钱欣博士
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美国化学文摘社北京代表处

SciFinder^{n}专题培训

---药理/药代信息检索

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SciFinder^{n}登陆平台

https://scifinder-n.cas.org

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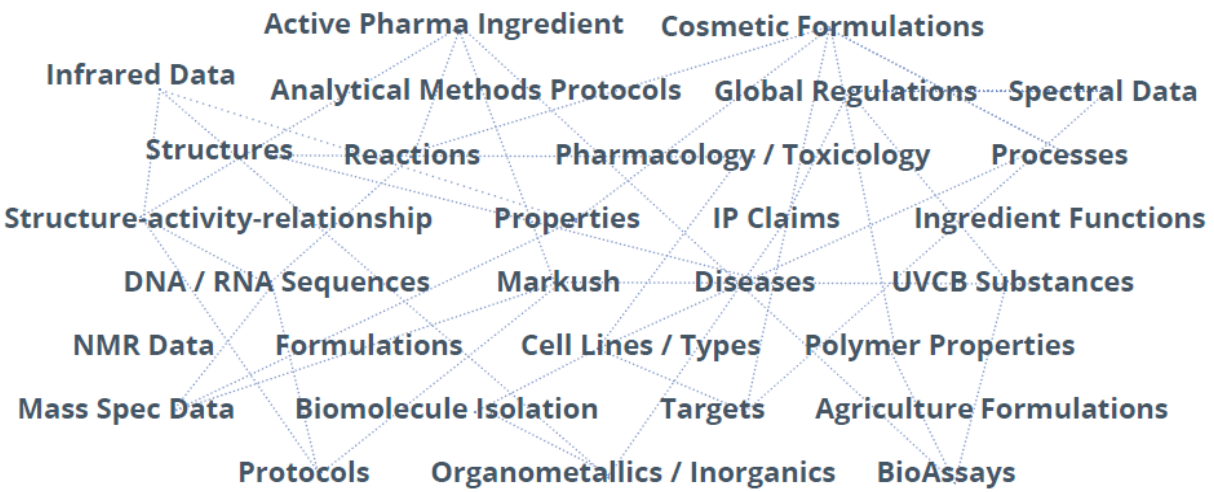
SciFinder^{n}涵盖内容的独特性

54 Million scientific journals and documents

64 PATENT OFFICES worldwide

180 MILLION substances

50 LANGUAGES translated



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SciFinder Discovery平台涵盖内容的独特性

- 化学物质数量全球领先。目前收录的化学物质数量已超过1.80亿个，是进行新化合物确认的唯一可用资源。
- 生物大分子数量全球领先。目前收录来自期刊和专利中的约5.8亿条序列（包括蛋白、核酸）
- 由CAS创建的CAS登记号是化学物质的黄金标准；是对物质进行确认的唯一身份识别号；是在进行化学品进出口交易时，必须向相关国家管控机构提供的身份识别号；是在申报课题项目时，需向评议组提供的身份识别号
- CAS几乎收录了从高分子聚合物到纳米颗粒的所有类别的物质，包括有机物、无机物、聚合物、合金、矿物质、配合物、混合物、生物序列等

Sources: https://www.cas.org/about/cas-content

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SciFinder Discovery平台涵盖内容的独特性

- CAS不但收录专利中报道的确定结构的物质，还收录专利中的通式结构（马库什结构），帮助用户在使用CAS的数据后能够最大程度的避免专利法律风险
- 化学反应数量全球领先，目前收录的化学反应数量超过1.34亿条，是确认新的化学反应、工艺和方法时必不可缺的资源
- 近千名科学家每天阅读来自全球的科技文献，并根据CAS制定的规则和标准、从信息专家和科学家的角度对原文中重要的信息进行改写和标引，从而节省CAS的用户花在阅读、理解、总结科技原文文献所需的时间，将更多的时间投入到其他的工作中

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大纲

- 疾病模型研究信息
- 药物与受体的相互作用研究
- 药代动力学研究
- 副作用研究

人类疾病动物模型研究信息

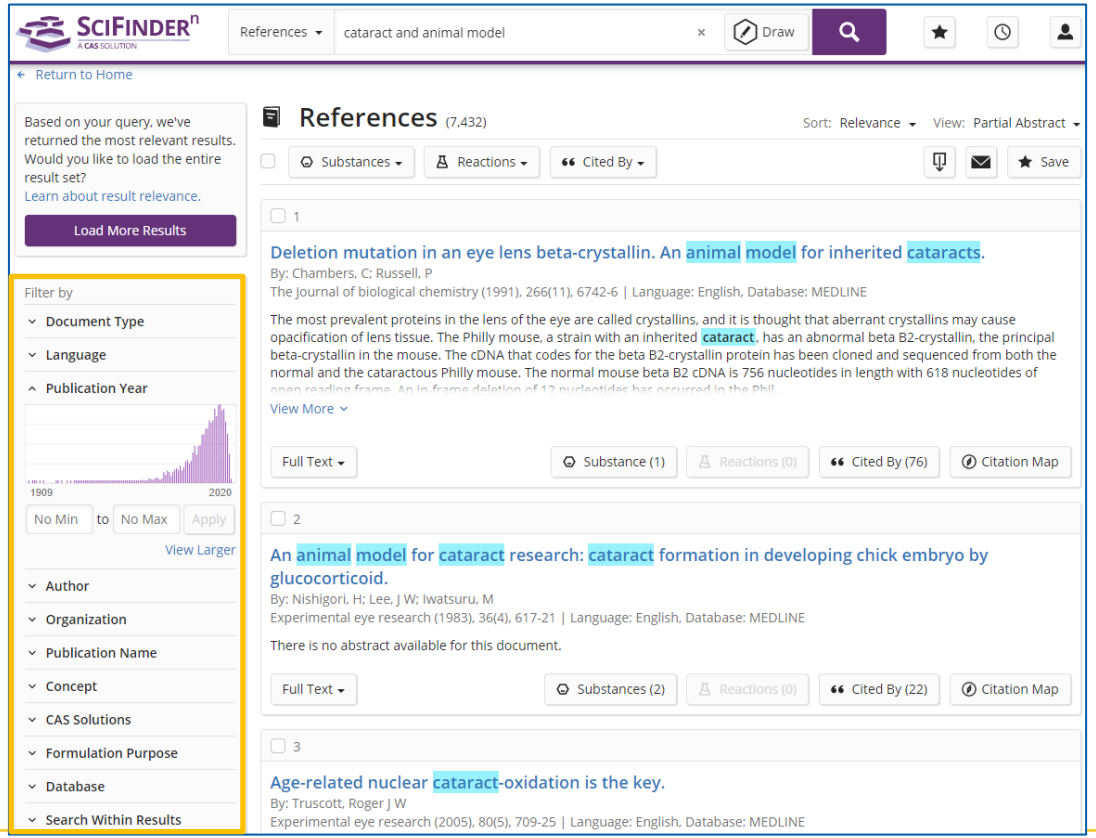
用于研究发病机制、药物筛选、药效评价等。

信息的检索方法

构建检索主题

关联文献和物质信息

人类疾病动物模型研究信息



cataract and animal model

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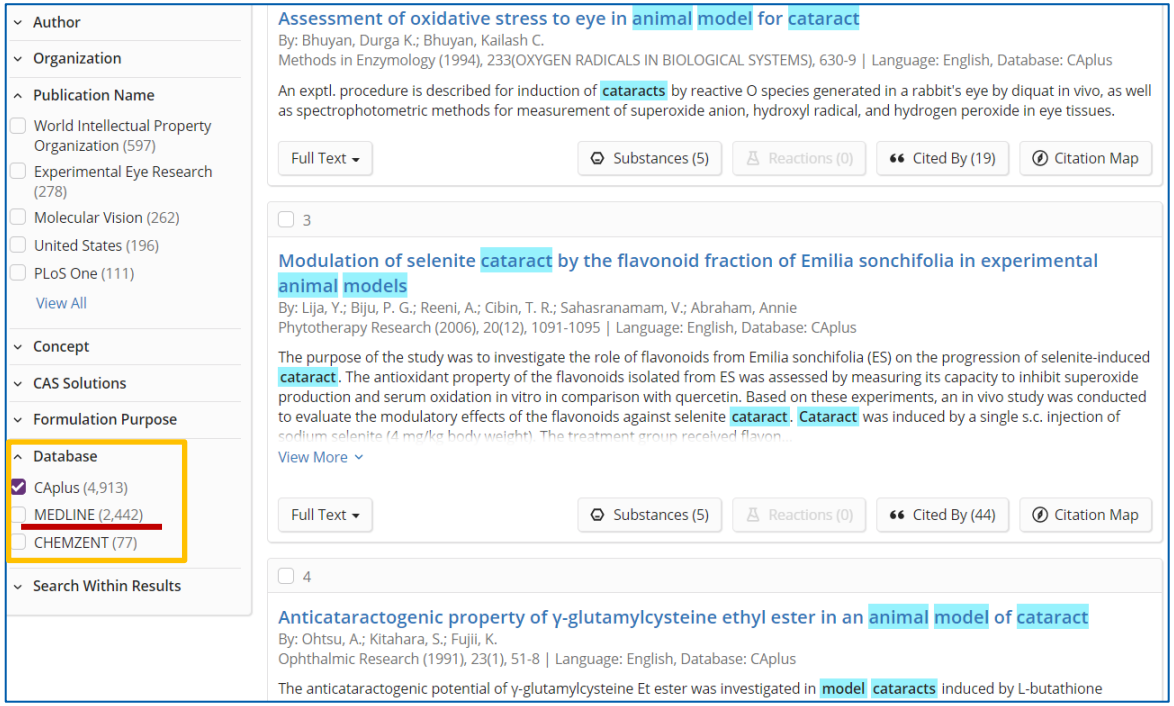
广泛的覆盖范围确保尽可能全面地获取文献研究信息



CAplus是CAS核心文献库，同时SciFinder-n中也收录了1946年以来的，来自Medline的文献。

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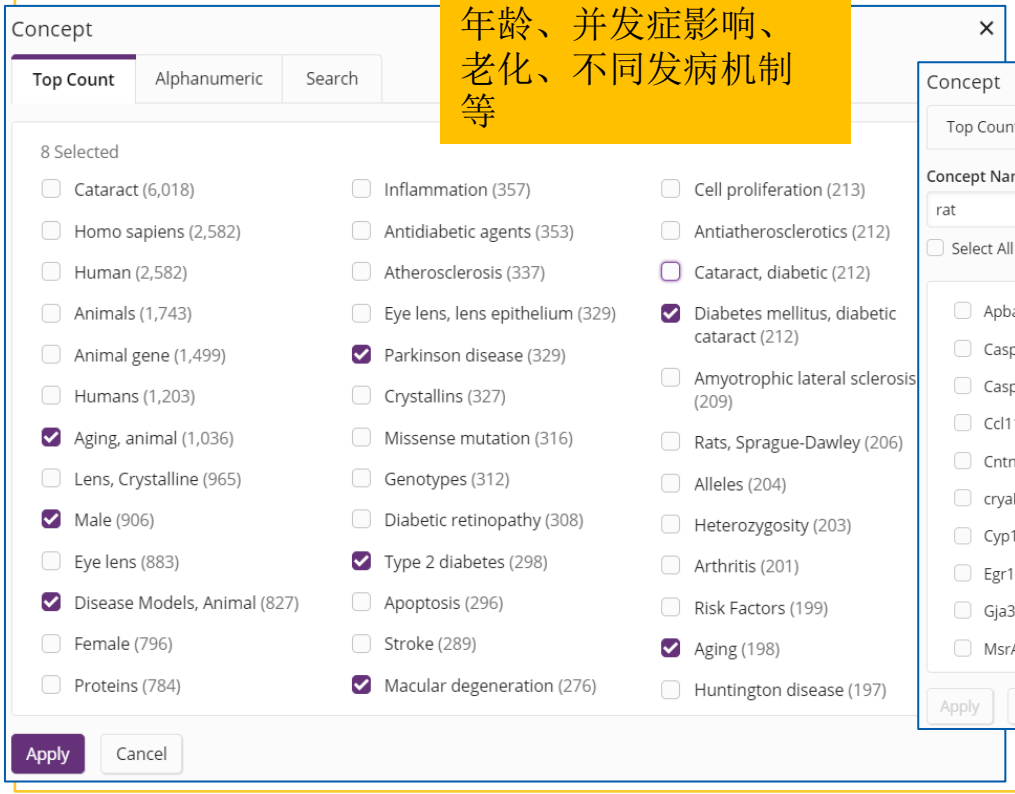
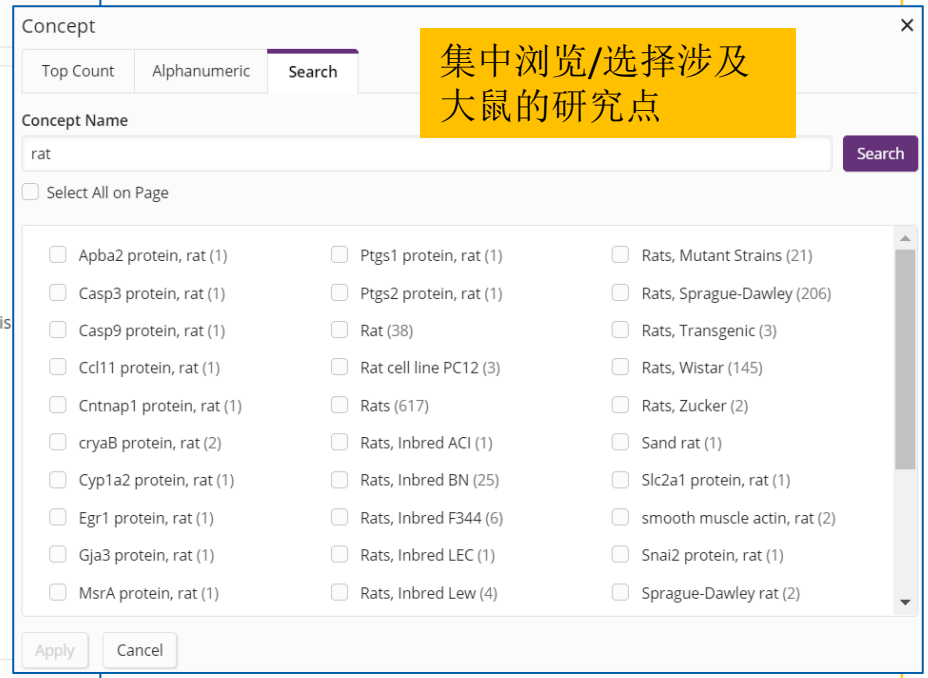
通过Concept标准概念词库，细化模型中涉及的研究点

年龄、并发症影响、老化、不同发病机制等



集中浏览/选择涉及大鼠的研究点



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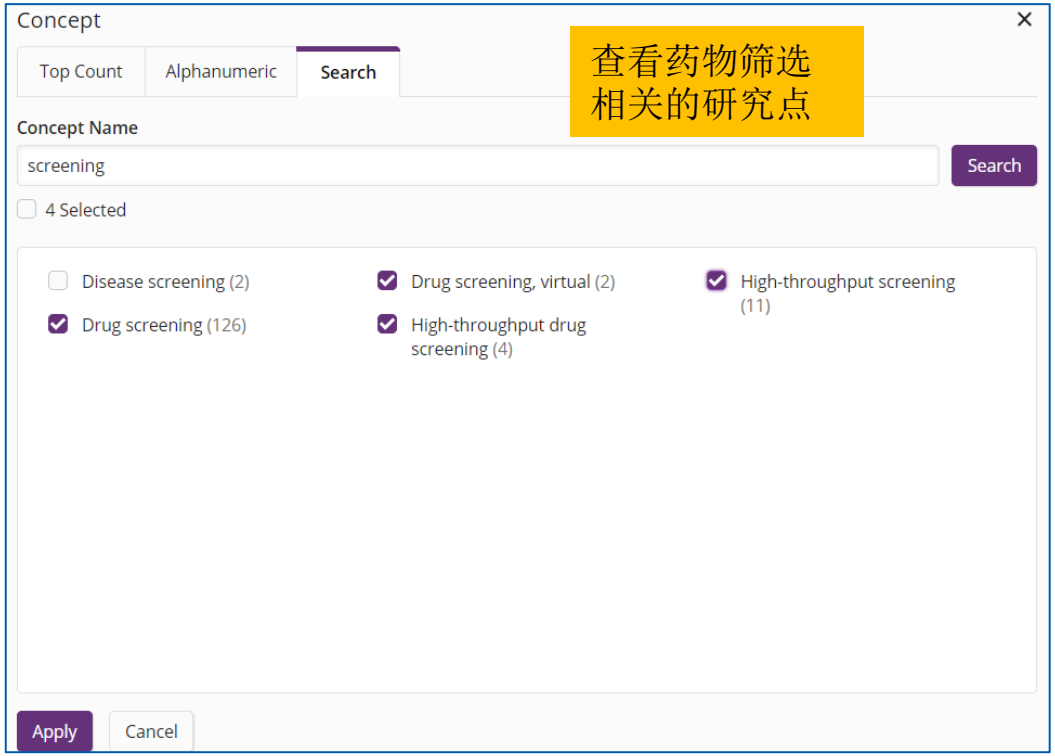
通过Concept标准概念词库，细化模型中涉及的研究点



