Number: 723-46-6

30K | 1,050 | 110 | View in CAS BioFinder



$C_{10}H_{11}N_3O_3S$

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm³	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra

Experimental Spectra

实验谱图

^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman | UV and Visible

	Solvent	Source
View Carbon-13 NMR Spectrum (Image Available)	DMSO-d_6	(1) WSS
View Carbon-13 NMR Spectrum (Image Available)	DMSO-d_6	(2) WSS
View Carbon-13 NMR Spectrum (Image Available)	-	(2) WSS
View Carbon-13 NMR Spectrum (Image Available)	-	(3) BIORAD
View Carbon-13 NMR Spectrum (Image Available)	DMSO-d_6	(4) AIST
View Carbon-13 NMR Spectrum	DMSO-d_6	(5) CAS
View Carbon-13 NMR Spectrum	Methanol-d_4	(6) CAS
Carbon-13 NMR Spectrum - 1 Source	-	(7) CAS

Sources

(1) Kartashov, V. S.; Khimiko-Farmatsevtiche
(2) Fruttero, Roberta; Journal of the Chemica
(3) Copyright Bio-Rad Laboratories. All Right
(4) "Integrated Spectral Data Base System of
(5) Sunduru, Naresh; European Journal of M
(6) Ham, Won Seok; Angewandte Chemie, In
(7) Blasioli, Sonia; Journal of Colloid and Inte

723-46-6

$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Solvent
DMSO-d_6 (2206-27-1)

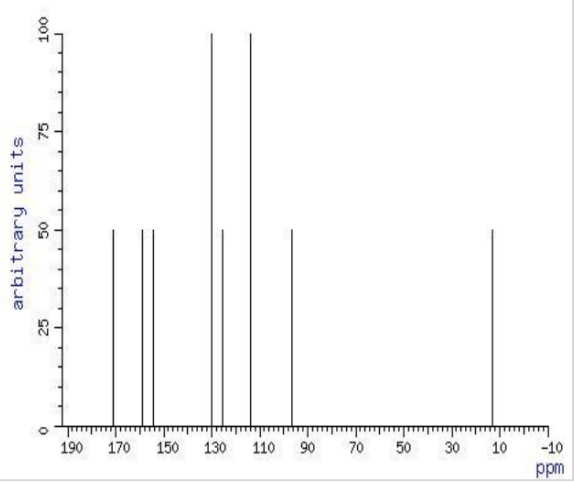
Temperature
30 °C

Spectrum Summary

Spectrum ID
CC-03-C_SPC-17694

Spectrometer
BRUKER WH-90

Source
Spectral data were obtained from John Wiley & Sons, Inc.



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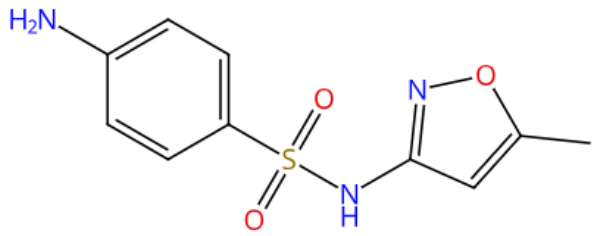
物质的生命科学数据



$C_{10}H_{11}N_3O_3S$

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm³	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Pharmacological Data
- ADME
- Toxicity

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Pharmacological Data

药理数据

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Knowledge Graph

Target ⌄1	Function	Parameter ⌃2	Value	Disease	Organism	Assay	Source
Yersinia enterocolitica	-	MBC50	304 mg/mL	bacterial infectious disease	Yersinia enterocolitica	View Detail	(1) CAS
Yersinia enterocolitica	-	MBC90	1216 mg/mL	bacterial infectious disease	Yersinia enterocolitica	View Detail	(1) CAS
Yersinia enterocolitica	-	MIC50	38 mg/L	bacterial infectious disease	Yersinia enterocolitica	View Detail	(1) CAS

ADME

代谢数据

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Target ⌃2	Function	Parameter ⌃1	Value	Disease	Organism	Assay	Source
-	Inhibitor	Absorption	Rapid	-	-	View Detail	(1)
-	-	AUC	796.3 μg.hr/mL	-	-	View Detail	(2) CAS
-	-	AUC	930.2 μg.hr/mL	-	-	View Detail	(2) CAS
-	Inhibitor	AUC	342.6 - 796.3 μg.hr/mL	-	-	View Detail	(2) CAS
-	Inhibitor	AUC	273 - 930.2 μg.hr/mL	-	-	View Detail	(2) CAS

Toxicity

毒性数据

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Target ⌃1	Function	Parameter ⌃2	Value	Disease	Organism	Assay	Source
C8166 cell line	-	TD50	> 240 μg/mL	-	Homo sapiens	View Detail	(1)
Dihydropteroate synthase	-	Acute toxicity	3.61 mol/L	bacterial infectious disease	DHPS	View Detail	(2) CAS
Dihydropteroate synthase	-	Chronic toxicity	5.03 mol/L	bacterial infectious disease	DHPS	View Detail	(2) CAS
Vero cell line	-	TD50	4.25×10^3 μg/mL	-	Macaca mulatta	View Detail	(1)
-	-	IC25	1×10^3 mg/L	-	-	View Detail	(3)
-	-	IC25	1×10^3 mg/L	-	-	View Detail	(3)
-	-	IC50	200 mg/L	-	-	View Detail	(3)

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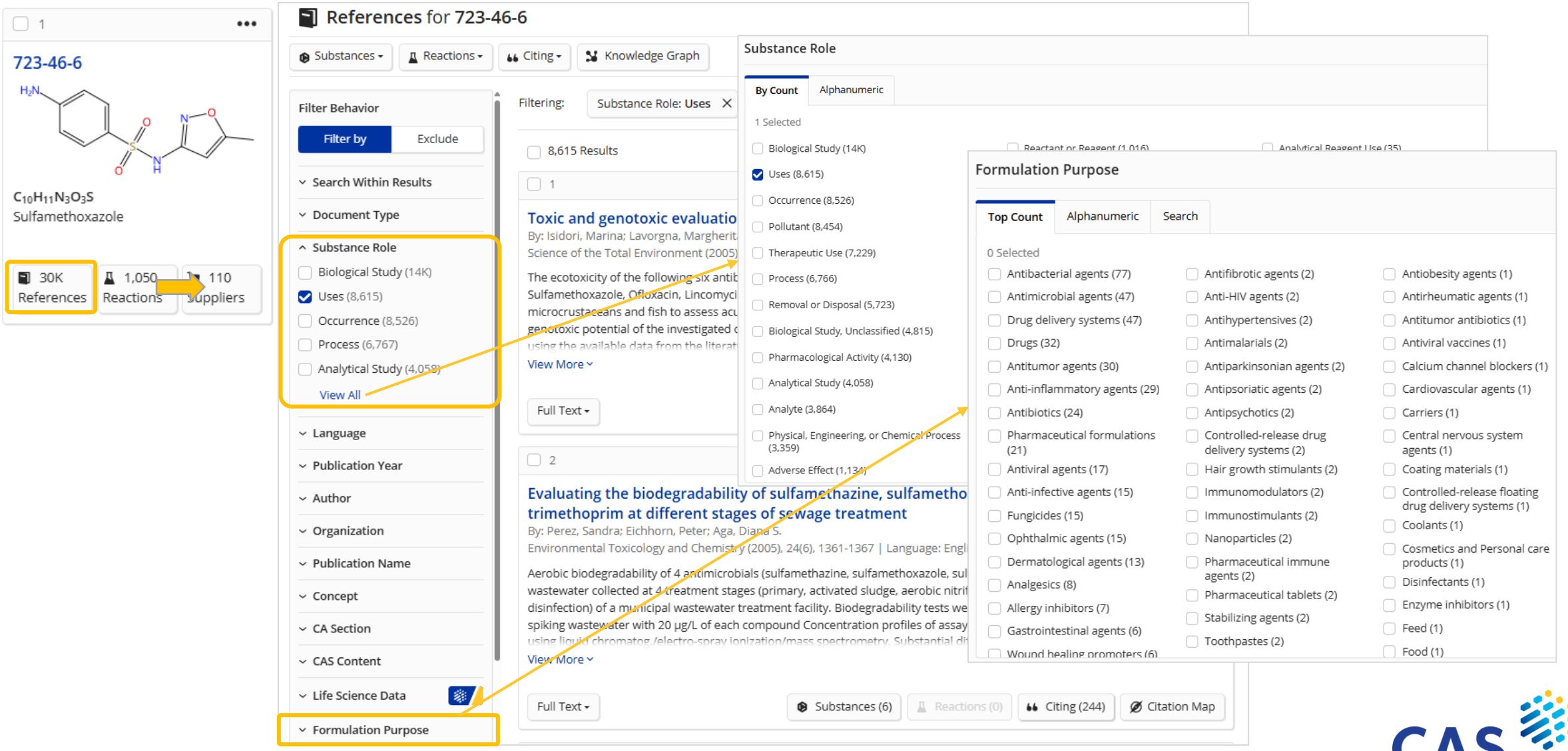
拓展关注结构的其他应用研究