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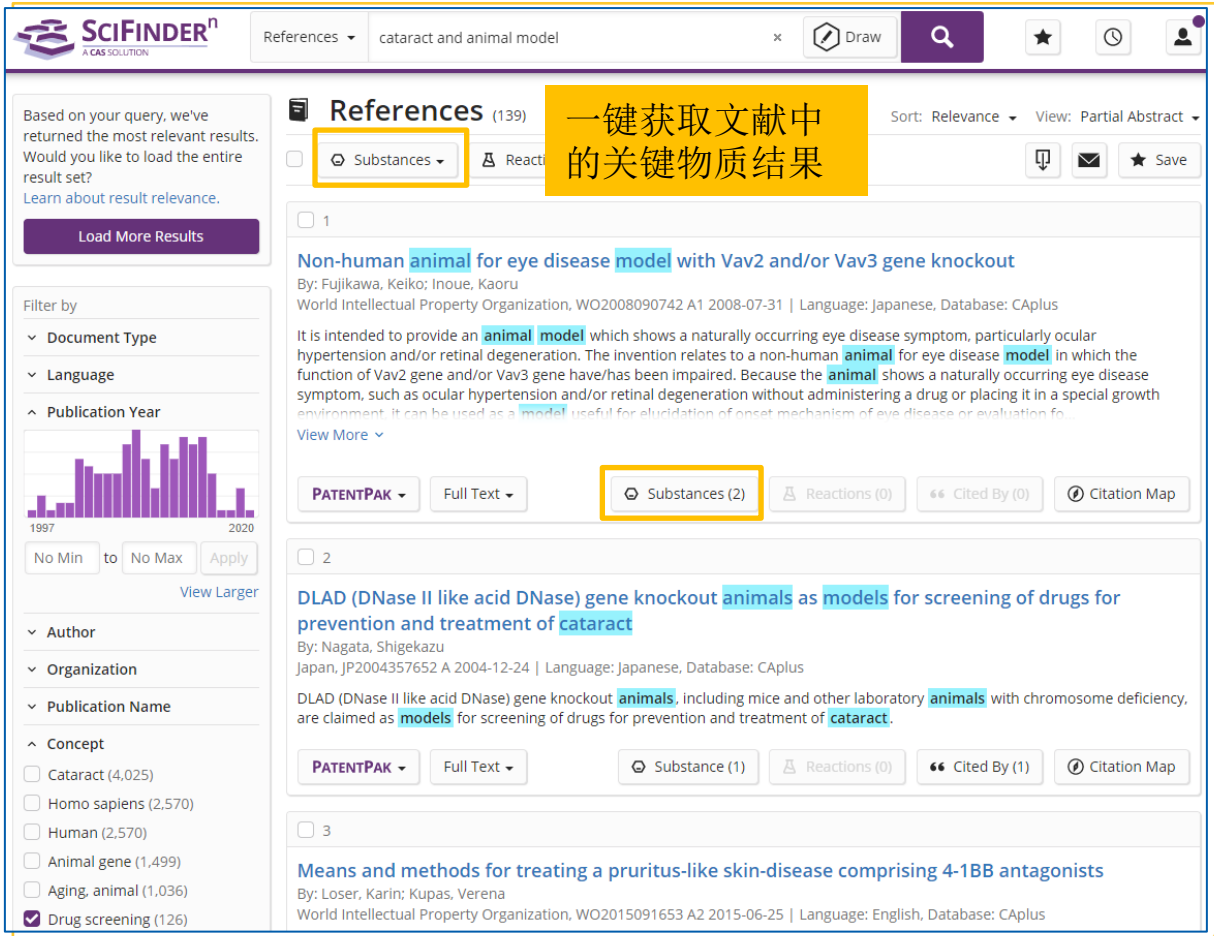

通过文献获取关联的物质结果

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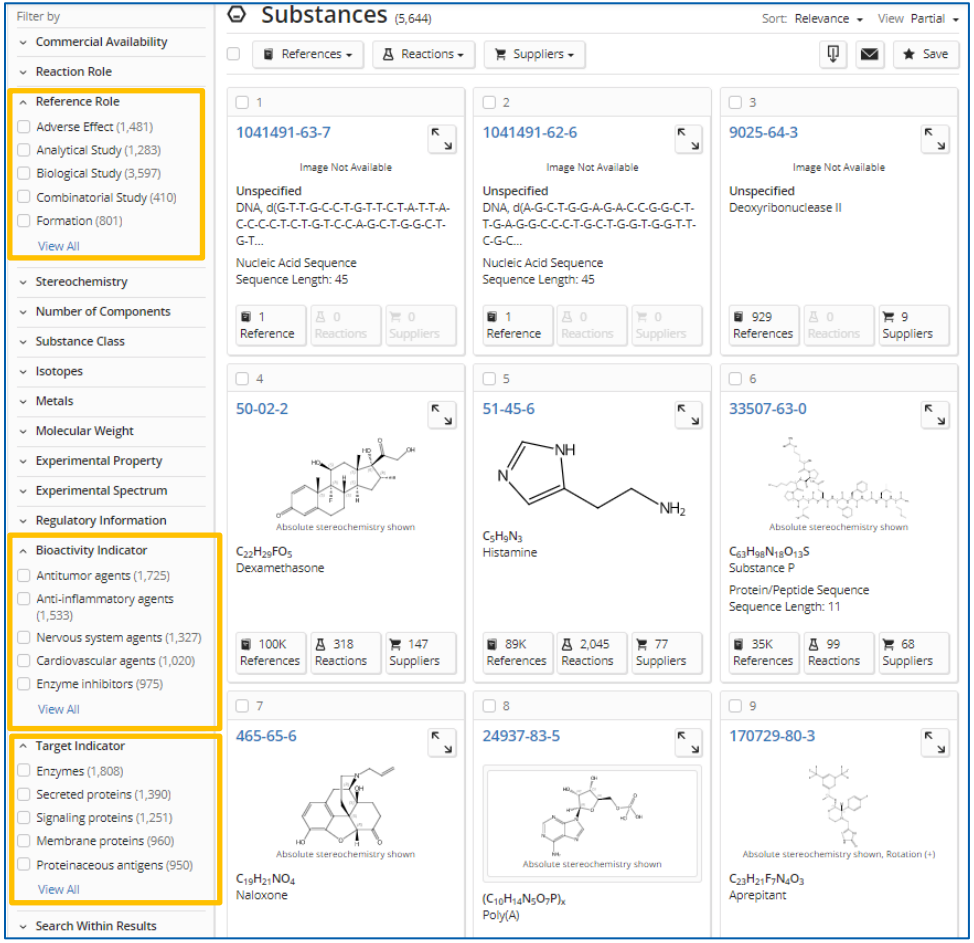

分析文献中的物质结果

研究角色

生物活性

靶点信息

物质类型

属性

谱图

等等

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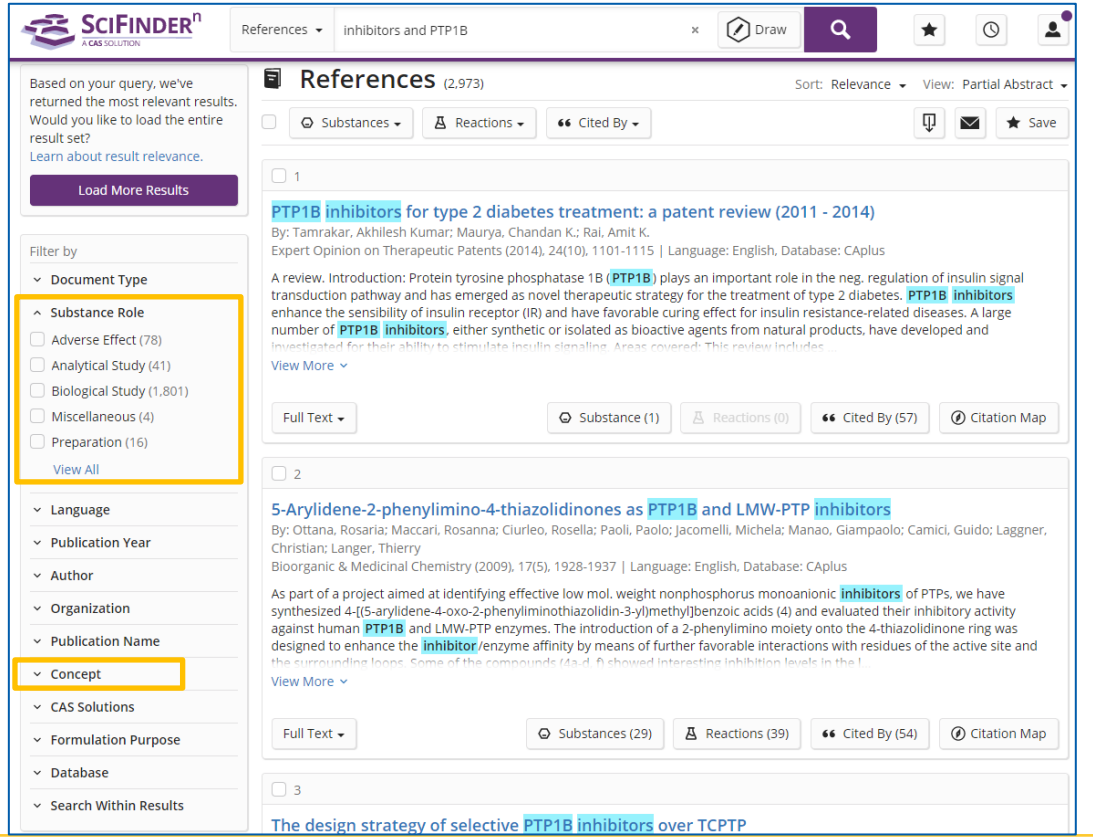
大纲

- 疾病模型研究信息
- 药物与受体的相互作用研究
- DMPK药代药动学研究
- 副作用研究

例1：PTP1B和小分子抑制剂的作用研究



inhibitors and PTP1B

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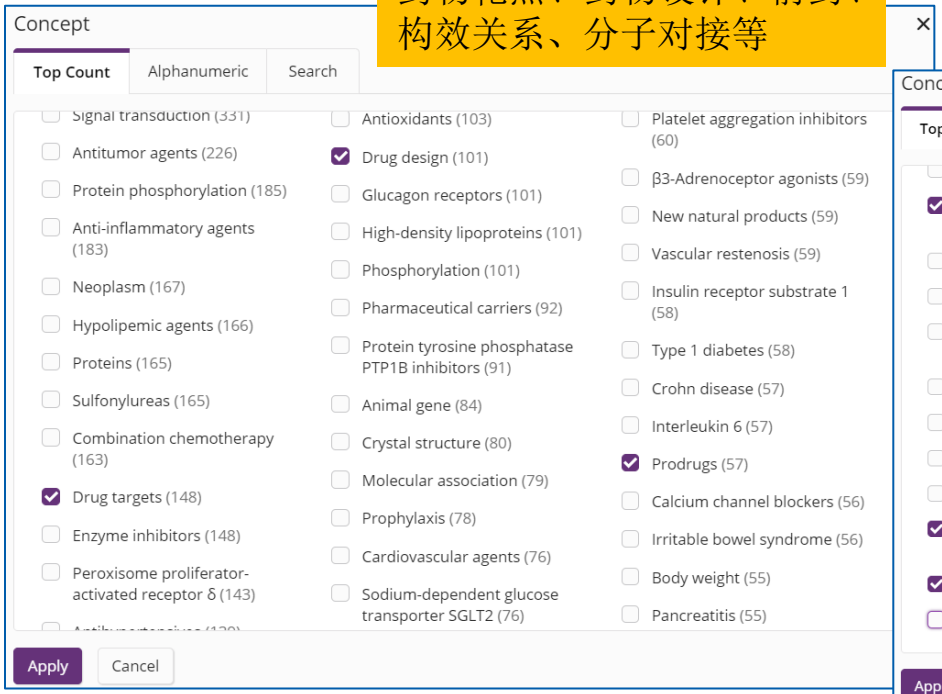
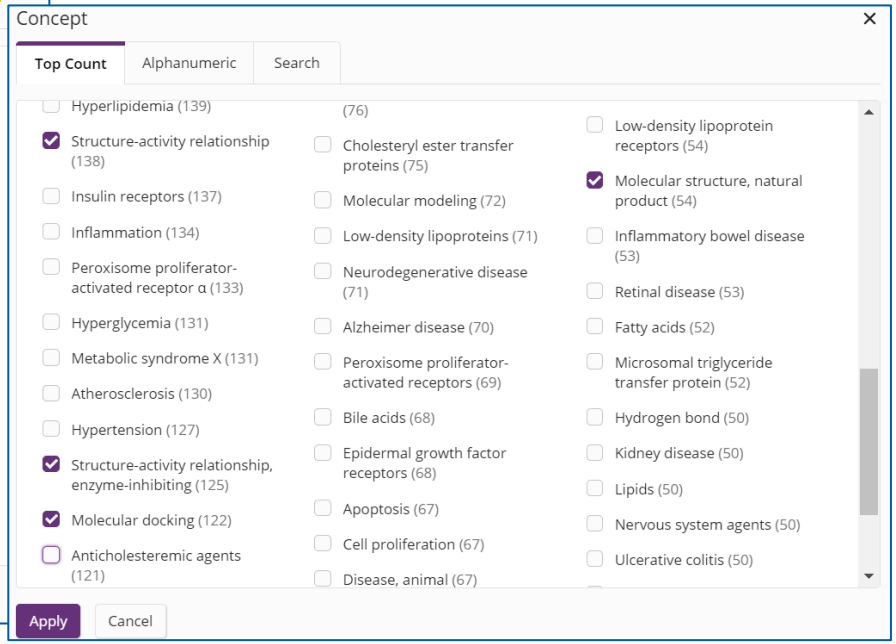
通过Concept概念词库，细化具体的研究点

药物靶点、药物设计、前药、构效关系、分子对接等





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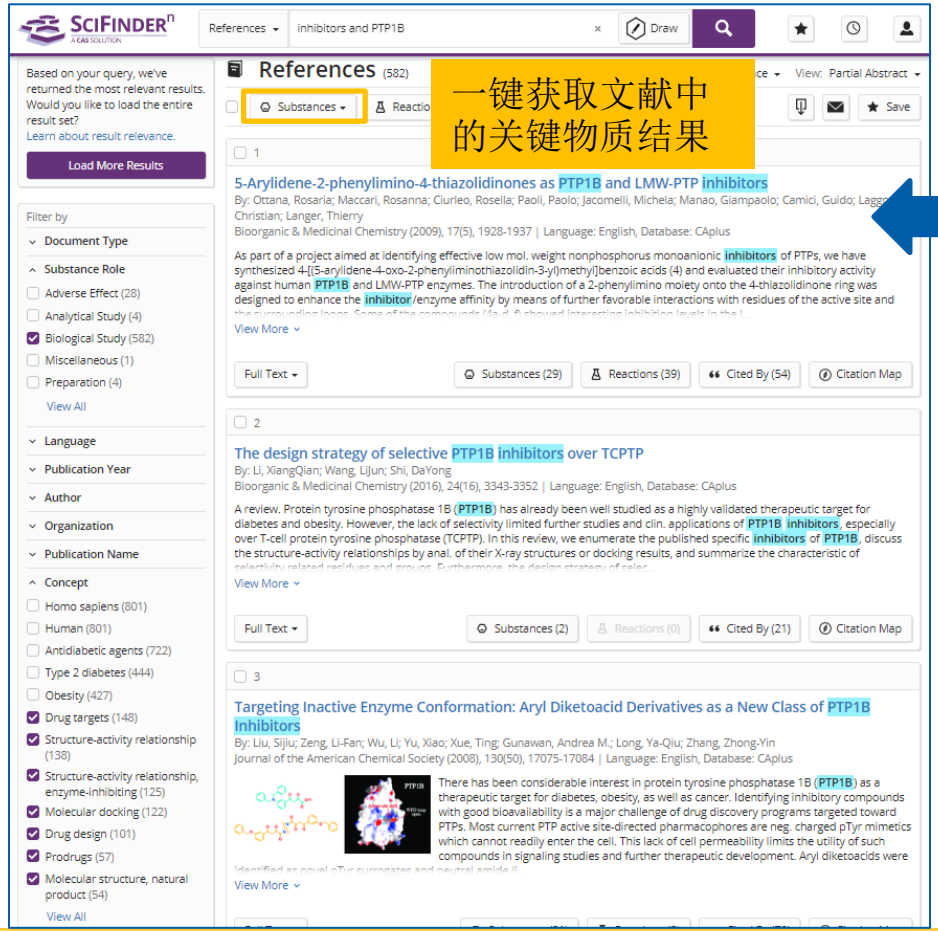

锁定感兴趣的文献，通过文献详情快速了解文献主旨，并获取关联的物质信息

点击标题，快速获取文献主旨

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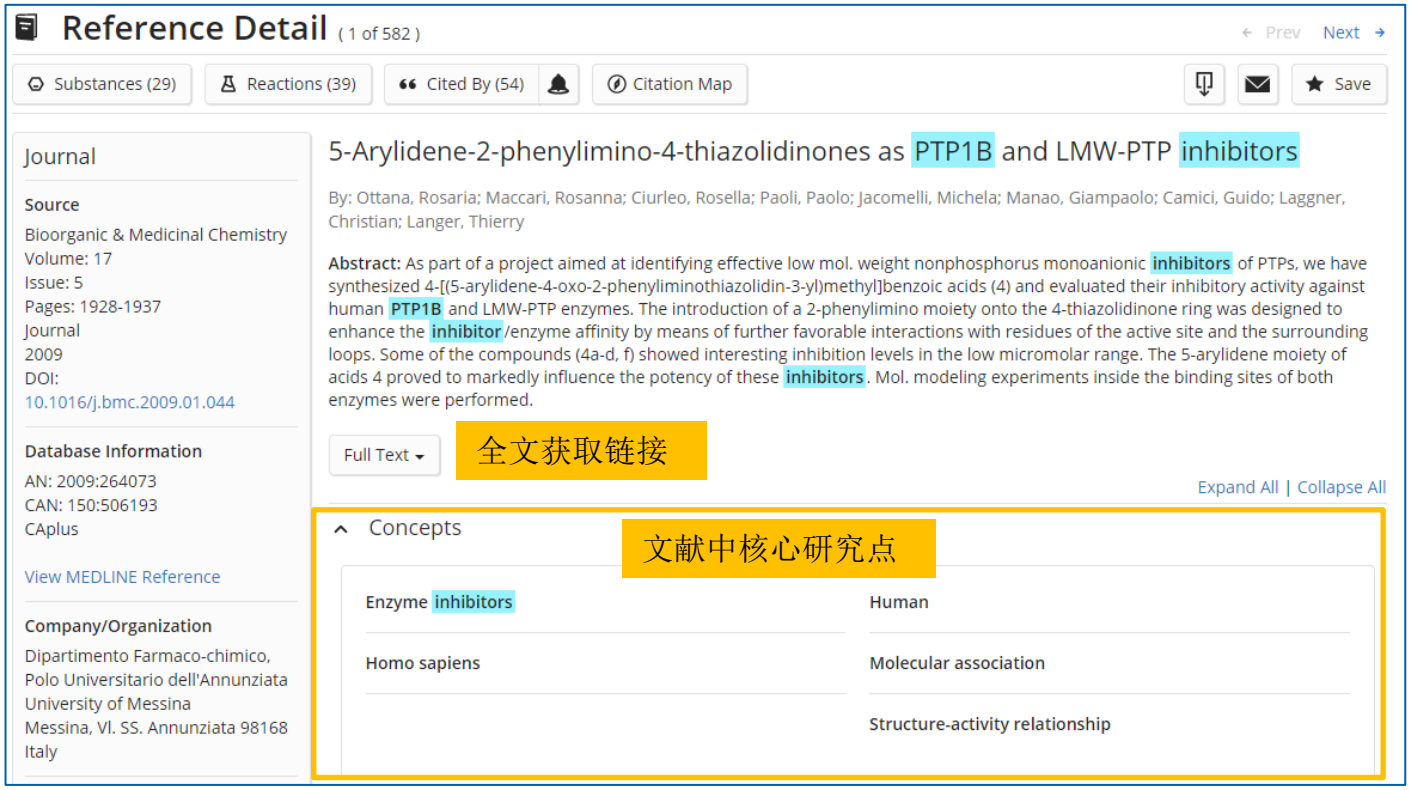
充分利用文献详情中人工标引的信息，快速了解文献主旨