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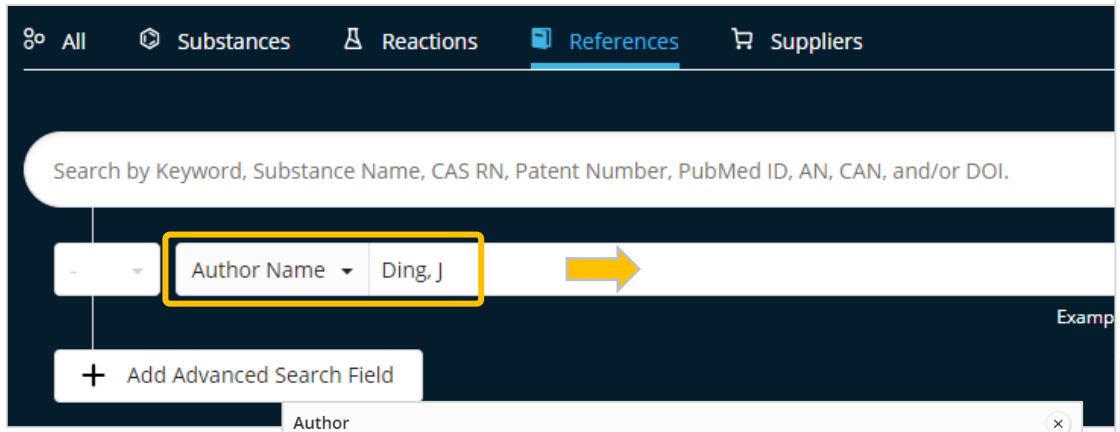
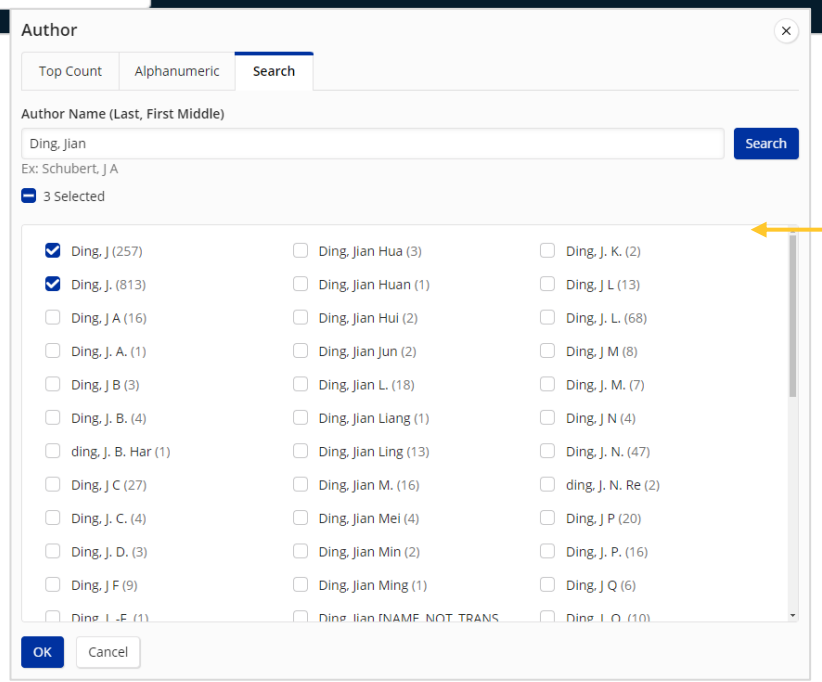
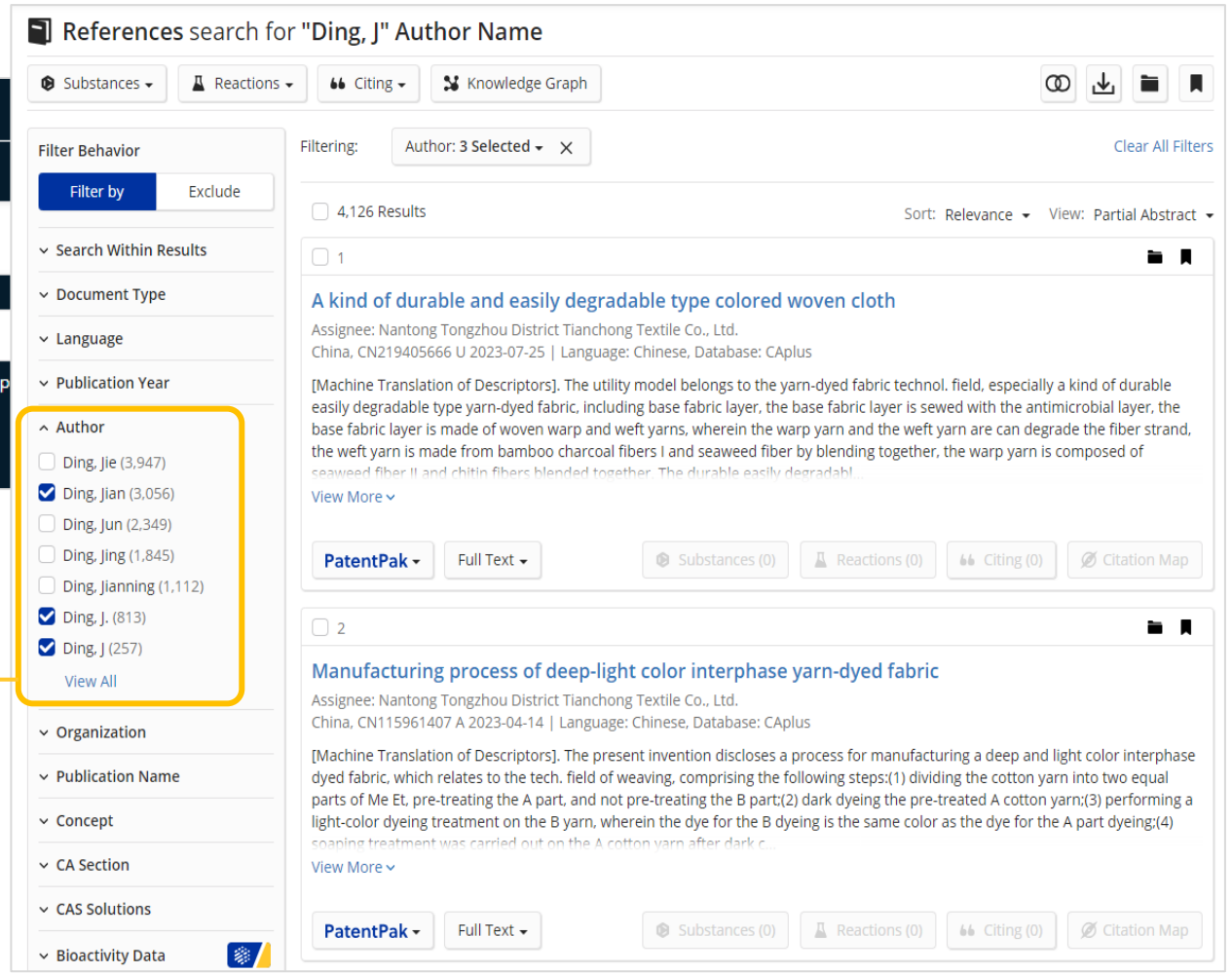
查阅知名学者的研究