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Substances

Substances (29)

300865-11-6

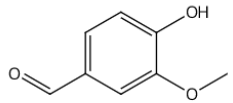
Image Not Available

Unspecified

PTP1B

Role: Biological Study, Unclassified, Biological Study

121-33-5

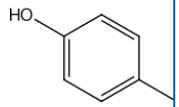


$C_8H_8O_3$

Vanillin

Role: Reactant, Reactant or Reagent

123-08-0

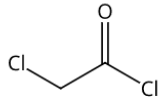


$C_7H_6O_2$

4-Hydroxybenzaldehyde

Role: Reactant, Reactant or Reage

79-04-9

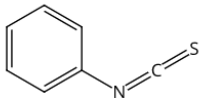


$C_2H_2Cl_2O$

Chloroacetyl chloride

Role: Reactant, Reactant or Reagent

103-72-0

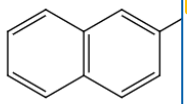


C_7H_5NS

Phenyl isothiocyanate

Role: Reactant, Reactant or Reagent

66-99-9

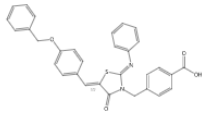


$C_{11}H_8O$

2-Naphthalenecarboxaldeh

Role: Reactant, Reactant or Reage

1148126-96-8



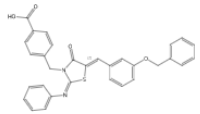
E/Z labels describe double bond geometry

$C_{31}H_{24}N_2O_4S$

Benzoic acid, 4-[[(5*Z*)-4-oxo-2-(phenylimino)-5-[[4-(phenylmethoxy)phenyl]methylene]-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-95-7



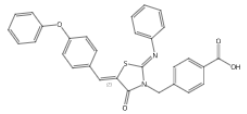
E/Z labels describe double bond geometry

$C_{31}H_{24}N_2O_4S$

Benzoic acid, 4-[[(5*Z*)-4-oxo-2-(phenylimino)-5-[[3-(phenylmethoxy)phenyl]methylene]-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-93-5



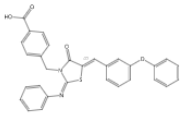
E/Z labels describe double bond geometry

$C_{30}H_{22}N_2O_4S$

Benzoic acid, 4-[[(5*Z*)-4-oxo-5-[(4-phenoxyphenyl)methylene]-2-(phenylimino)-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-91-3



E/Z labels describe double bond geometry

$C_{30}H_{22}N_2O_4S$

Benzoic acid, 4-[[(5*Z*)-4-oxo-5-[(3-phenoxyphenyl)methylene]-2-(phenylimino)-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

352548-19-7

Image Not Available

Unspecified

Low-mol.-wt. protein tyrosine phosphatase

Role: Biological Study, Unclassified, Biological Study

文献中重要物质列表及研究角色

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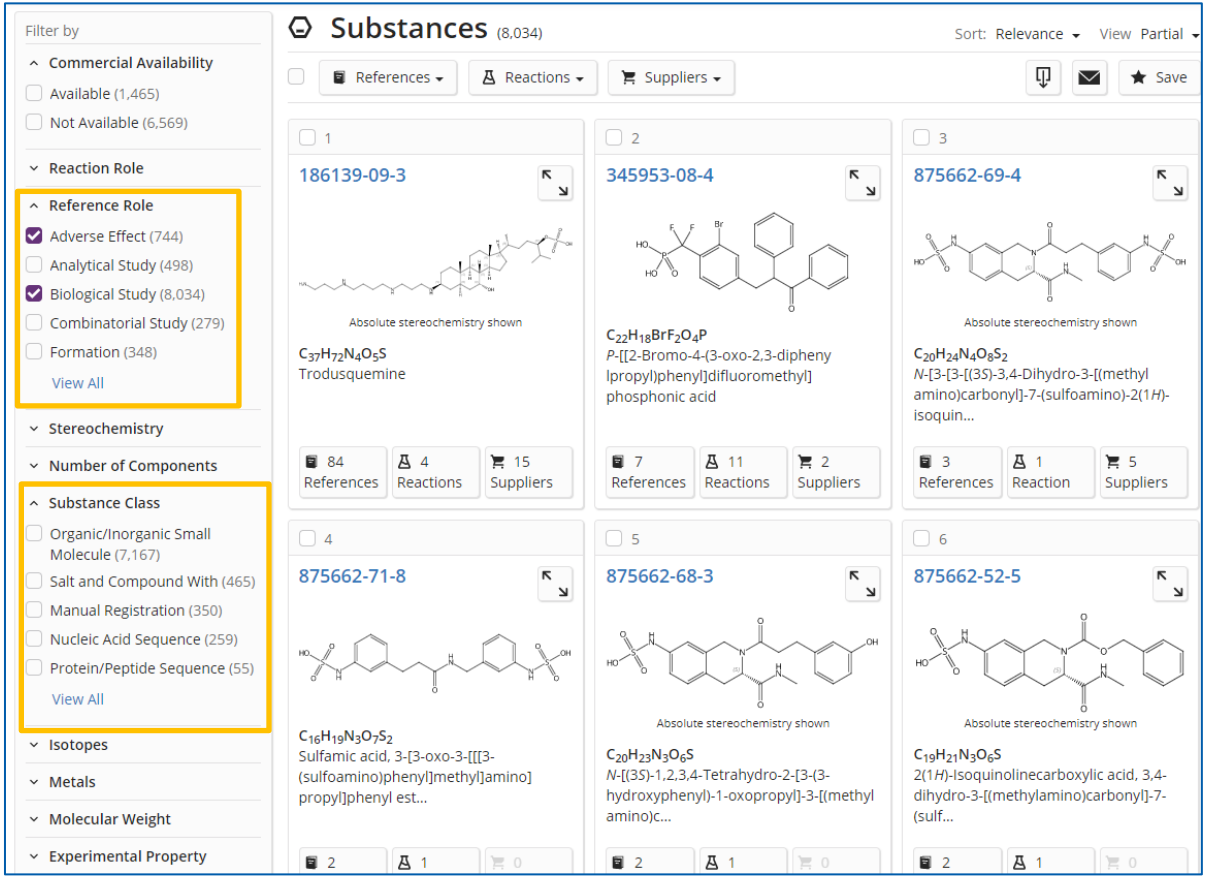
物质在文献中的研究角色

物质类型



通过文献获取关联的物质结果

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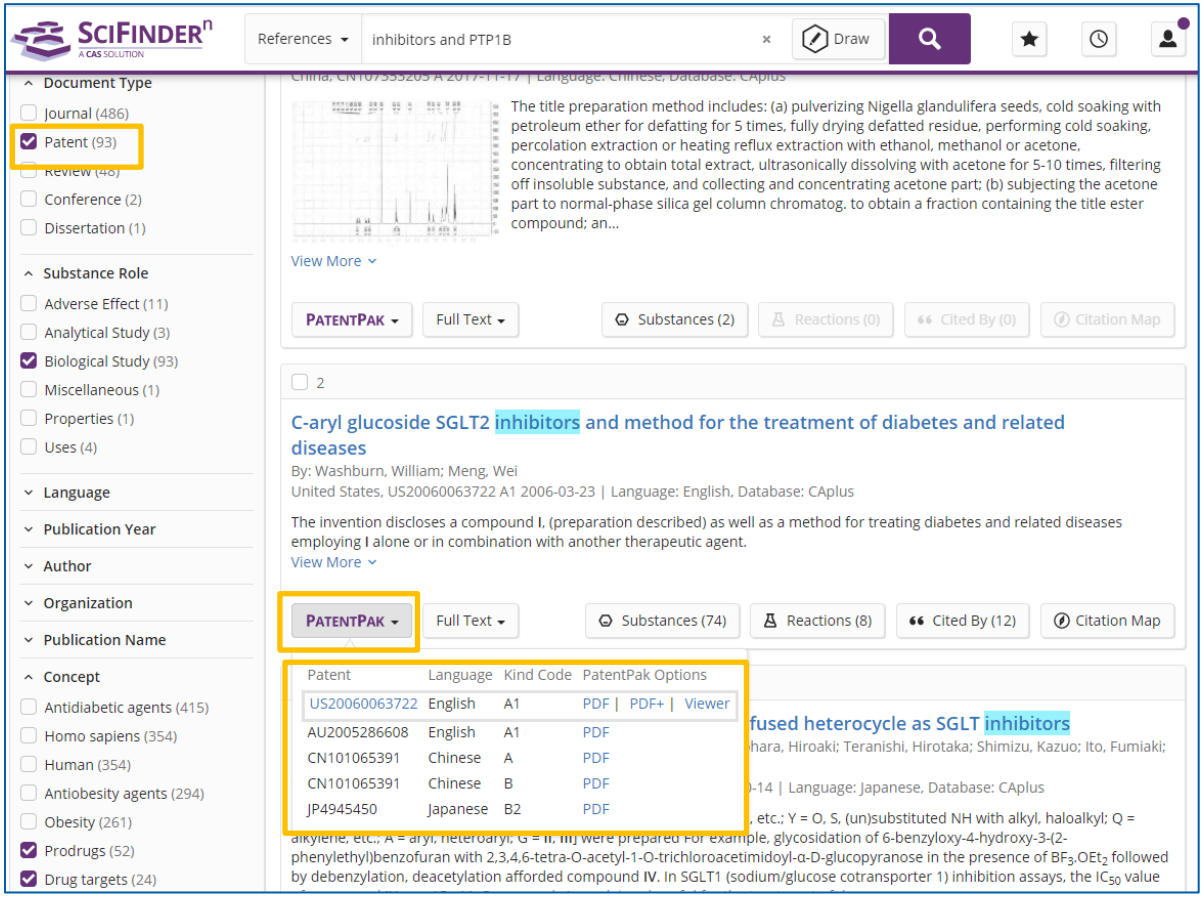

对于专利文献，可直接通过PatentPak高效获取全文及人工标引的物质信息

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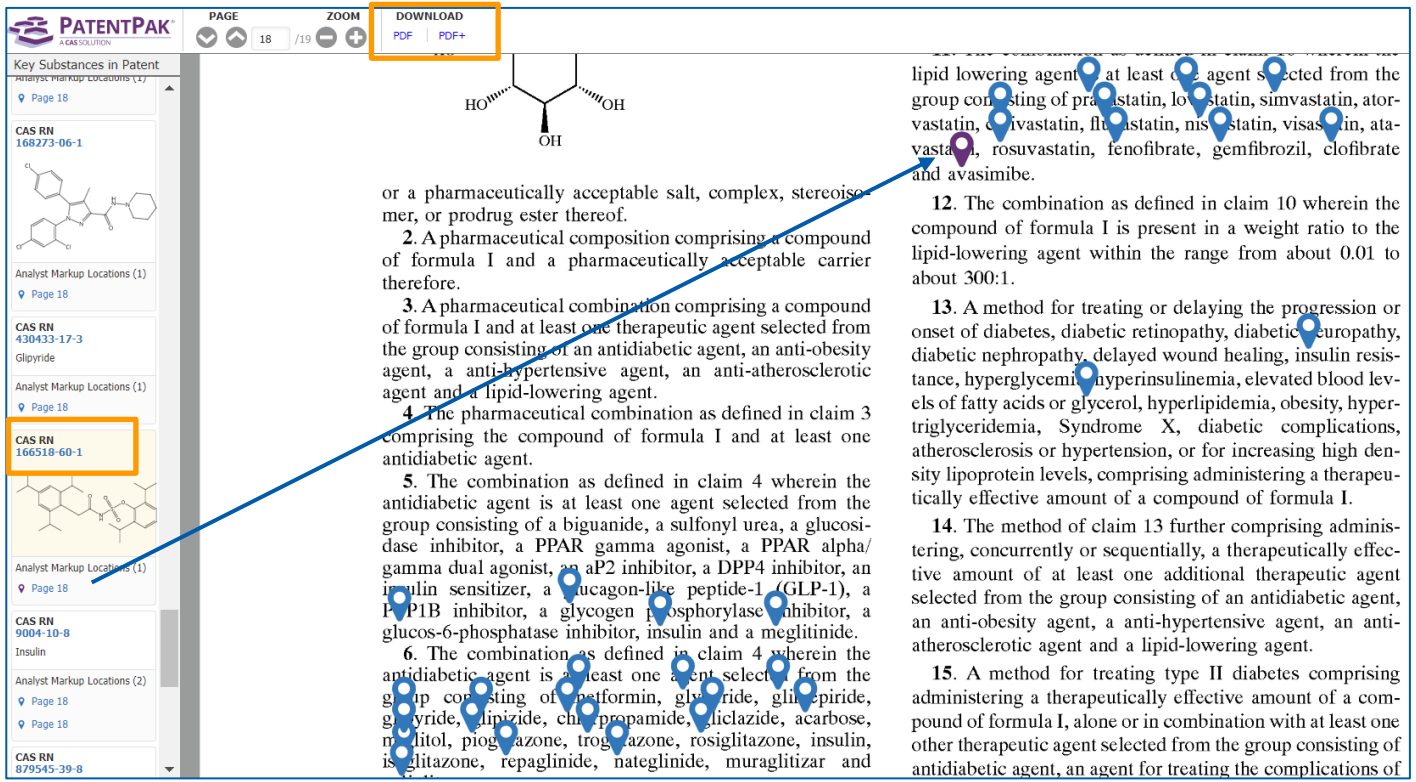
通过PatentPak，高效获取专利中重要的化学信息



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大纲

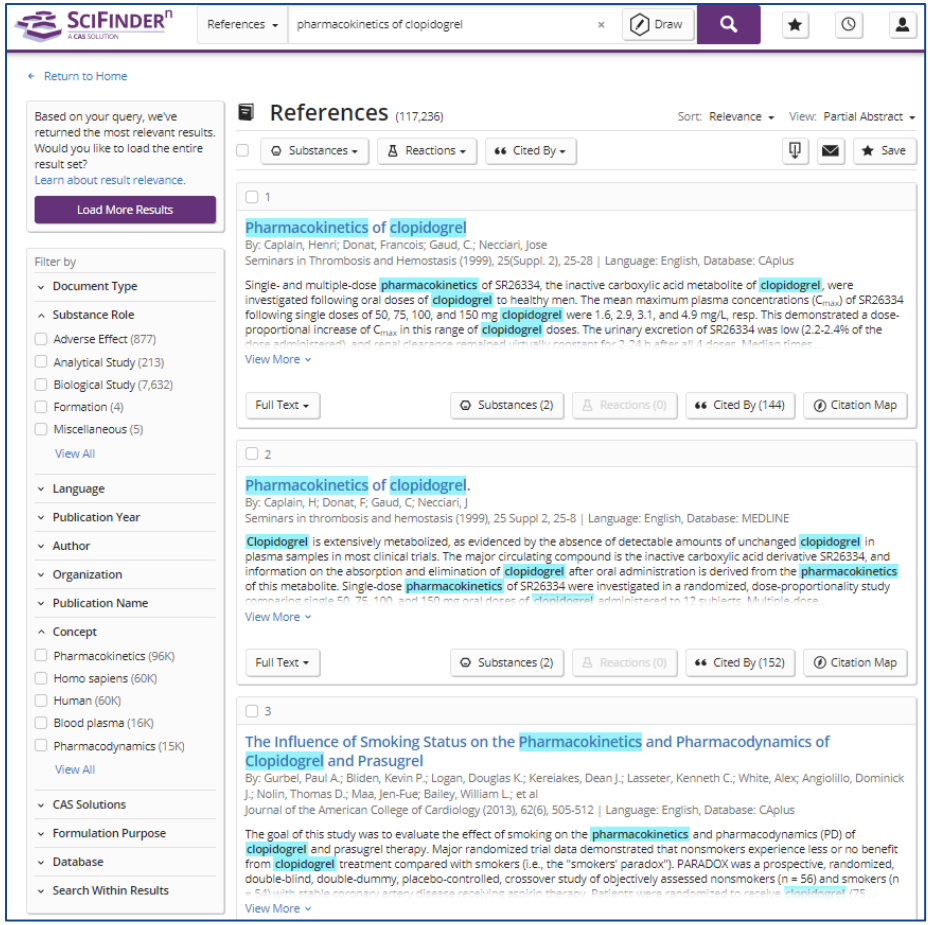
- 疾病模型研究信息
- 药物与受体的相互作用研究
- **药代动力学研究**
- 副作用研究

关于药代动力学研究信息检索

检索方法：

方法一、通过主题词进行文献检索

方法二、先进行物质检索，再获取相关文献研究信息



方法一：通过主题词进行文献检索

Pharmacokinetics and clopidogrel

Pharmacokinetics not clopidogrel

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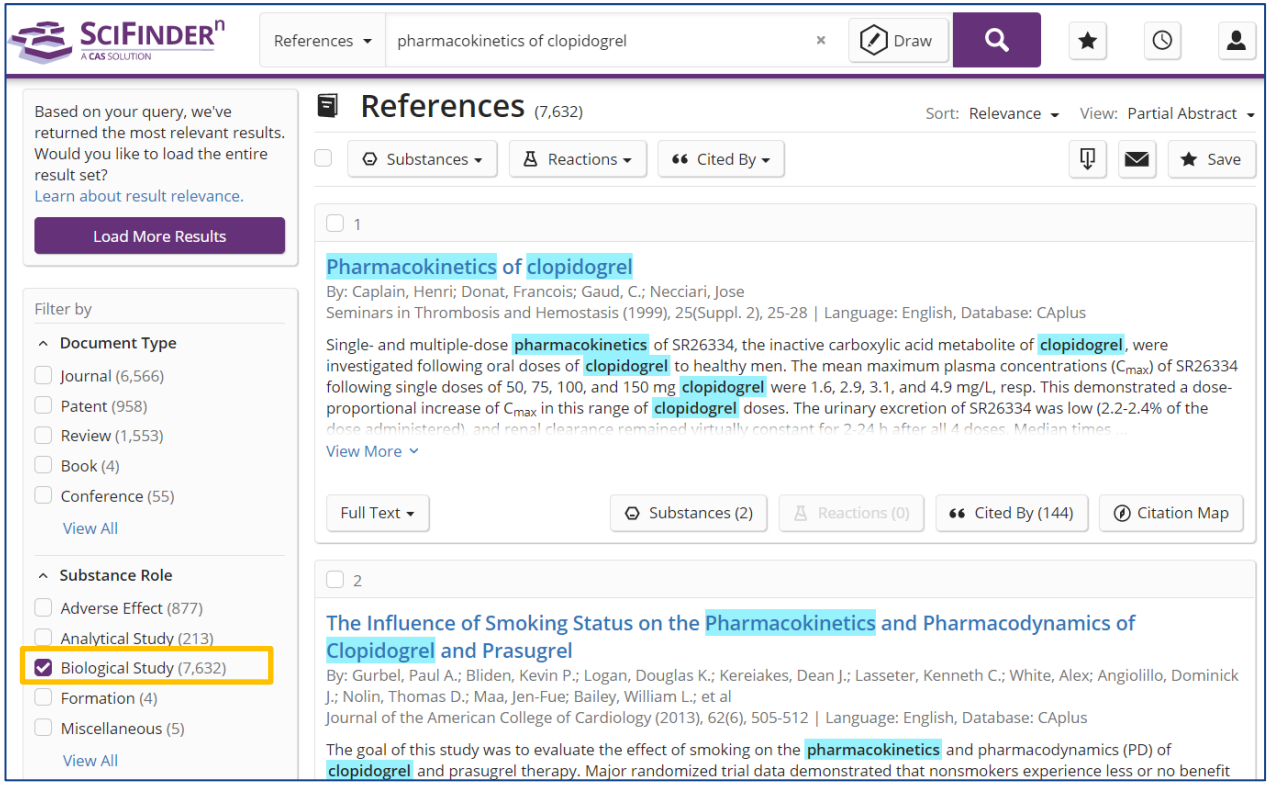
通过Substance Role可筛选相关研究方向的文献，如Biological Study