先全面检索，再筛选精炼

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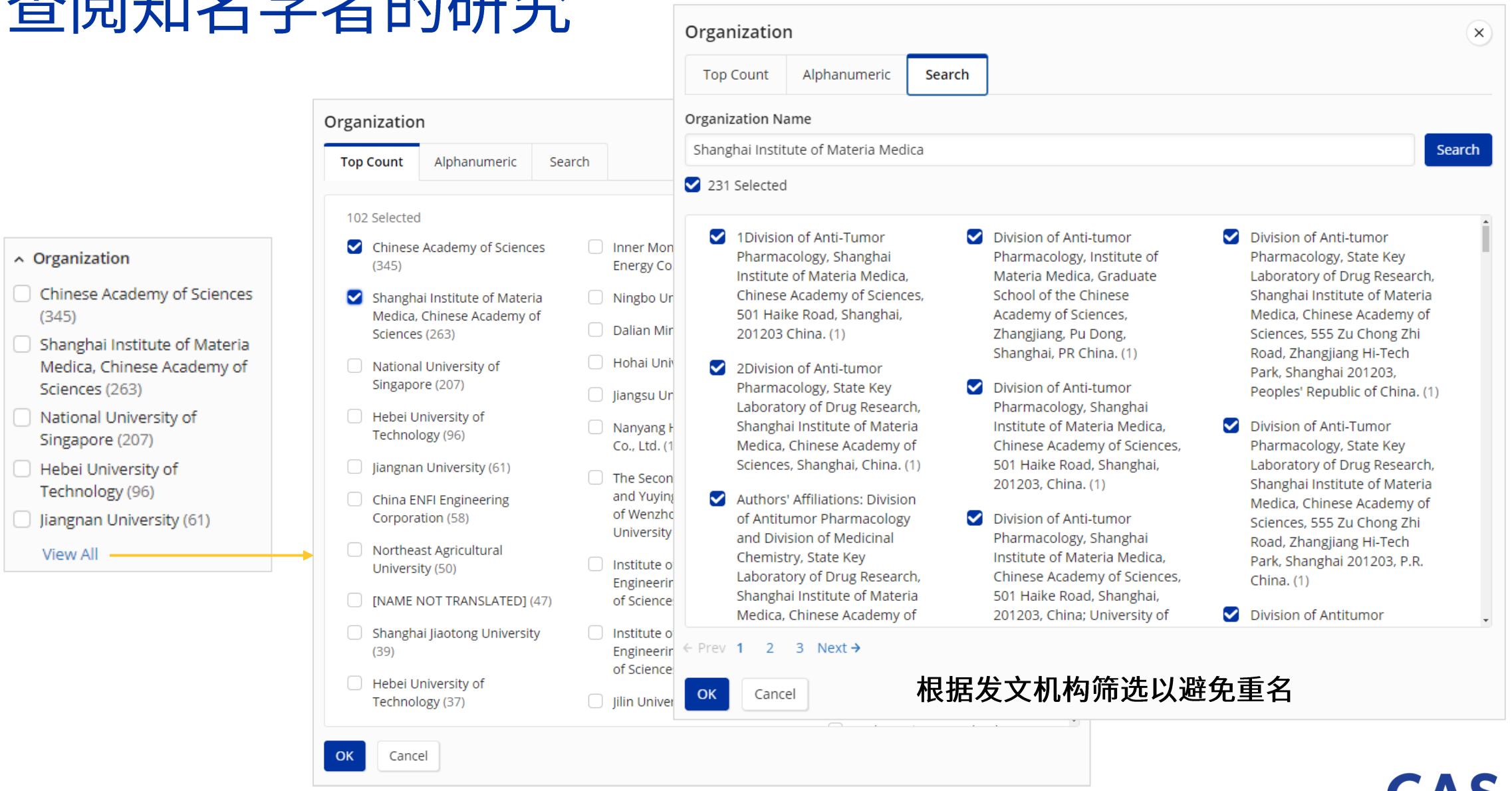

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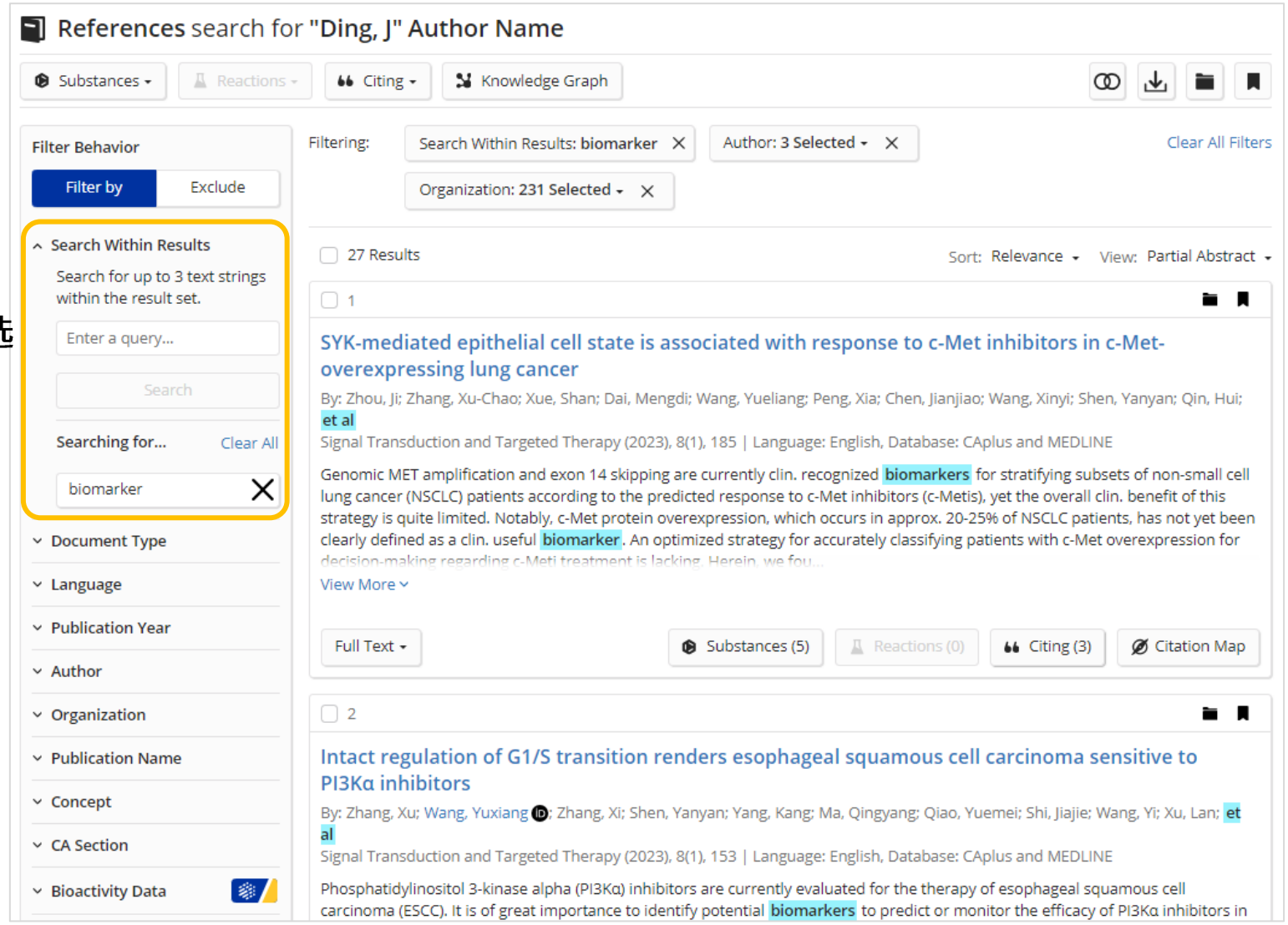
查阅知名学者在某特定方向的研究