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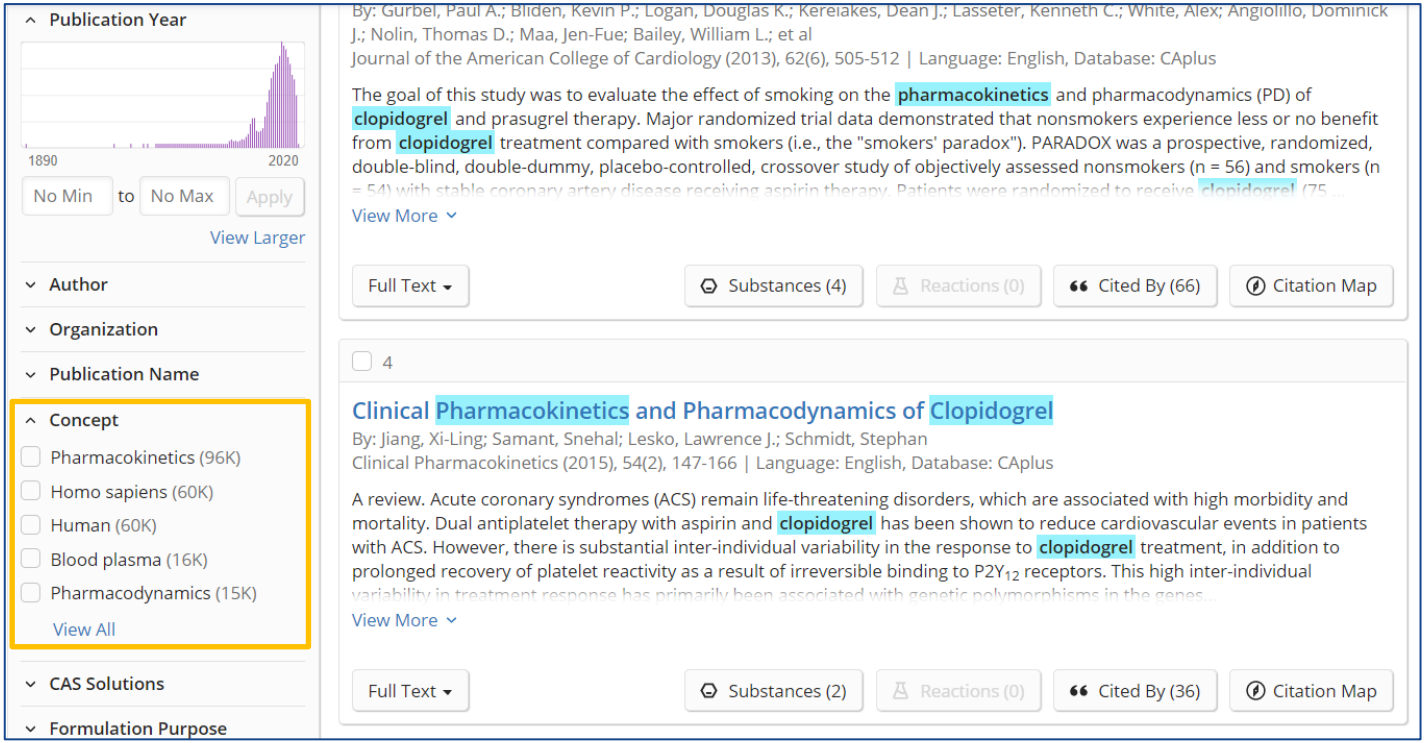
通过Concept标准概念词库，筛选感兴趣的研究点



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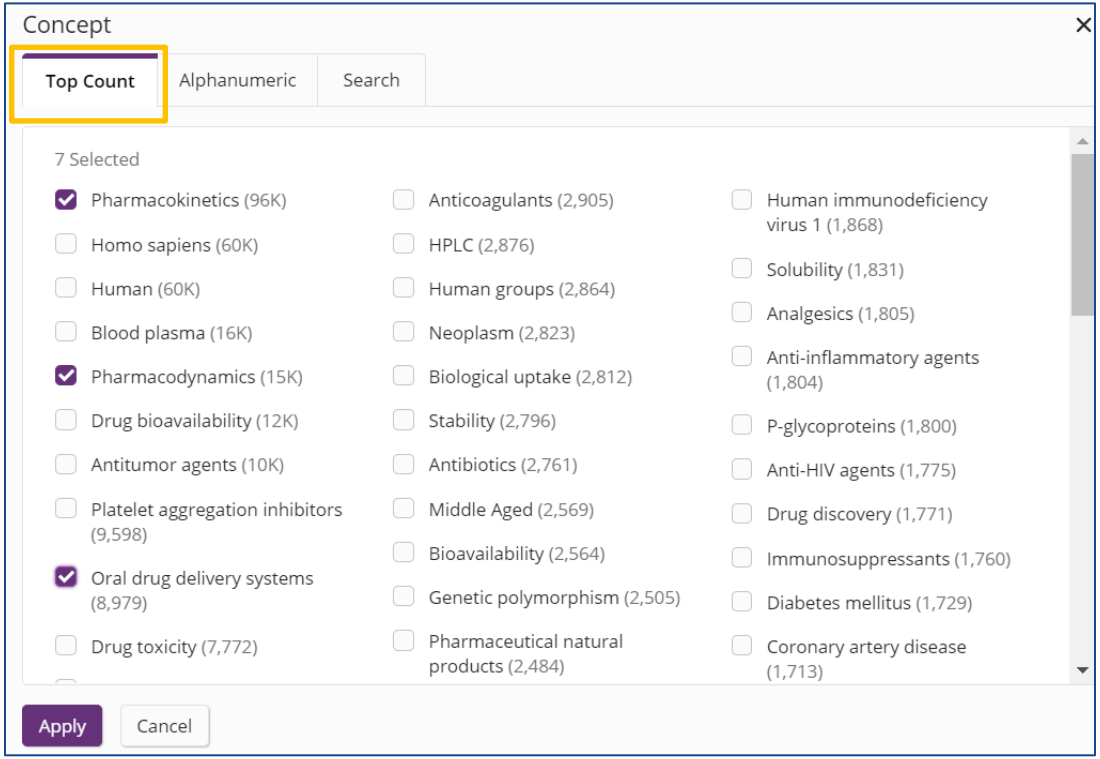
如，药代动力学、药物传递系统，药物相互作用等



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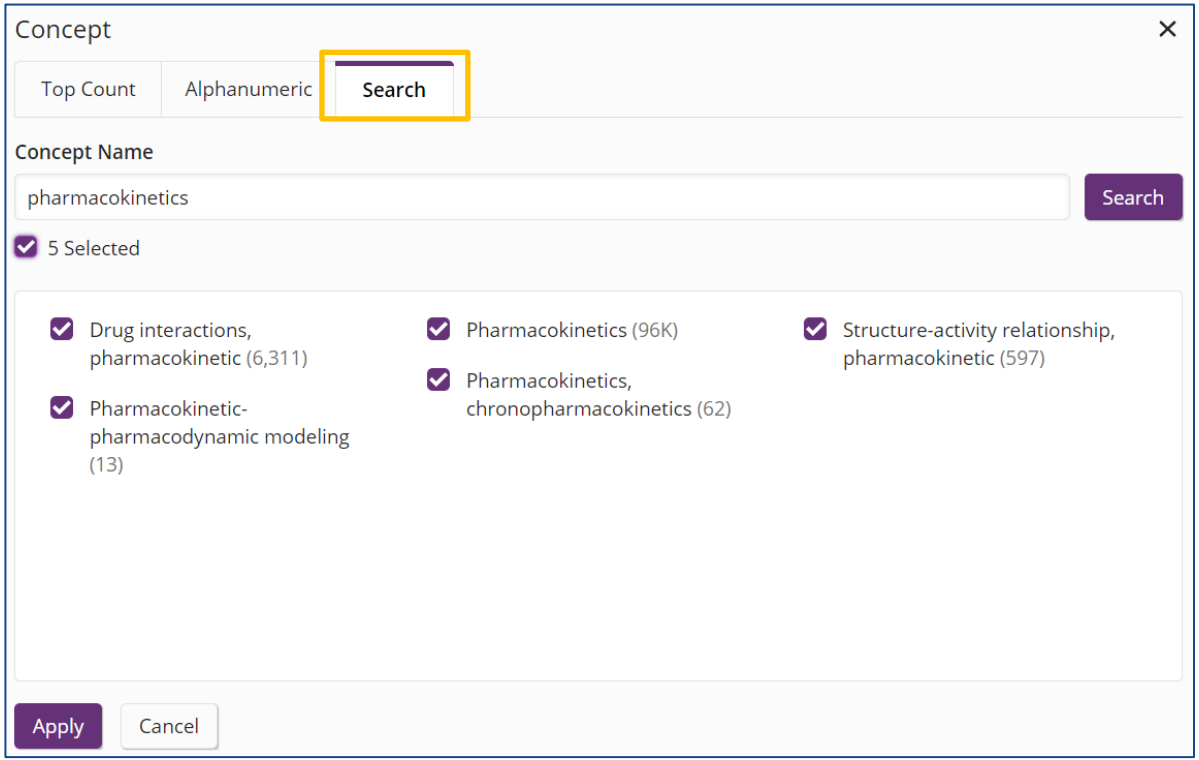
可通过Find在Concept中筛选概念词， 如药代动力学



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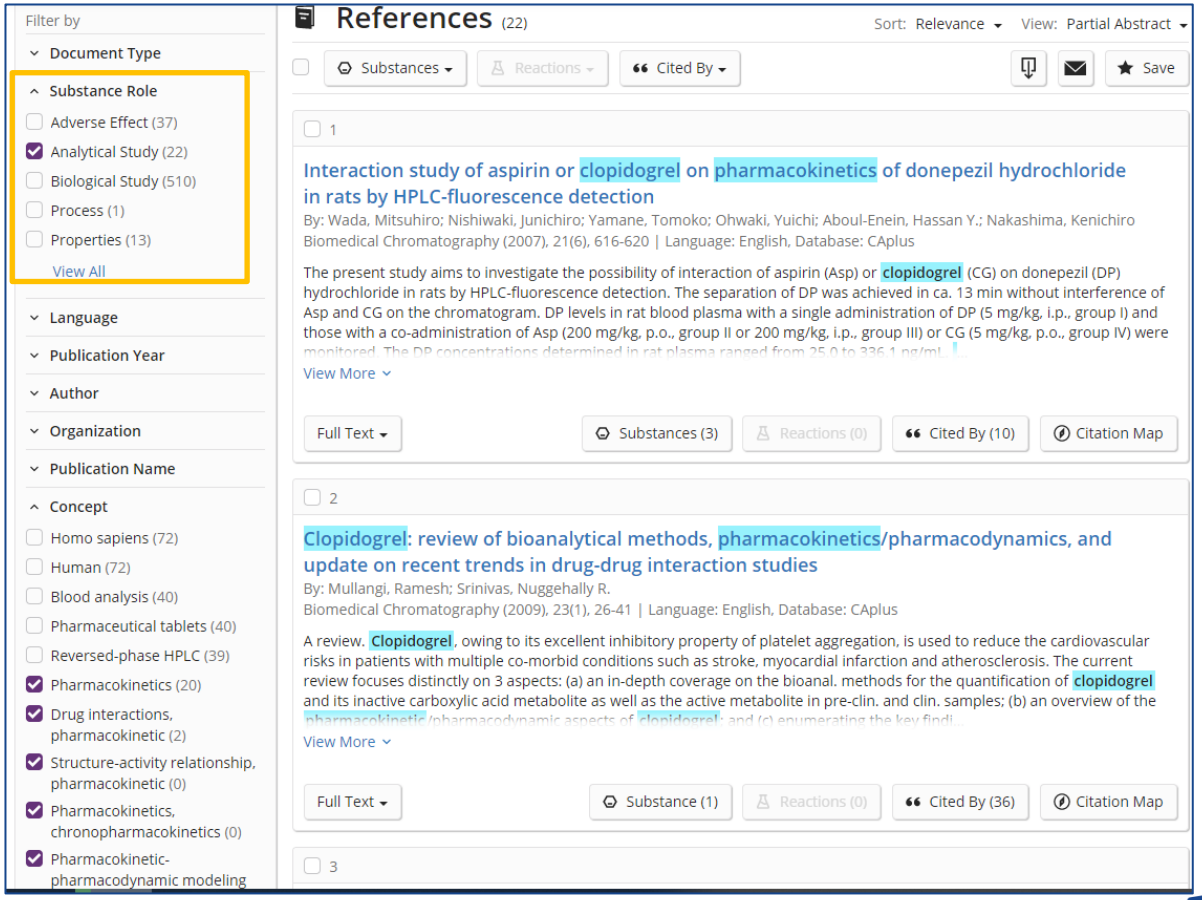

通过Substance Role，可继续选择Analytical Study获取分析相关信息

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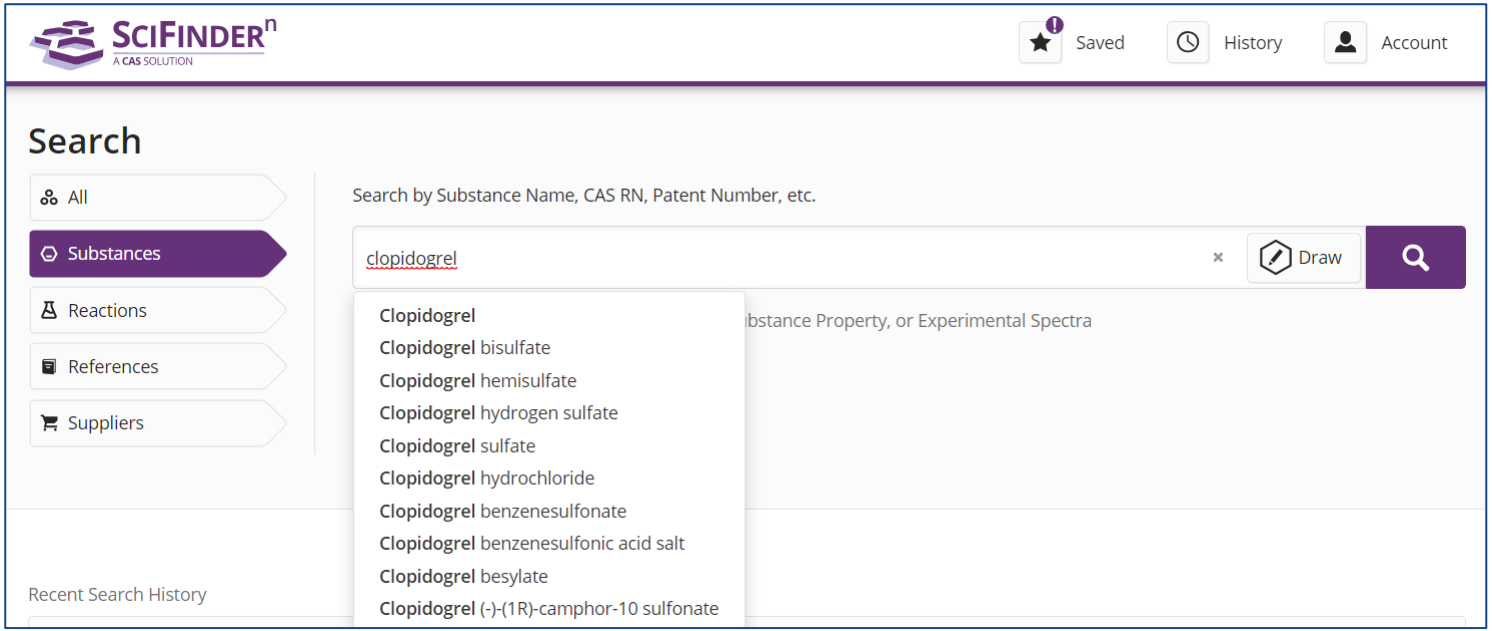
方法二：先获取物质，再获取相关研究文献



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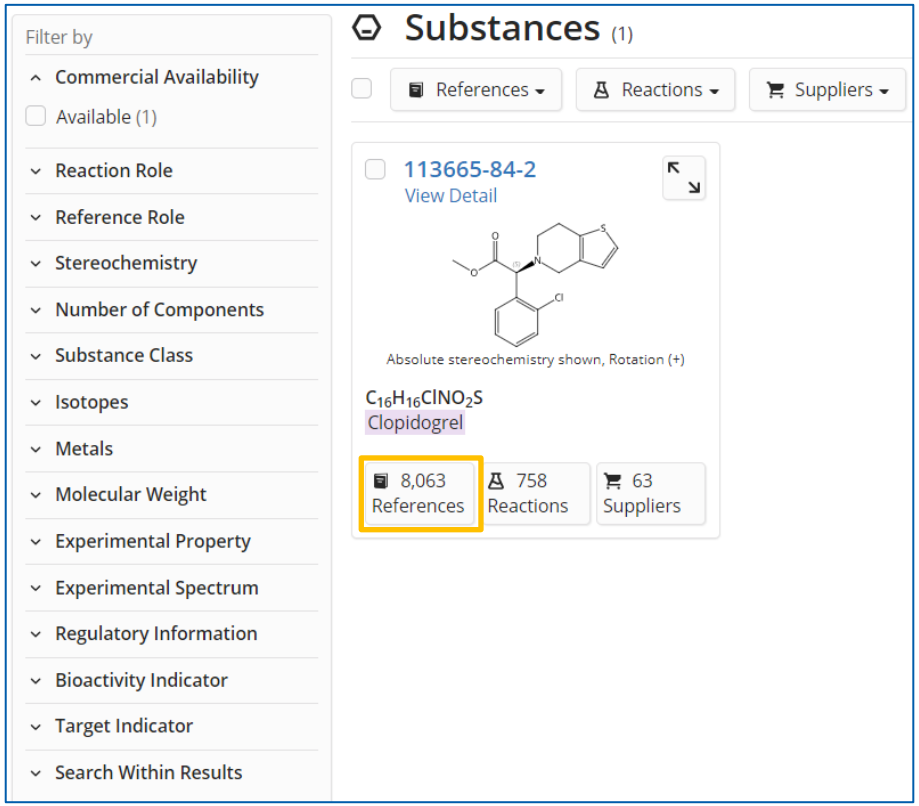
方法二：先获取物质，再获取相关研究文献



点击物质结构下方的文本图标，获取其对应的研究文献

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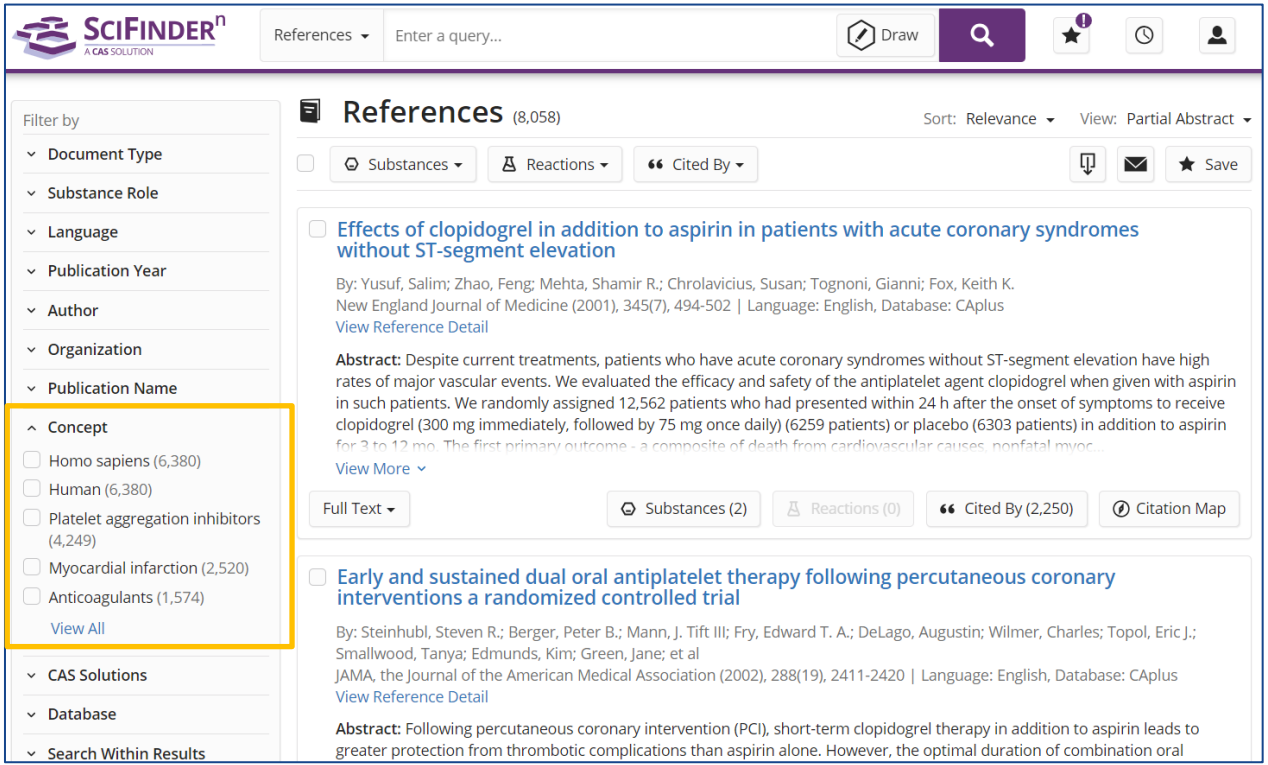
通过Concept词库，选择精炼的研究点



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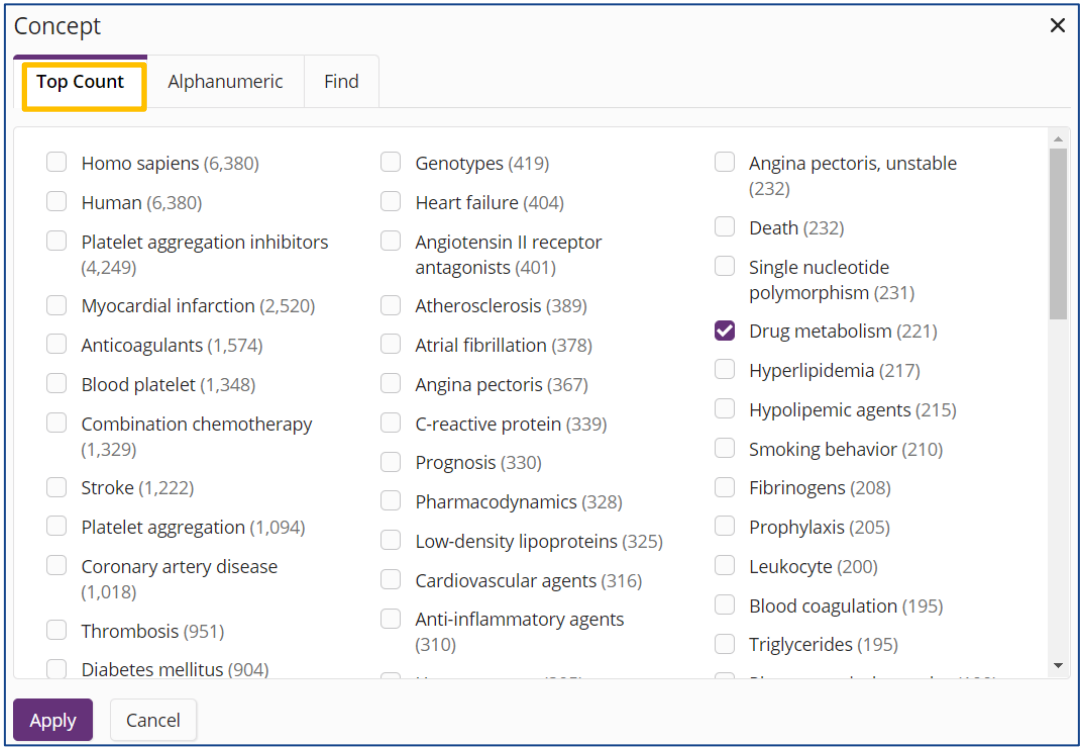
如，药物代谢



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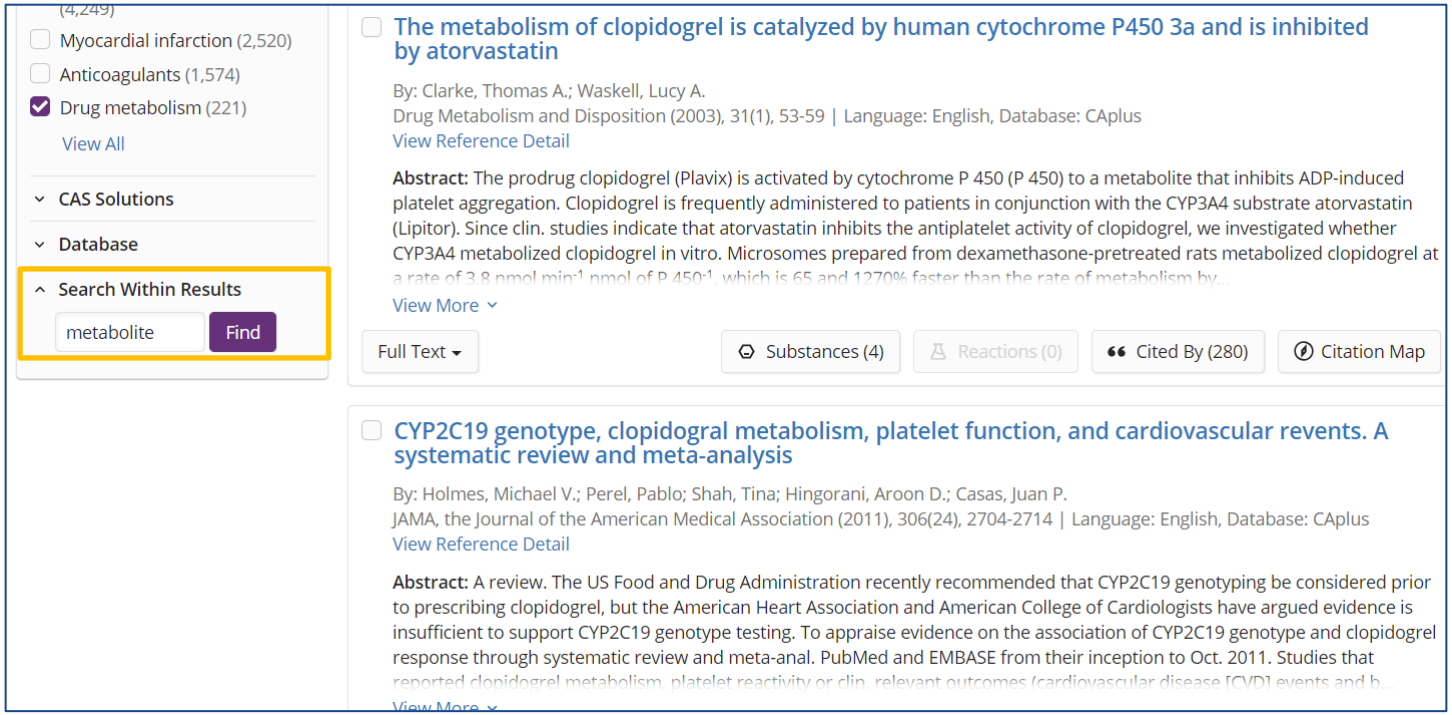
通过Search Within Results，可全面筛选文献中出现的词/短语，如代谢物



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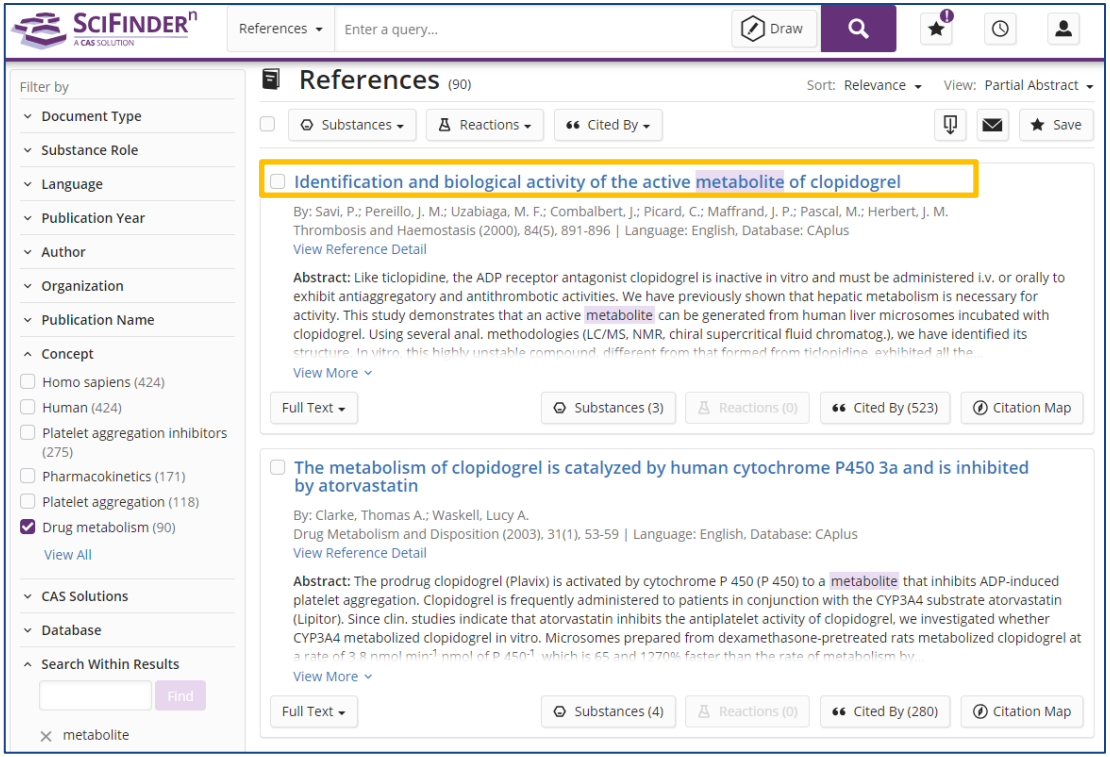
点击文献标题，获取文献详情



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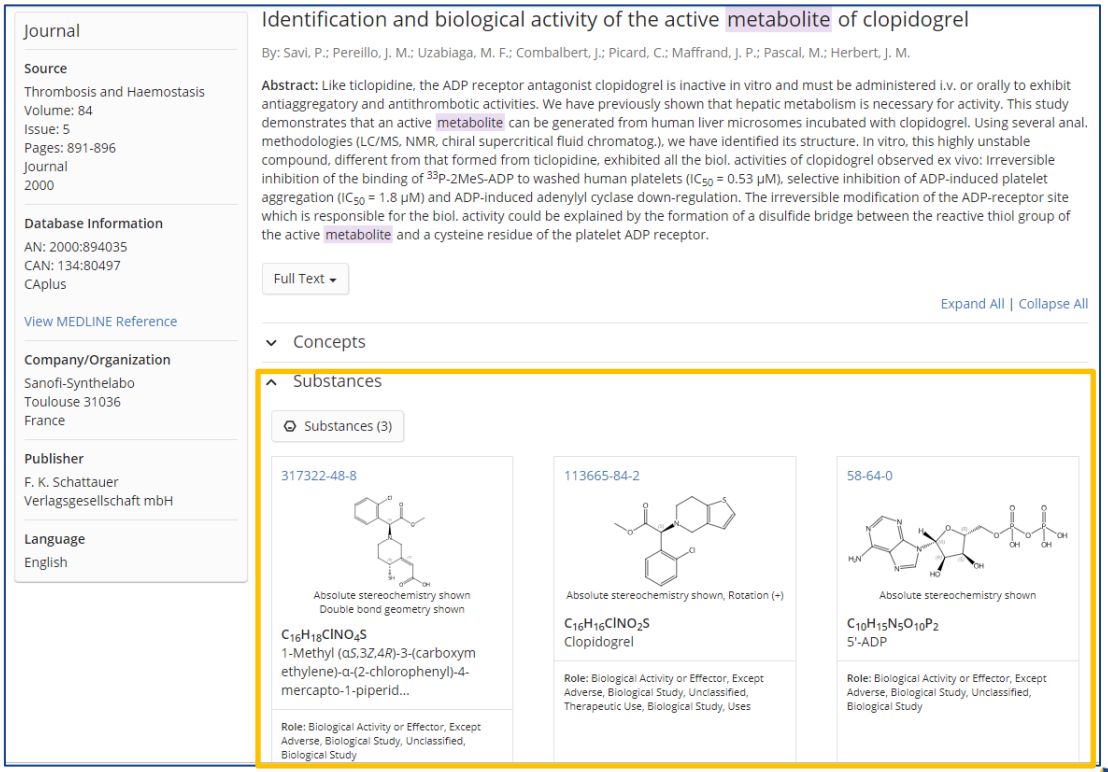
在物质列表中，通过Substances列表查看文献涉及的物质及角色描述



Journal

Source

Thrombosis and Haemostasis
Volume: 84
Issue: 5
Pages: 891-896
Journal
2000

Database Information

AN: 2000:894035
CAN: 134:80497
CAplus

View MEDLINE Reference

Company/Organization

Sanofi-Synthelabo
Toulouse 31036
France

Publisher

F. K. Schattauer
Verlagsgesellschaft mbH

Language

English

Identification and biological activity of the active metabolite of clopidogrel

By: Savi, P.; Pereillo, J. M.; Uzabiaga, M. F.; Combalbert, J.; Picard, C.; Maffrand, J. P.; Pascal, M.; Herbert, J. M.

Abstract: Like ticlopidine, the ADP receptor antagonist clopidogrel is inactive in vitro and must be administered i.v. or orally to exhibit antiaggregatory and antithrombotic activities. We have previously shown that hepatic metabolism is necessary for activity. This study demonstrates that an active metabolite can be generated from human liver microsomes incubated with clopidogrel. Using several anal. methodologies (LC/MS, NMR, chiral supercritical fluid chromatog.), we have identified its structure. In vitro, this highly unstable compound, different from that formed from ticlopidine, exhibited all the biol. activities of clopidogrel observed ex vivo: Irreversible inhibition of the binding of ^{33}P-2MeS-ADP to washed human platelets (IC_{50} = 0.53 μM), selective inhibition of ADP-induced platelet aggregation (IC_{50} = 1.8 μM) and ADP-induced adenylyl cyclase down-regulation. The irreversible modification of the ADP-receptor site which is responsible for the biol. activity could be explained by the formation of a disulfide bridge between the reactive thiol group of the active metabolite and a cysteine residue of the platelet ADP receptor.

Full Text

Expand All | Collapse All

Concepts

Substances

Substances (3)

317322-48-8

Absolute stereochemistry shown
Double bond geometry shown

$C_{16}H_{18}ClNO_4S$
1-Methyl (αS,3Z,4R)-3-(carboxymethylene)-α-(2-chlorophenyl)-4-mercapto-1-piperid...