检索结果的二次筛选

示例：生物标志物



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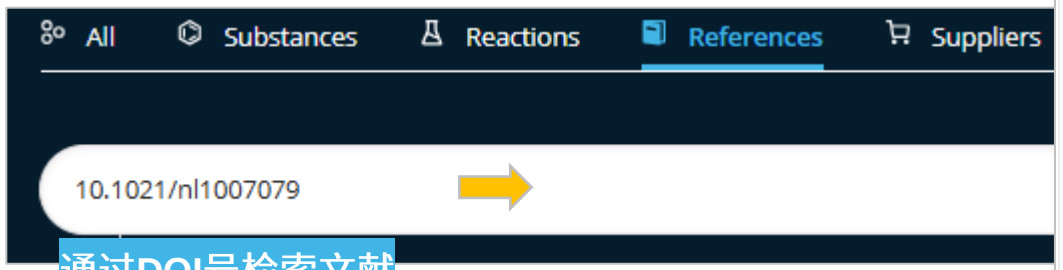
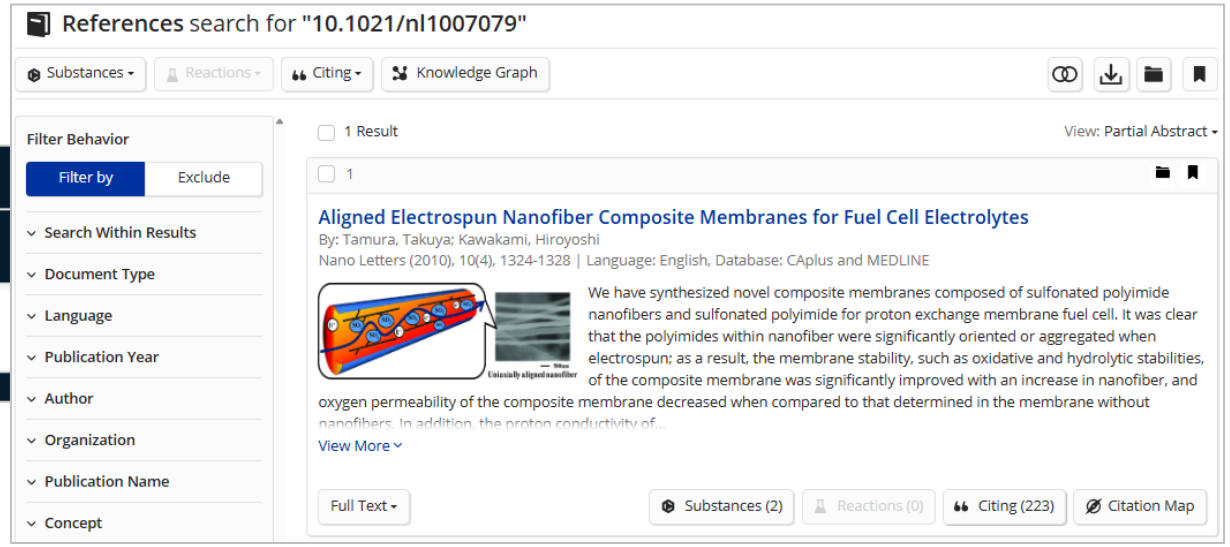
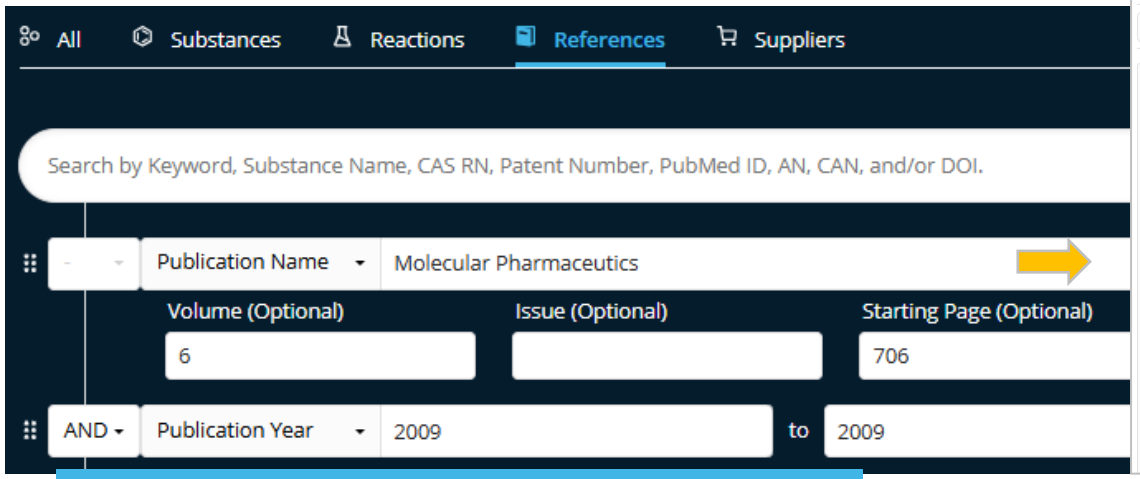
查看导师/审稿人推荐的研究工作

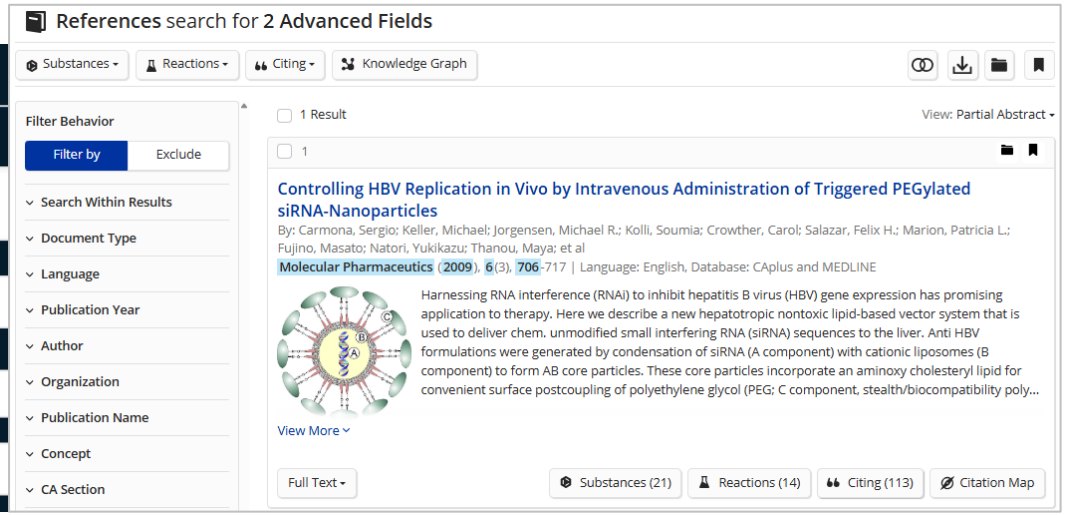


通过DOI号检索文献





通过期刊名、卷号、页码、发表年份等检索文献



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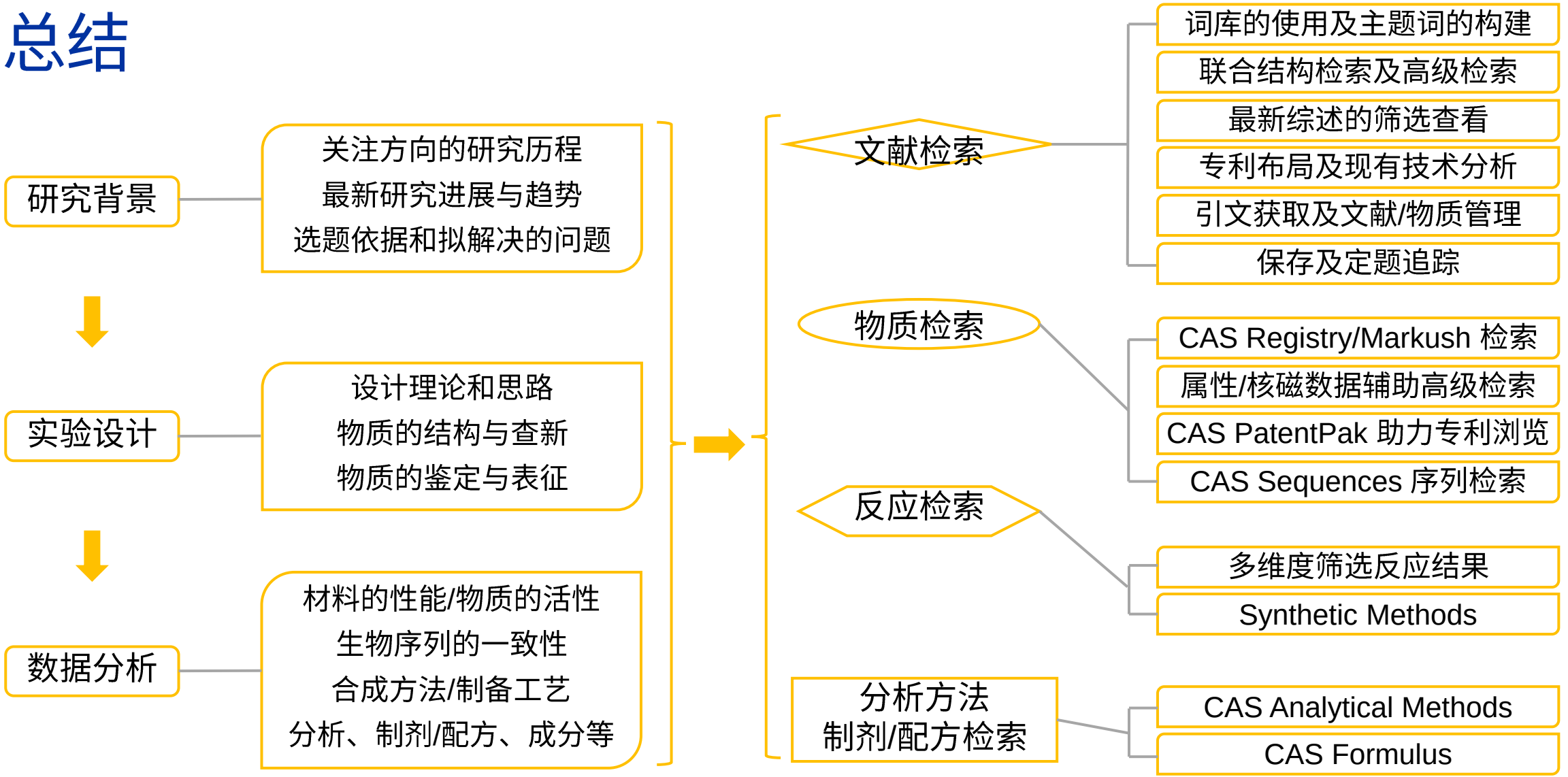
总结



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Between problems and progress are connections that matter

are connections that matter

谢 谢!

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