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Biological Study

113665-84-2

Absolute stereochemistry shown, Rotation (+)

$C_{16}H_{16}ClNO_2S$
Clopidogrel

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Therapeutic Use, Biological Study, Uses

58-64-0

Absolute stereochemistry shown

$C_{10}H_{15}N_5O_{10}P_2$
5'-ADP

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Biological Study

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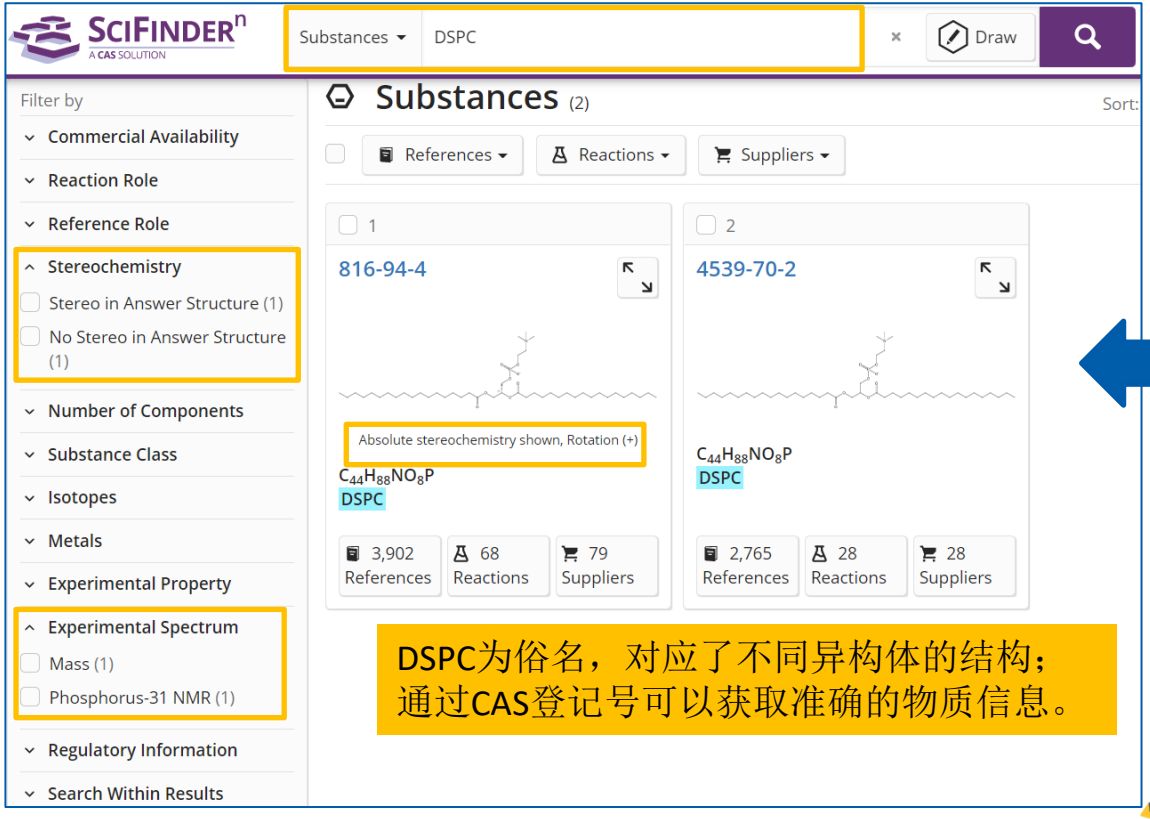
例2：如何获取代谢小分子磷脂(DSPC)的谱图研究信息？



点击CAS登记号，
查看物质详情

DSPC为俗名，对应了不同异构体的结构；
通过CAS登记号可以获取准确的物质信息。

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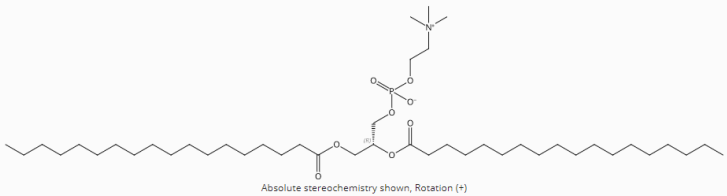
通过物质详情，获取物质属性、谱图和管控等信息

Substance Detail (1 of 2)

Prev Next

References (3,902) | Reactions (68) | Suppliers (79) | Save

CAS Registry Number
816-94-4



$C_{44}H_{88}NO_8P$

3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-*N*,*N*,*N*-trimethyl-10-oxo-7-[(1-oxooctadecyl)oxy]-, inner salt, 4-oxide, (7*R*)-

Key Physical Properties	Value	Condition
Melting Point (Experimental)	230.5-231.5 °C	-

Experimental Properties | Spectra

Expand All

Other Names

Experimental Properties

Chemical | Interface | Optical and Scattering | Thermal

Property	Value	Condition	Source
Melting Point	230.5-231.5 °C	-	(1) CAS
Melting Point	55 °C	-	(2) CAS
Enthalpy - 1 Source	See Full Text		(3) CAS
Entropy - 1 Source	See Full Text		(4) CAS
Liquid Crystal Transition Temperature - 1 Source	See Full Text		(5) CAS

Sources

(1) Shvets, V. I.; Zhurnal Obshchei Khimii, (1964), 34(6), 1908-11, CAplus

(2) Greenough, Kelly P.; Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy, (2009), 71A(5), 2050-2056, CAplus

(3) Matsuki, Hitoshi; Chemistry Letters, (2005), 34(2), 270-271, CAplus

(4) Matsuki, Hitoshi; Chemistry Letters, (2005), 34(2), 270-271, CAplus

(5) Kalmbach, Rolf; Journal of Molecular Biology, (2007), 371(3), 639-648, CAplus

Experimental Spectra

Hetero NMR | IR | Mass | Raman | X-Ray | Additional Spectra

	Source
NMR Spectrum - 1 Source	(1) CAS
Phosphorus-31 NMR Spectrum - 1 Source	(2) CAS

Sources

(1) Matsuoka, Shigeru; Biochemistry, (2005), 44(2), 704-710, CAplus

(2) Ledo, D. Correia; ECS Transactions, (2009), 19(33), 1-10, CAplus

Regulatory Information

Additional Details

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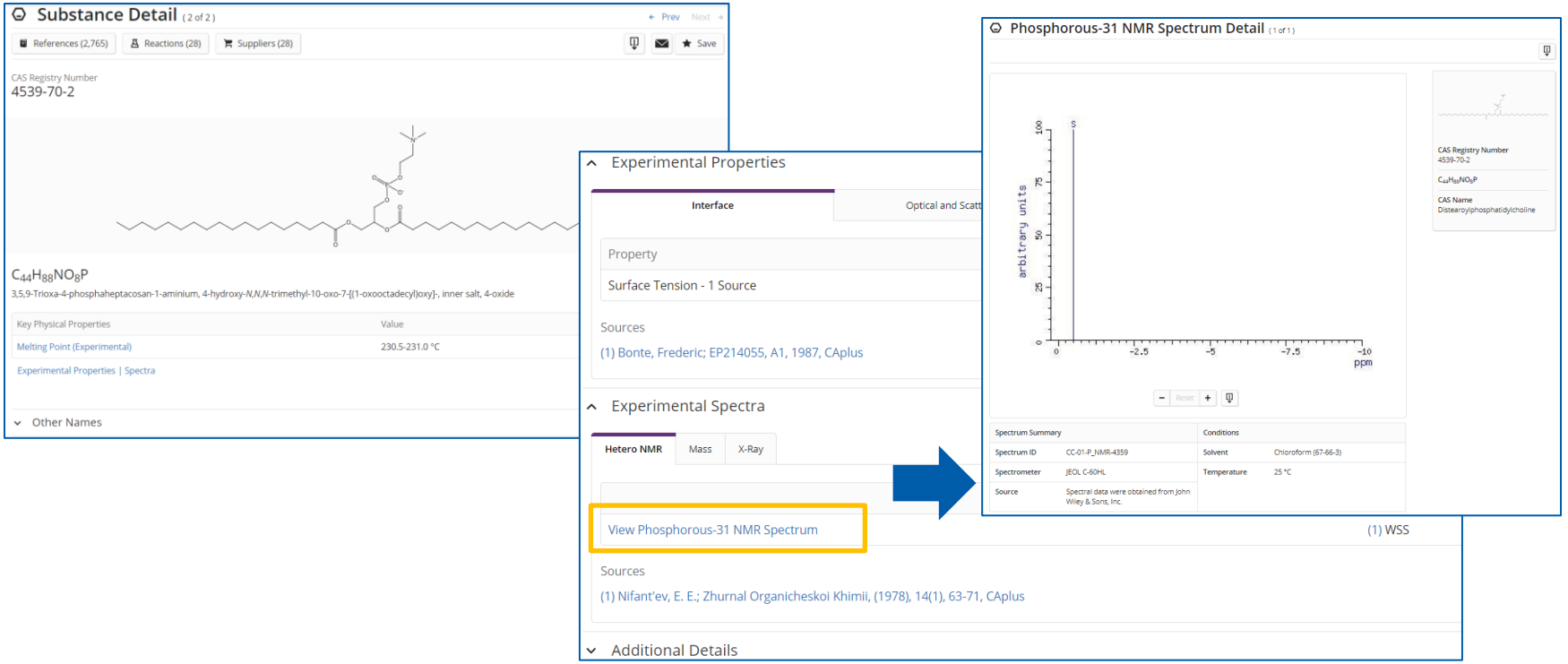
通过物质详情，获取物质属性、谱图和管控等信息



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大纲

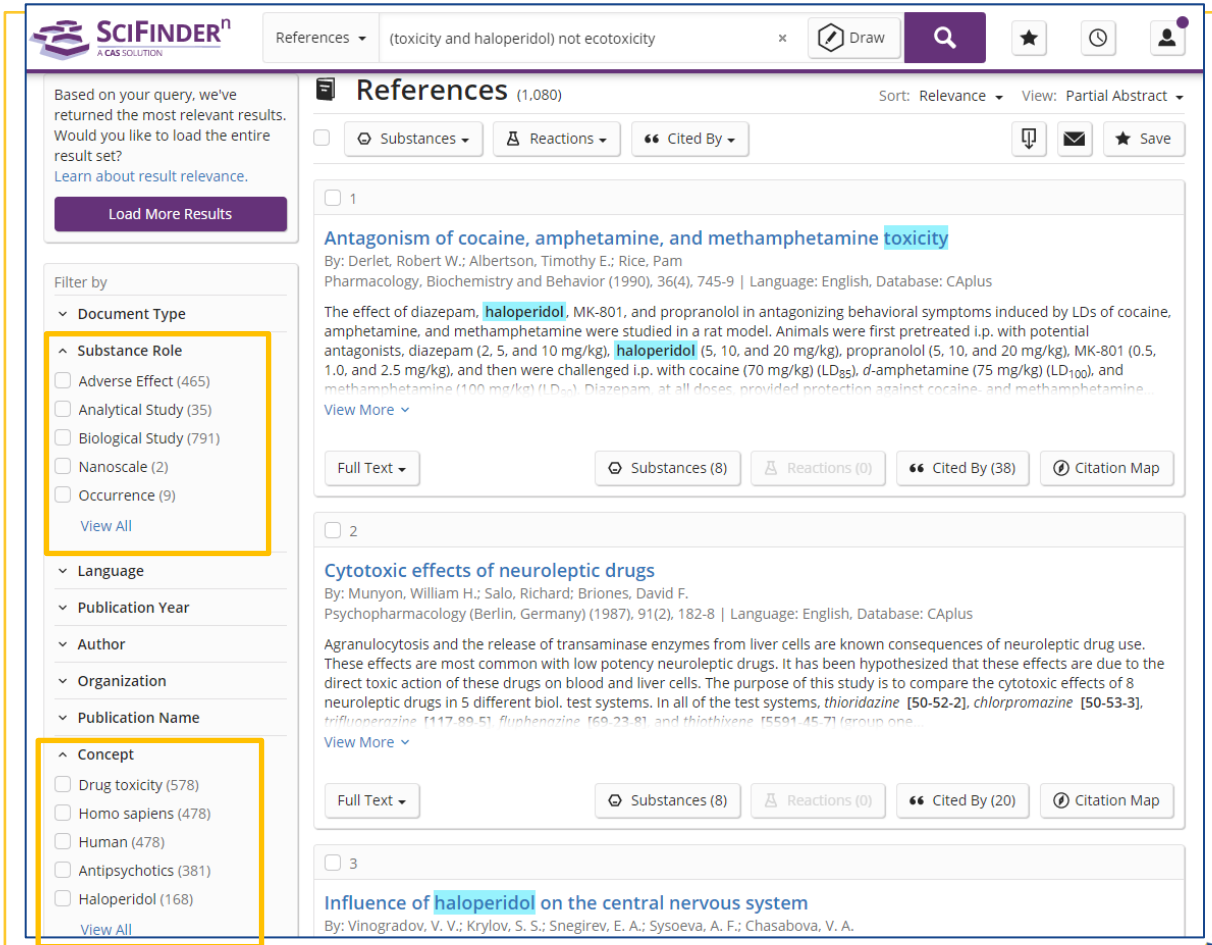
- 疾病模型研究信息
- 药物与受体的相互作用研究
- 药代动力学研究
- 副作用研究

例：药物毒副作用研究信息的获取

检索方法：

方法一、通过主题词进行检索

方法二、先进行物质检索，再获取其毒性研究方面的信息



方法一、通过主题词进行检索

主题词 (toxicity and haloperidol) not ecotoxicity

通过Substance role分析研究方向，concept分析具体的研究点

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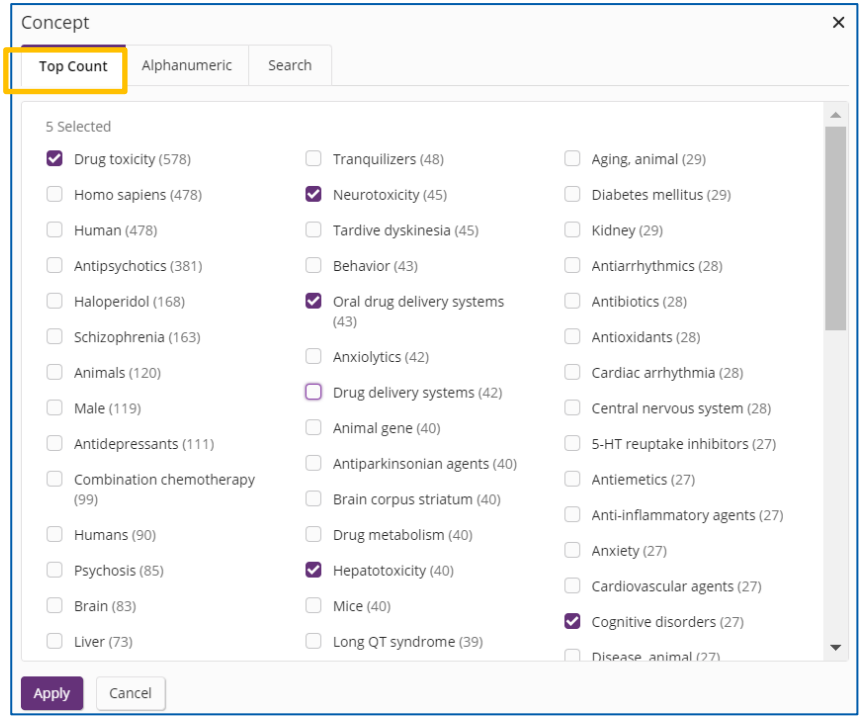
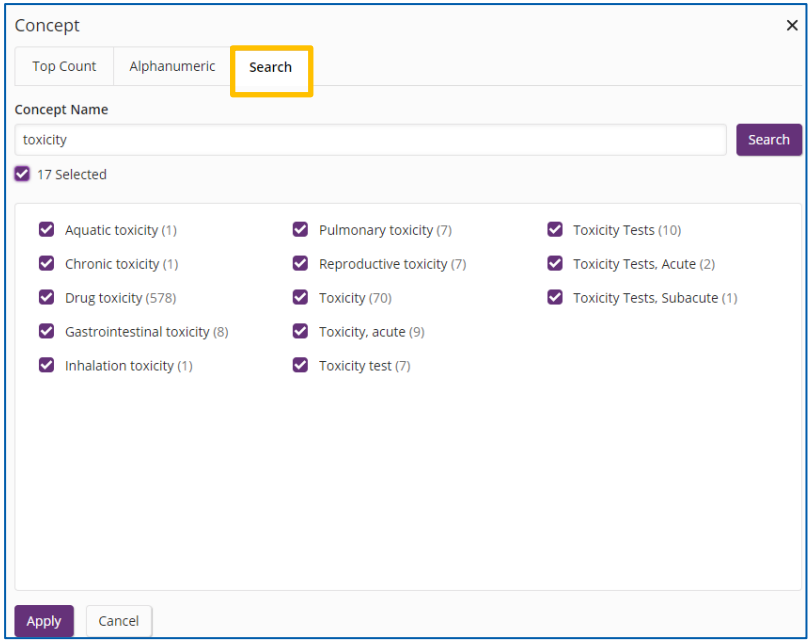
可以直接选择Top Count中涉及toxicity的概念词，或者通过Find在Concept词库中检索toxicity





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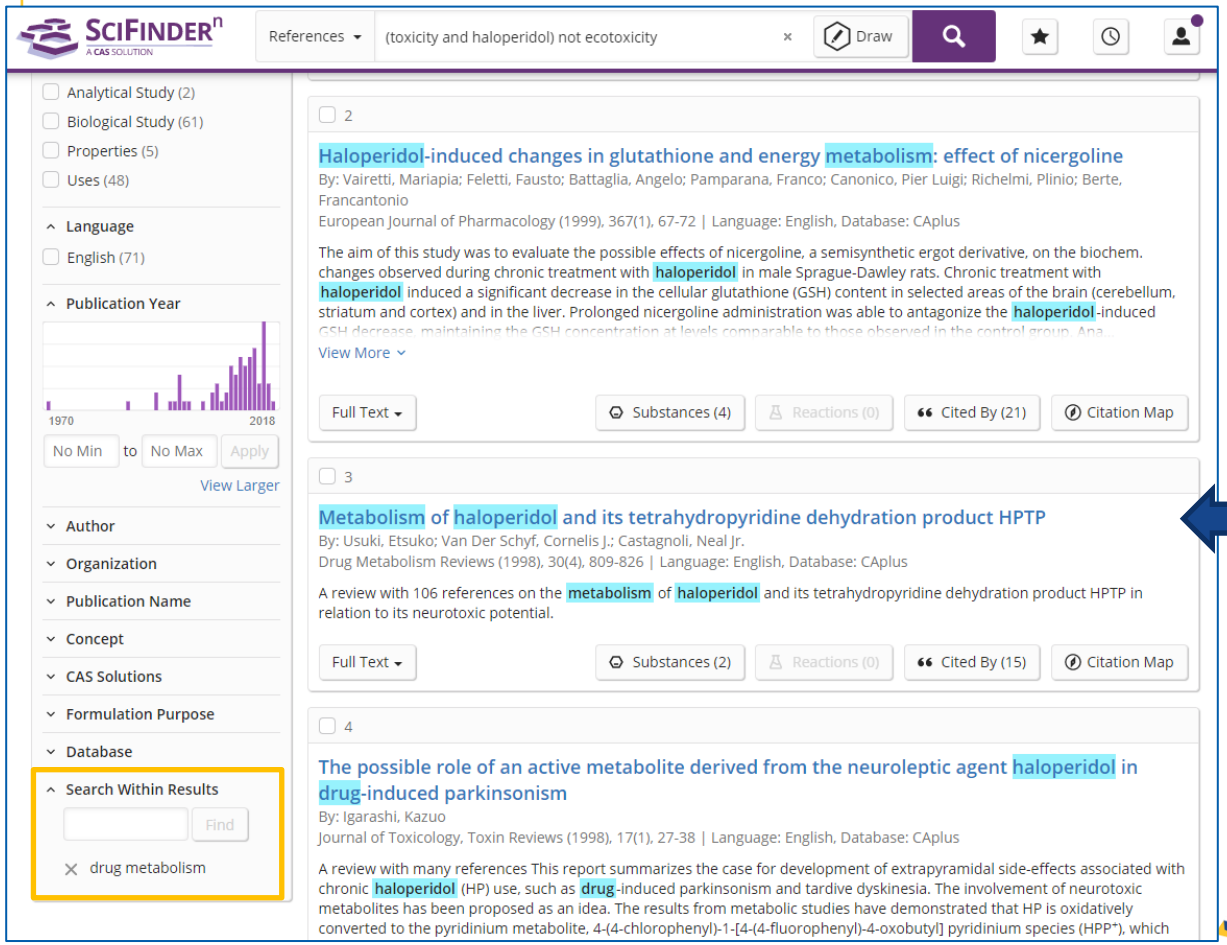

也可在Search Within Results中输入关键词，比如drug metabolism，进一步精炼所需信

点击标题，查看文献详情

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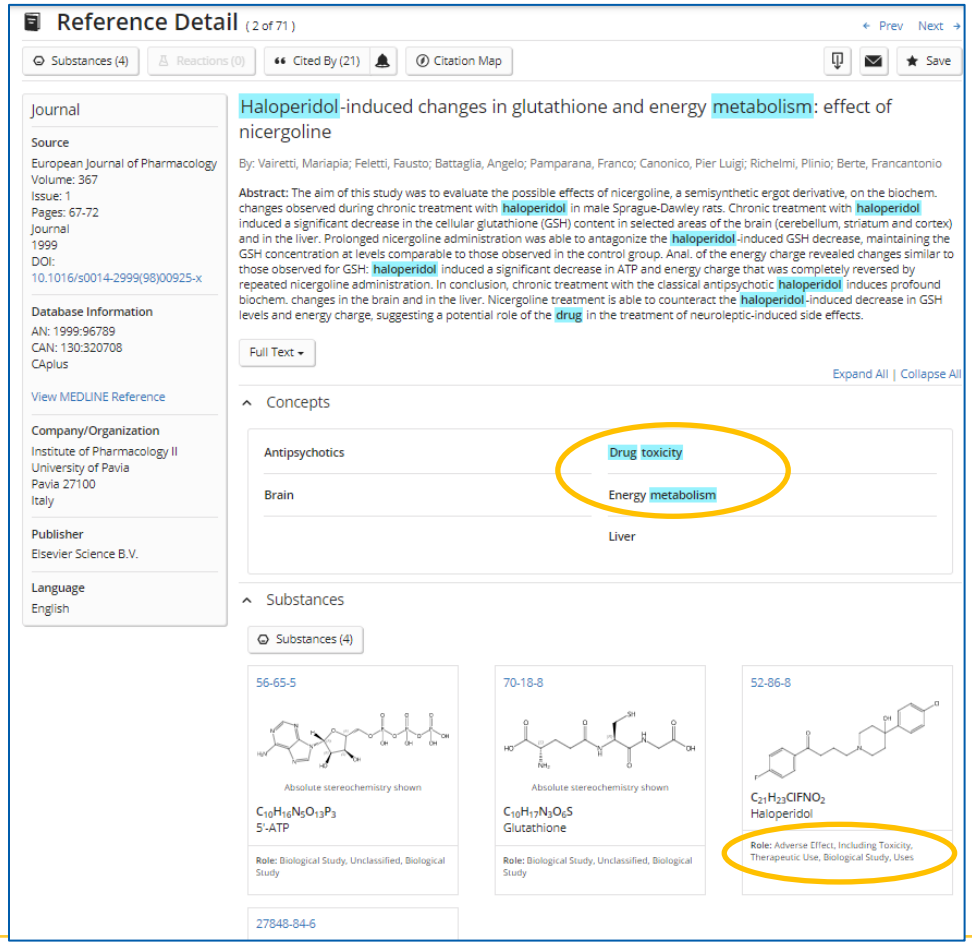

文献详情：可以查看摘要及CAS科学家人工标引信息，如Concepts（概念词库）及Substances（物质列表）等

Concepts、Substances及其Role（研究角色）有助于快速判断文献的研究主旨

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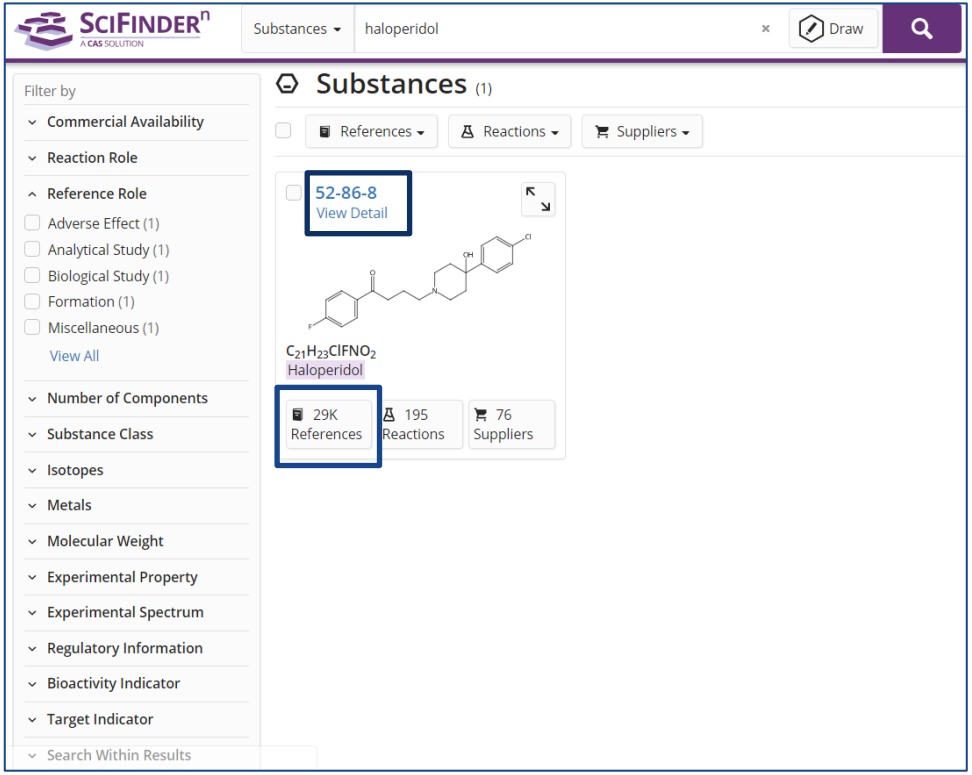
方法二、先进行物质检索，再获取其毒性研究方面的信息



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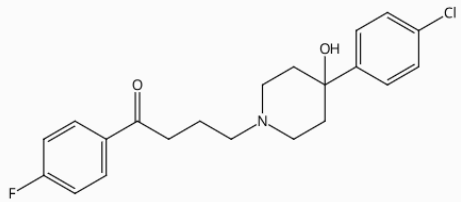
物质详情中的标引信息

Substance Detail (1 of 4)

← Prev Next →

References (29K) | Reactions (195) | Suppliers (81) | Save

CAS Registry Number
52-86-8



$C_{21}H_{23}ClFNO_2$

1-Butanone, 4-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-

Key Physical Properties	Value	Condition
Molecular Weight	375.86	-
Melting Point (Experimental)	151.5 °C	-
Boiling Point (Predicted)	529.0±50.0 °C	Press: 760 Torr
Density (Predicted)	1.239±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.86±0.20	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names

结构式、理化属性、名称等

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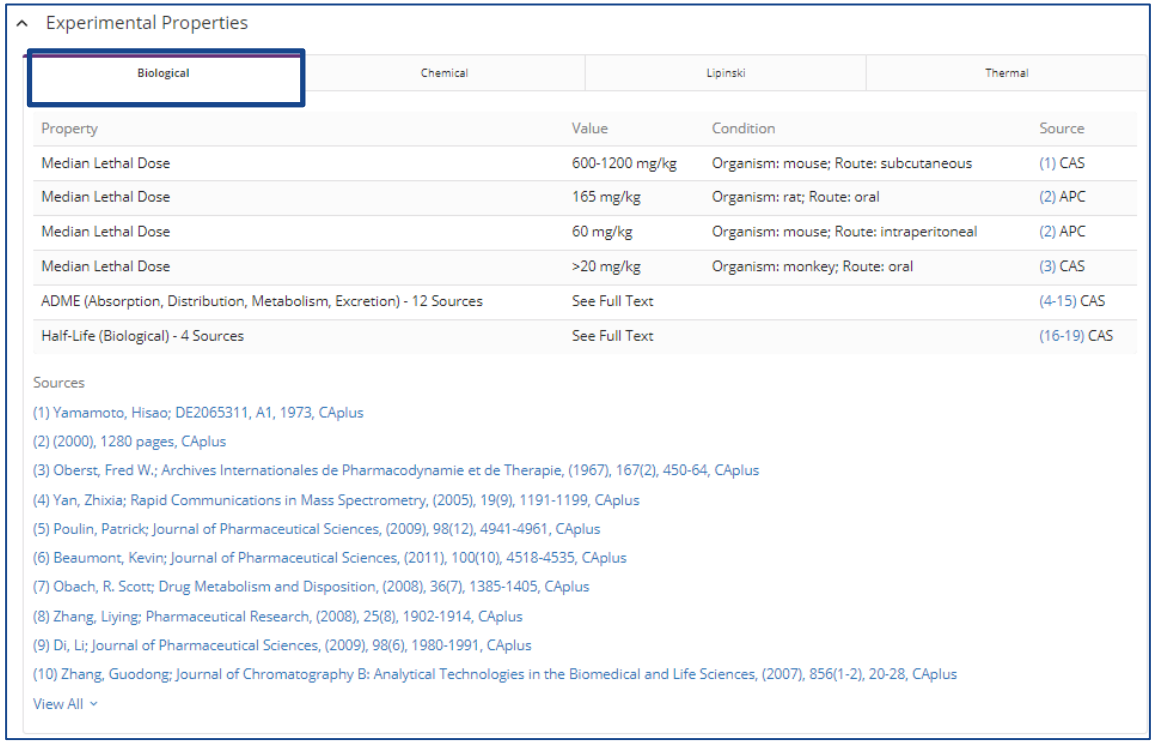
物质详情中的标引信息



Experimental Properties

Biological | Chemical | Lipinski | Thermal

Property	Value	Condition	Source
Median Lethal Dose	600-1200 mg/kg	Organism: mouse; Route: subcutaneous	(1) CAS
Median Lethal Dose	165 mg/kg	Organism: rat; Route: oral	(2) APC
Median Lethal Dose	60 mg/kg	Organism: mouse; Route: intraperitoneal	(2) APC
Median Lethal Dose	>20 mg/kg	Organism: monkey; Route: oral	(3) CAS
ADME (Absorption, Distribution, Metabolism, Excretion) - 12 Sources	See Full Text		(4-15) CAS
Half-Life (Biological) - 4 Sources	See Full Text		(16-19) CAS

Sources

(1) Yamamoto, Hisao; DE2065311, A1, 1973, CAplus

(2) (2000), 1280 pages, CAplus

(3) Oberst, Fred W.; Archives Internationales de Pharmacodynamie et de Therapie, (1967), 167(2), 450-64, CAplus

(4) Yan, Zhixia; Rapid Communications in Mass Spectrometry, (2005), 19(9), 1191-1199, CAplus

(5) Poulin, Patrick; Journal of Pharmaceutical Sciences, (2009), 98(12), 4941-4961, CAplus

(6) Beaumont, Kevin; Journal of Pharmaceutical Sciences, (2011), 100(10), 4518-4535, CAplus

(7) Obach, R. Scott; Drug Metabolism and Disposition, (2008), 36(7), 1385-1405, CAplus

(8) Zhang, Liying; Pharmaceutical Research, (2008), 25(8), 1902-1914, CAplus

(9) Di, Li; Journal of Pharmaceutical Sciences, (2009), 98(6), 1980-1991, CAplus

(10) Zhang, Guodong; Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, (2007), 856(1-2), 20-28, CAplus

View All

实验属性、实验谱图、预测属性、预测谱图、生物活性、靶点信息、管控信息等

- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- Additional Details

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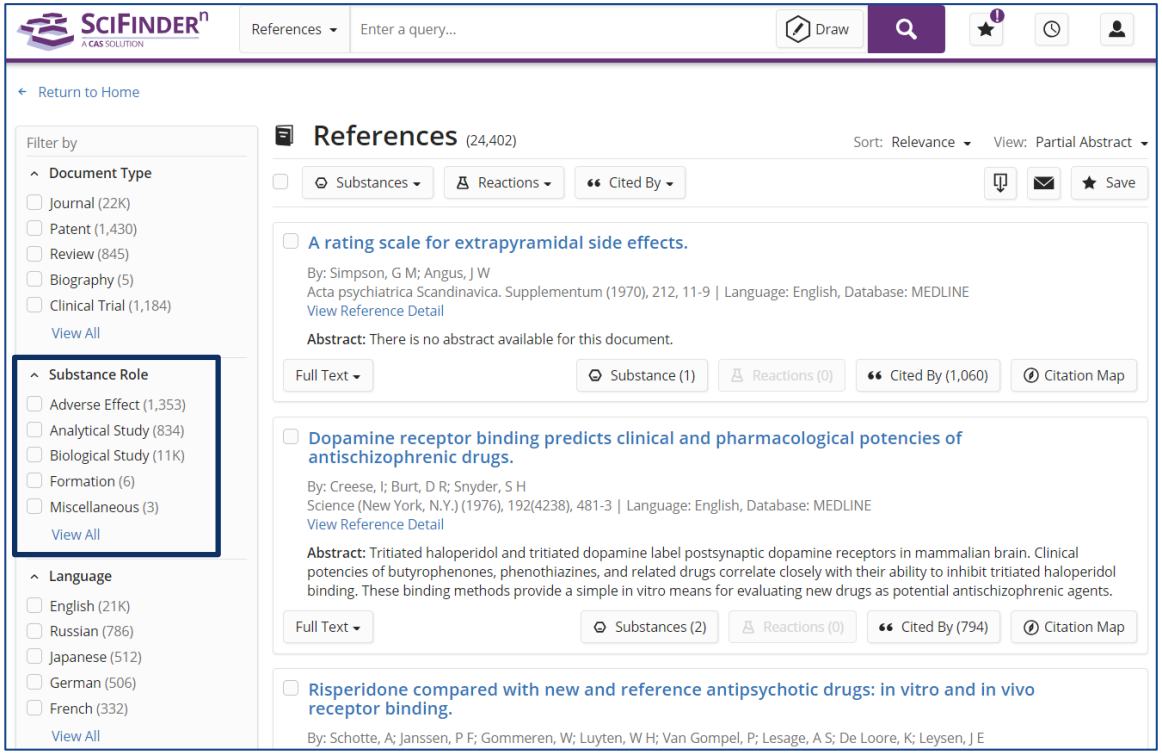
在文献结果的基础上，通过Substance Role，获取物质在文献中的研究角色



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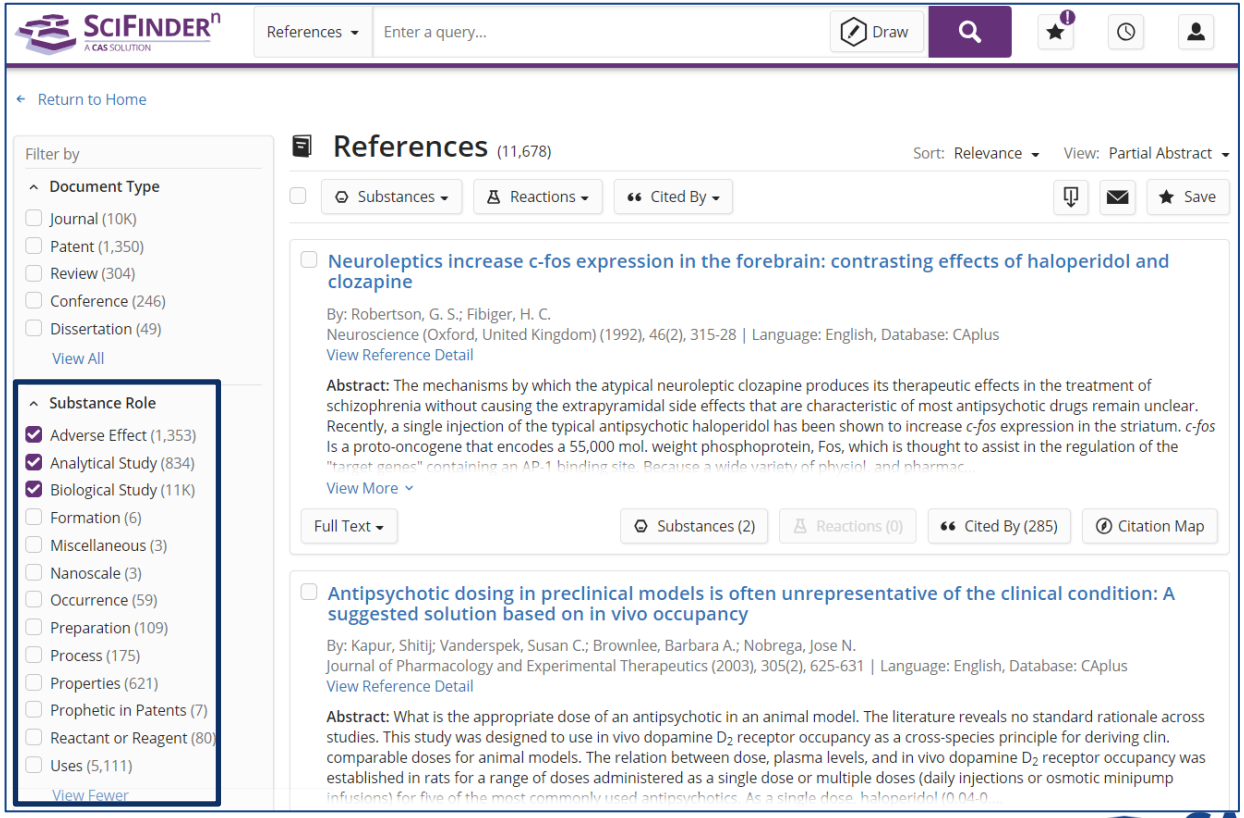
根据检索需要，选择Substance Role



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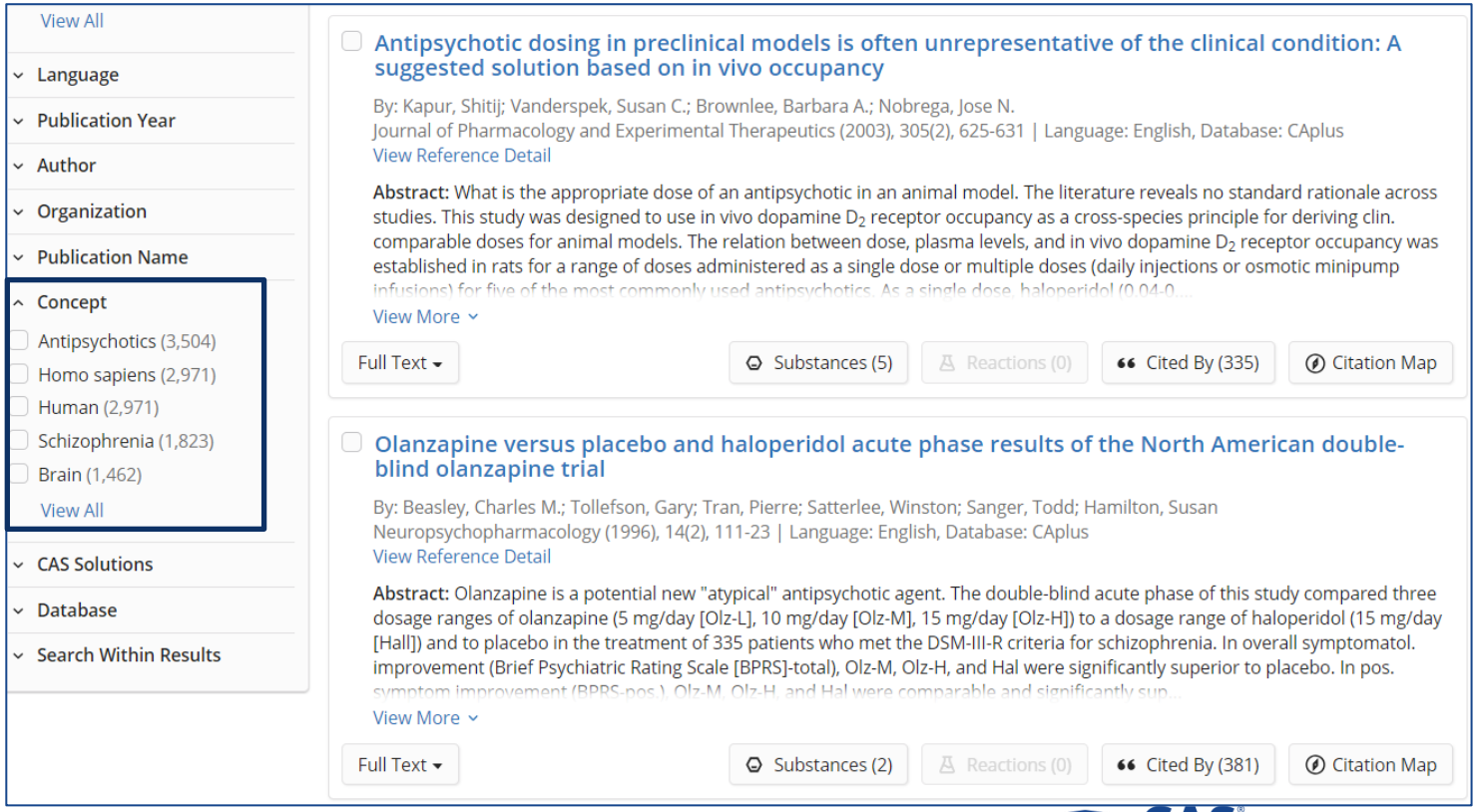
也可根据Concept，精炼具体的毒性研究方向



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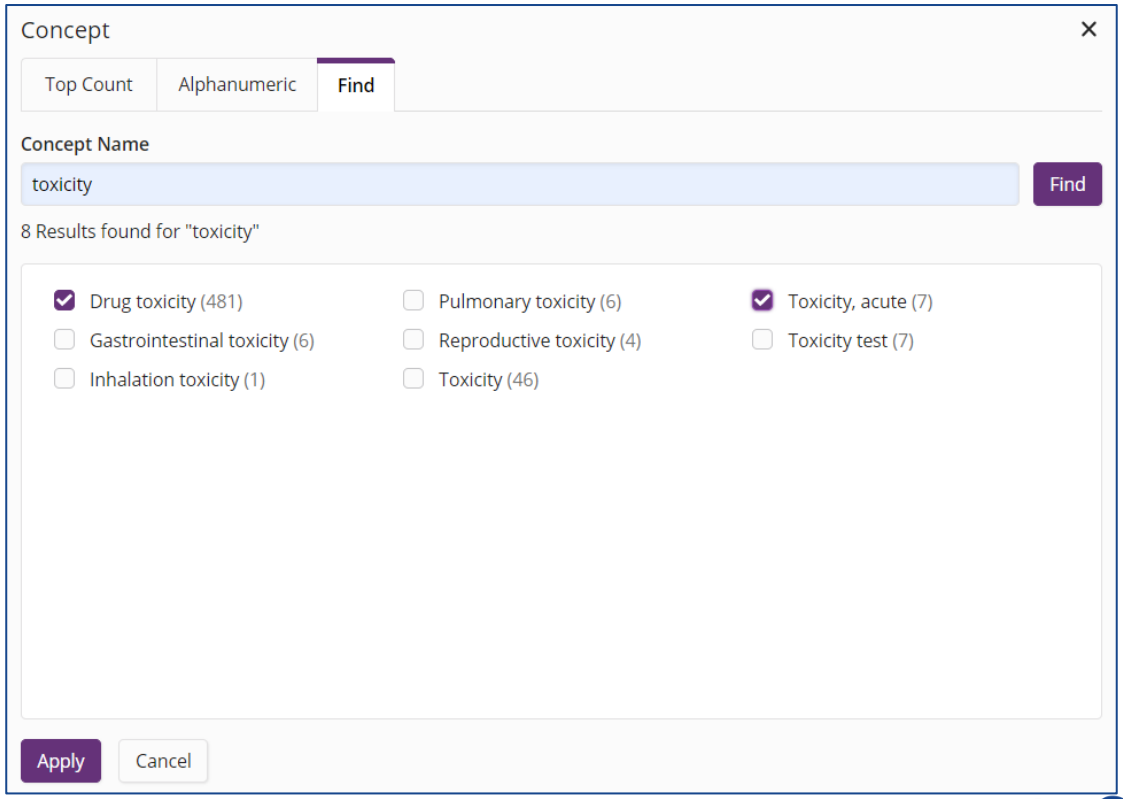
根据需要，在Concept中选择具体的毒性研究方向



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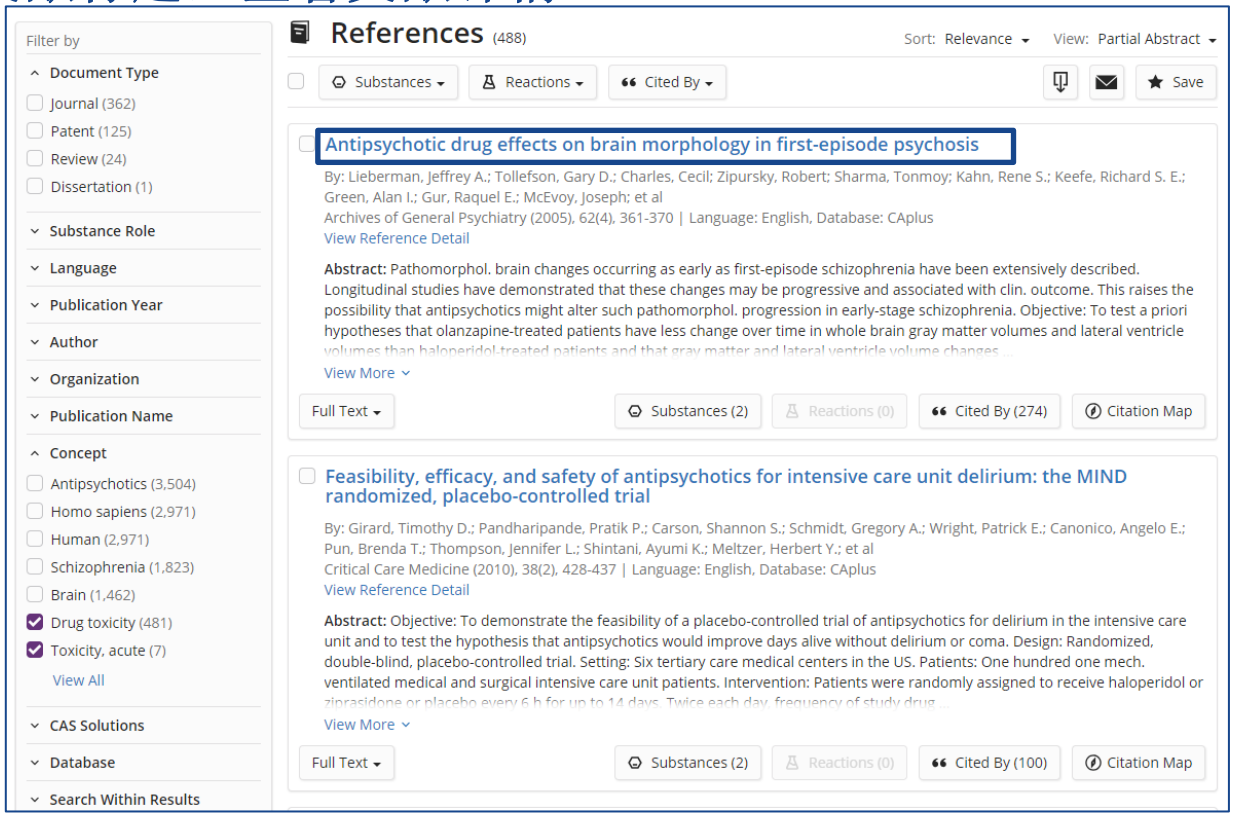
点击文献标题，查看文献详情



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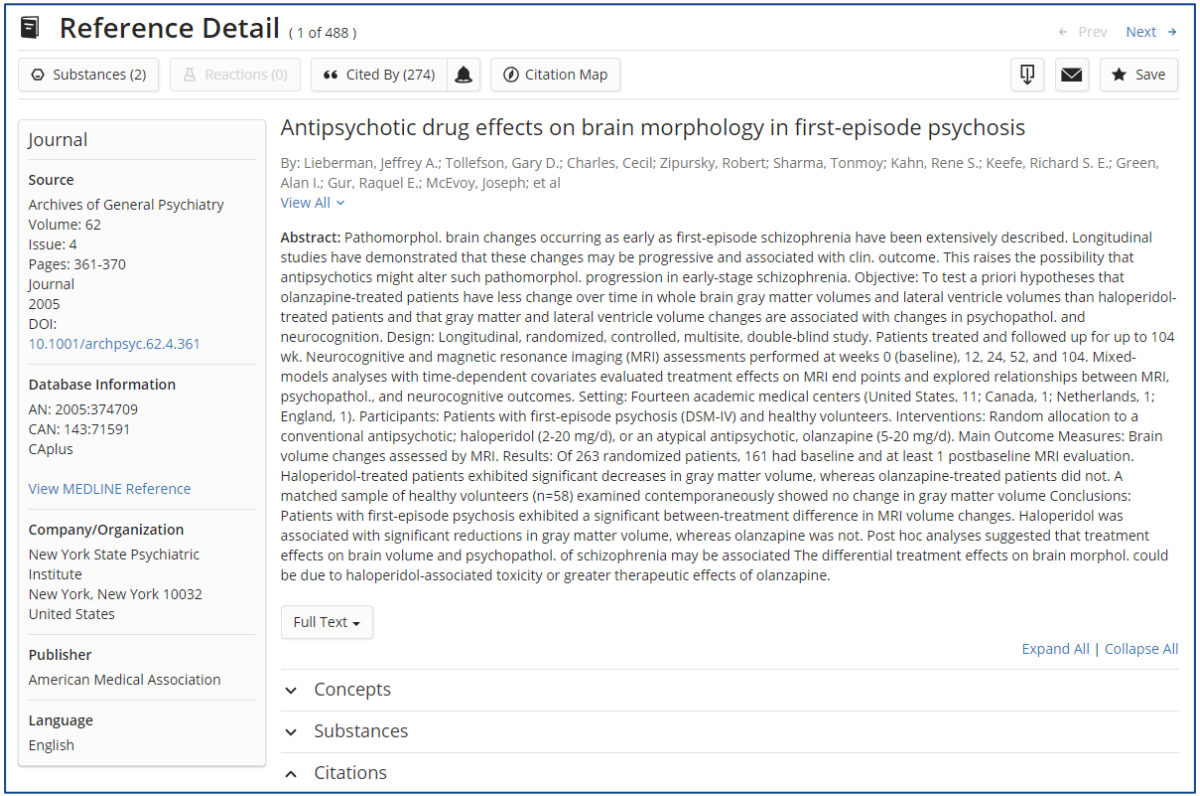
根据摘要、Concepts、Substance Role判断文献研究主旨



Reference Detail (1 of 488)

Prev Next

Substances (2) Reactions (0) Cited By (274) Citation Map Save

Journal

Source

Archives of General Psychiatry
Volume: 62
Issue: 4
Pages: 361-370
Journal
2005
DOI:
10.1001/archpsyc.62.4.361

Database Information

AN: 2005:374709
CAN: 143:71591
CAplus

View MEDLINE Reference

Company/Organization

New York State Psychiatric Institute
New York, New York 10032
United States

Publisher

American Medical Association

Language

English

Antipsychotic drug effects on brain morphology in first-episode psychosis

By: Lieberman, Jeffrey A.; Tollefson, Gary D.; Charles, Cecil; Zipursky, Robert; Sharma, Tonmoy; Kahn, Rene S.; Keefe, Richard S. E.; Green, Alan I.; Gur, Raquel E.; McEvoy, Joseph; et al
View All

Abstract: Pathomorphol. brain changes occurring as early as first-episode schizophrenia have been extensively described. Longitudinal studies have demonstrated that these changes may be progressive and associated with clin. outcome. This raises the possibility that antipsychotics might alter such pathomorphol. progression in early-stage schizophrenia. Objective: To test a priori hypotheses that olanzapine-treated patients have less change over time in whole brain gray matter volumes and lateral ventricle volumes than haloperidol-treated patients and that gray matter and lateral ventricle volume changes are associated with changes in psychopathol. and neurocognition. Design: Longitudinal, randomized, controlled, multisite, double-blind study. Patients treated and followed up for up to 104 wk. Neurocognitive and magnetic resonance imaging (MRI) assessments performed at weeks 0 (baseline), 12, 24, 52, and 104. Mixed-models analyses with time-dependent covariates evaluated treatment effects on MRI end points and explored relationships between MRI, psychopathol., and neurocognitive outcomes. Setting: Fourteen academic medical centers (United States, 11; Canada, 1; Netherlands, 1; England, 1). Participants: Patients with first-episode psychosis (DSM-IV) and healthy volunteers. Interventions: Random allocation to a conventional antipsychotic; haloperidol (2-20 mg/d), or an atypical antipsychotic, olanzapine (5-20 mg/d). Main Outcome Measures: Brain volume changes assessed by MRI. Results: Of 263 randomized patients, 161 had baseline and at least 1 postbaseline MRI evaluation. Haloperidol-treated patients exhibited significant decreases in gray matter volume, whereas olanzapine-treated patients did not. A matched sample of healthy volunteers (n=58) examined contemporaneously showed no change in gray matter volume Conclusions: Patients with first-episode psychosis exhibited a significant between-treatment difference in MRI volume changes. Haloperidol was associated with significant reductions in gray matter volume, whereas olanzapine was not. Post hoc analyses suggested that treatment effects on brain volume and psychopathol. of schizophrenia may be associated The differential treatment effects on brain morphol. could be due to haloperidol-associated toxicity or greater therapeutic effects of olanzapine.

Full Text

Expand All | Collapse All

Concepts

Substances

Citations

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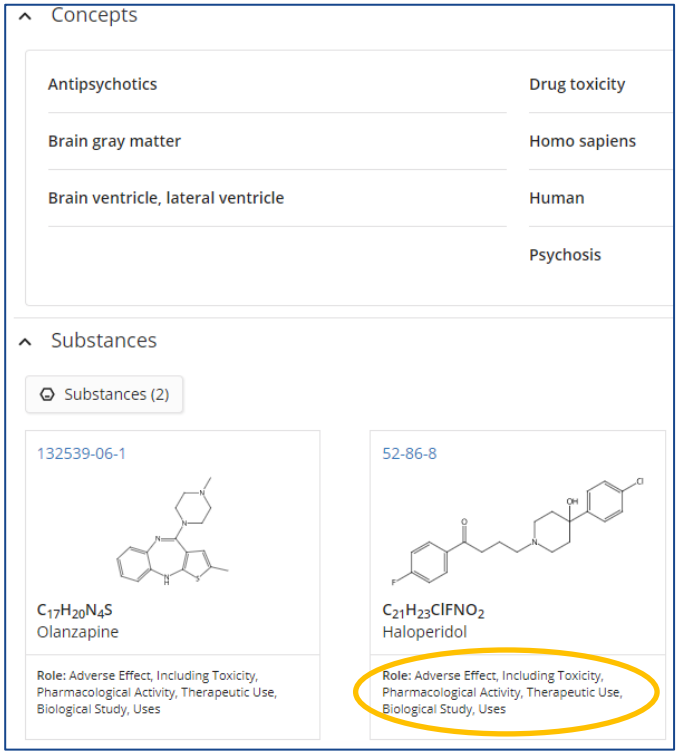
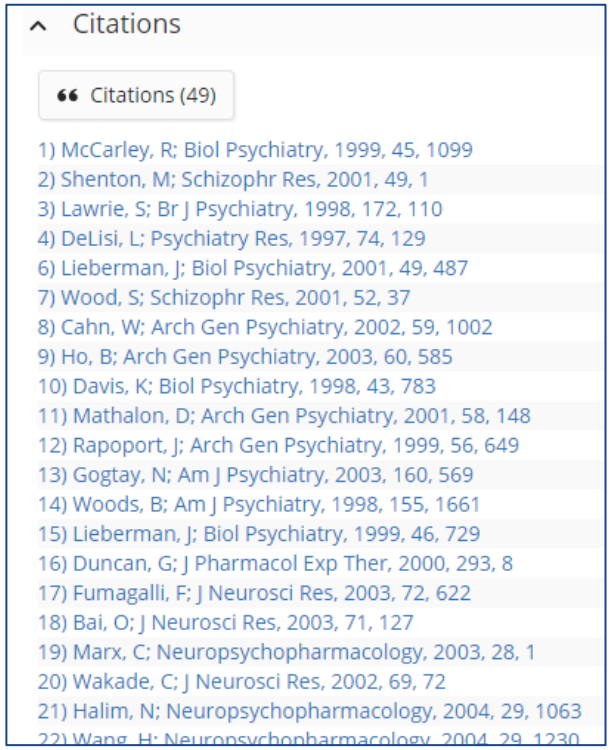
Substance Role有助快速确认物质在文献中的研究主旨





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在线学习资源

1.CAS官网上的培训资料
https://www.cas.org/support/training/scifinder-n

2.SciFinder-n Help使用指南
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

3.SciFinder-n What's New功能更新动态
https://scifinder-n.cas.org/help/#t=About_SciFinder-n%2FSciFinderN_Release_Notes%2FSciFinderN_Release_Notes.htm

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